Supporting Information

Practical Chemoselective Aromatic Substitution: Synthesis of *N*-(4-halo-2-nitrophenyl)benzenesulfonamide through Efficient Nitration and Halogenation of *N*-phenylbenzenesulfonamide

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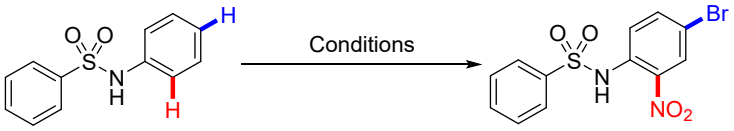
1. Optimization of Reaction Conditions

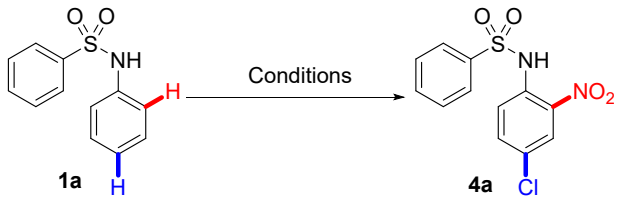
1.1 Optimization of reaction conditions to synthetize **3a**.[a]



Entry	Solvent	Base	Nitro source	Halogen	Yield(%)[b]
1	DCE	C_5H_5N	$Co(NO_3)_2•6H_2O$	TBAB	62[c]
2	DCE	-	$Co(NO_3)_2•6H_2O$	TBAB	nr[c]
3	DCE	C_5H_5N	$Co(NO_3)_2•6H_2O$	TBAB	76
4	DCE	C_5H_5N	$Fe(NO_3)_3•9H_2O$	TBAB	74, 80[d]
5	DCE	C_5H_5N	$Bi(NO_3)_3•5H_2O$	TBAB	66, 78[d]
6	**DCE**	**C_5H_5N**	**$Cu(NO_3)_2•3H_2O$**	**TBAB**	**86**
7	**DCE**	**C_5H_5N**	**NH_4NO_3**	**TBAB**	nr, 13[e], **84**[e,f]
8	CH_3CN	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	trace
9	EtOH	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	nr
10	THF	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	nr
11	1,4-dioxane	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	26
12	DCE	Cs_2CO_3	$Cu(NO_3)_2•3H_2O$	TBAB	nr
13	DCE	*t*-BuOK	$Cu(NO_3)_2•3H_2O$	TBAB	80
14	DCE	DBU	$Cu(NO_3)_2•3H_2O$	TBAB	nr
15	DCE	CH_3COOK	$Cu(NO_3)_2•3H_2O$	TBAB	76
16	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	NH_4Br	62
17	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	CuBr	32
18	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	$CuBr_2$	40, 43[f]
19	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	NaBr	29
20	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	KBr	31
21	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	79[g], 81[h]
22	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	13[i], 75[j], nr[k]
23	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	74[l], 79[m], 69[n]
24	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	83[o], 78[p]
25	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	79[q], 78[r]
26	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAB	82[s], 69[t]

[a] Reaction conditions: **1a** (0.2 mmol), base (0.3 mmol), nitrate (0.3 mmol), halogen (0.4 mmol) and solvent (2.0 mL) in a sealed tube with an air atmosphere at 110 °C stirred for 12 h. [b] Isolated yield. [c] $Pd(OAc)_2$ (0.1 equiv.) was additionally added. [d] Nitrate (0.2 mmol). [e] NH_4NO_3 (0.6 mmol) and $CuBr_2$ (0.2 equiv.) were additionally added. [f] Halogen (0.2 mmol). [g] C_5H_5N (1.0 equiv.). [h] C_5H_5N (2.0 equiv.). [i] $Cu(NO_3)_2•3H_2O$ (0.5 equiv.). [j] $Cu(NO_3)_2•3H_2O$ (1.0 equiv.). [k] $Cu(NO_3)_2•3H_2O$ (2.0 equiv.). [l] TBAB (1.0 equiv.). [m] TBAB (1.5 equiv.). [n] TBAB (2.5 equiv.). [o] 100 °C. [p] 120 °C. [q] 8h. [r] 16h. [s] N_2. [t] O_2.

1.2 Optimization of reaction conditions to synthetize **4a**.[a]



Entry	Solvent	Base	Nitro source	Halogen	Yield(%)[b]
1	DCE	C_5H_5N	$Cu(NO_3)_2•3H_2O$	TBAC	trace
2	DCE	Et_3N	$Cu(NO_3)_2•3H_2O$	TBAC	nr
3	DCE	DBU	$Cu(NO_3)_2•3H_2O$	TBAC	nr
4	DCE	Cs_2CO_3	$Cu(NO_3)_2•3H_2O$	TBAC	nr
5	DCE	*t*-BuOK	$Cu(NO_3)_2•3H_2O$	TBAC	67
6	DCE	CH_3COONa	$Cu(NO_3)_2•3H_2O$	TBAC	62
7	**DCE**	**CH_3COOK**	**$Cu(NO_3)_2•3H_2O$**	**TBAC**	**71**
8	DCE	-	$Cu(NO_3)_2•3H_2O$	TBAC	nr
9	CH_3CN	CH_3COOK	$Cu(NO_3)_2•3H_2O$	TBAC	nr
10	THF	CH_3COOK	$Cu(NO_3)_2•3H_2O$	TBAC	nr
11	1,4-dioxane	CH_3COOK	$Cu(NO_3)_2•3H_2O$	TBAC	nr
12	DCE	CH_3COOK	$Bi(NO_3)_3•5H_2O$	TBAC	nr, nr[c]
13	DCE	CH_3COOK	$Fe(NO_3)_3•9H_2O$	TBAC	nr, nr[c]
14	DCE	CH_3COOK	$Co(NO_3)_2•6H_2O$	TBAC	nr
15	**DCE**	**CH_3COOK**	**NH_4NO_3**	**TBAC**	nr, **70**[d], 35[d, e]
16	DCE	CH_3COOK	$Cu(NO_3)_2•3H_2O$	KCl	nr
17	DCE	CH_3COOK	$Cu(NO_3)_2•3H_2O$	NH_4Cl	trace
18	DCE	CH_3COOK	$Cu(NO_3)_2•3H_2O$	CuCl	nr
19	DCE	CH_3COOK	$Cu(NO_3)_2•3H_2O$	$CuCl_2$	nr, nr[e]
20	DCE	CH_3COOK	$Cu(NO_3)_2•3H_2O$	TBAC	66[f], nr[g]

[a] Reaction conditions: **1a** (0.2 mmol) base (0.3 mmol), nitrate (0.3 mmol), halogen (0.4 mmol) and solvent (2.0 mL) in a sealed tube with an air atmosphere at 100 °C stirred for 12 h.

[b] Isolated yield.

[c] Nitrate (0.2 mmol).

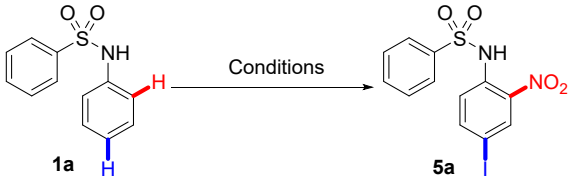
[d] NH_4NO_3 (0.6 mmol) and $CuCl_2$ (0.2 equiv.) were additionally added.

[e] Halogen (0.2 mmol).

[f] 110 °C.

[g] 120 °C.

1.3 Optimization of reaction conditions to synthetize **5a**.[a]



Entry	Solvent	Base	Nitro source	Halogen	Yield(%)[b]
1	DCE	C_5H_5N	$Fe(NO_3)_3•9H_2O$	TBAI	36
2	DCE	Et_3N	$Fe(NO_3)_3•9H_2O$	TBAI	nr
3	DCE	DBU	$Fe(NO_3)_3•9H_2O$	TBAI	trace
4	DCE	Cs_2CO_3	$Fe(NO_3)_3•9H_2O$	TBAI	nr
5	DCE	*t*-BuOK	$Fe(NO_3)_3•9H_2O$	TBAI	67
6	DCE	CH_3COONa	$Fe(NO_3)_3•9H_2O$	TBAI	60
7	**DCE**	**CH_3COOK**	**$Fe(NO_3)_3•9H_2O$**	**TBAI**	**73**
8	CH_3CN	CH_3COOK	$Fe(NO_3)_3•9H_2O$	TBAI	nr
9	1,4-dioxane	CH_3COOK	$Fe(NO_3)_3•9H_2O$	TBAI	nr
10	THF	CH_3COOK	$Fe(NO_3)_3•9H_2O$	TBAI	nr
11	DCE	CH_3COOK	$Fe(NO_3)_3•9H_2O$	TBAI	31[c]
12	DCE	CH_3COOK	$Bi(NO_3)_3•5H_2O$	TBAI	58, 23[c]
13	DCE	CH_3COOK	$Cu(NO_3)_2•3H_2O$	TBAI	67
14	DCE	CH_3COOK	$Co(NO_3)_2•6H_2O$	TBAI	26
15	DCE	CH_3COOK	NH_4NO_3	TBAI	nr, 50[e], 44[d, e]
16	**DCE**	**CH_3COOK**	**NH_4NO_3**	**TBAI**	**62**[f], 53[d, f]
17	DCE	CH_3COOK	$Fe(NO_3)_3•9H_2O$	NH_4I	nr
18	DCE	CH_3COOK	$Fe(NO_3)_3•9H_2O$	CuI	nr
19	DCE	CH_3COOK	$Fe(NO_3)_3•9H_2O$	KI	nr
20	DCE	CH_3COOK	$Fe(NO_3)_3•9H_2O$	TBAI	66[g], 70[h]

[a] Reaction conditions: **1a** (0.2 mmol) base (0.3 mmol), nitrate (0.3 mmol), halogen (0.4 mmol) and solvent (2.0 mL) in a sealed tube with an air atmosphere at 120 °C stirred for 12 h.

[b] Isolated yield.

[c] Nitrate (0.2 mmol).

[d] Halogen (0.2 mmol).

[e] NH_4NO_3 (0.6 mmol) and $Fe(NO_3)_3•9H_2O$ (0.2 equiv.) were additionally added.

[f] NH_4NO_3 (0.6 mmol) and $Cu(NO_3)_2•3H_2O$ (0.2 equiv.) were additionally added.

[g] 110 °C.

[h] 130 °C.

2. Experimental Section ＆ Characterization data of the products

General Experiment Information: ^{1}H NMR (400 MHz) and ^{13}C NMR spectra (101 MHz) were recorded on the Bruker Ascend™ 400 spectrometer using $CDCl_3$ and DMSO-d_6 as the solvent. Chemical shifts are given in ppm and coupling constants in Hz. ^{1}H spectra were calibrated in relation to the reference measurement of TMS (0.000 ppm). The following abbreviations were used for ^{1}H NMR spectra to indicate the signal multiplicity: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiple) as well as combinations of them. Flash chromatography was performed on silica gel 200-300 mesh (purchased from Qingdao Haiyang Chemical, China). MS spectra were recorded on Agilent 6546 LC/Q-TOF and AB SCIEX Triple Quad™ 4500MD.

General procedure for synthesis of *N*-phenylbenzenesulfonamide: Benzenesulfonyl chloride (0.55 mmol, 1.1 eq.) was added to a solution of appropriate aniline (0.5 mmol, 1 eq.) in pyridine (30 ml) at 0 °C. After stirring at room temperature for 24 hours, pyridine was removed by a rotary evaporator and the reaction mixture was poured into water. The product was extracted with DCM, dried over $MgSO_4$ and concentrated in vacuum. The residue was purified by silica gel column chromatography to obtain the corresponding product.

General procedure for synthesis of 3a-3aj: A mixture of the **1a** (0.2 mmol), C_5H_5N (0.3 mmol), $Cu(NO_3)_2$•$3H_2O$ (0.3 mmol), TBAB (0.4 mmol) and DCE (2.0 mL) was in a sealed tube with an air atmosphere at 110 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a short silica gel to afford the product **3a-3aj**.

***N*-(4-bromo-2-nitrophenyl)benzenesulfonamide (3a).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **3a**. Yellow solid, 61 mg, 86 % yield, m. p. = 98-99 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), 8.12 (d, *J* = 2.4 Hz, 1H), 7.81 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.80 – 7.71 (m, 2H), 7.70 – 7.63 (m, 1H), 7.62 – 7.52 (m, 2H), 7.22 (d, *J* = 8.7 Hz, 1H).**^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.61, 139.40, 137.22, 133.95, 129.94, 129.76, 128.45, 128.06, 127.21, 118.43. **HRMS** (ESI+):

Calculated for $C_{12}H_9BrN_2O_4S$, $[M-H]^-$ 354.9388. Found 354.9334.

***N*-(4-bromo-2-nitrophenyl)-4-methylbenzenesulfonamide (3b).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **3b**. Yellow solid, 65 mg, 88 % yield, m. p. = 109-110 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 8.12 (d, J = 2.3 Hz, 1H), 7.81 (dd, J = 8.7, 2.4 Hz, 1H), 7.64 (d, J = 8.3 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.7 Hz, 1H), 2.34 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.42, 144.13, 137.26, 136.54, 130.32, 130.10, 128.41, 127.57, 127.32, 118.07, 21.47. **HRMS** (ESI+): Calculated for $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9509.

***N*-(4-bromo-2-nitrophenyl)-4-methoxybenzenesulfonamide (3c).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:60) to afford the product **3c**. Yellow liquid, 65 mg, 84 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.26 (s, 1H), 8.13 (d, J = 2.3 Hz, 1H), 7.82 (dd, J = 8.7, 2.4 Hz, 1H), 7.72 – 7.65 (m, 2H), 7.23 (d, J = 8.7 Hz, 1H), 7.11 – 7.05 (m, 2H), 3.82 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 163.36, 144.08, 137.27, 130.83, 130.22, 129.61, 128.40, 127.49, 117.95, 115.03, 56.19. **HRMS** (ESI+): Calculated for $C_{13}H_{11}BrN_2O_5S$, $[M+Na]^+$ 408.9470. Found 408.9464.

***N*-(4-bromo-2-nitrophenyl)-4-fluorobenzenesulfonamide (3d).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **3d**. Yellow liquid, 63 mg, 85 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.74 (s, 1H), 8.25 (d, J = 2.1 Hz, 1H), 7.90 – 7.84 (m, 2H), 7.72 (dt, J = 9.0, 5.5 Hz, 2H), 7.17 (t, J = 8.5 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 165.75 (d, J = 257.4 Hz), 138.84, 137.49, 134.42 (d, J = 3.2 Hz), 132.63, 130.11 (d, J = 9.8 Hz), 128.85, 122.58, 116.96 (d, J = 23.0 Hz), 116.63. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -102.28. **HRMS** (ESI+): Calculated for $C_{12}H_8BrFN_2O_4S$, $[M-H]^-$ 372.9294. Found 372.9295.

***N*-(4-bromo-2-nitrophenyl)-4-chlorobenzenesulfonamide (3e).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **3e**. Yellow liquid, 62 mg, 80 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.56 (s, 1H), 8.14 (d, J = 2.3 Hz, 1H), 7.84 (dd, J = 8.7, 2.4 Hz, 1H), 7.74 – 7.70 (m, 2H), 7.67 – 7.64 (m, 2H), 7.21 (d, J = 8.7 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.92, 138.81, 138.34, 137.27, 130.07, 129.39, 129.18, 128.61, 128.45, 118.82. **HRMS** (ESI+): Calculated for $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8967.

4-bromo-*N*-(4-bromo-2-nitrophenyl)benzenesulfonamide (3f). The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3f**. Yellow liquid, 71 mg, 82 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.57 (s, 1H), 8.15 (d, *J* = 2.4 Hz, 1H), 7.85 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.83 – 7.79 (m, 2H), 7.66 – 7.61 (m, 2H), 7.20 (d, *J* = 8.7 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.97, 138.75, 137.27, 133.03, 129.34, 129.22, 128.62, 128.48, 127.85, 118.85. **HRMS** (ESI+): Calculated for $C_{12}H_8Br_2N_2O_4S$, $[M+Na]^+$ 458.8449. Found 458.8443.

***N*-(4-bromo-2-nitrophenyl)-3-methylbenzenesulfonamide (3i).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3i**. Yellow liquid, 58.4mg, 79 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.24 (d, *J* = 2.3 Hz, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.66 (ddd, *J* = 12.6, 8.1, 2.1 Hz, 3H), 7.43 – 7.34 (m, 2H), 2.40 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 140.03, 138.75, 138.26, 137.24, 134.83, 133.05, 129.36, 128.73, 127.46, 124.39, 122.31, 116.11, 21.36. **HRMS** (ESI+): Calculated for $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9515.

***N*-(4-bromo-2-nitrophenyl)-3-fluorobenzenesulfonamide (3j).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3j**. Yellow liquid, 62 mg, 83 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.27 (d, *J* = 2.2 Hz, 1H), 7.79 – 7.69 (m, 2H), 7.65 (ddd, *J* = 7.9, 1.8, 1.0 Hz, 1H), 7.56 (ddd, *J* = 7.9, 2.6, 1.8 Hz, 1H), 7.51 (td, *J* = 8.1, 5.2 Hz, 1H), 7.31 (tdd, *J* = 8.3, 2.5, 1.0 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.41 (d, *J* = 253.4 Hz), 140.36 (d, *J* = 6.8 Hz), 138.90, 137.48, 136.05, 131.52 (d, *J* = 7.9 Hz), 128.88, 122.97 (d, *J* = 3.4 Hz), 122.53, 121.33 (d, *J* = 21.1 Hz), 116.77, 114.73 (d, *J* = 24.7 Hz). **^{19}F NMR** (377 MHz, $CDCl_3$) δ -108.08. **HRMS** (ESI+): Calculated for $C_{12}H_8BrFN_2O_4S$, $[M+Na]^+$ 396.9270. Found 396.9259.

***N*-(4-bromo-2-nitrophenyl)-3-chlorobenzenesulfonamide (3k).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3k**. Yellow liquid, 64 mg, 82 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.81 (s, 1H), 8.27 (d, *J* = 1.9 Hz, 1H), 7.84 (t, *J* = 1.8 Hz, 1H), 7.76 – 7.70 (m, 3H), 7.60 – 7.55 (m, 1H), 7.45 (t, *J* = 8.0 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 140.13, 138.93, 137.40, 135.82, 134.16, 132.47, 130.90, 128.91, 127.32, 125.24, 122.34, 116.70. **HRMS** (ESI+): Calculated for $C_{12}H_8BrClN_2O_4S$, $[M-H]^-$ 388.8998. Found 388.8996.

3-bromo-*N*-(4-bromo-2-nitrophenyl)benzenesulfonamide (3l). The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3l**. Yellow liquid, 71 mg, 82 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.81 (s, 1H), 8.29 – 8.26 (m, 1H), 7.99 (t, *J* = 1.8 Hz, 1H), 7.78 (ddd, *J* = 7.9, 1.8, 1.0 Hz, 1H), 7.73 (tdd, *J* = 3.2, 1.9, 1.0 Hz, 3H), 7.39 (t, *J* = 8.0 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 140.26, 138.93, 137.40, 137.07, 132.46, 131.08, 130.13, 128.92, 125.66, 123.53, 122.34, 116.71. **HRMS** (ESI+): Calculated for $C_{12}H_8Br_2N_2O_4S$, $[M+Na]^+$ 458.8449. Found 458.8418.

***N*-(4-bromo-2-nitrophenyl)-2-methylbenzenesulfonamide (3o).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3o**. Yellow liquid, 62 mg, 84 % yield (eluent: ethyl acetate / petroleum ether = 1:100); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.29 – 8.25 (m, 1H), 8.04 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.60 (s, 2H), 7.49 (td, *J* = 7.5, 1.2 Hz, 1H), 7.37 – 7.29 (m, 2H), 2.65 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.83, 137.62, 136.46, 136.35, 134.13, 133.25, 130.02, 128.83, 126.54, 120.83, 115.37, 20.17. **HRMS** (ESI+): Calculated for $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9515.

***N*-(4-bromo-2-nitrophenyl)-2-fluorobenzenesulfonamide (3p).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **3p**. Yellow liquid, 64 mg, 86 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.29 (d, *J* = 2.3 Hz, 1H), 7.96 (td, *J* = 7.8, 1.7 Hz, 1H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.66 – 7.60 (m, 2H), 7.31 (td, *J* = 7.8, 0.9 Hz, 1H), 7.22 – 7.16 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.80 (d, *J* = 257.3 Hz), 138.74, 137.04, 136.57 (d, *J* = 8.7 Hz), 132.50, 130.73, 128.88, 126.38 (d, *J* = 13.1 Hz), 124.81 (d, *J* = 3.8 Hz), 121.43, 117.60 (d, *J* = 20.7 Hz), 116.17. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -108.94. **HRMS** (ESI+): Calculated for $C_{12}H_8BrFN_2O_4S$, $[M+Na]^+$ 396.9270. Found 396.9270.

***N*-(4-bromo-2-nitrophenyl)-2-chlorobenzenesulfonamide (3q).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **3q**. Yellow liquid, 66 mg, 85 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.34 (s, 1H), 8.27 (d, *J* = 2.2 Hz, 1H), 8.18 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.64 (d, *J* = 9.0 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.55 – 7.52 (m, 1H), 7.49 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.45 (td, *J* = 7.8, 1.4 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.76, 136.63, 135.56, 135.13, 132.56, 132.36, 132.13, 132.04, 128.99,

127.37, 120.42, 115.70. **HRMS** (ESI+): Calculated for $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8992.

2-bromo-*N*-(4-bromo-2-nitrophenyl)benzenesulfonamide (3r). The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **3r**. Yellow liquid, 72 mg, 83 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.44 (s, 1H), 8.29 (d, *J* = 2.1 Hz, 1H), 8.25 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.71 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.60 (dt, *J* = 9.0, 5.6 Hz, 2H), 7.51 (td, *J* = 7.6, 1.4 Hz, 1H), 7.45 (td, *J* = 7.6, 1.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.74, 137.25, 136.53, 135.90, 135.04, 132.54, 132.37, 129.03, 127.92, 120.36, 120.22, 115.58. **HRMS** (ESI+): Calculated for $C_{12}H_8Br_2N_2O_4S$, $[M+Na]^+$ 458.8449. Found 458.8471.

***N*-(4-bromo-5-methyl-2-nitrophenyl)benzenesulfonamide (3u).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3u**. Yellow liquid, 55 mg, 70 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 8.14 (s, 1H), 7.78 – 7.73 (m, 2H), 7.70 – 7.65 (m, 1H), 7.61 – 7.55 (m, 2H), 7.27 (s, 1H), 2.33 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 145.08, 141.95, 139.52, 133.90, 129.89, 129.00, 127.96, 127.24, 120.73, 23.11. **HRMS** (ESI+): Calculated for $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9528.

***N*-(4-bromo-5-methoxy-2-nitrophenyl)benzenesulfonamide (3v).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:60) to afford the product **3v**.Yellow liquid, 59 mg, 76 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.40 (s, 1H), 8.23 (s, 1H), 7.85 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.60 (dd, *J* = 8.2, 7.0 Hz, 2H), 6.95 (s, 1H), 3.84 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 159.96, 139.25, 135.12, 134.19, 133.32, 130.48, 130.02, 127.52, 107.17, 106.83, 57.69. **HRMS** (ESI+): Calculated for $C_{13}H_{11}BrN_2O_5S$, $[M+Na]^+$ 408.9470. Found 408.9480.

***N*-(4-bromo-5-chloro-2-nitrophenyl)benzenesulfonamide (3w).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **3w**. Yellow liquid, 51 mg, 65 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.84 (s, 1H), 8.37 (s, 1H), 8.01 (s, 1H), 7.91 – 7.84 (m, 2H), 7.68 – 7.60 (m, 1H), 7.58 – 7.49 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.08, 138.20, 135.10, 134.23, 133.56, 130.65, 129.71, 127.26,

121.64, 116.69. **HRMS** (ESI+): Calculated for $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8963.

***N*-(4-bromo-2-nitrophenyl)-2,5-dimethylbenzenesulfonamide (3ab).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3ab**. Yellow liquid, 66 mg, 86 % yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.42 (s, 1H), 8.15 (d, J = 2.3 Hz, 1H), 7.83 (dd, J = 8.8, 2.4 Hz, 1H), 7.60 (s, 1H), 7.38 – 7.35 (m, 1H), 7.31 (d, J = 7.8 Hz, 1H), 7.26 (d, J = 8.8 Hz, 1H), 2.51 (s, 3H), 2.29 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.06, 137.58, 137.30, 136.42, 134.55, 134.42, 133.24, 130.06, 129.50, 128.36, 127.72, 117.96, 20.77, 19.87. **HRMS** (ESI+): Calculated for $C_{14}H_{13}BrN_2O_4S$, $[M+Na]^+$ 406.9677. Found 406.9686.

***N*-(4-bromo-2-nitrophenyl)naphthalene-2-sulfonamide (3ac).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3ac**. Yellow liquid, 73 mg, 90 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.56 (s, 1H), 8.44 (d, J = 1.7 Hz, 1H), 8.15 (dd, J = 10.2, 4.8 Hz, 3H), 8.05 (d, J = 8.3 Hz, 1H), 7.80 (dd, J = 4.2, 2.2 Hz, 1H), 7.78 (dd, J = 4.2, 2.1 Hz, 1H), 7.76 – 7.70 (m, 1H), 7.70 – 7.65 (m, 1H), 7.24 (d, J = 8.7 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.62, 137.23, 136.59, 134.94, 132.04, 130.12, 129.87, 129.84, 129.70, 128.53, 128.44, 128.34, 128.25, 128.05, 122.48, 118.39. **HRMS** (ESI+): Calculated for $C_{16}H_{11}BrN_2O_4S$, $[M+Na]^+$ 428.9521. Found 428.9522.

***N*-(4-bromo-2-nitrophenyl)-2,4,6-trimethylbenzenesulfonamide (3ad).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **3ad**. Yellow solid, 65 mg, 82 % yield, m. p. = 129-130 ℃ ; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.21 (s, 1H), 8.15 (d, J = 2.3 Hz, 1H), 7.86 (dd, J = 8.7, 2.4 Hz, 1H), 7.17 (d, J = 8.7 Hz, 1H), 7.03 (s, 2H), 2.42 (s, 6H), 2.25 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.75, 143.14, 139.20, 137.29, 133.95, 132.40, 129.84, 128.74, 128.38, 118.46, 22.96, 20.90. **HRMS** (ESI+): Calculated for $C_{15}H_{15}BrN_2O_4S$, $[M-H]^-$ 396.9858. Found 396.9851.

***N*-(4-bromo-2-nitrophenyl)thiophene-2-sulfonamide (3ag).** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:70) to afford the product **3ag**. Yellow liquid, 53 mg, 74 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.60 (s, 1H), 8.18 (d, J = 2.3 Hz, 1H), 7.99 (dd, J = 5.0, 1.3 Hz, 1H), 7.89 (dd, J = 8.7, 2.4 Hz, 1H), 7.55 (dd, J = 3.8, 1.3 Hz, 1H), 7.26 (d, J = 8.7 Hz, 1H), 7.17 (dd, J = 5.0, 3.8 Hz, 1H). **^{13}C NMR** (101 MHz,

DMSO-d_6) δ 145.17, 139.58, 137.22, 134.81, 133.56, 129.40, 128.72, 128.46, 128.44, 119.02. **HRMS** (ESI+): Calculated for $C_{10}H_7BrN_2O_4S_2$, $[M+Na]^+$ 384.8928. Found 384.8926.

General procedure for synthesis of 4a-4aj: A mixture of the **1a** (0.2 mmol), CH_3COOK (0.3 mmol), $Cu(NO_3)_2•3H_2O$ (0.3 mmol), TBAC (0.4 mmol) and DCE (2.0 mL) was in a sealed tube with an air atmosphere at 100 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a short silica gel to afford the product **4a-4aj**.

***N*-(4-chloro-2-nitrophenyl)benzenesulfonamide (4a)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **4a**. Yellow solid, 44.3 mg, 71 % yield, m. p. = 112-113 ℃ ; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.44 (s, 1H), 8.05 (d, *J* = 2.5 Hz, 1H), 7.71 (td, *J* = 7.1, 3.5 Hz, 3H), 7.67 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.24 (d, *J* = 8.8 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.60, 139.47, 134.31, 133.93, 130.75, 129.93, 129.40, 128.02, 127.20, 125.73. **HRMS** (ESI+): Calculated for $C_{12}H_9ClN_2O_4S$, $[M-H]^-$ 310.9893. Found 310.9894.

***N*-(4-chloro-2-nitrophenyl)-4-methylbenzenesulfonamide (4b)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **4b**. Yellow solid, 45 mg, 69 % yield, m. p. = 101-102 ℃ ; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 8.05 (d, *J* = 2.5 Hz, 1H), 7.71 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.64 – 7.60 (m, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.8 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.39, 144.31, 136.58, 134.34, 130.51, 130.34, 129.61, 127.65, 127.30, 125.72, 21.49. **HRMS** (ESI+): Calculated for $C_{13}H_{11}ClN_2O_4S$, $[M-H]^-$ 325.0050 Found 325.0052.

***N*-(4-chloro-2-nitrophenyl)-4-methoxybenzenesulfonamide (4c)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:60) to afford the product **4c**. Yellow solid, 51 mg, 75 % yield, m. p. = 113-114 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.04 (d, *J* = 2.4 Hz, 1H), 7.71 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.67 (d, *J* = 8.8 Hz, 2H), 7.28 (d, *J* = 8.8 Hz, 1H), 7.09 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 3H). **^{13}C NMR** (101 MHz,

DMSO-d_6) δ 163.35, 144.16, 134.35, 130.92, 130.34, 129.82, 129.59, 127.50, 125.69, 115.04, 56.21. **HRMS** (ESI+): Calculated for $C_{13}H_{11}ClN_2O_5S$, $[M+Na]^+$ 364.9975. Found 364.9970.

***N*-(4-chloro-2-nitrophenyl)-4-fluorobenzenesulfonamide (4d)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4d**. Yellow liquid, 42 mg, 64 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.49 (s, 1H), 8.06 (d, *J* = 2.5 Hz, 1H), 7.80 – 7.76 (m, 2H), 7.73 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.27 (d, *J* = 8.7 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 165.10 (d, *J* = 252.2 Hz), 144.85, 135.87 (d, *J* = 2.7 Hz), 135.87 (d, *J* = 2.7 Hz), 130.99, 130.40 (d, *J* = 9.7 Hz), 129.16, 128.43, 125.73, 117.14 (d, *J* = 22.9 Hz). **^{19}F NMR** (377 MHz, DMSO-d_6) δ -105.29. **HRMS** (ESI+): Calculated for $C_{12}H_8ClFN_2O_4S$, $[M-H]^-$ 328.9799. Found 328.9802.

4-chloro-*N*-(4-chloro-2-nitrophenyl)benzenesulfonamide (4e) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4e**. Yellow liquid, 47 mg, 68 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.56 (s, 1H), 8.06 (d, *J* = 2.5 Hz, 1H), 7.75 – 7.69 (m, 3H), 7.69 – 7.65 (m, 2H), 7.26 (d, *J* = 8.7 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.98, 138.78, 138.37, 134.36, 131.16, 130.08, 129.17, 128.96, 128.60, 125.77. **HRMS** (ESI+): Calculated for $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9503.

4-bromo-*N*-(4-chloro-2-nitrophenyl)benzenesulfonamide (4f) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4f**. Yellow liquid, 51 mg, 66 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.57 (s, 1H), 8.06 (d, *J* = 2.5 Hz, 1H), 7.84 – 7.79 (m, 2H), 7.73 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.66 – 7.61 (m, 2H), 7.30 – 7.25 (m, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.94, 138.79, 134.37, 133.02, 131.17, 129.22, 128.94, 128.58, 127.84, 125.78. **HRMS** (ESI+): Calculated for $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8969.

***N*-(4-chloro-2-nitrophenyl)-3-methylbenzenesulfonamide (4i)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4i**. Yellow liquid, 38 mg, 58 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.39 (s, 1H), 8.05 (d, *J* = 2.5 Hz, 1H), 7.71 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.57 (s, 1H), 7.52 (d, *J* = 7.2 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.24 (d, *J* = 8.8 Hz, 1H), 2.36 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.43,

139.70, 139.45, 134.54, 134.32, 130.59, 129.75, 129.54, 127.77, 127.35, 125.73, 124.40, 21.26. **HRMS** (ESI+): Calculated for $C_{13}H_{11}ClN_2O_4S$, $[M+Na]^+$ 349.0026. Found 349.0019.

***N*-(4-chloro-2-nitrophenyl)-3-fluorobenzenesulfonamide (4j)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4j**. Yellow liquid, 43 mg, 65 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.62 (s, 1H), 8.07 (d, J = 2.5 Hz, 1H), 7.73 (dd, J = 8.8, 2.5 Hz, 1H), 7.66 (ddd, J = 13.2, 7.2, 3.4 Hz, 1H), 7.57 (ddd, J = 11.8, 5.2, 3.0 Hz, 3H), 7.28 (d, J = 8.8 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 162.16 (d, J = 249.1 Hz), 144.88, 141.55 (d, J = 7.0 Hz), 134.37, 132.40 (d, J = 8.1 Hz), 131.14, 128.92, 128.47, 125.76, 123.54 (d, J = 3.2 Hz), 121.13 (d, J = 21.1 Hz), 114.23 (d, J = 24.7 Hz). **^{19}F NMR** (377 MHz, DMSO-d_6) δ -109.99. **HRMS** (ESI+): Calculated for $C_{12}H_8ClFN_2O_4S$, $[M-H]^-$ 328.9799. Found 328.9798.

3-chloro-*N*-(4-chloro-2-nitrophenyl)benzenesulfonamide (4k) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4k**. Yellow liquid, 46 mg, 66 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.64 (s, 1H), 8.07 (d, J = 2.5 Hz, 1H), 7.80 – 7.72 (m, 3H), 7.68 – 7.59 (m, 2H), 7.27 (d, J = 8.8 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.91, 141.40, 134.47, 134.38, 133.87, 131.99, 131.17, 128.87, 128.50, 126.75, 125.95, 125.78. **HRMS** (ESI+): Calculated for $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9498.

3-bromo-*N*-(4-chloro-2-nitrophenyl)benzenesulfonamide (4l) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4l**. Yellow liquid, 51 mg, 65 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.62 (s, 1H), 8.07 (d, J = 2.5 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.88 (t, J = 1.7 Hz, 1H), 7.74 (dd, J = 8.7, 2.5 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.54 (t, J = 7.9 Hz, 1H), 7.27 (d, J = 8.8 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.91, 141.50, 136.74, 134.38, 132.16, 131.16, 129.53, 128.89, 128.47, 126.26, 125.79, 122.72. **HRMS** (ESI+): Calculated for $C_{12}H_8BrClN_2O_4S$, $[M-H]^-$ 388.8998. Found 388.8988.

***N*-(4-chloro-2-nitrophenyl)-2-methylbenzenesulfonamide (4o)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **4o**. Yellow liquid, 44 mg, 68 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), 8.04 (d, J = 2.5 Hz, 1H), 7.74 – 7.69 (m, 2H), 7.56 (td, J = 7.5, 1.3 Hz, 1H), 7.43 (d, J = 7.6 Hz,

1H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.29 (d, *J* = 8.8 Hz, 1H), 2.56 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.36, 137.85, 137.56, 134.33, 133.97, 133.33, 130.54, 129.51, 129.30, 128.05, 126.98, 125.63, 20.35. **HRMS** (ESI+): Calculated for $C_{13}H_{11}ClN_2O_4S$, $[M-H]^-$ 325.0050. Found 325.0046.

***N*-(4-chloro-2-nitrophenyl)-2-fluorobenzenesulfonamide (4p)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:70) to afford the product **4p**. Yellow liquid, 48 mg, 73 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.73 (s, 1H), 8.06 (d, *J* = 2.5 Hz, 1H), 7.78 – 7.71 (m, 3H), 7.49 – 7.41 (m, 1H), 7.42 – 7.34 (m, 2H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 158.78 (d, *J* = 255.0 Hz), 145.06, 136.77 (d, *J* = 8.6 Hz), 134.25, 131.35, 130.20, 129.38, 128.82, 127.61 (d, *J* = 14.3 Hz), 125.58, 125.54 (d, *J* = 3.7 Hz), 117.88 (d, *J* = 21.0 Hz). **^{19}F NMR** (377 MHz, DMSO-d_6) δ -108.99. **HRMS** (ESI+): Calculated for $C_{12}H_8ClFN_2O_4S$, $[M+Na]^+$ 352.9775. Found 352.9768.

2-chloro-*N*-(4-chloro-2-nitrophenyl)benzenesulfonamide (4q) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:65) to afford the product **4q**. Yellow liquid, 48 mg, 70 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.68 (s, 1H), 8.08 (d, *J* = 2.5 Hz, 1H), 7.96 – 7.88 (m, 1H), 7.75 – 7.66 (m, 3H), 7.53 (ddd, *J* = 8.1, 6.4, 2.2 Hz, 1H), 7.33 (d, *J* = 8.8 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.67, 137.22, 135.46, 134.42, 132.56, 131.38, 131.32, 131.05, 129.19, 128.66, 128.40, 125.67. **HRMS** (ESI+): Calculated for $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9494.

2-bromo-*N*-(4-chloro-2-nitrophenyl)benzenesulfonamide (4r) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:70) to afford the product **4r**. Yellow liquid, 55 mg, 71 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.62 (s, 1H), 8.09 (d, *J* = 2.5 Hz, 1H), 7.98 (dd, *J* = 6.1, 3.5 Hz, 1H), 7.88 (dd, *J* = 5.8, 3.3 Hz, 1H), 7.73 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.62 – 7.53 (m, 2H), 7.34 (d, *J* = 8.8 Hz, 1H).**^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.08, 138.83, 136.15, 135.42, 134.59, 131.63, 130.79, 129.47, 128.91, 128.04, 125.75, 119.83. **HRMS** (ESI+): Calculated for $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8969.

***N*-(4-chloro-5-methyl-2-nitrophenyl)benzenesulfonamide (4u)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4u**. Yellow liquid, 38.5 mg, 59 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 8.03 (s, 1H), 7.74 (dd, *J* = 5.3, 3.3 Hz, 2H), 7.70 – 7.65 (m, 1H), 7.61 – 7.55 (m, 2H), 7.27 (s, 1H), 2.32 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 143.21, 142.10, 139.55, 133.89,

130.89, 129.89, 129.33, 128.44, 127.23, 125.99, 20.30. **HRMS** (ESI+): Calculated for $C_{13}H_{11}ClN_2O_4S$, $[M+Na]^+$ 349.0026. Found 349.0014.

***N*-(4-chloro-5-methoxy-2-nitrophenyl)benzenesulfonamide (4v)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:50) to afford the product **4v**. Yellow liquid, 42 mg, 62 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.18 (s, 1H), 7.90 – 7.83 (m, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.39 (s, 1H), 3.99 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.66, 138.49, 135.09, 134.05, 129.69, 129.58, 127.77, 127.21, 118.26, 102.41, 57.09. **HRMS** (ESI+): Calculated for $C_{13}H_{11}ClN_2O_5S$, $[M+Na]^+$ 364.9975. Found 364.9958.

***N*-(4, 5-dichloro-2-nitrophenyl)benzenesulfonamide (4w)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **4w**. Yellow solid, 39 mg, 56 % yield, m. p. = 102-103 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.58 (s, 1H), 8.28 (s, 1H), 7.75 (dd, *J* = 5.2, 3.3 Hz, 2H), 7.72 – 7.67 (m, 1H), 7.60 (dd, *J* = 10.5, 4.7 Hz, 2H), 7.44 (s, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 142.68, 139.33, 136.78, 134.08, 130.68, 130.01, 128.81, 127.68, 127.22. **HRMS** (ESI+): Calculated for $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9491.

***N*-(4-chloro-2-nitrophenyl)-2, 5-dimethylbenzenesulfonamide (4ab)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4ab**. Yellow liquid, 50 mg, 74 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.40 (s, 1H), 8.05 (d, *J* = 2.5 Hz, 1H), 7.71 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.58 (s, 1H), 7.37 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.31 (s, 1H), 7.30 (d, *J* = 2.2 Hz, 1H), 2.49 (s, 3H), 2.28 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.16, 137.61, 136.42, 134.54, 134.41, 134.39, 133.25, 130.42, 129.60, 129.47, 127.80, 125.64, 20.77, 19.87. **HRMS** (ESI+): Calculated for $C_{14}H_{13}ClN_2O_4S$, $[M+Na]^+$ 363.0182. Found 363.0171.

***N*-(4-chloro-2-nitrophenyl)naphthalene-2-sulfonamide (4ac)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **4ac**. Yellow liquid, 53 mg, 73 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.55 (s, 1H), 8.42 (d, *J* = 1.8 Hz, 1H), 8.15 (t, *J* = 7.6 Hz, 2H), 8.07 – 8.03 (m, 2H), 7.77 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.72 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.69 (t, *J* = 1.9 Hz, 1H), 7.67 – 7.65 (m, 1H), 7.28 (d, *J* = 8.8 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.64, 136.60, 134.94, 134.33, 132.04, 130.76,

130.12, 129.87, 129.70, 129.42, 128.50, 128.35, 128.25, 128.05, 125.73, 122.48. **HRMS** (ESI+): Calculated for $C_{16}H_{11}ClN_2O_4S$, $[M+Na]^+$ 385.0026. Found 385.0005.

***N*-(4-chloro-2-nitrophenyl)-2, 4, 6-trimethylbenzenesulfonamide (4ad)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **4ad**. Yellow solid, 47 mg, 66 % yield, m. p. = 131-132 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.22 (s, 1H), 8.06 (d, *J* = 2.5 Hz, 1H), 7.74 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.23 (d, *J* = 8.8 Hz, 1H), 7.03 (s, 2H), 2.42 (s, 6H), 2.25 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.82, 143.11, 139.19, 134.37, 133.98, 132.39, 130.84, 129.42, 128.79, 125.65, 22.96, 20.90. **HRMS** (ESI+): Calculated for $C_{15}H_{15}ClN_2O_4S$, $[M-H]^-$ 353.0363. Found 353.0349.

***N*-(4-chloro-2-nitrophenyl)thiophene-2-sulfonamide (4ag)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:75) to afford the product **4ag**. Yellow liquid, 41 mg, 65 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.60 (s, 1H), 8.08 (d, *J* = 2.5 Hz, 1H), 7.98 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.77 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.54 (dd, *J* = 3.8, 1.4 Hz, 1H), 7.32 (d, *J* = 8.7 Hz, 1H), 7.17 (dd, *J* = 5.0, 3.8 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 145.15, 139.61, 134.79, 134.30, 133.53, 131.31, 129.01, 128.67, 128.43, 125.76. **HRMS** (ESI+): Calculated for $C_{10}H_7ClN_2O_4S_2$, $[M-H]^-$ 316.9458. Found 316.9448.

General procedure for synthesis of 5a-5ad: A mixture of the **1a** (0.2 mmol), CH_3COOK (0.3 mmol), $Fe(NO_3)_3$•$9H_2O$ (0.3 mmol), TBAI (0.4 mmol) and DCE (2.0 mL) was in a sealed tube with an air atmosphere at 120 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a short silica gel to afford the product **5a-5ad**.

***N*-(4-iodo-2-nitrophenyl)benzenesulfonamide (5a)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **5a**. Yellow liquid, 59 mg, 73 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.41 (s, 1H), 8.21 (d, *J* = 2.0 Hz, 1H), 7.95 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.74 (dd, *J* = 5.3, 3.3 Hz, 2H), 7.66 (dd, *J* = 5.0, 3.7 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.04 (d, *J* = 8.6 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO) δ 144.39, 142.96, 139.48, 133.92, 133.78, 130.19, 129.92, 127.80, 127.22, 90.62. **HRMS** (ESI+):

Calculated for $C_{12}H_9IN_2O_4S$, $[M+Na]^+$ 426.9225. Found 426.9218.

***N*-(4-iodo-2-nitrophenyl)-4-methylbenzenesulfonamide (5b)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **5b**. Yellow liquid, 63 mg, 75 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.31 (s, 1H), 8.21 (d, J = 2.0 Hz, 1H), 7.95 (dd, J = 8.6, 2.0 Hz, 1H), 7.67 – 7.59 (m, 2H), 7.38 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 8.6 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.39, 144.15, 142.96, 136.60, 133.77, 130.71, 130.41, 130.34, 128.18, 127.42, 127.31, 90.29, 21.49. **HRMS** (ESI+): Calculated for $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9375.

***N*-(4-iodo-2-nitrophenyl)-4-methoxybenzenesulfonamide (5c)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:60) to afford the product **5c**. Yellow liquid, 61 mg, 70 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.22 (s, 1H), 8.21 (d, J = 2.0 Hz, 1H), 7.96 (dd, J = 8.6, 2.0 Hz, 1H), 7.72 – 7.65 (m, 2H), 7.12 – 7.04 (m, 3H), 3.82 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 163.34, 143.98, 142.98, 133.76, 130.90, 130.59, 129.61, 127.25, 115.03, 90.09, 56.20. **HRMS** (ESI+): Calculated for $C_{13}H_{11}IN_2O_5S$, $[M+Na]^+$ 456.9331. Found 456.9324.

4-fluoro-*N*-(4-iodo-2-nitrophenyl)benzenesulfonamide (5d) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **5d**. Yellow liquid, 56 mg, 66 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), 8.22 (d, J = 2.0 Hz, 1H), 7.97 (dd, J = 8.5, 2.0 Hz, 1H), 7.79 (ddd, J = 8.3, 5.2, 2.6 Hz, 2H), 7.47 – 7.38 (m, 2H), 7.04 (d, J = 8.5 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 165.09 (d, J = 252.3 Hz), 144.71, 142.98, 135.87 (d, J = 3.0 Hz), 133.77, 130.41 (d, J = 9.9 Hz), 129.90, 128.24, 117.14 (d, J = 23.0 Hz), 91.00. **^{19}F NMR** (377 MHz, DMSO-d_6) δ -105.25. **HRMS** (ESI+): Calculated for $C_{12}H_8FIN_2O_4S$, $[M+Na]^+$ 444.9131. Found 444.9123.

4-chloro-*N*-(4-iodo-2-nitrophenyl)benzenesulfonamide (5e) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **5e.** Yellow liquid, 60 mg, 68 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.51 (s, 1H), 8.21 (d, J = 2.0 Hz, 1H), 7.97 (dd, J = 8.5, 2.0 Hz, 1H), 7.74 – 7.69 (m, 2H), 7.68 – 7.64 (m, 2H), 7.03 (d, J = 8.5 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.84, 142.99, 138.77, 138.40, 133.79, 130.08, 129.74, 129.17, 128.41, 91.17. **HRMS** (ESI+): Calculated for $C_{12}H_8ClIN_2O_4S$, $[M+Na]^+$ 460.8836. Found 460.8829.

4-bromo-*N*-(4-iodo-2-nitrophenyl)benzenesulfonamide (5f) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **5f.** Yellow liquid, 67 mg, 70 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.55 (s, 1H), 8.22 (d, *J* = 2.0 Hz, 1H), 7.97 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.91 – 7.70 (m, 2H), 7.71 – 7.53 (m, 2H), 7.04 (d, *J* = 8.5 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.81, 142.99, 138.79, 133.80, 133.01, 129.75, 129.22, 128.37, 127.83, 91.20. **HRMS** (ESI+): Calculated for $C_{12}H_8BrIN_2O_4S$, $[M+Na]^+$ 504.8331. Found 504.8330.

***N*-(4-iodo-2-nitrophenyl)-3-methylbenzenesulfonamide (5i)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **5i.** Yellow liquid, 45 mg, 54 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.38 (s, 1H), 8.21 (d, *J* = 2.1 Hz, 1H), 7.95 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.58 (d, *J* = 2.0 Hz, 1H), 7.56 – 7.41 (m, 3H), 7.03 (d, *J* = 8.6 Hz, 1H), 2.35 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.24, 142.96, 139.69, 139.43, 134.54, 133.78, 130.33, 129.74, 127.52, 127.37, 124.42, 90.42, 21.28. **HRMS** (ESI+): Calculated for $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9375.

3-chloro-*N*-(4-iodo-2-nitrophenyl)benzenesulfonamide (5j) The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **5j.** Yellow liquid, 58 mg, 66 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.59 (s, 1H), 8.23 (d, *J* = 2.0 Hz, 1H), 7.98 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.77 (dt, *J* = 2.9, 1.9 Hz, 2H), 7.66 (dt, *J* = 7.9, 1.4 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.04 (d, *J* = 8.5 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.78, 143.01, 141.44, 134.46, 133.86, 133.80, 131.98, 129.68, 128.29, 126.76, 125.95, 91.17. **HRMS** (ESI+): Calculated for $C_{12}H_8ClIN_2O_4S$, $[M-H]^-$ 436.8860 Found 436.8839.

***N*-(4-iodo-2-nitrophenyl)-2-methylbenzenesulfonamide (5m)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:70) to afford the product **5m.**Yellow liquid, 62 mg, 74 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.44 (s, 1H), 8.21 (d, *J* = 2.0 Hz, 1H), 7.95 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.73 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.56 (td, *J* = 7.5, 1.4 Hz, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.35 (td, *J* = 7.7, 1.3 Hz, 1H), 7.07 (d, *J* = 8.6 Hz, 1H), 2.56 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.18, 142.96, 137.79, 137.56, 133.98, 133.71, 133.33, 130.26, 129.32, 127.81, 126.98, 90.39, 20.35. **HRMS** (ESI+): Calculated for $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9376.

2-fluoro-*N*-(4-iodo-2-nitrophenyl)benzenesulfonamide (5n) The residue was purified by flash

chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:70) to afford the product **5n.** Yellow liquid, 60 mg, 71 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.70 (s, 1H), 8.22 (d, J = 2.0 Hz, 1H), 8.00 (dd, J = 8.5, 2.1 Hz, 1H), 7.74 (dddd, J = 8.7, 7.3, 3.2, 1.5 Hz, 2H), 7.50 – 7.40 (m, 1H), 7.40 – 7.32 (m, 1H), 7.15 (d, J = 8.6 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.77 (d, J = 255.0 Hz), 144.98, 142.90, 136.76 (d, J = 8.7 Hz), 133.64, 130.21, 129.60, 129.25, 127.60 (d, J = 14.4 Hz), 125.53 (d, J = 3.6 Hz), 117.89 (d, J = 20.7 Hz), 91.47. **^{19}F NMR** (377 MHz, DMSO-d_6) δ -108.98. **HRMS** (ESI+): Calculated for $C_{12}H_8FIN_2O_4S$, $[M+Na]^+$ 444.9131. Found 444.9121.

***N*-(4-iodo-5-methyl-2-nitrophenyl)benzenesulfonamide (5q)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **5q.** Yellow liquid, 50 mg, 60 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.31 (s, 1H), 8.28 (s, 1H), 7.77 – 7.73 (m, 2H), 7.67 (dd, J = 10.5, 4.3 Hz, 1H), 7.57 (dd, J = 10.5, 4.7 Hz, 2H), 7.22 (s, 1H), 2.35 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 148.63, 141.63, 139.59, 135.00, 133.90, 130.50, 129.90, 127.25, 126.43, 96.90, 28.09. **HRMS** (ESI+): Calculated for $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9371.

***N*-(5-chloro-4-iodo-2-nitrophenyl)benzenesulfonamide (5r)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **5r.** Yellow liquid, 45 mg, 52 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.55 (s, 1H), 7.98 (s, 1H), 7.88 (dd, J = 5.3, 3.4 Hz, 2H), 7.63 (dt, J = 8.6, 1.1 Hz, 1H), 7.54 (t, J = 7.7 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 147.02, 138.23, 137.00, 134.44, 134.22, 129.70, 127.27, 120.33, 90.05. **HRMS** (ESI+): Calculated for $C_{12}H_8ClIN_2O_4S$, $[M-H]^-$ 436.8860. Found 436.8861.

***N*-(4-iodo-2-nitrophenyl)-2,5-dimethylbenzenesulfonamide (5w)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **5w.** Yellow liquid, 64.8 mg, 75 % yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.45 (d, J = 2.1 Hz, 1H), 7.86 (s, 1H), 7.78 (dd, J = 8.9, 2.0 Hz, 1H), 7.46 (d, J = 8.9 Hz, 1H), 7.29 (d, J = 7.7 Hz, 1H), 7.18 (d, J = 7.7 Hz, 1H), 2.59 (s, 3H), 2.38 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.44, 136.60, 136.34, 136.19, 134.85, 134.58, 134.39, 133.97, 133.13, 130.27, 120.84, 84.43, 20.91, 19.67. **HRMS** (ESI+): Calculated for $C_{14}H_{13}IN_2O_4S$, $[M+Na]^+$ 454.9538. Found 454.9532.

***N*-(4-iodo-2-nitrophenyl)naphthalene-2-sulfonamide (5x)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **5x**. Yellow liquid, 69 mg, 76 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.53 (s, 1H), 8.43 (d, *J* = 1.9 Hz, 1H), 8.20 (d, *J* = 2.0 Hz, 1H), 8.18 – 8.10 (m, 2H), 8.04 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.92 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.77 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.72 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.66 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 1H), 7.06 (d, *J* = 8.5 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.48, 142.96, 136.59, 134.93, 133.79, 132.02, 130.20, 130.12, 129.88, 129.71, 128.53, 128.34, 128.26, 127.83, 122.49, 90.65. **HRMS** (ESI+): Calculated for $C_{16}H_{11}IN_2O_4S$, $[M+Na]^+$ 476.9382. Found 476.9372.

***N*-(4-iodo-2-nitrophenyl)thiophene-2-sulfonamide (5aa)** The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:70) to afford the product **5aa**. Yellow liquid, 52 mg, 64 % yield; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.56 (s, 1H), 8.24 (d, *J* = 2.0 Hz, 1H), 8.01 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.98 (dd, *J* = 4.9, 1.4 Hz, 1H), 7.54 (dd, *J* = 3.8, 1.4 Hz, 1H), 7.17 (dd, *J* = 5.0, 3.8 Hz, 1H), 7.09 (d, *J* = 8.5 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 145.03, 142.94, 139.65, 134.77, 133.78, 133.52, 129.80, 128.49, 128.42, 91.36. **HRMS** (ESI+): Calculated for $C_{10}H_7IN_2O_4S_2$, $[M+Na]^+$ 432.8790. Found 432.8780.

General procedure for synthesis of 4-methoxy-2-nitroaniline

Synthesis of *N*-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide (7a): A mixture of the **6a** (2 mmol), C_5H_5N (3 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (3 mmol), TBAB (4 mmol) and DCE (20 mL) was in a sealed tube with an air atmosphere at 110 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a silica gel (eluent: ethyl acetate / petroleum ether = 1:50) to afford the product 7**a**. Orange solid, 503 mg, 78 % yield, m. p. = 104-105 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.98 (s, 1H), 7.53 (d, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 3.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.19 (dd, *J* = 8.9, 3.0 Hz, 1H), 7.05 (d, *J* = 8.9 Hz, 1H), 3.79 (s, 3H), 2.36 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 157.93, 146.45, 143.92, 136.94, 130.16, 129.62, 127.21, 122.49, 120.17, 110.29, 56.52, 21.45. **HRMS** (ESI+): Calculated for $C_{14}H_{14}N_2O_5S$, $[M+Na]^+$ 345.0521. Found 345.0524.

Synthesis of 4-methoxy-2-nitroaniline (8a): A sealed tube equipped with a rubber septum was charged with **7a** (1 mmol), TfOH (2 mmol), and DCE (10 ml) at 0 °C under argon. The mixture was stirred at 90 °C for 8 h and then quenched with 6 drops of neat Et_3N and subsequently diluted with 1.0 M NaOH aq solution. The biphasing resulting mixture was extracted with EA (3 times); the combined organic extracts were dried over $MgSO_4$, filtered, and then concentrated in vacuum. The residue was purified by silica gel flash column chromatography (eluent: ethyl acetate / petroleum ether = 1:10) to afford the product **8a**. Orange solid, 155 mg, 92 % yield, m. p. = 119-120 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.36 (d, J = 3.0 Hz, 1H), 7.28 (s, 2H), 7.16 (dd, J = 9.2, 3.0 Hz, 1H), 7.00 (d, J = 9.2 Hz, 1H), 3.72 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 149.63, 142.45, 129.48, 127.67, 121.27, 105.25, 55.94. **HRMS** (ESI+): Calculated for $C_7H_8N_2O_3$, $[M+H]^+$ 169.0613. Found 169.0602.

General procedure for synthesis of 4,5-dichloro-2-nitroaniline

Synthesis of *N*-(4,5-dichloro-2-nitrophenyl)benzenesulfonamide (4w): A mixture of the *N*-(3-chlorophenyl)benzenesulfonamide (2 mmol), CH_3COOK (3 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (3 mmol), TBAC (4 mmol) and DCE (20 mL) was in a sealed tube with an air atmosphere at 100 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **4w**. Yellow solid, 368 mg, 53 % yield, m. p. = 102-103 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.58 (s, 1H), 8.28 (s, 1H), 7.75 (dd, J = 5.2, 3.3 Hz, 2H), 7.72 – 7.67 (m, 1H), 7.60 (dd, J = 10.5, 4.7 Hz, 2H), 7.44 (s, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 142.68, 139.33, 136.78, 134.08, 130.68, 130.01, 128.81, 127.68, 127.22. **HRMS** (ESI+): Calculated for $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9491.

Synthesis of 4,5-dichloro-2-nitroaniline (8b): A sealed tube equipped with a rubber septum was charged with **4w** (1 mmol), DCE (10 ml), and TfOH (3 mmol) at 0 °C under argon. The mixture was stirred at 100 °C for 8 h and then quenched with 6 drops of neat Et_3N and subsequently diluted with 1.0 M NaOH aq solution. The biphasing resulting mixture was extracted with EA (3 times); the combined organic extracts were dried over $MgSO_4$, filtered, and then concentrated in

vacuum. The product was purified by silica gel flash column chromatography (eluent: ethyl acetate / petroleum ether = 1:10) to afford the product **8b**. Orange solid, 182 mg, 88 %, 160-161 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.09 (s, 1H), 7.61 (s, 2H), 7.25 (s, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 145.67, 138.72, 129.67, 126.92, 120.26, 116.82. **HRMS** (ESI+): Calculated for $C_6H_4Cl_2N_2O_2$, $[M-H]^-$ 204.9572. Found 204.9571.

General procedure for synthesis of 4-bromo-2-nitroaniline

Synthesis of *N*-(4-bromo-2-nitrophenyl)benzenesulfonamide (3a): A mixture of the **1a** (20 mmol), C_5H_5N (30 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (30 mmol), TBAB (40 mmol) and DCE (100 mL) was in reaction kettle with an air atmosphere at 110 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **3a**. Yellow solid, 5.43 g, 76 % yield, m. p. = 98-99 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), 8.12 (d, J = 2.4 Hz, 1H), 7.81 (dd, J = 8.8, 2.4 Hz, 1H), 7.80 – 7.71 (m, 2H), 7.70 – 7.63 (m, 1H), 7.62 – 7.52 (m, 2H), 7.22 (d, J = 8.7 Hz, 1H).**^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.61, 139.40, 137.22, 133.95, 129.94, 129.76, 128.45, 128.06, 127.21, 118.43. **HRMS** (ESI+): Calculated for $C_{12}H_9BrN_2O_4S$, $[M-H]^-$ 354.9388. Found 354.9334.

Synthesis of 4-bromo-2-nitroaniline (8c): The mixture charged with **3a** (15 mmol), TfOH (45 mmol), and DCE (60 ml) was stirred at 100 °C for 10 h under argon and subsequently diluted with 1.0 M NaOH aq solution. The biphasing resulting mixture was extracted with EA (3 times); the combined organic extracts were dried over $MgSO_4$, filtered, and then concentrated in vacuum. The product was purified by silica gel flash column chromatography (eluent: ethyl acetate / petroleum ether = 1:10) to afford the product **8c**. Orange solid, 2.86 g, 88 % yield, m. p. = 109-110 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 (d, J = 2.3 Hz, 1H), 7.43 (dd, J = 8.9, 2.3 Hz, 1H), 6.74 (d, J = 8.9 Hz, 1H), 6.03 (s, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.59, 138.50, 132.48, 128.33, 120.35, 107.85. **HRMS** (ESI+): Calculated for $C_6H_5BrN_2O_2$, $[M-H]^-$ 214.9456. Found 214.9470.

General procedure for synthesis of *N*-(2-nitrophenyl)benzenesulfonamide (11): A mixture of

the **1a** (0.2 mmol), C_5H_5N (0.3 mmol), $Cu(NO_3)_2$•$3H_2O$ (0.3 mmol) and DCE (2.0 mL) was in a sealed tube with an air atmosphere at 110 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:80) to afford the product **11**. Yellow solid, 24 mg, 43 % yield, m. p. = 100-101 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 7.92 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.78 – 7.73 (m, 2H), 7.68 – 7.62 (m, 1H), 7.58 (ddd, *J* = 13.7, 7.4, 1.3 Hz, 3H), 7.40 – 7.34 (m, 1H), 7.27 (dd, *J* = 8.2, 1.2 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 143.82, 139.65, 134.63, 133.81, 130.57, 129.84, 127.22, 126.90, 126.16, 125.95. **HRMS** (ESI+): Calculated for $C_{12}H_{10}N_2O_4S$, $[M-H]^-$ 277.0283. Found 277.0288.

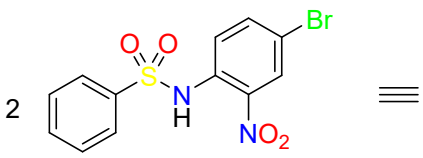
General procedure for synthesis of 4-methyl-*N*-(4-methyl-2-nitrophenyl)benzenesulfonamide (13): A mixture of the **12** (0.2 mmol), C_5H_5N (0.3 mmol), $Cu(NO_3)_2$•$3H_2O$ (0.3 mmol), TBAB (0.4 mmol) and DCE (2.0 mL) was in a sealed tube with an air atmosphere at 110 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:60) to afford the product **13**. Yellow solid, 49 mg, 80 % yield, m. p. = 145-146 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.11 (s, 1H), 7.72 (d, *J* = 1.3 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.37 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.3 Hz, 1H), 2.33 (s, 3H), 2.28 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.12, 143.83, 137.14, 136.85, 135.09, 130.18, 128.07, 127.27, 126.36, 125.79, 21.41, 20.38. **HRMS** (ESI+): Calculated for $C_{14}H_{14}N_2O_4S$, $[M+Na]^+$ 329.0572. Found 329.0576.

General procedure for synthesis of *N*-(2-nitrophenyl)benzamide (18): A mixture of the **17** (0.2 mmol), C_5H_5N (0.3 mmol), $Cu(NO_3)_2$•$3H_2O$ (0.3 mmol), TBAB (0.4 mmol) and DCE (2.0 mL) was in a sealed tube with an air atmosphere at 110 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:90) to afford the product **18**. Yellow solid, 22 mg, 45 % yield, 95-96 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.77 (s, 1H), 8.03 (dd, *J* =

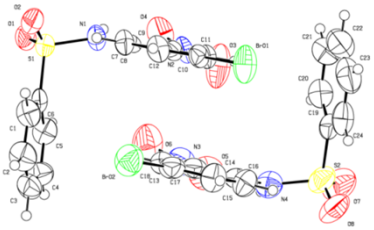
8.2, 1.4 Hz, 1H), 7.99 – 7.95 (m, 2H), 7.79 (dtd, *J* = 9.6, 8.2, 1.5 Hz, 2H), 7.68 – 7.63 (m, 1H), 7.61 – 7.55 (m, 2H), 7.43 (ddd, *J* = 8.6, 7.2, 1.6 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 165.82, 143.31, 134.52, 134.01, 132.79, 132.05, 129.16, 128.18, 126.39, 126.05, 125.47. **HRMS** (ESI+): Calculated for $C_{13}H_{10}N_2O_3$, $[M+Na]^+$ 265.0589. Found 265.0581.

General procedure for synthesis of (2-nitroethene-1,1-diyl)dibenzene (21): A mixture of the **1b** (0.2 mmol), ethene-1,1-diyldibenzene (0.2 mmol), C_5H_5N (0.3 mmol), $Cu(NO_3)_2$•$3H_2O$ (0.3 mmol), TBAB (0.4 mmol) and DCE (2.0 mL) was in a sealed tube with an air atmosphere at 110 ℃ stirred for 12 h. After that time, the media was acidified until pH = 6 and extracted with EA (3 times); the combined organic phase was dried over $MgSO_4$ and evaporated. The residue was purified by flash chromatography on a short silica gel (eluent: ethyl acetate / petroleum ether = 1:100) to afford the product **21**. Yellow solid, 20 mg, 46 % yield, m. p. = 81-82 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.95 (s, 1H), 7.52 – 7.40 (m, 6H), 7.36 (ddd, *J* = 7.2, 3.5, 1.9 Hz, 2H), 7.24 – 7.18 (m, 2H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 148.91, 136.78, 136.10, 131.28, 129.43, 129.35, 129.21, 129.04, 128.83. **HRMS** (ESI+): Calculated for $C_{14}H_{11}NO_2$, $[M+H]^+$ 226.0868. Found 226.0864.

3. Crystal data of 3a



3a

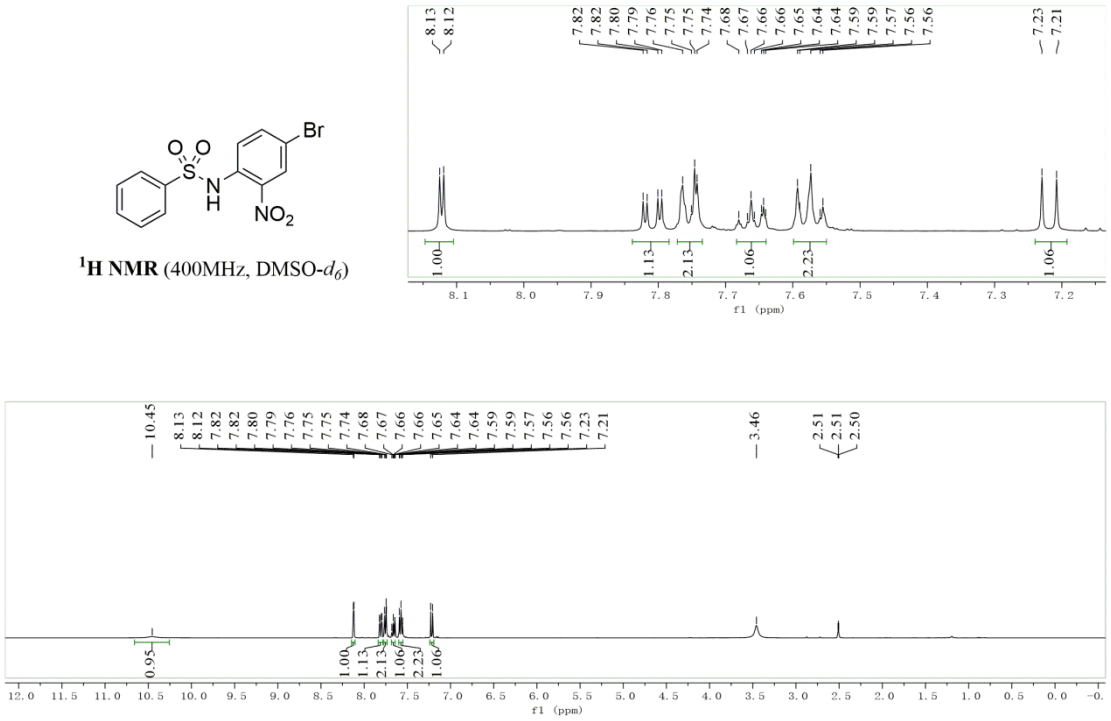


X-ray structure of **3a**
CCDC 2123138

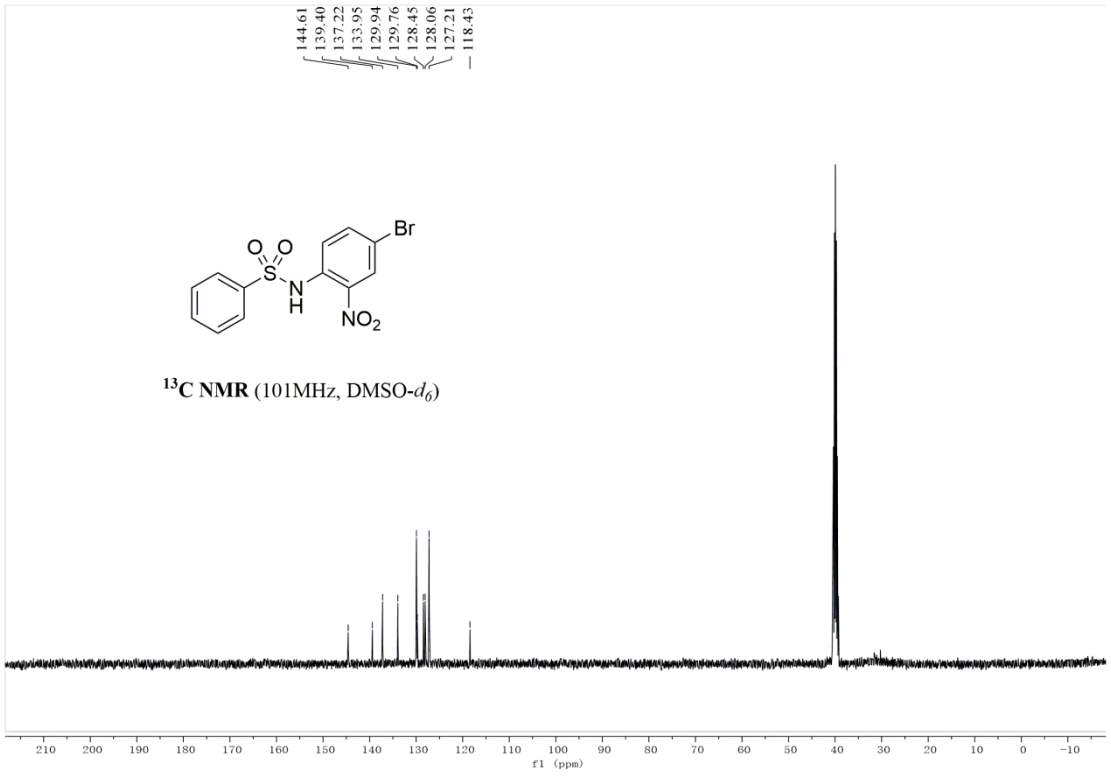
Empirical formula	$C_{24}H_{18}Br_2N_4O_8S_2$
Formula weight	714.36
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P 21/n
Unit cell dimensions	a = 10.609(6) Å α = 90°.
b = 8.728(5 Å	β = 91.652(12)°.
c = 29.627(17) Å	γ = 90°.
Volume	2742(3) $Å^3$
Z	4
Density (calculated)	1.730 g/cm^3
Absorption coefficient	3.164 mm^{-1}
F(000)	1424
Crystal size	0.260 x 0.250 x 0.210 mm^3
Theta range for data collection	2.43 to 21.42°
Index ranges	-11<=h<=12, -10<=k<=10, -35<=l<=30
Reflections collected / unique	13522 / 4825 [R(int) = 0.0393]
Completeness to theta = 24.999	99.6%
Absorption correction	None
Max. and min. transmission	0.7456 and 0.5220
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4825 / 1 / 361
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.1284
R indices (all data)	R1 = 0.0991, wR2 = 0.1410

4. Copies of NMR and HPLC-MS Spectra

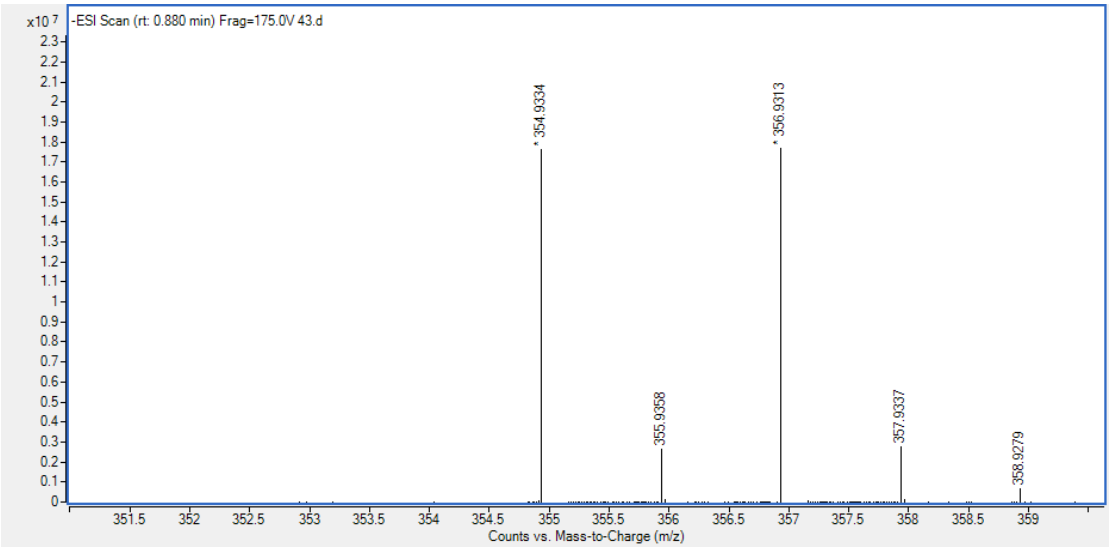
3a ^{1}H NMR



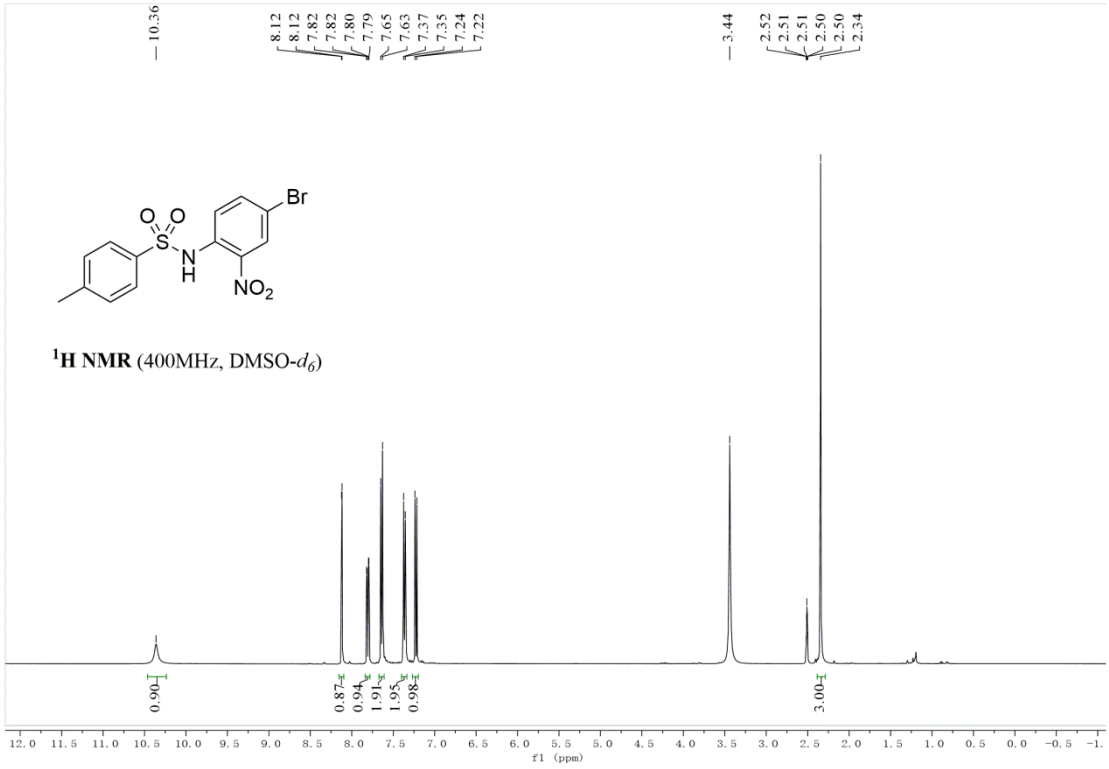
3a ^{13}C NMR



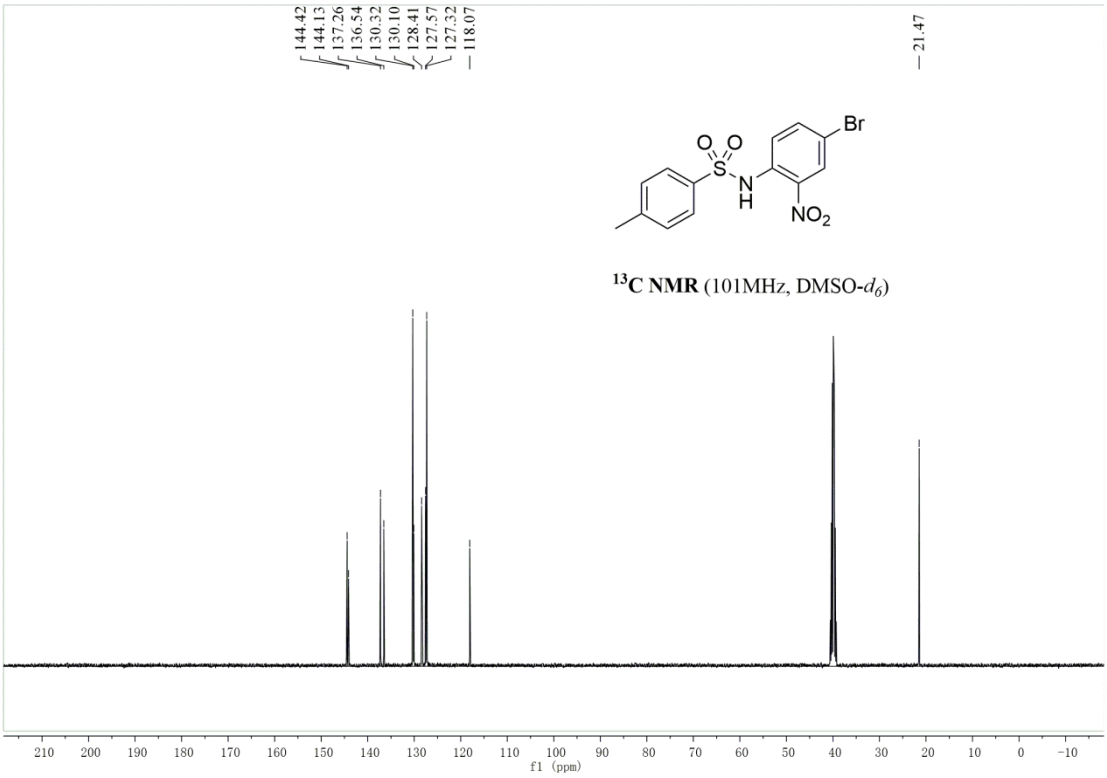
3a $C_{12}H_9BrN_2O_4S$, $[M-H]^-$ 354.9388. Found 354.9334.



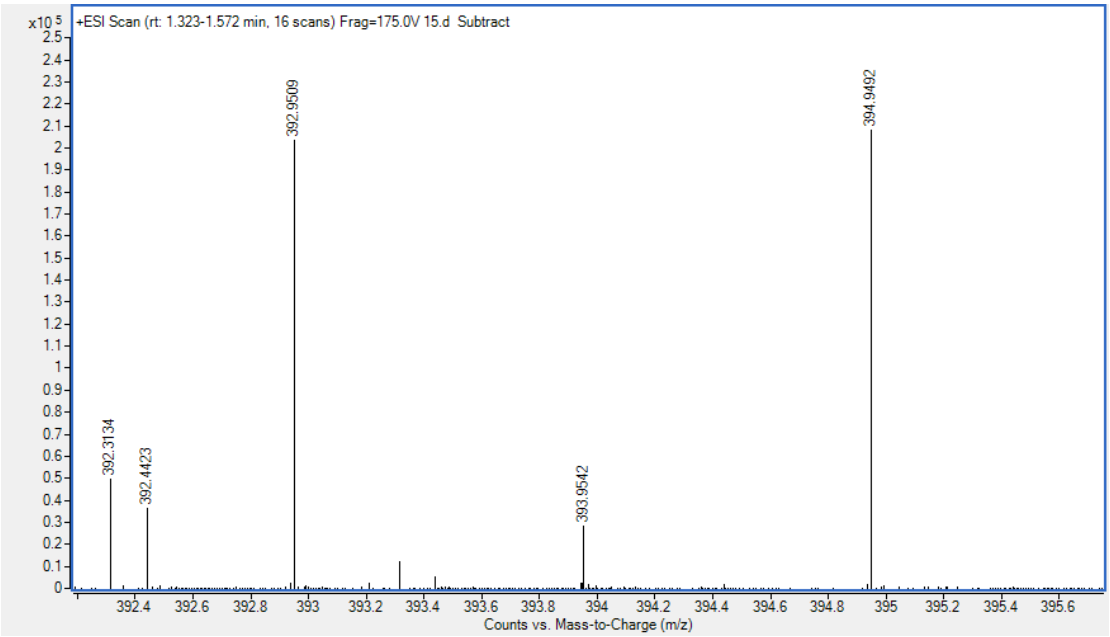
3b ^{1}H NMR



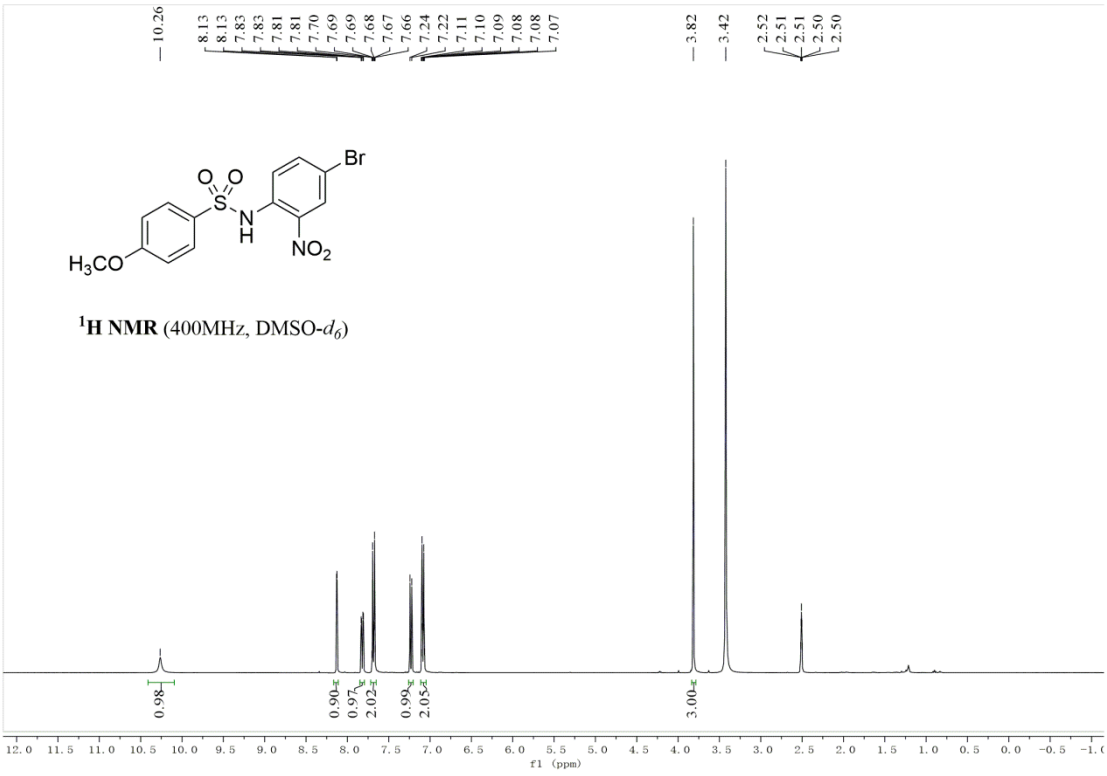
3b ^{13}C NMR



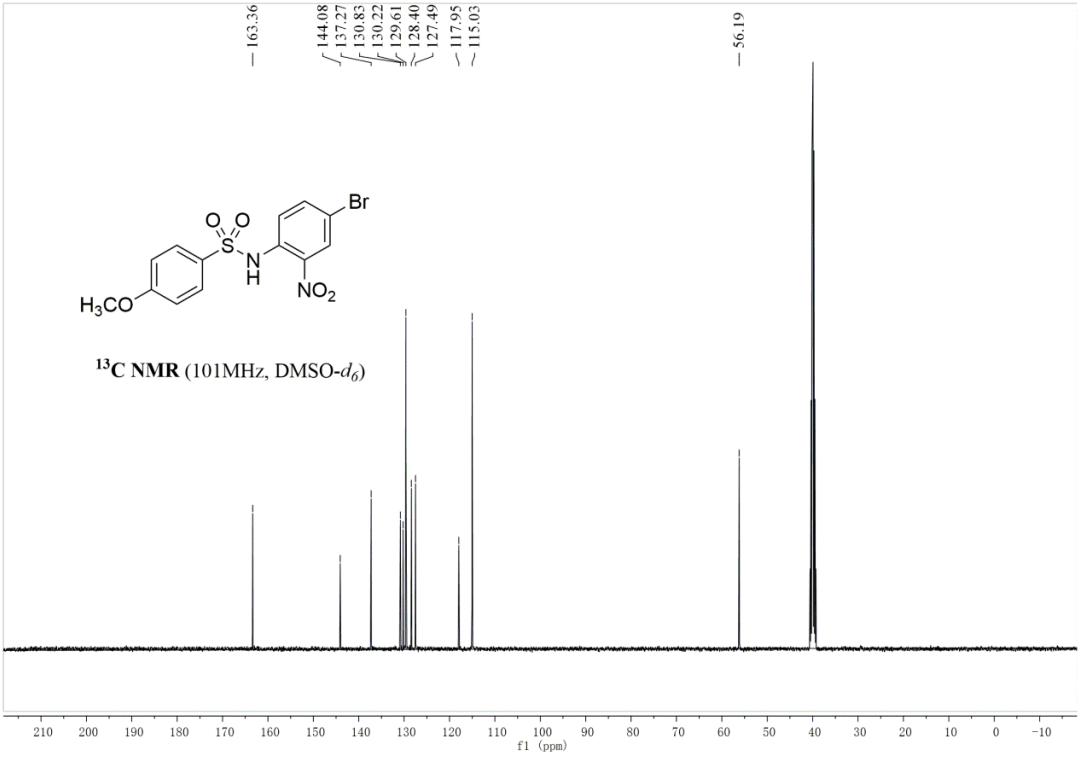
3b $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9509.



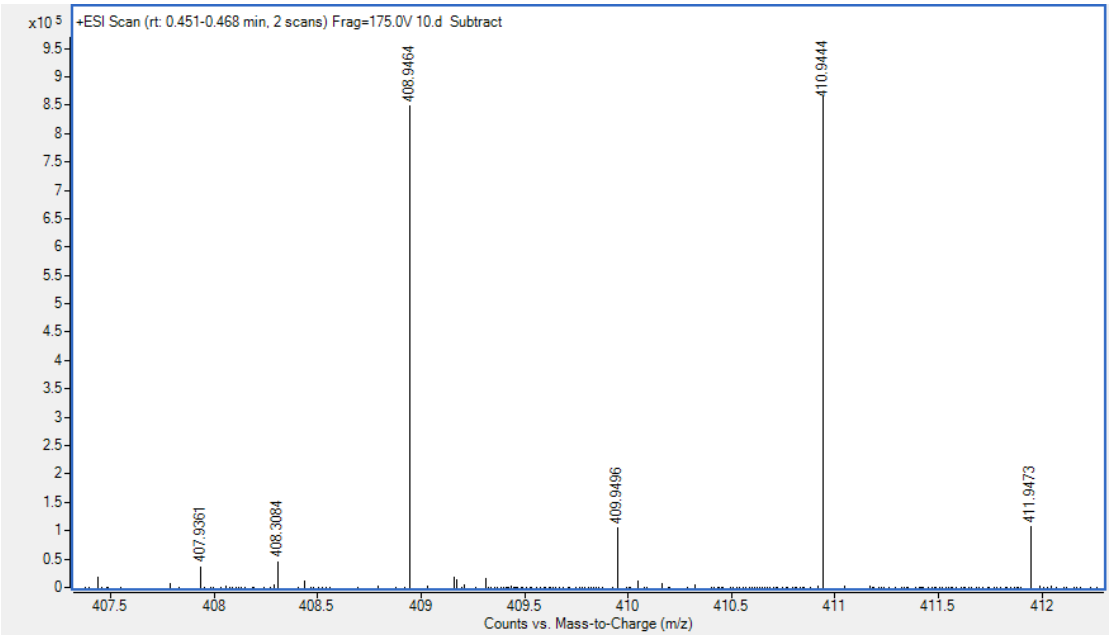
3c ^{1}H NMR



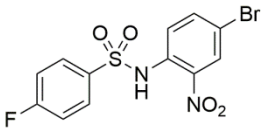
3c ^{13}C NMR



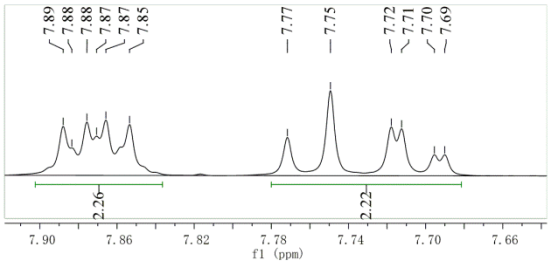
3c $C_{13}H_{11}BrN_2O_5S$, $[M+Na]^+$ 408.9470. Found 408.9464

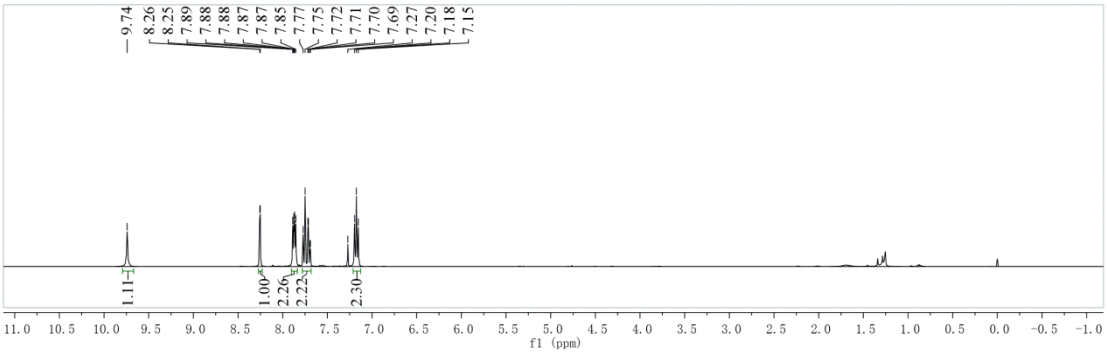


3d ^{1}H NMR

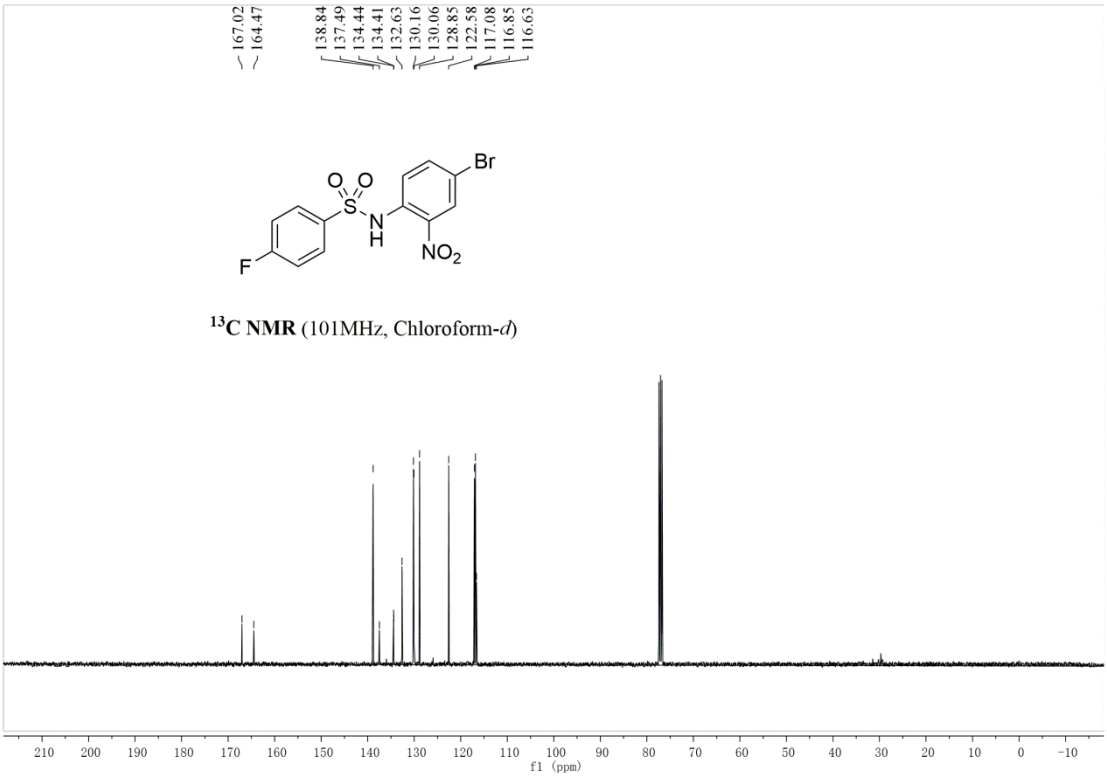


^{1}H NMR (400MHz, Chloroform-*d*)





3d ^{13}C NMR


167.02
164.47
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137.49
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134.41
132.63
130.16
130.06
128.85
122.58
117.08
116.85
116.63
Br
O
O
S
N
H
F
NO2
13C NMR (101MHz, Chloroform-d)
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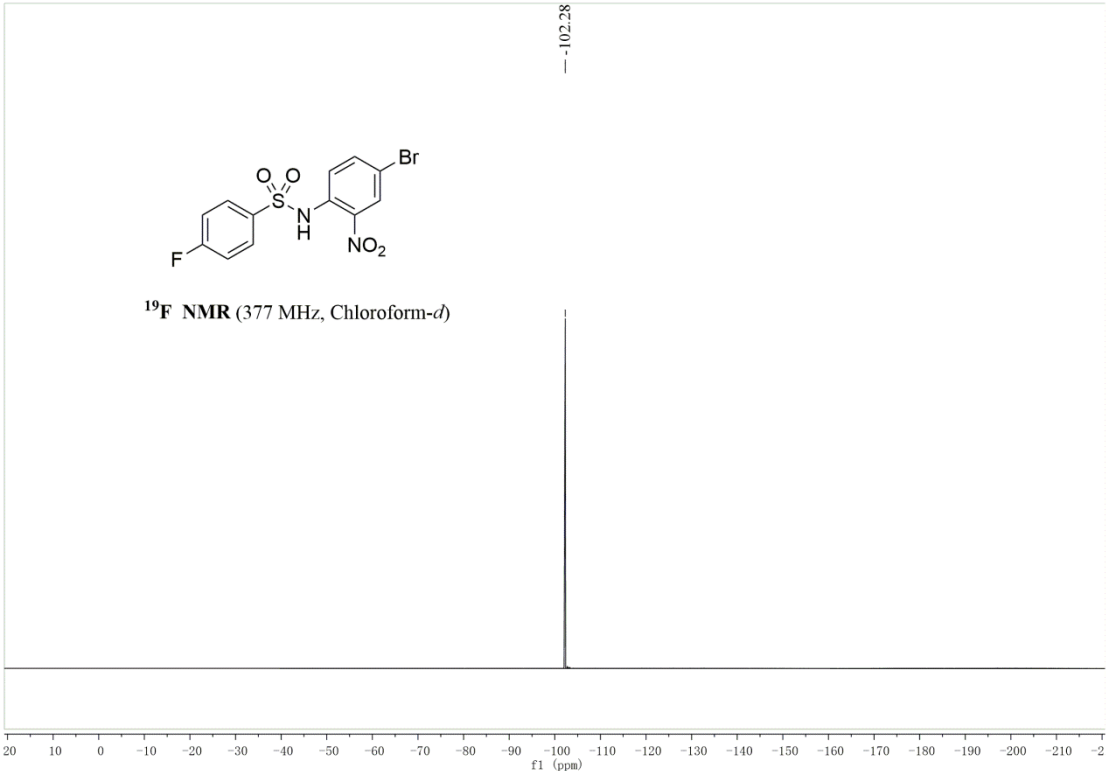
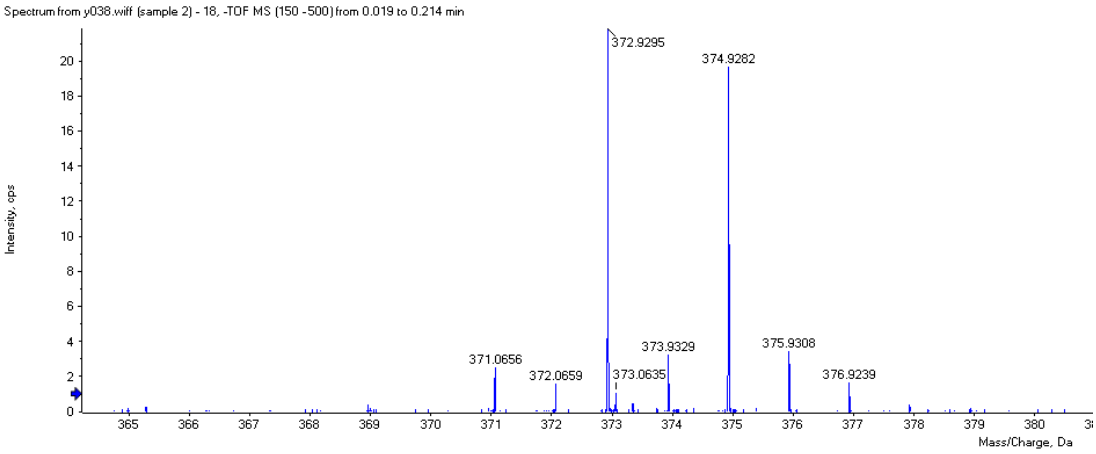
f1 (ppm)

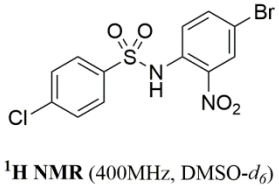
3d ^{19}F NMR


-102.28
Br
O
O
S
N
H
F
NO2
19F NMR (377 MHz, Chloroform-d)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -2
f1 (ppm)

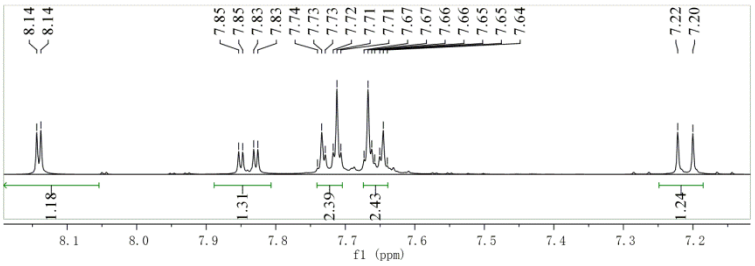
3d $C_{12}H_8BrFN_2O_4S$, $[M-H]^-$ 372.9294. Found 372.9295.

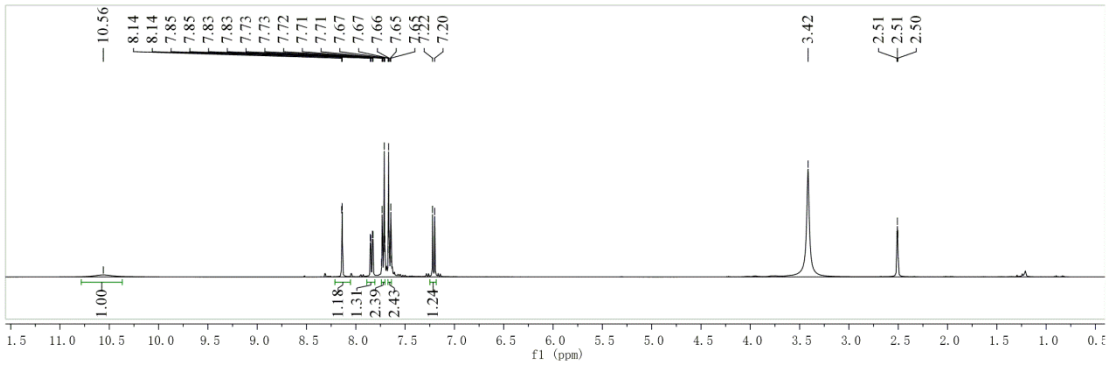


3e ^{1}H NMR

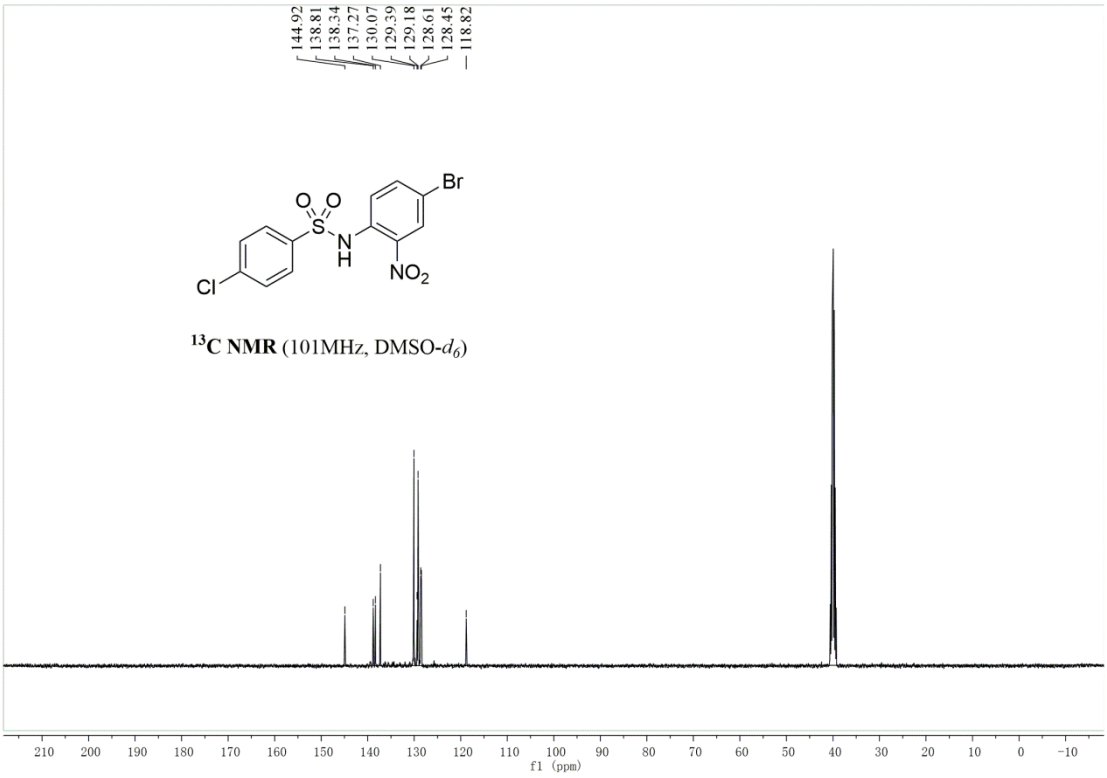


^{1}H NMR (400MHz, DMSO-d_6)

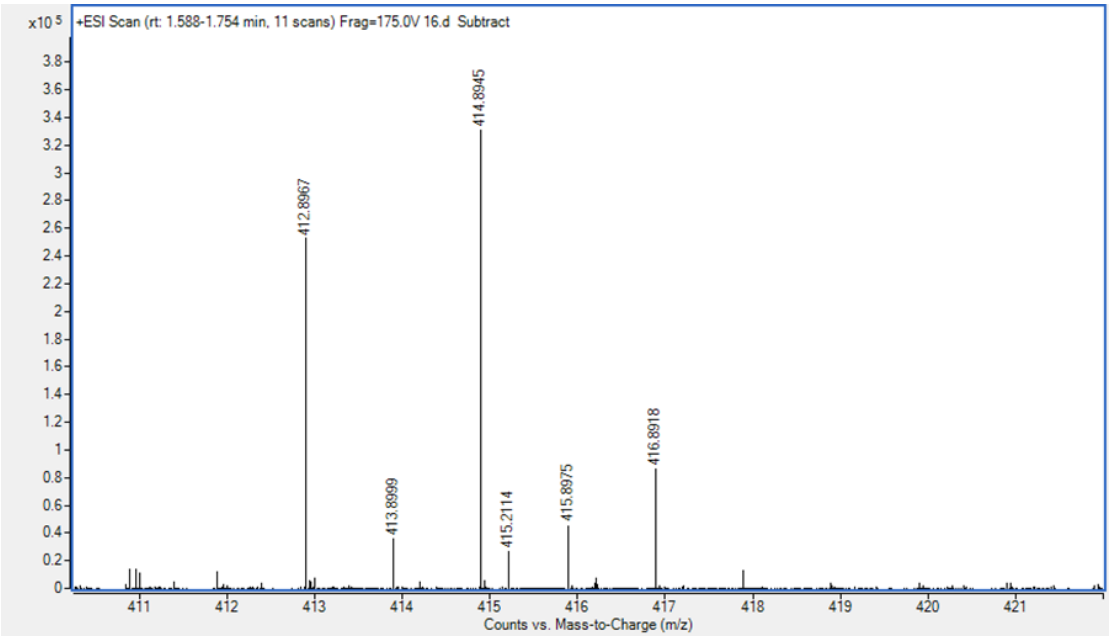




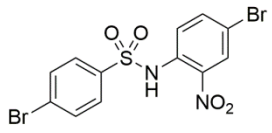
3e ^{13}C NMR



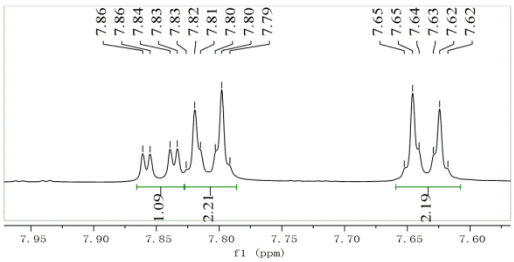
3e $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8967.

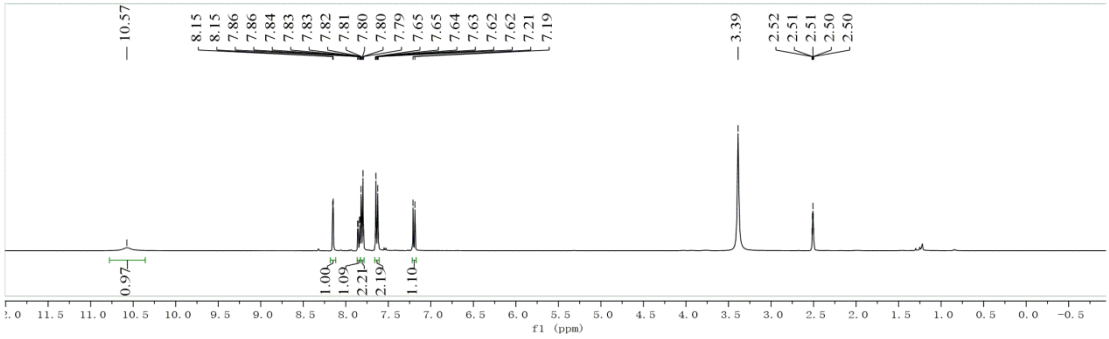


3f ^{1}H NMR

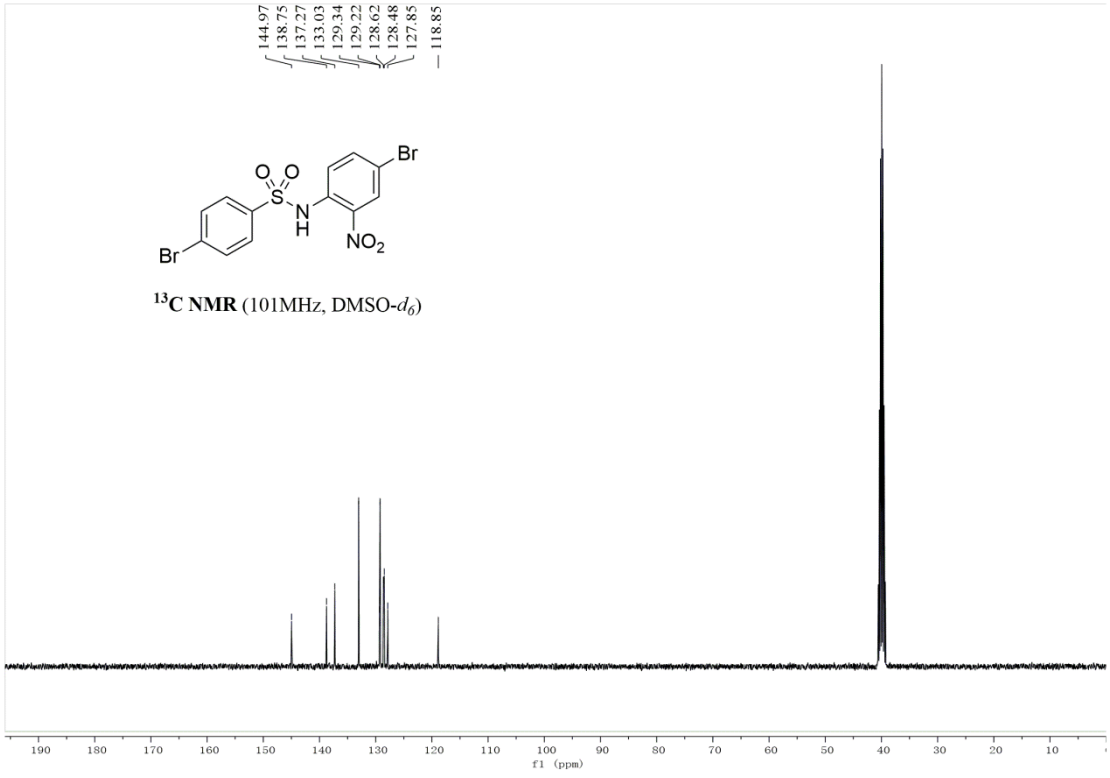


^{1}H NMR (400MHz, DMSO-d_6)



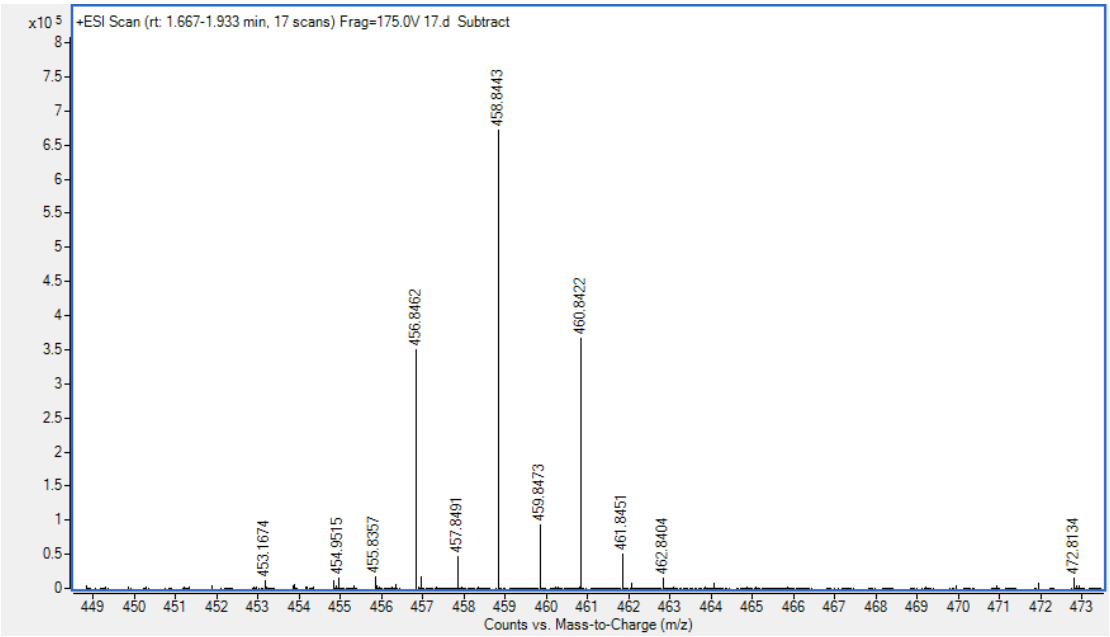


3f ^{13}C NMR

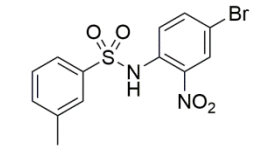


^{13}C NMR (101MHz, DMSO-d_6)

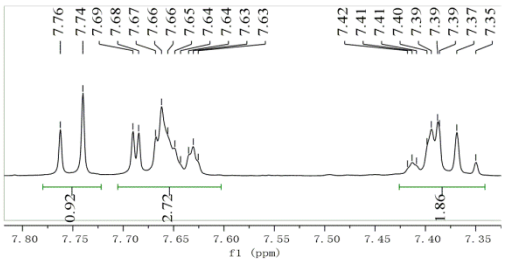
3f $C_{12}H_8Br_2N_2O_4S$, $[M+Na]^+$ 458.8449. Found 458.8443.

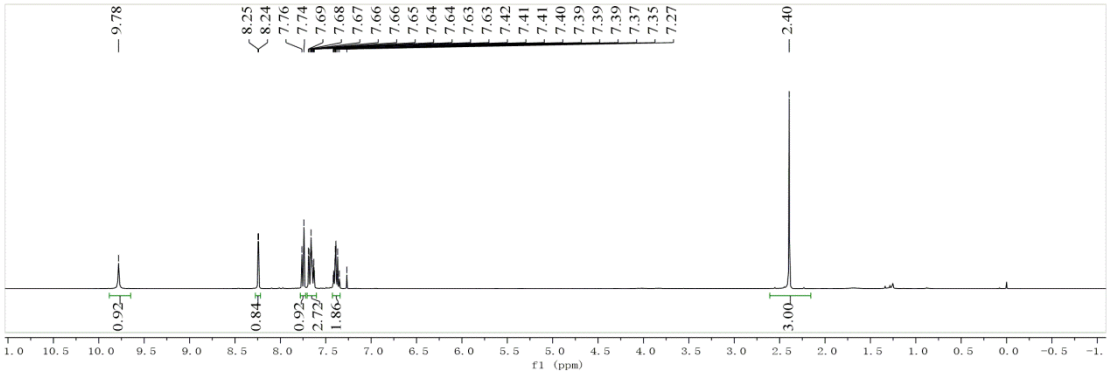


3i ^{1}H NMR

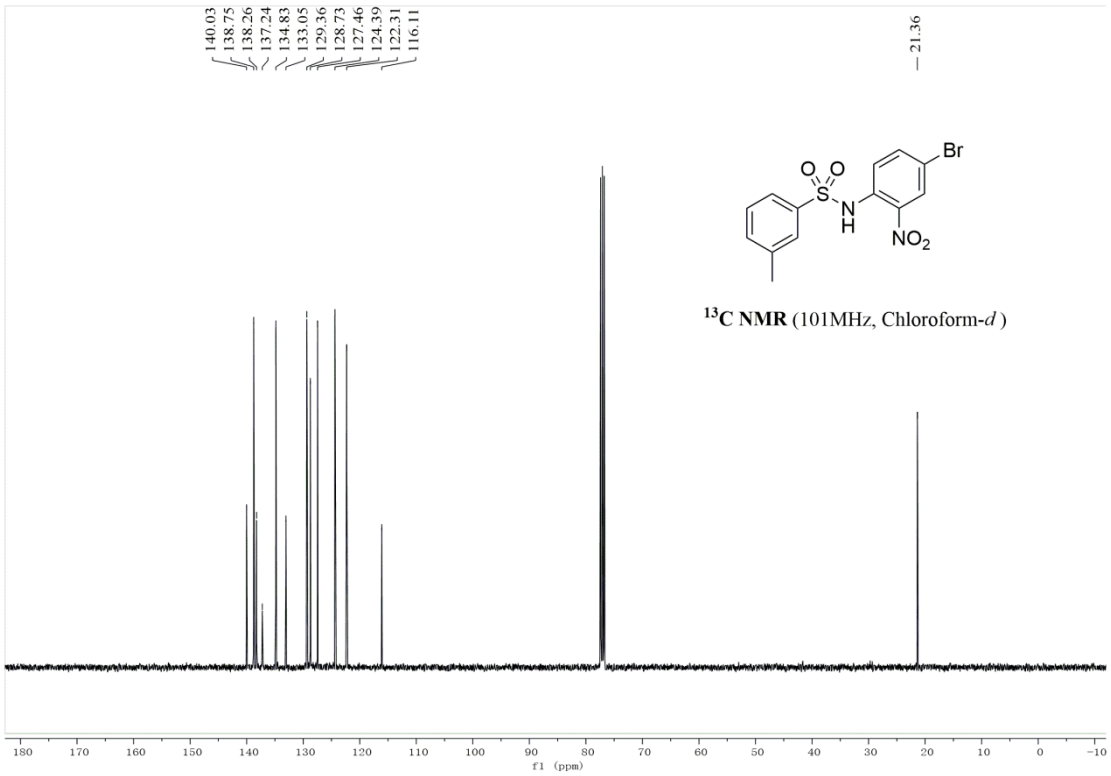


^{1}H NMR (400MHz, Chloroform-*d*)



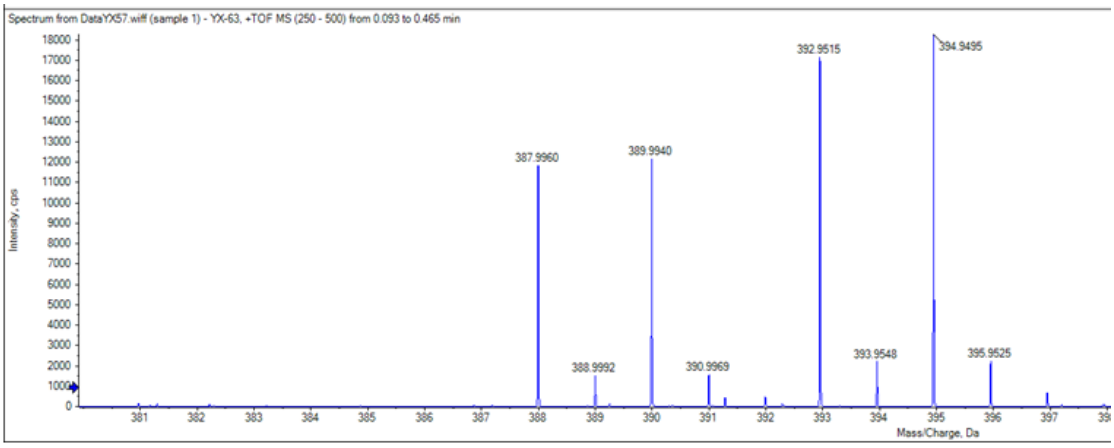


3i ^{13}C NMR

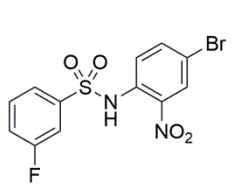


^{13}C NMR (101MHz, Chloroform-*d*)

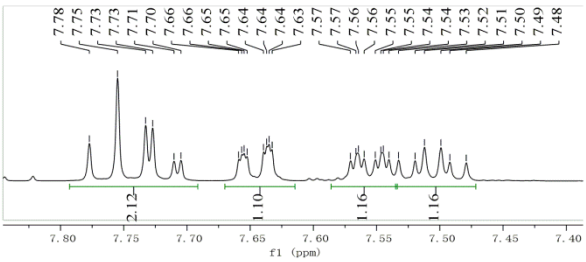
3i $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9515.

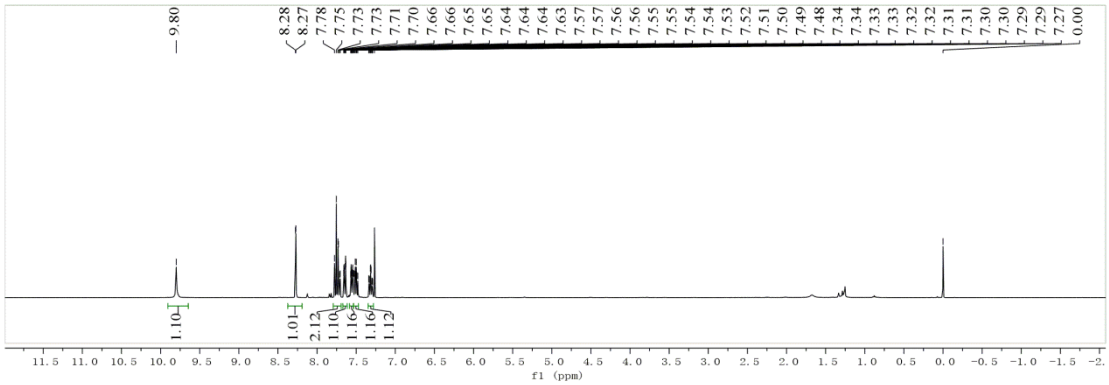


3j ^{1}H NMR

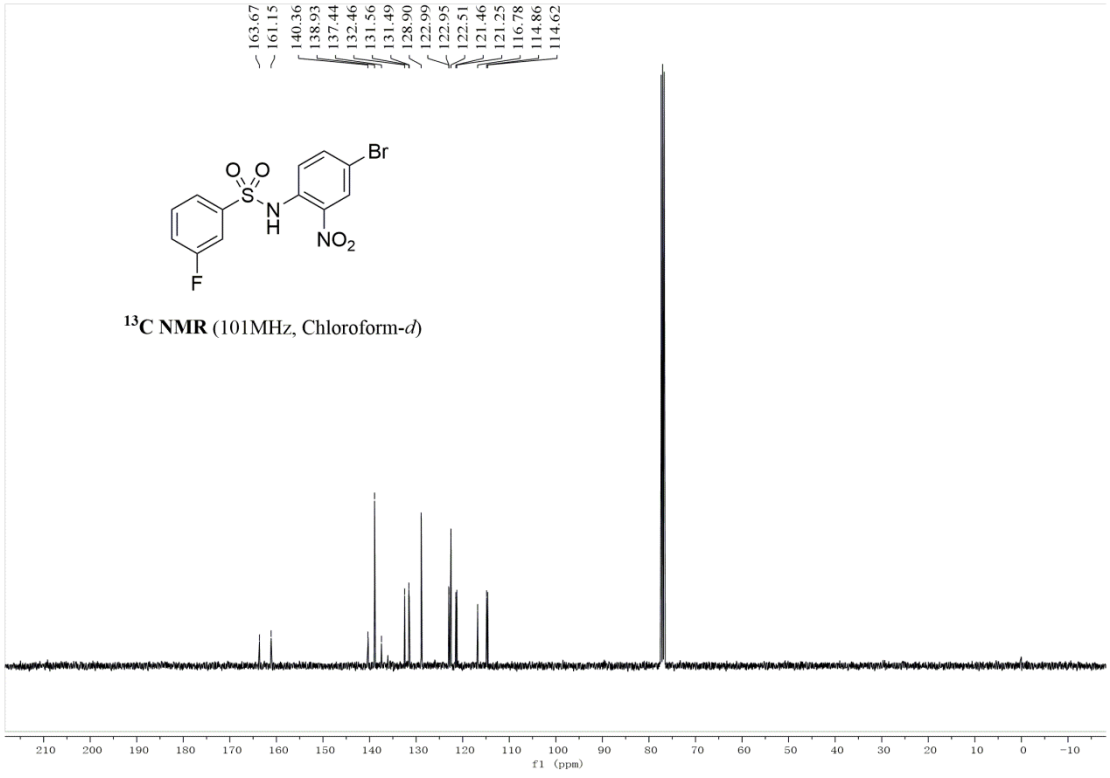


^{1}H NMR (400MHz, Chloroform-*d*)



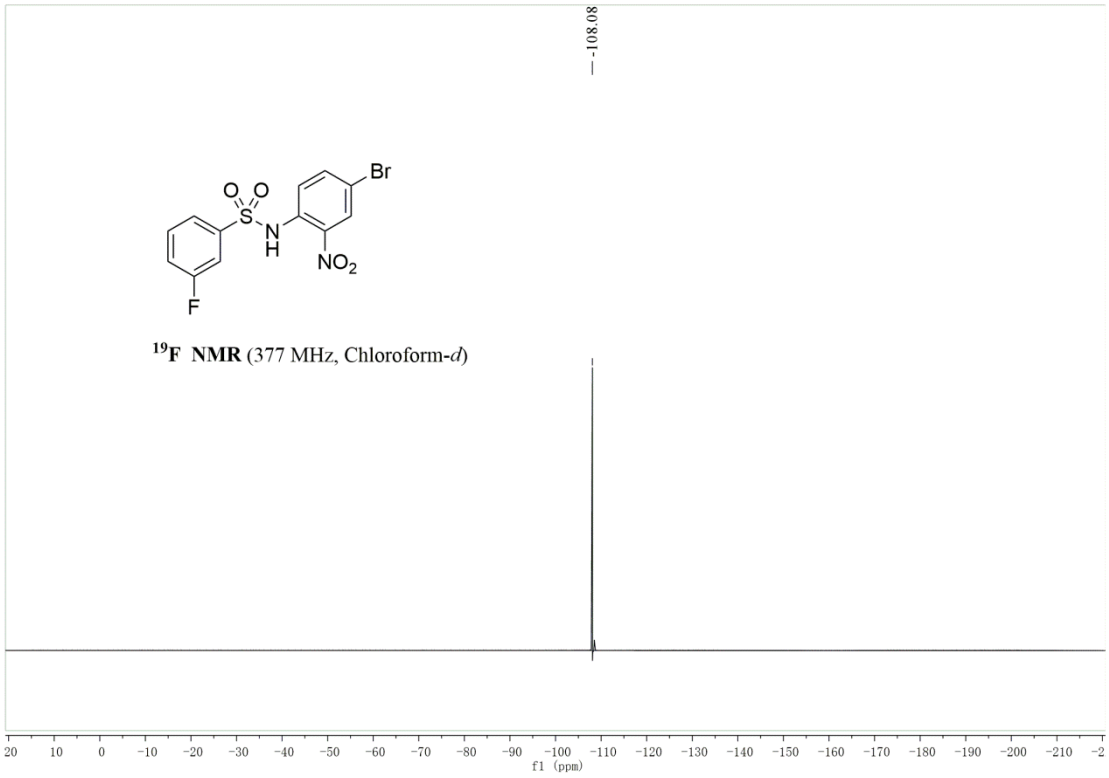


3j ^{13}C NMR

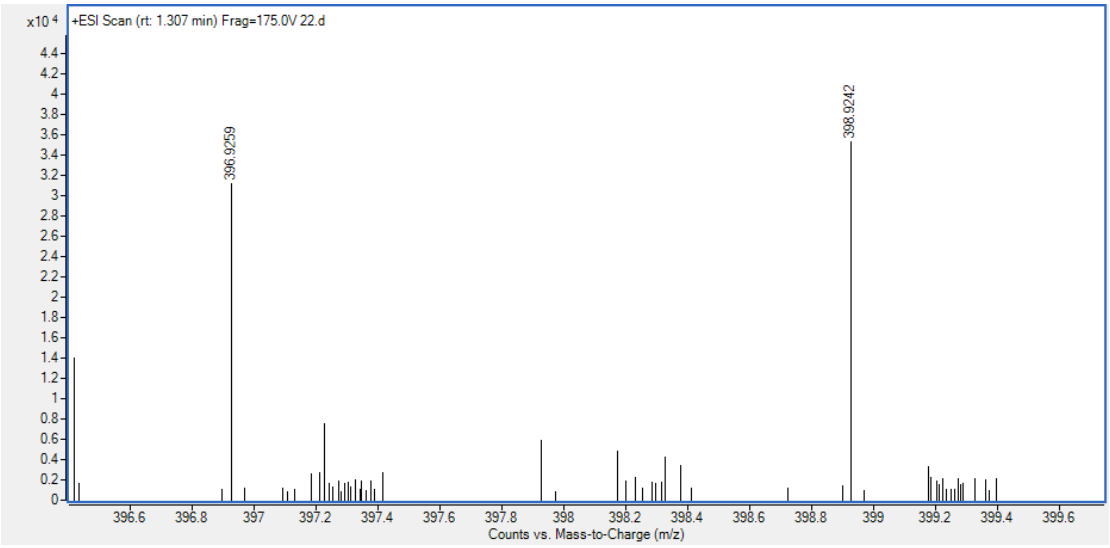


^{13}C NMR (101MHz, Chloroform-*d*)

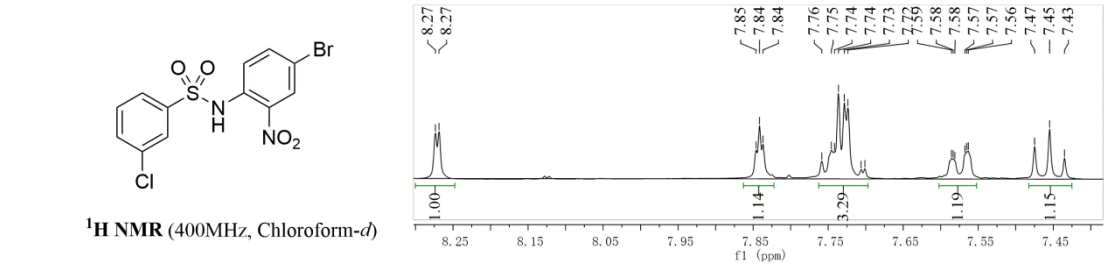
3j ^{19}F NMR



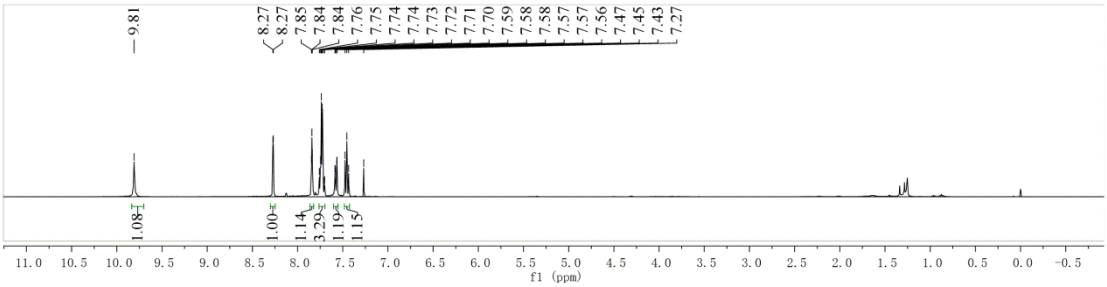
3j $C_{12}H_8BrFN_2O_4S$, $[M+Na]^+$ 396.9270. Found 396.9259.



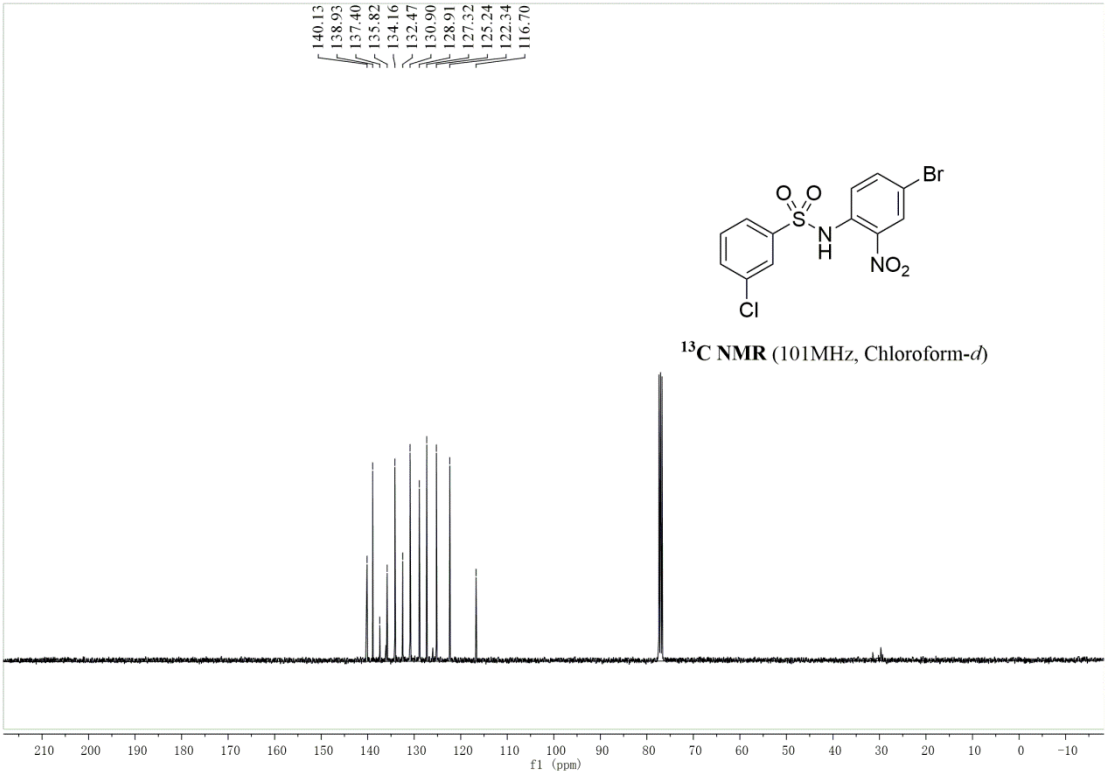
3k ^{1}H NMR



^{1}H NMR (400MHz, Chloroform-*d*)

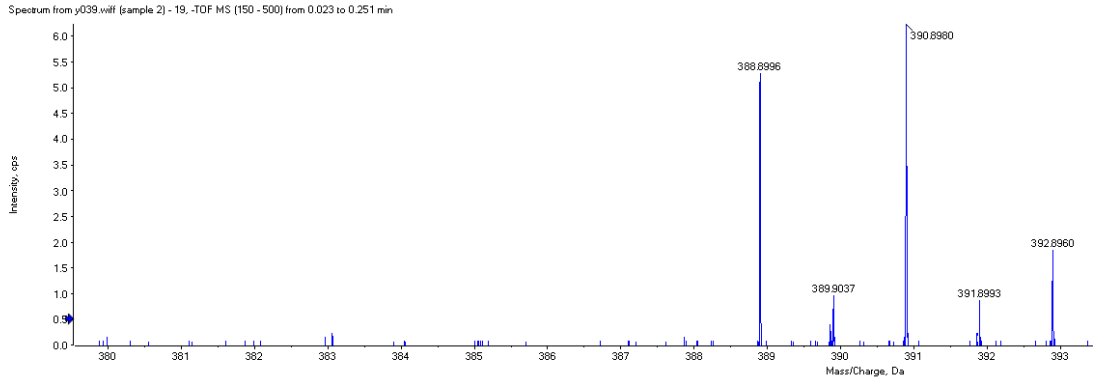


3k ^{13}C NMR

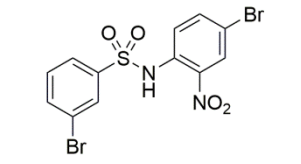


^{13}C NMR (101MHz, Chloroform-*d*)

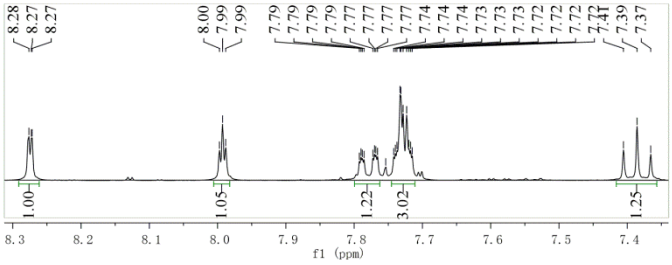
3k $C_{12}H_8BrClN_2O_4S$, $[M-H]^-$ 388.8998. Found 388.8996.

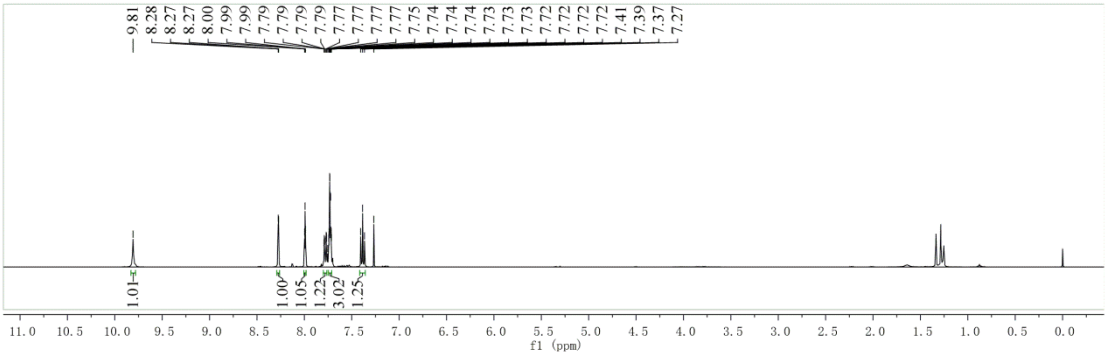


3l ^{1}H NMR

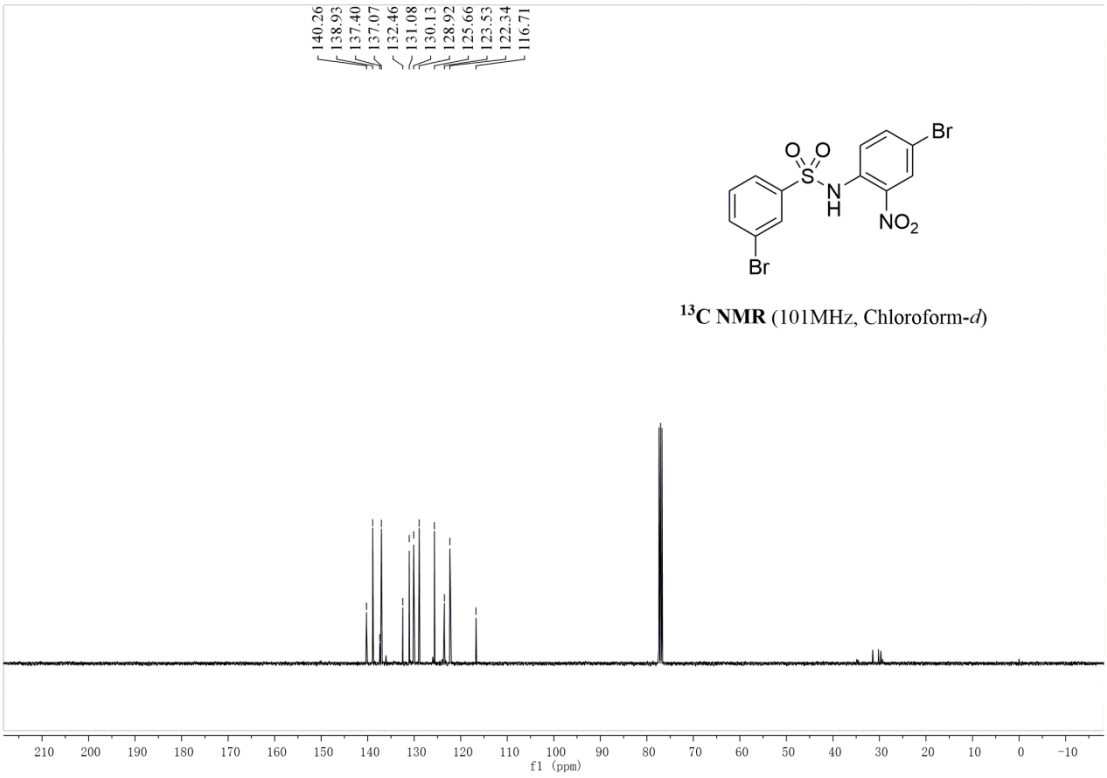


^{1}H NMR (400MHz, Chloroform-*d*)

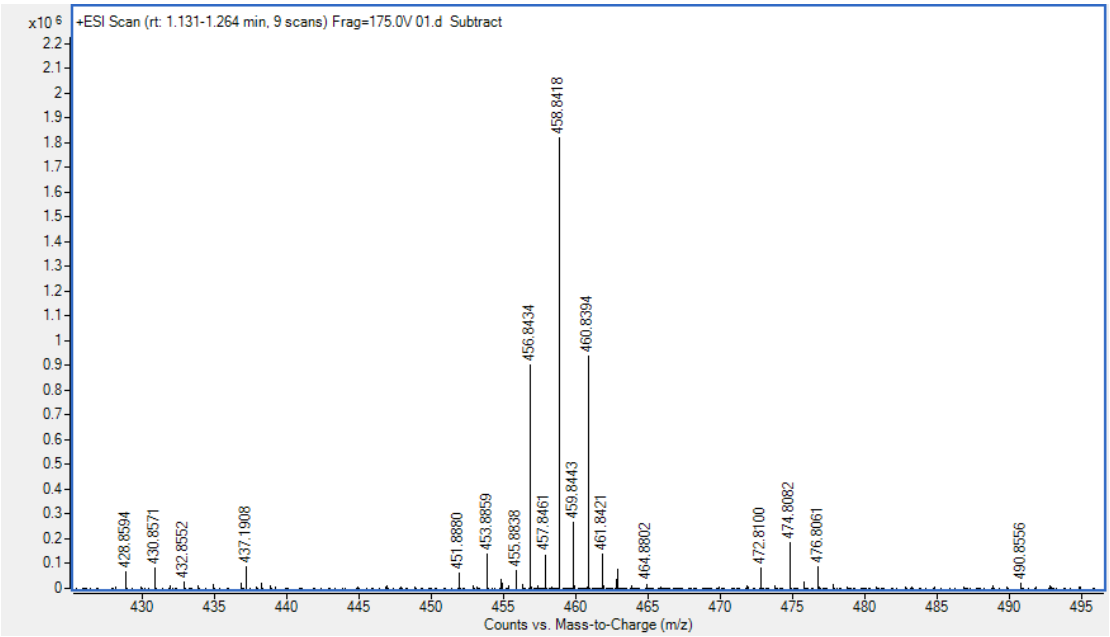




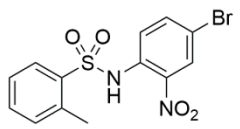
3l ^{13}C NMR



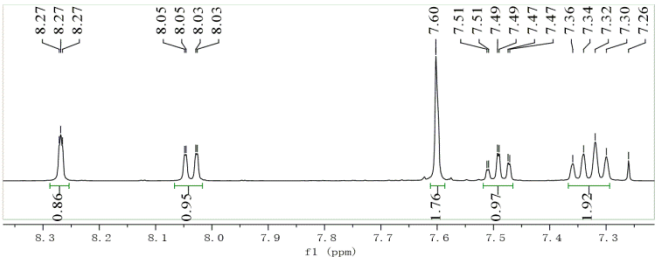
3l $C_{12}H_8Br_2N_2O_4S$, $[M+Na]^+$ 458.8449. Found 458.8418.

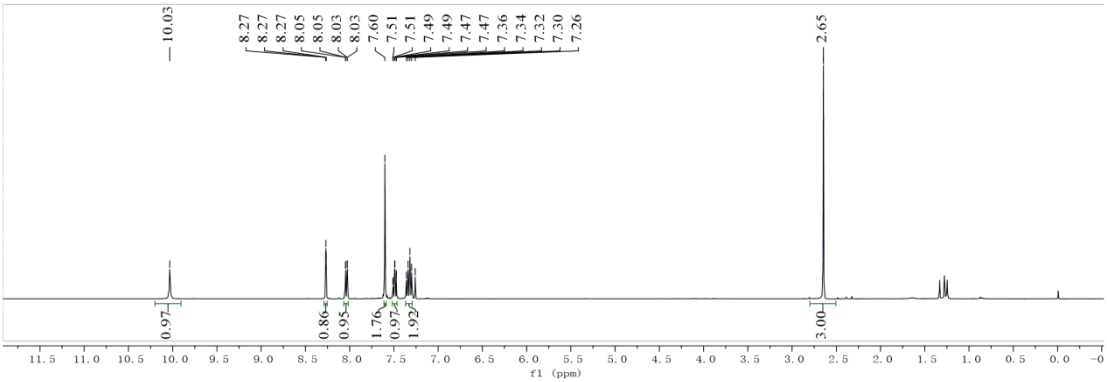


3o ^1H NMR

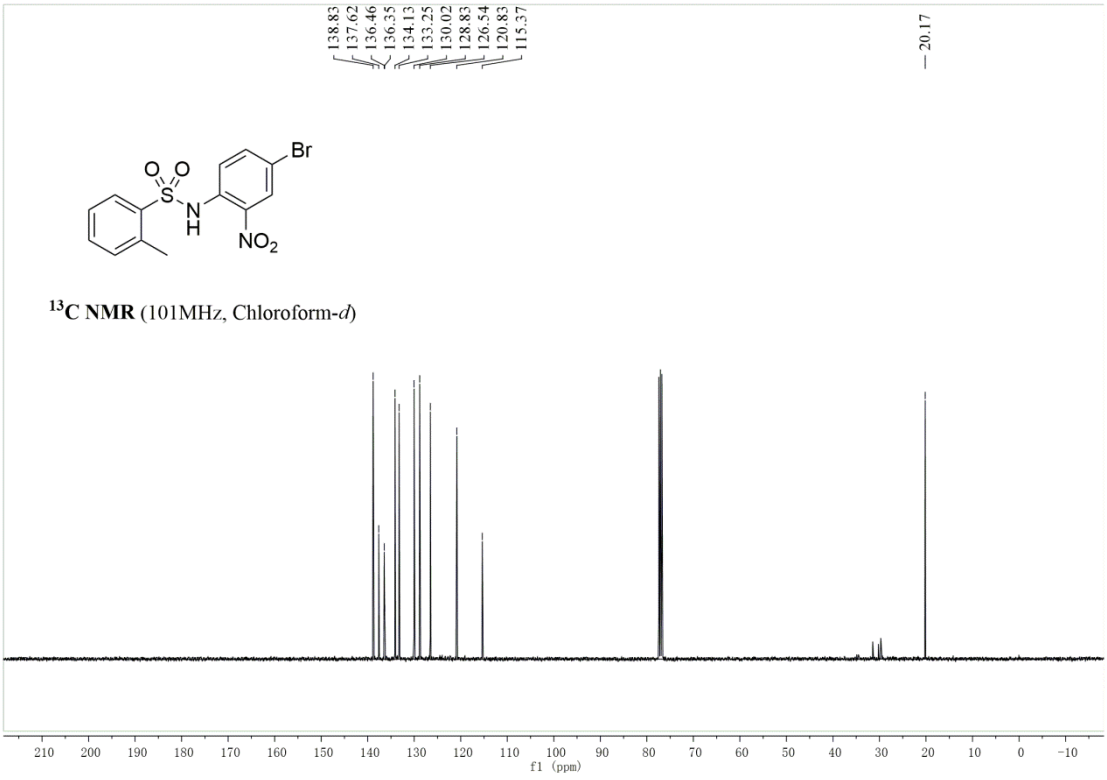


^{1}H NMR (400MHz, Chloroform-*d*)



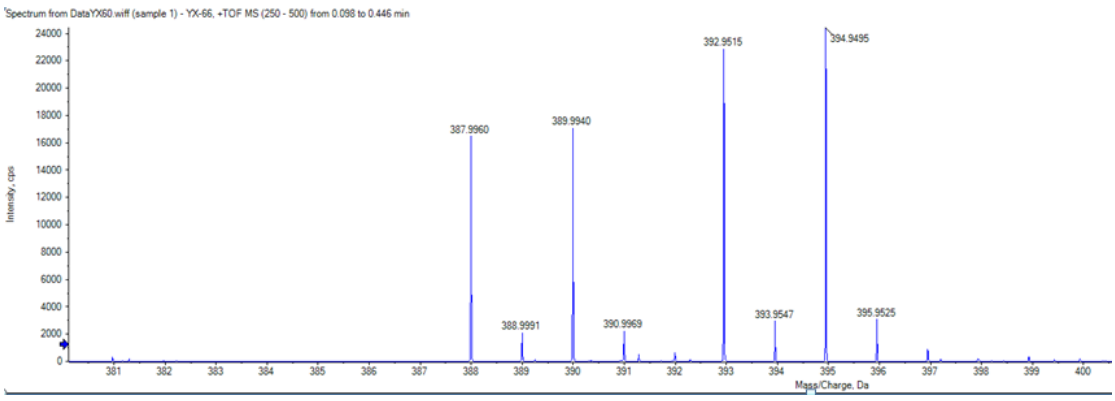


3o ^{13}C NMR

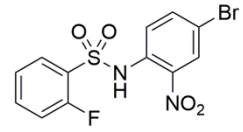


^{13}C NMR (101MHz, Chloroform-*d*)

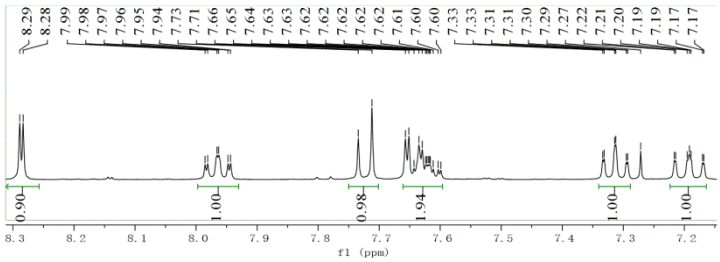
3o $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9515.

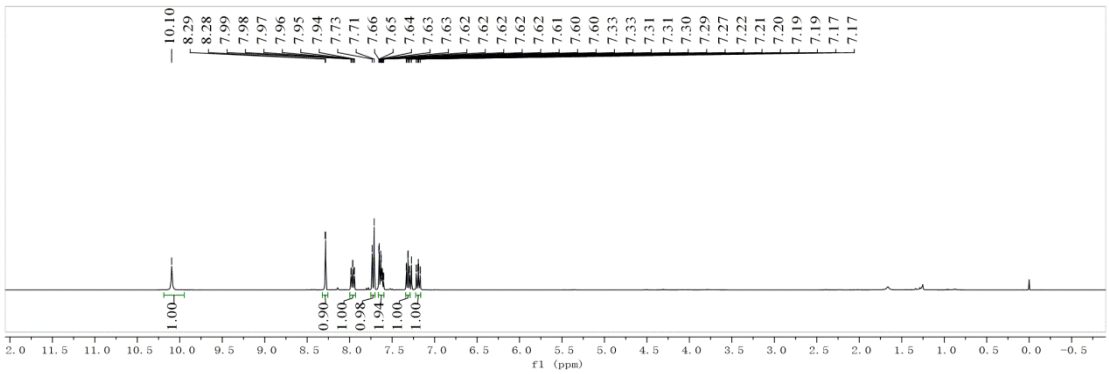


3p ^{1}H NMR

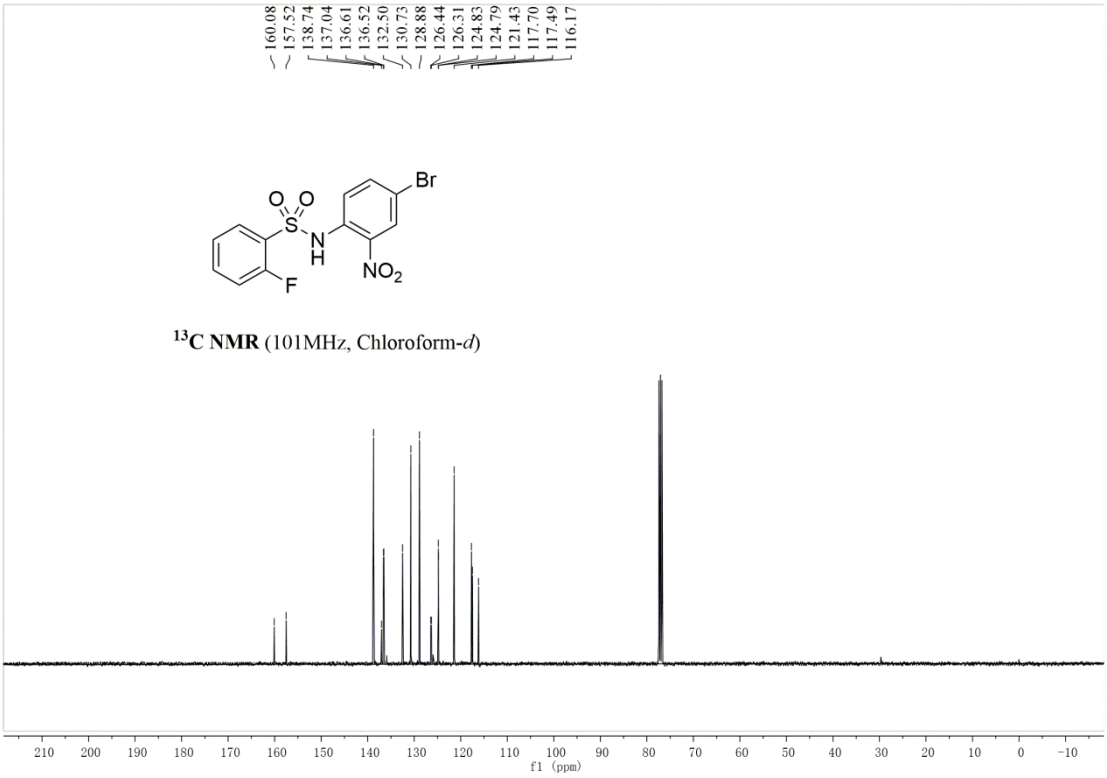


^{1}H NMR (400MHz, Chloroform-*d*)

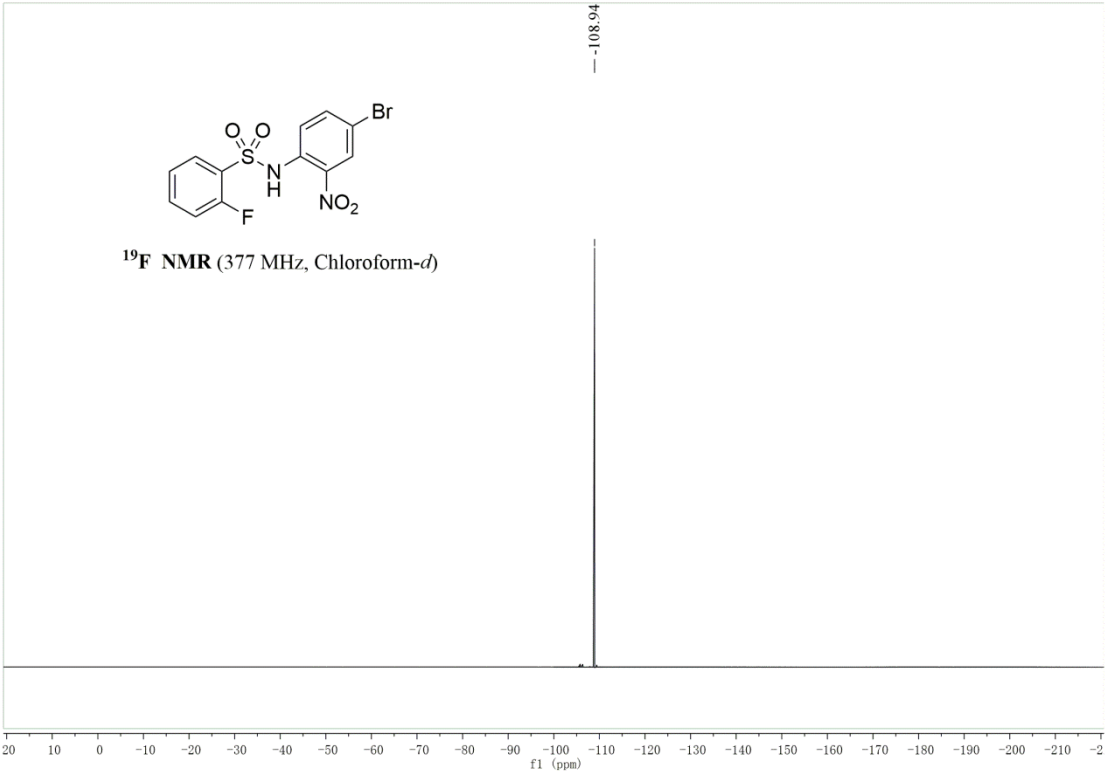




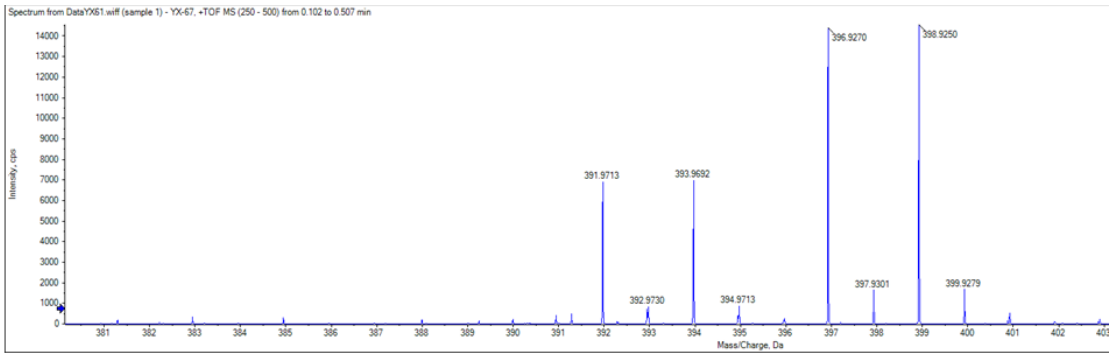
3p ^{13}C NMR


160.08
157.52
138.74
137.04
136.61
136.52
132.50
130.73
128.88
126.44
126.31
124.83
124.79
121.43
117.70
117.49
116.17
Br
O
O
S
N
H
NO2
F
13C NMR (101MHz, Chloroform-d)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

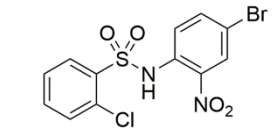
3p ^{19}F NMR


-108.94
Br
O
O
S
N
H
NO2
F
19F NMR (377 MHz, Chloroform-d)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -2
f1 (ppm)

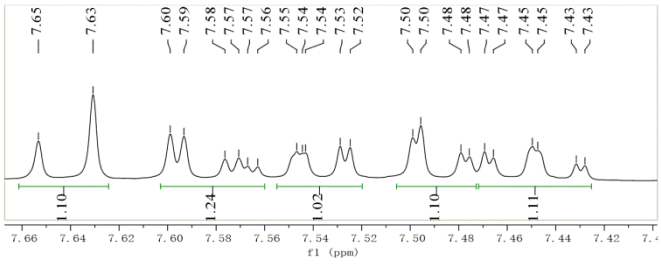
3p $C_{12}H_8BrFN_2O_4S$, $[M+Na]^+$ 396.9270. Found 396.9270.

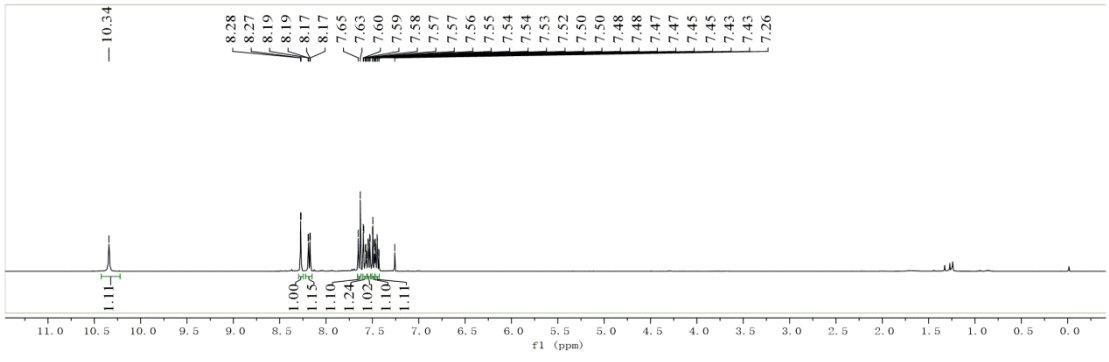


3q ^{1}H NMR

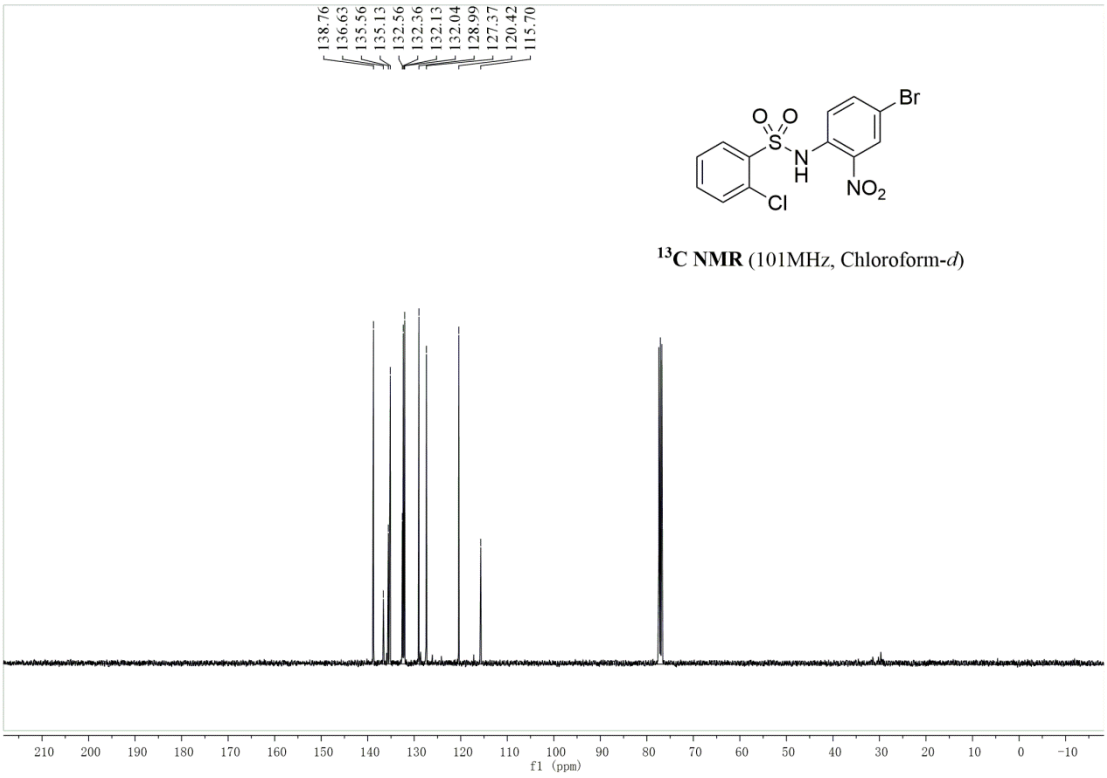


^{1}H NMR (400MHz, Chloroform-*d*)

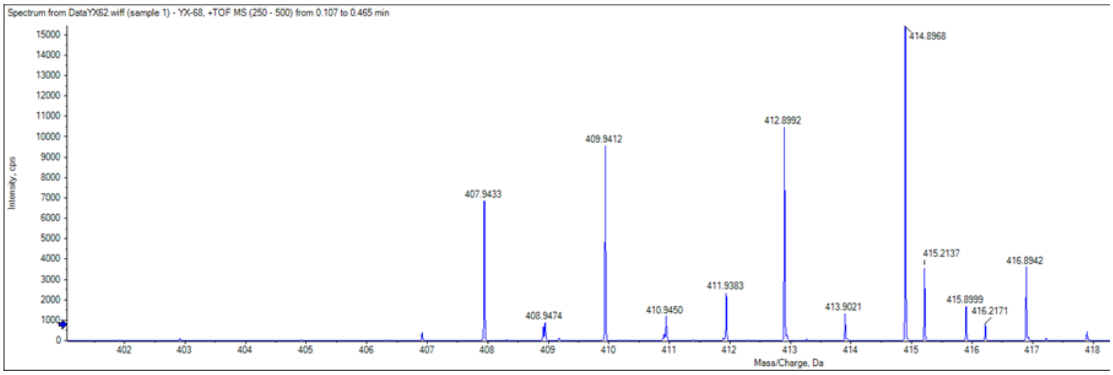




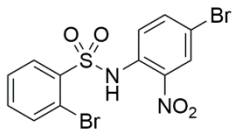
3q ^{13}C NMR



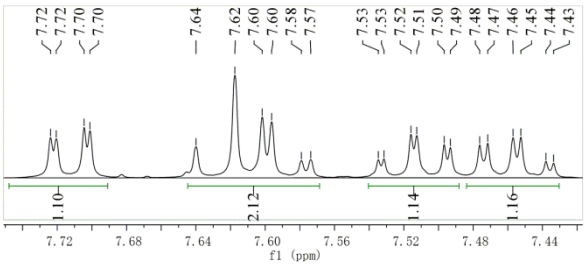
3q $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8992.

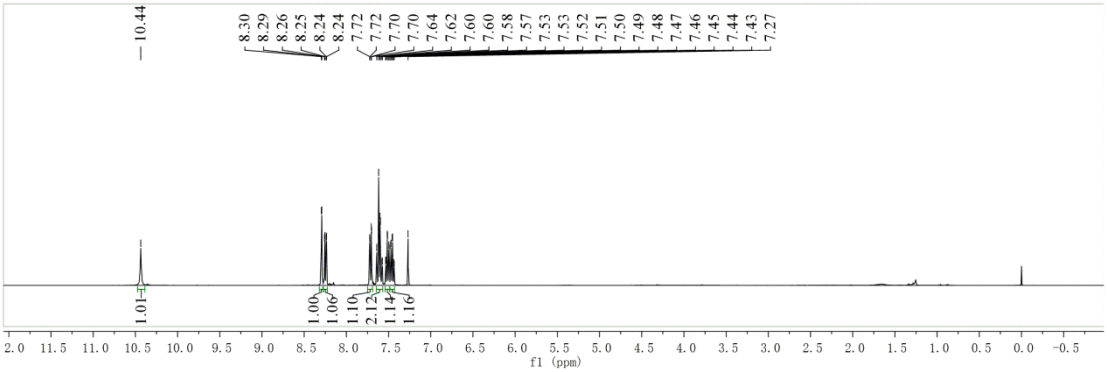


3r ^{1}H NMR

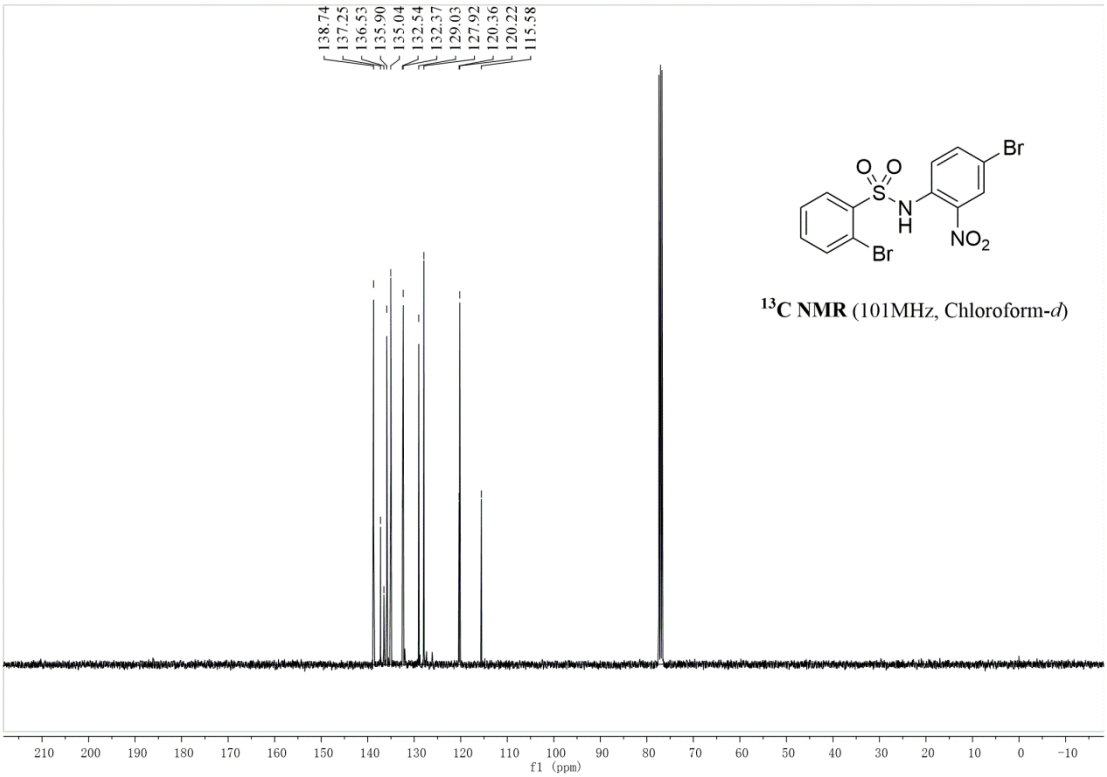


^{1}H NMR (400MHz, Chloroform-*d*)



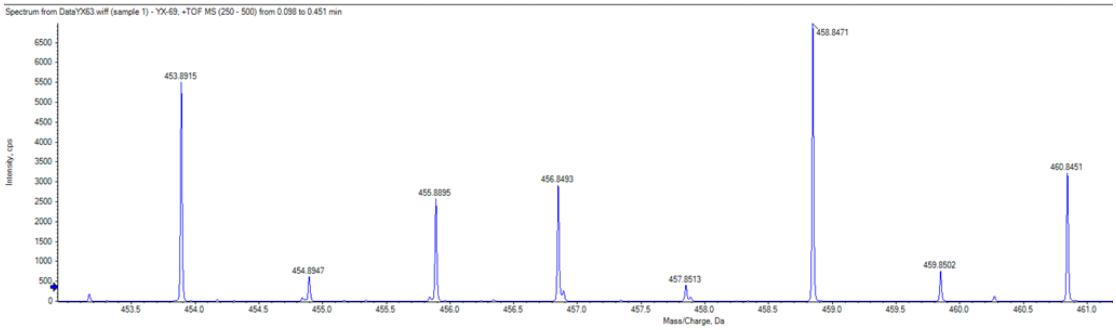


3r ^{13}C NMR

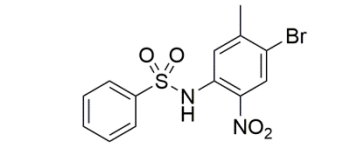


^{13}C NMR (101MHz, Chloroform-*d*)

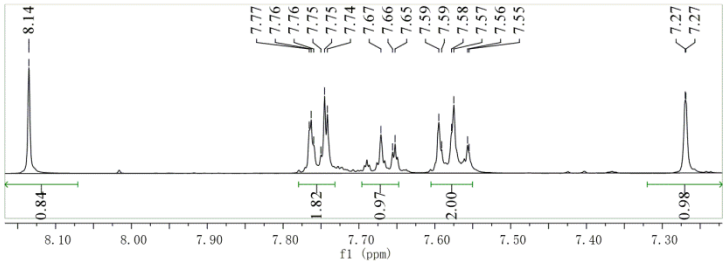
3r $C_{12}H_8Br_2N_2O_4S$, $[M+Na]^+$ 458.8449. Found 458.8471.

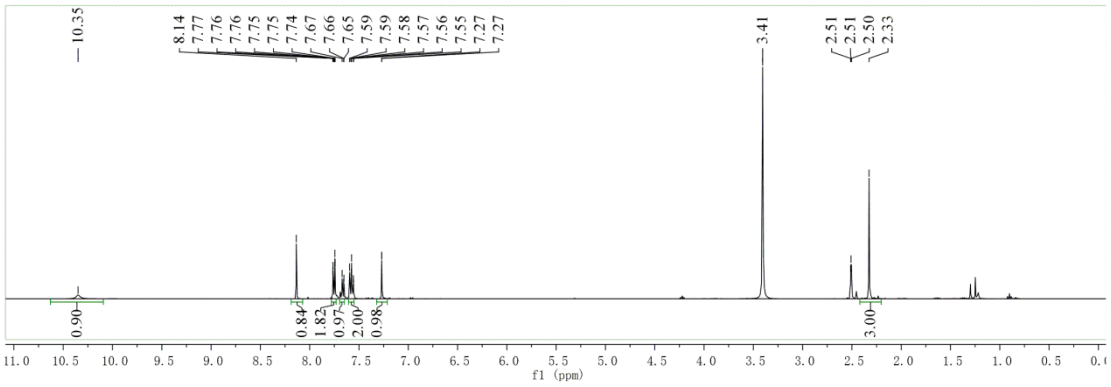


3u ^{1}H NMR

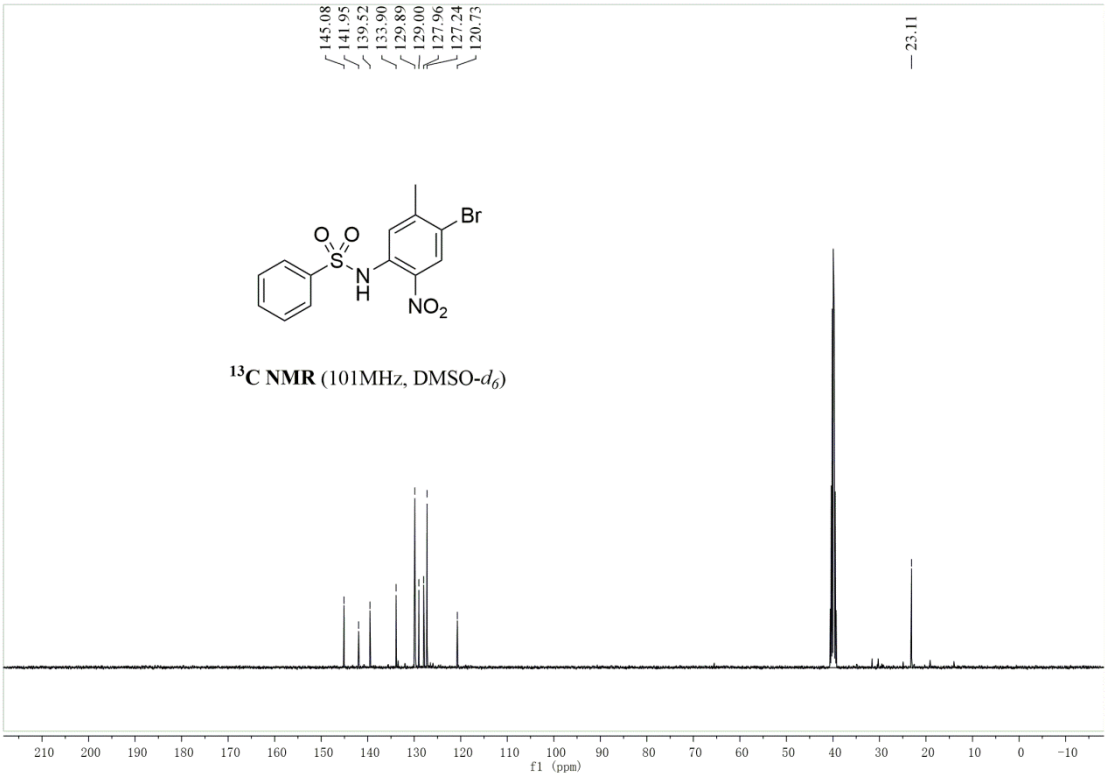


^{1}H NMR (400MHz, Chloroform-*d*)

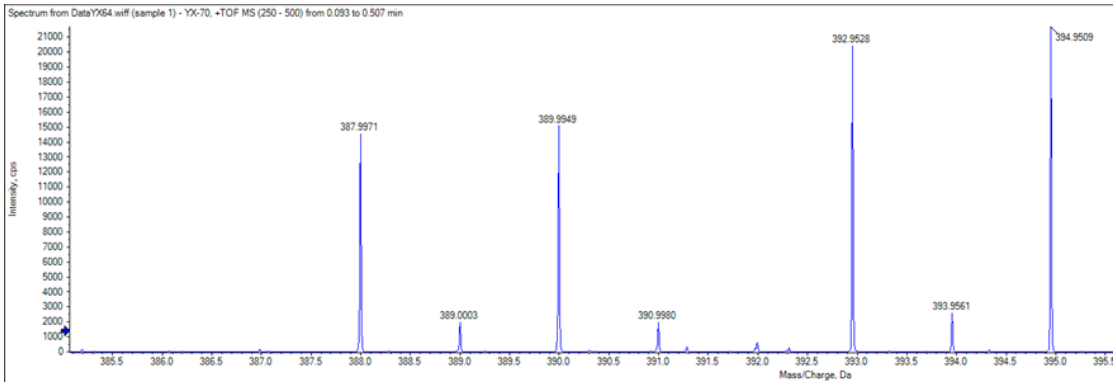




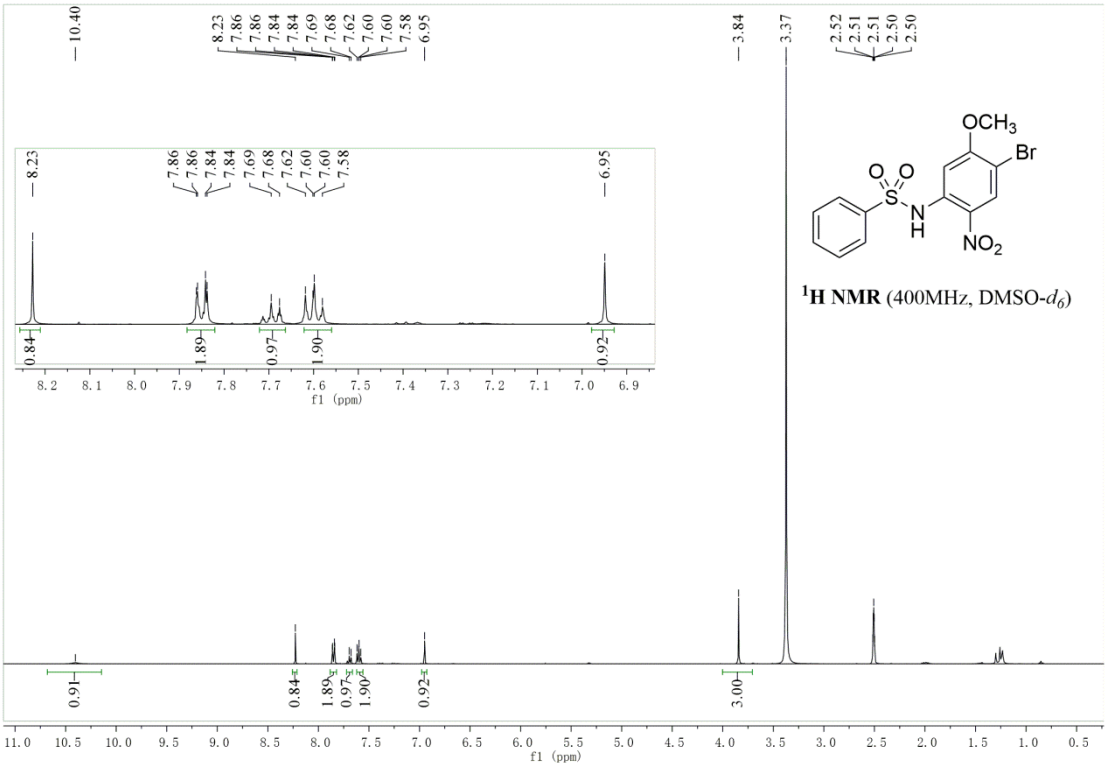
3u ^{13}C NMR



3u $C_{13}H_{11}BrN_2O_4S$, $[M+Na]^+$ 392.9521. Found 392.9528.

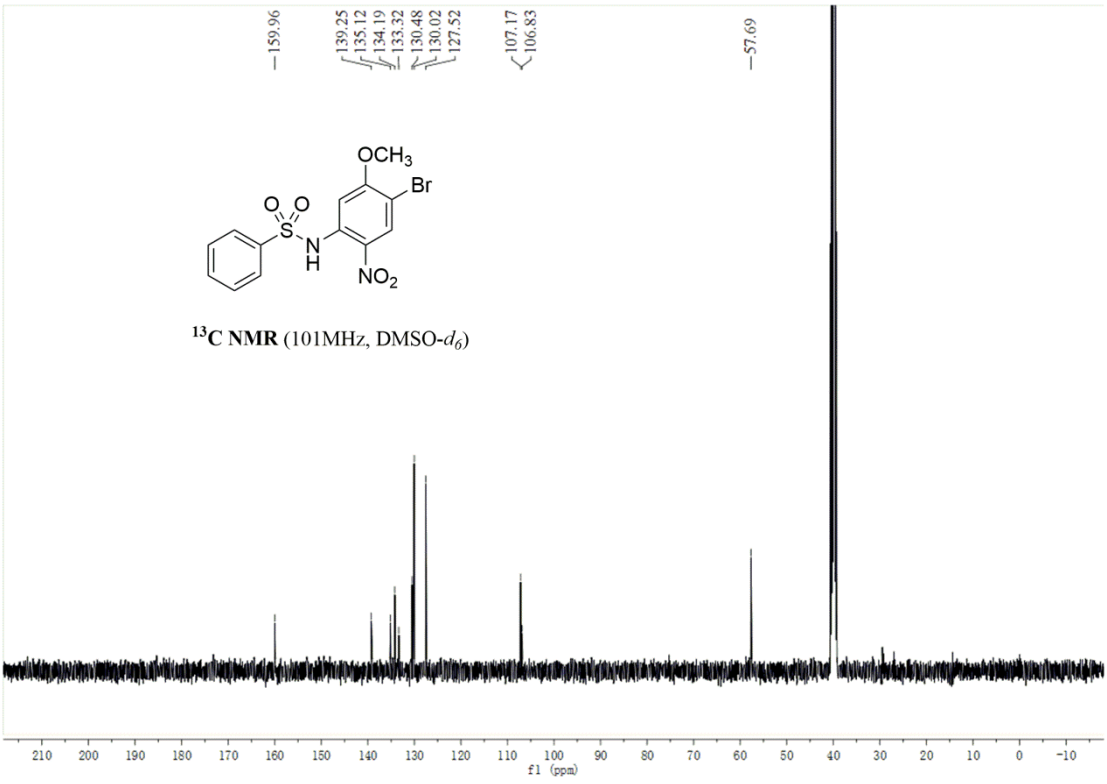


3v ^{1}H NMR



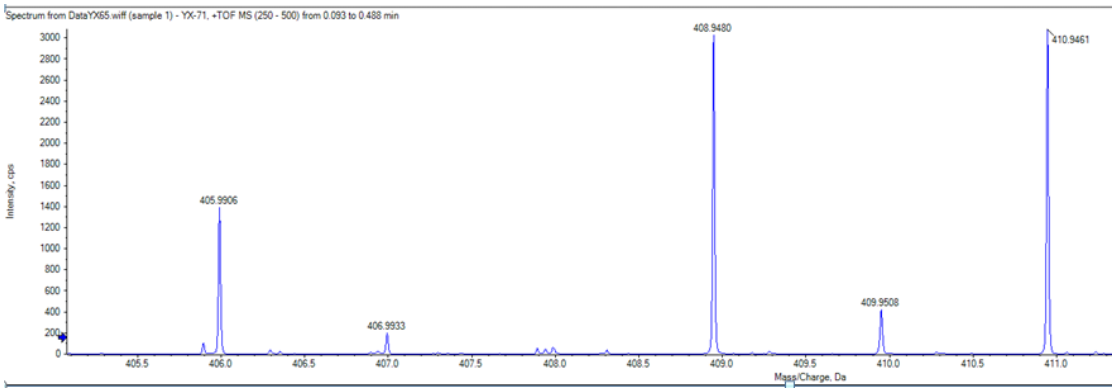
^{1}H NMR (400MHz, DMSO-d_6)

3v ^{13}C NMR

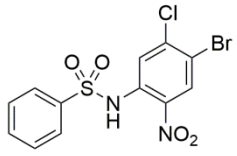


^{13}C NMR (101MHz, DMSO-d_6)

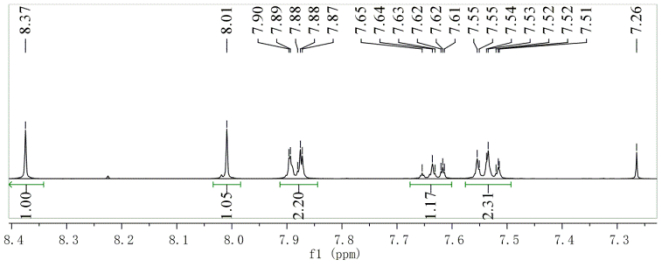
3v $C_{13}H_{11}BrN_2O_5S$, $[M+Na]^+$ 408.9470. Found 408.9480

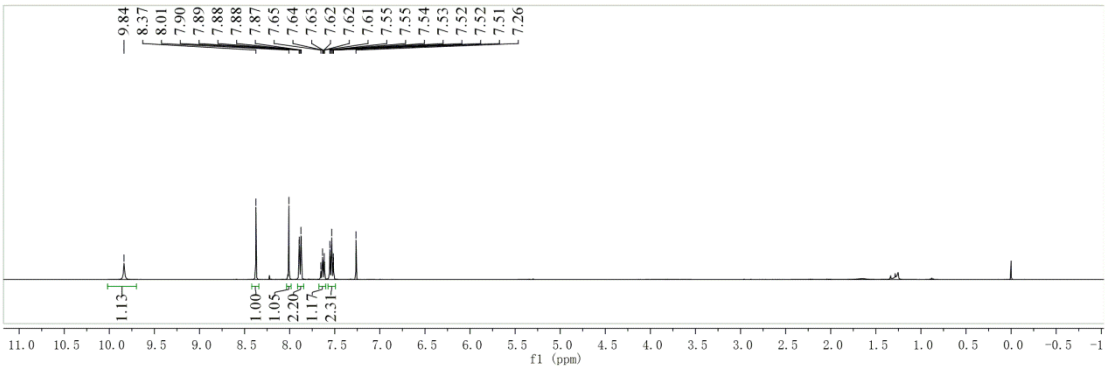


3w ^{1}H NMR

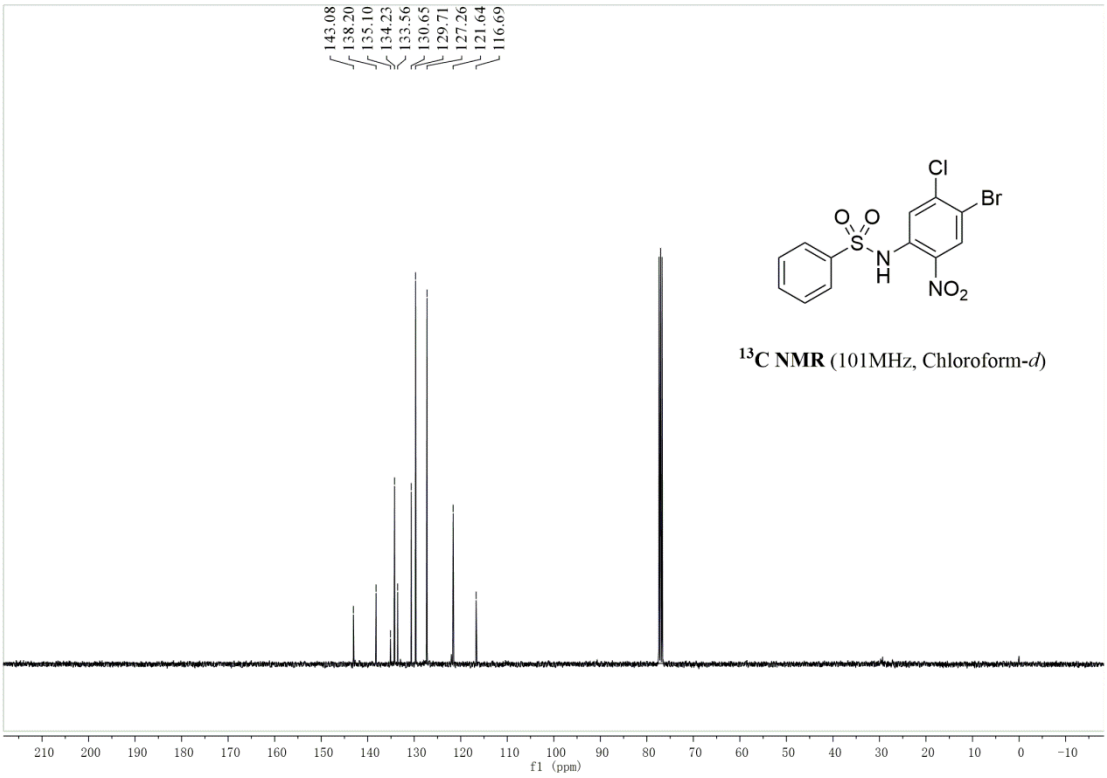


^{1}H NMR (400MHz, Chloroform-*d*)

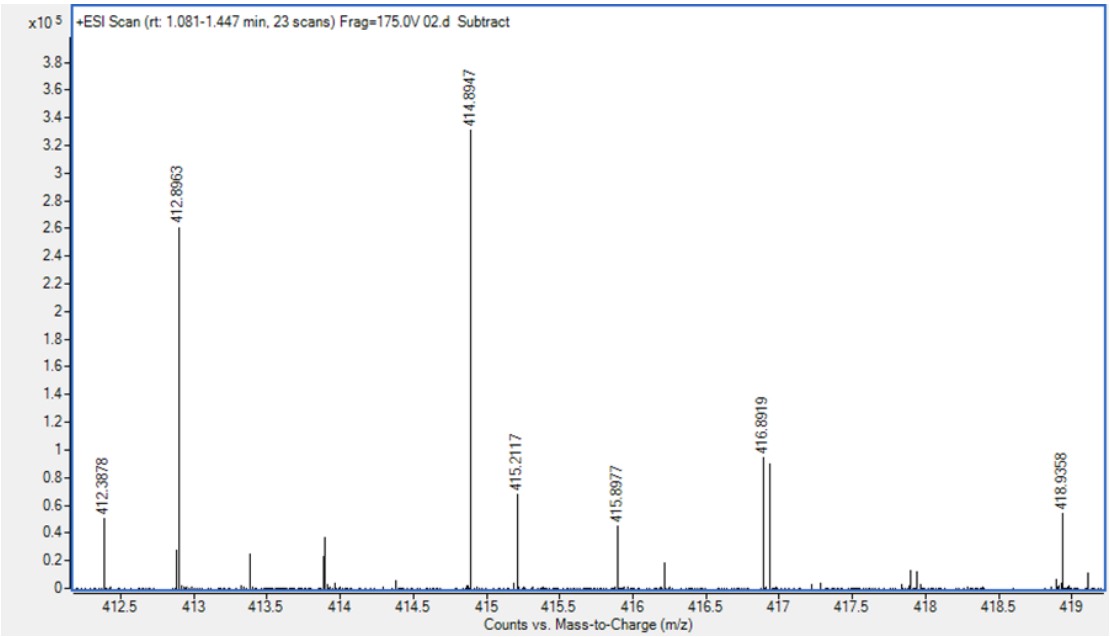




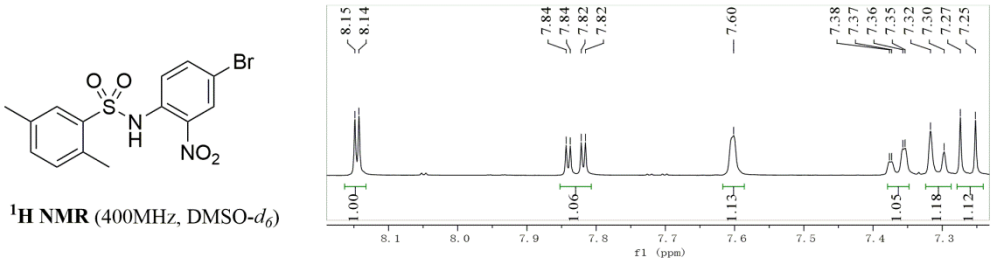
3w ^{13}C NMR



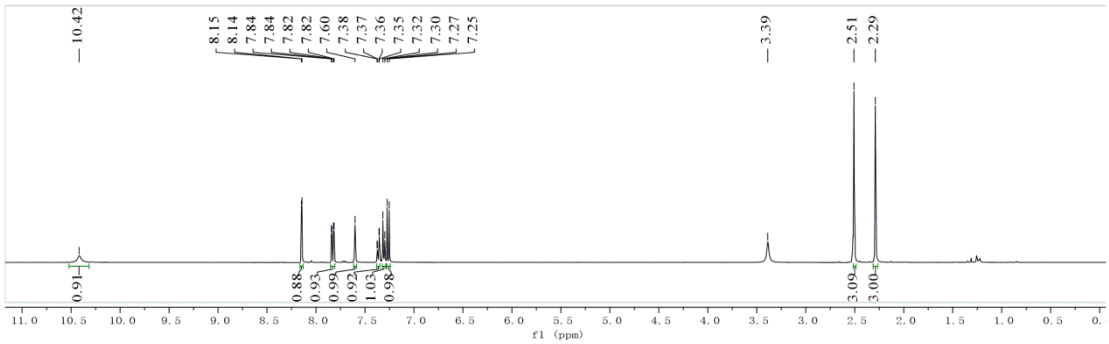
3w $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8963.



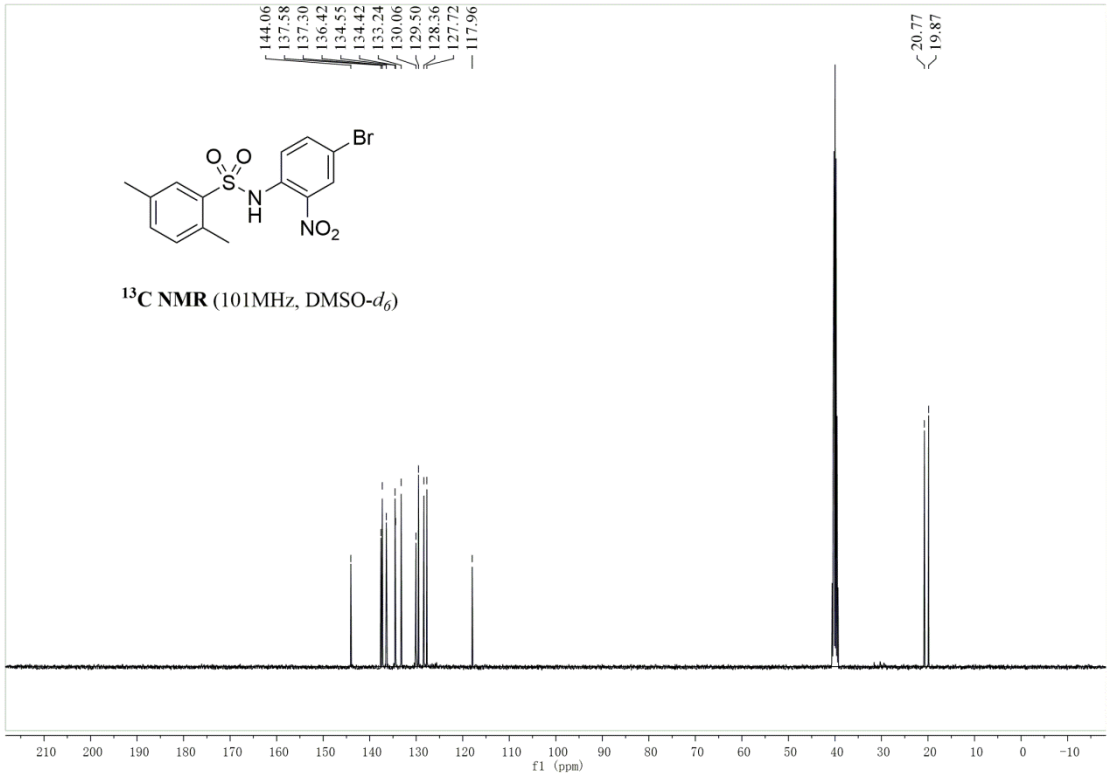
3ab ^{1}H NMR



^{1}H NMR (400MHz, DMSO-d_6)

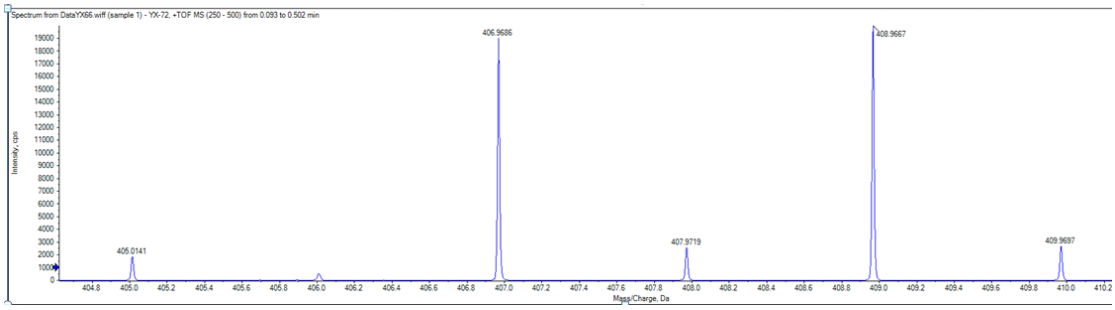


3ab ^{13}C NMR

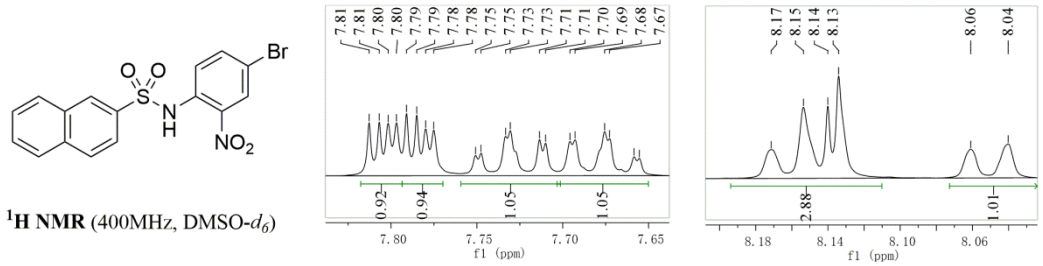


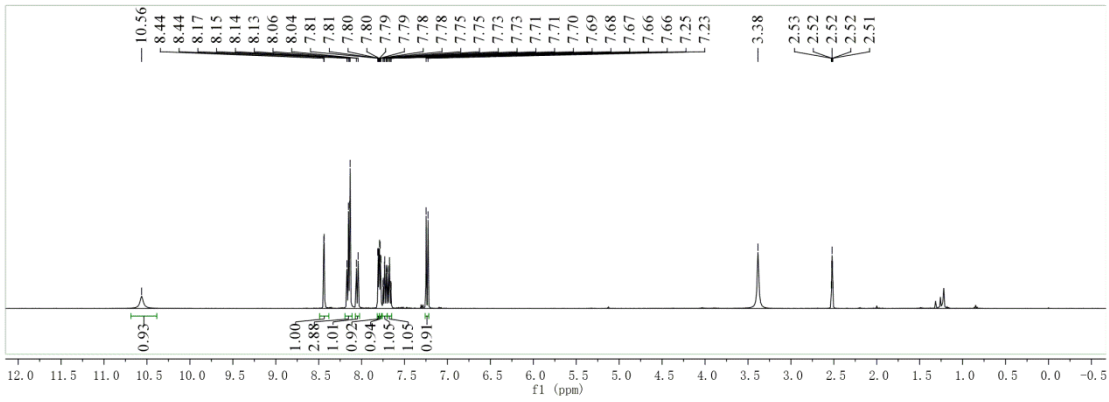
^{13}C NMR (101MHz, DMSO-d_6)

3ab $C_{14}H_{13}BrN_2O_4S$, $[M+Na]^+$ 406.9677. Found 406.9686.

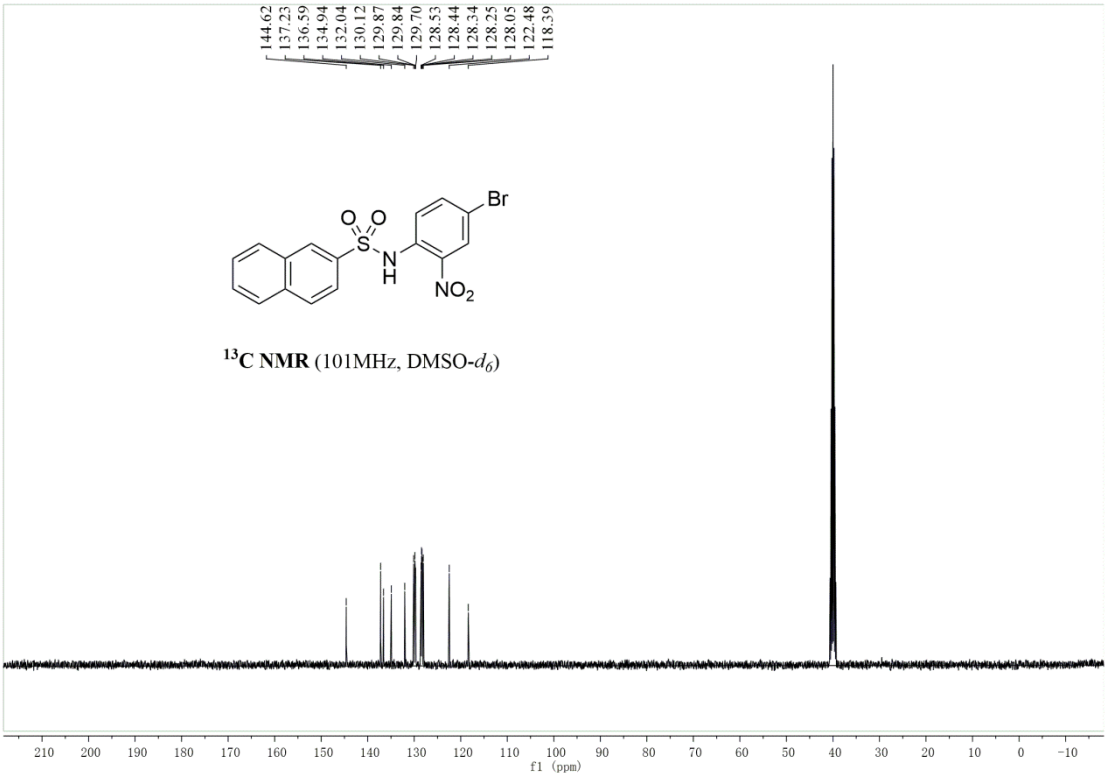


3ac ^{1}H NMR

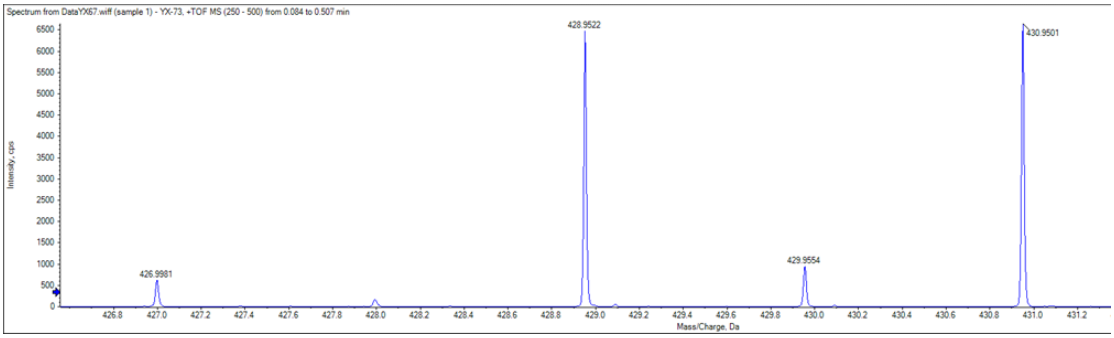




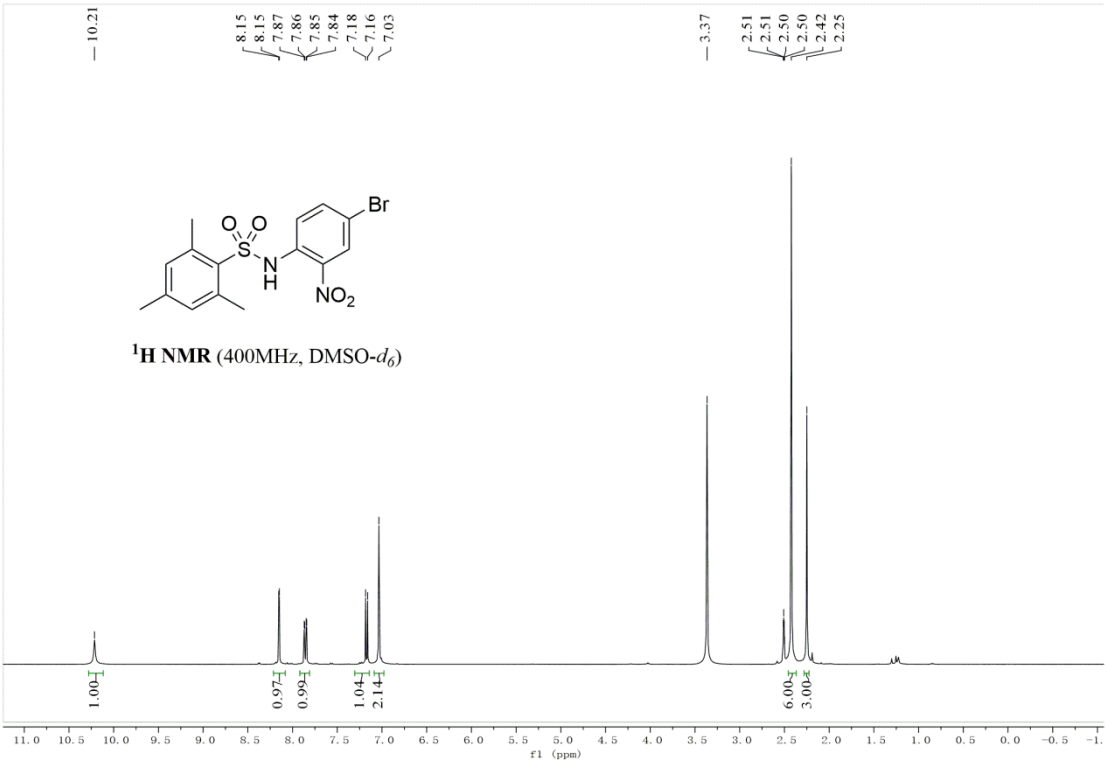
3ac ^{13}C NMR



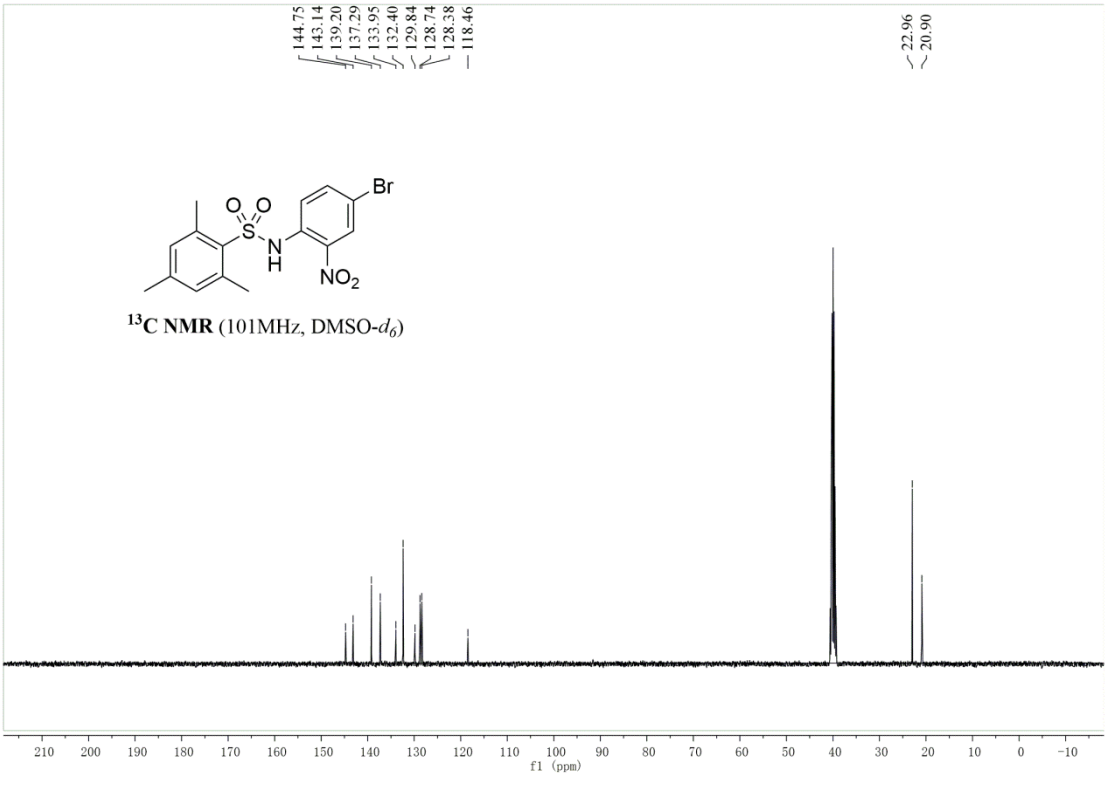
3ac $C_{16}H_{11}BrN_2O_4S$, $[M+Na]^+$ 428.9521. Found 428.9522.



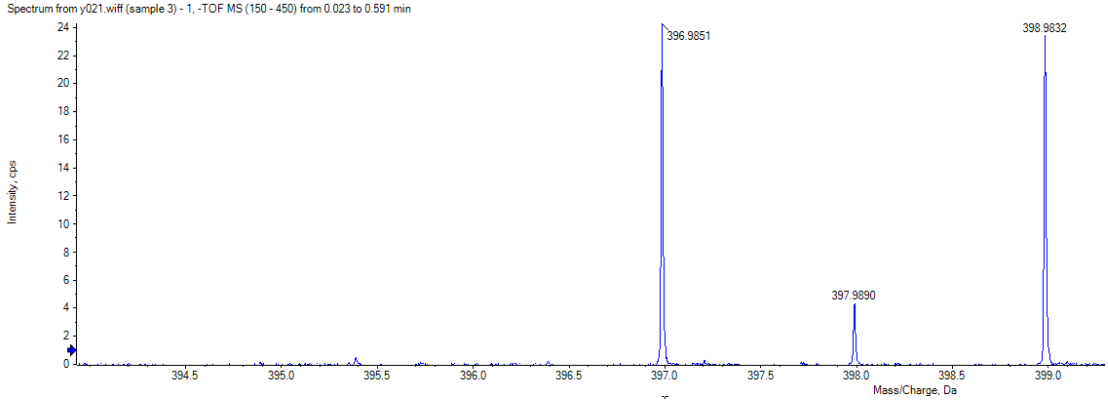
3ad ^{1}H NMR



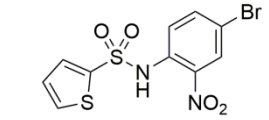
3ad ^{13}C NMR



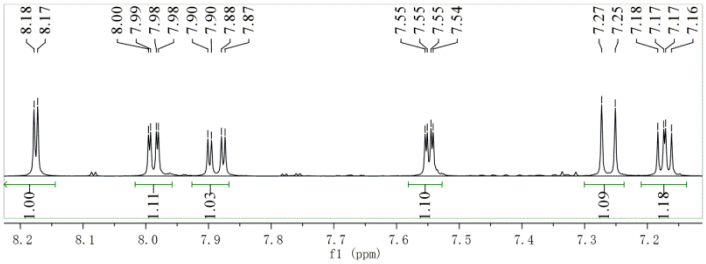
3ad $C_{15}H_{15}BrN_2O_4S$, $[M-H]^-$ 396.9858. Found 396.9851.

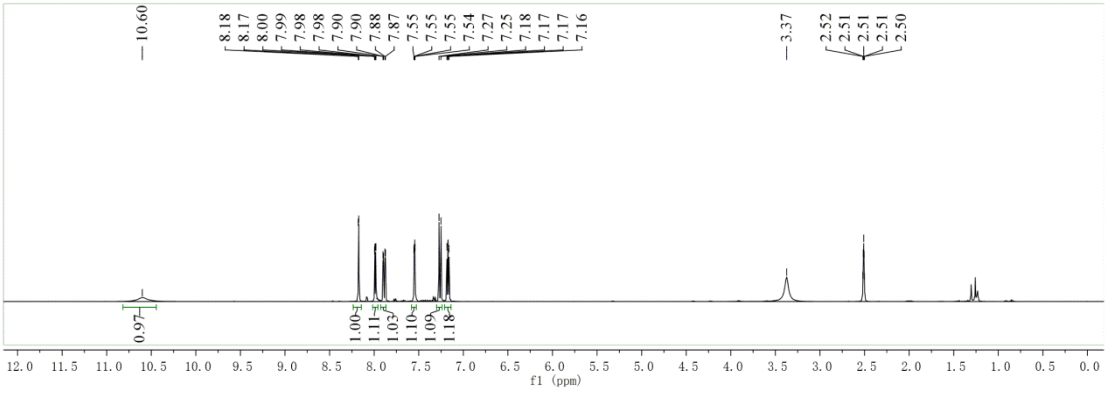


3ag ^{1}H NMR

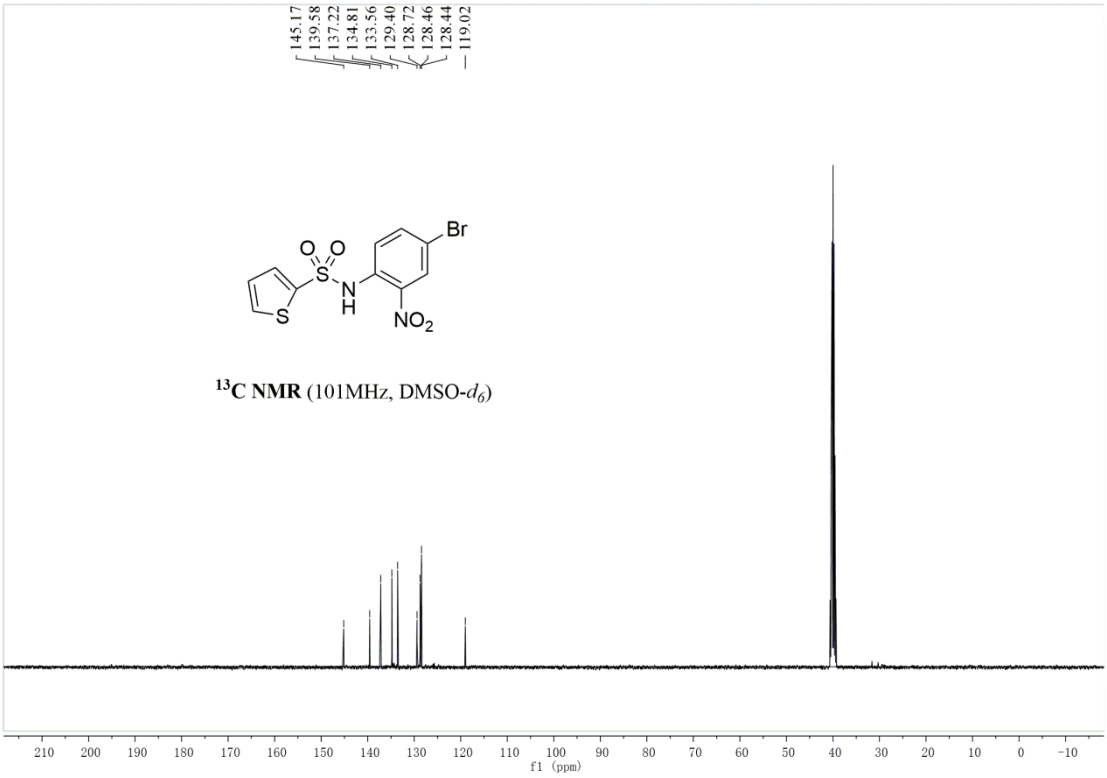


^{1}H NMR (400MHz, DMSO-d_6)

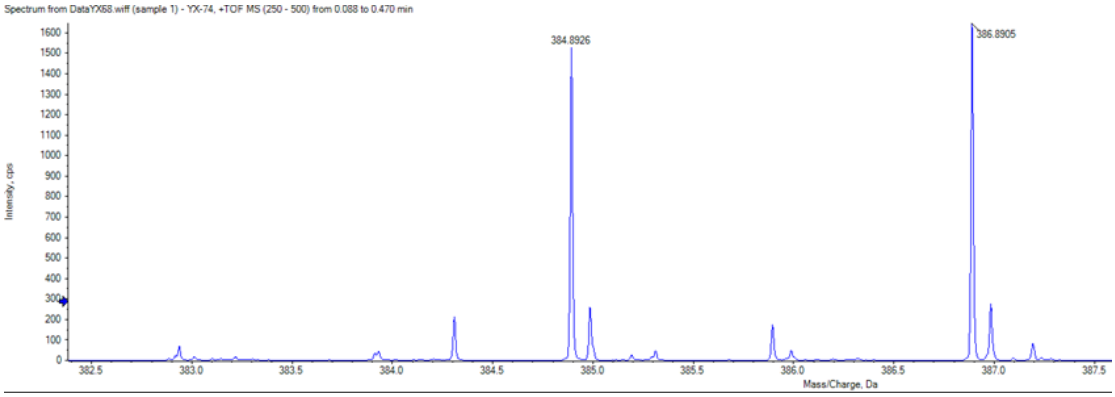




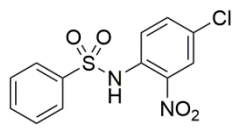
3ag ^{13}C NMR



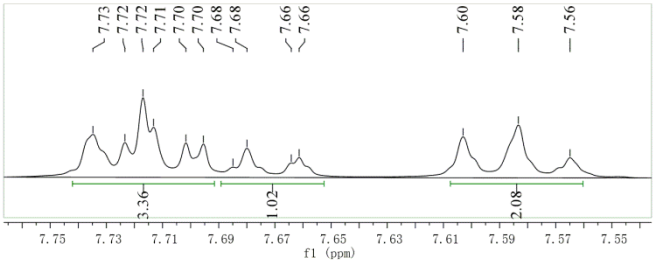
3ag $C_{10}H_7BrN_2O_4S_2$, $[M+Na]^+$ 384.8928. Found 384.8926.

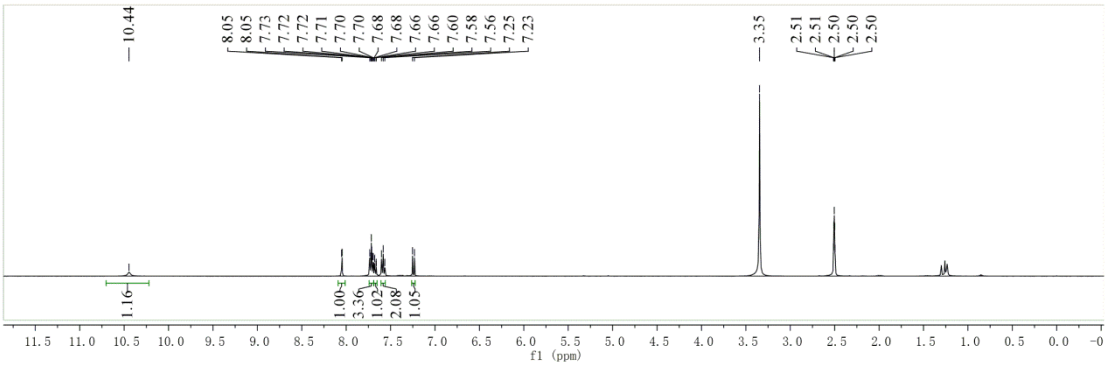


4a ^{1}H NMR

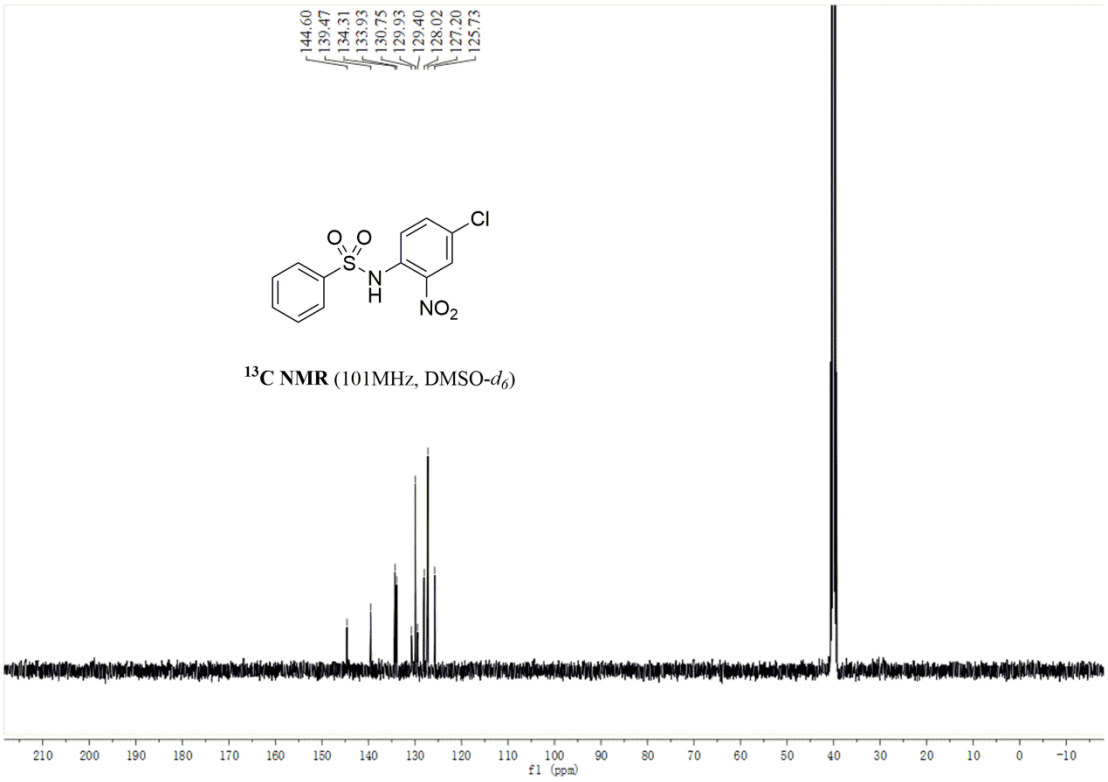


^{1}H NMR (400MHz, DMSO-d_6)



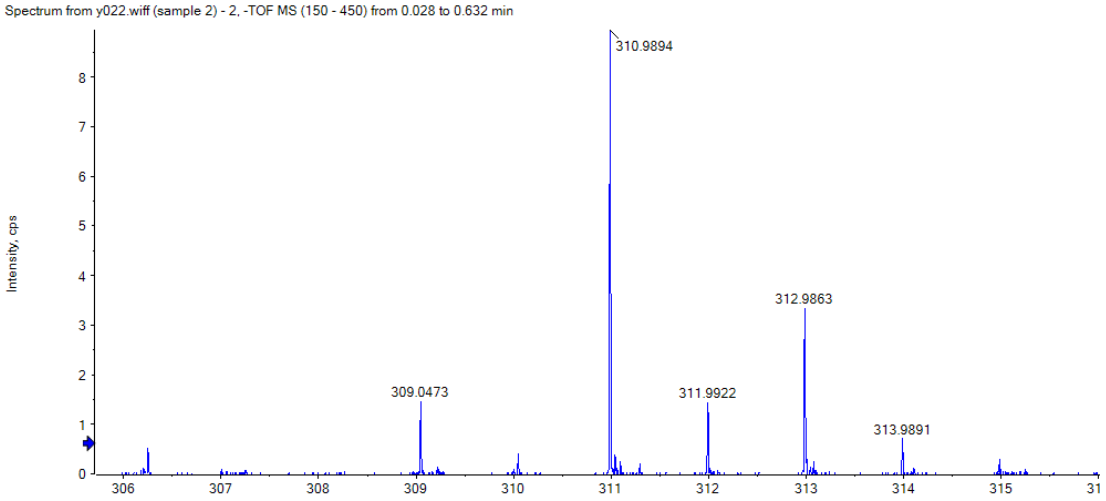


4a ^{13}C NMR

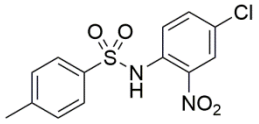


^{13}C NMR (101MHz, DMSO-d_6)

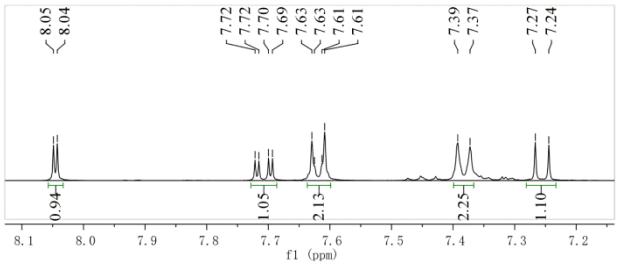
4a $C_{12}H_9ClN_2O_4S$, $[M-H]^-$ 310.9893. Found 310.9894.

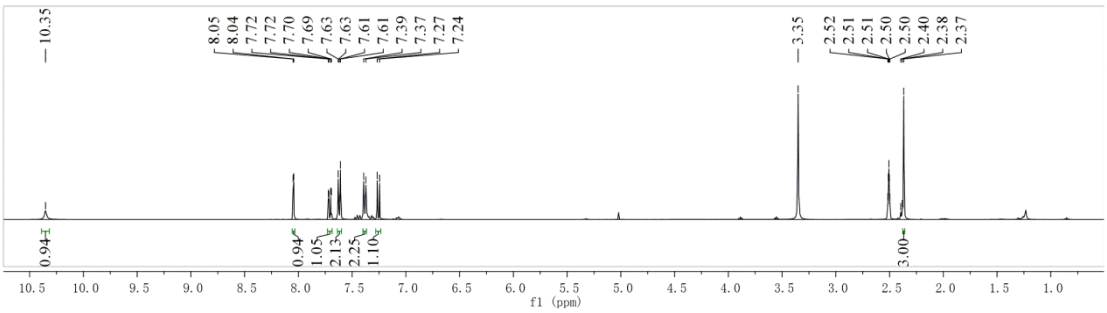


4b ^{1}H NMR

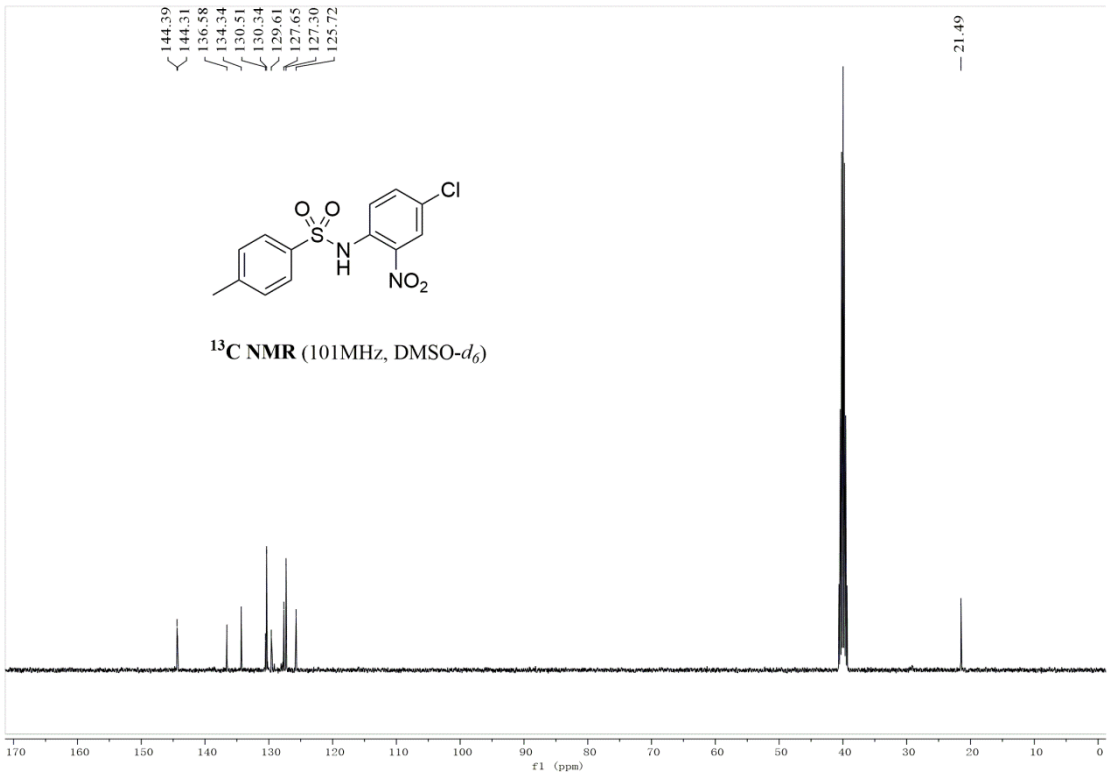


^{1}H NMR (400MHz, DMSO-d_6)



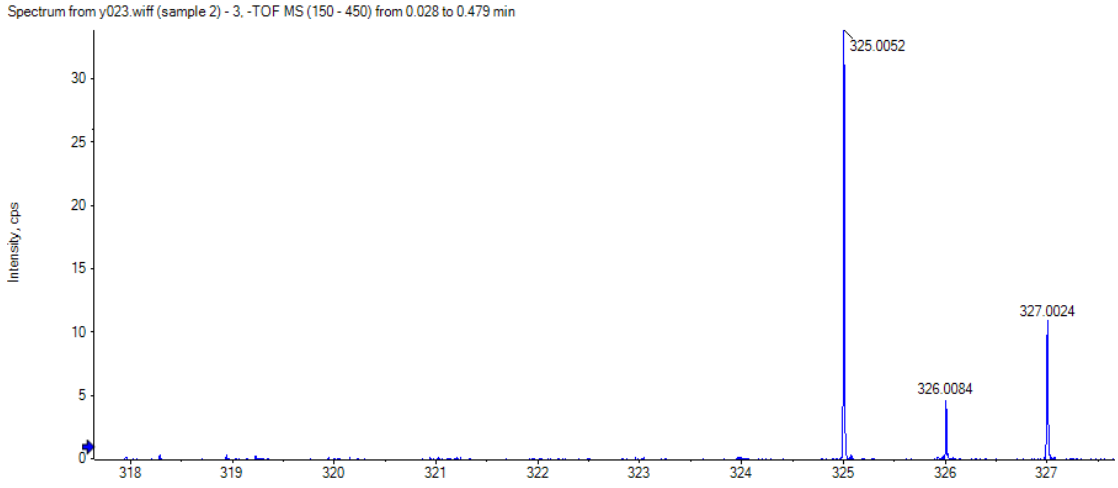


4b ^{13}C NMR

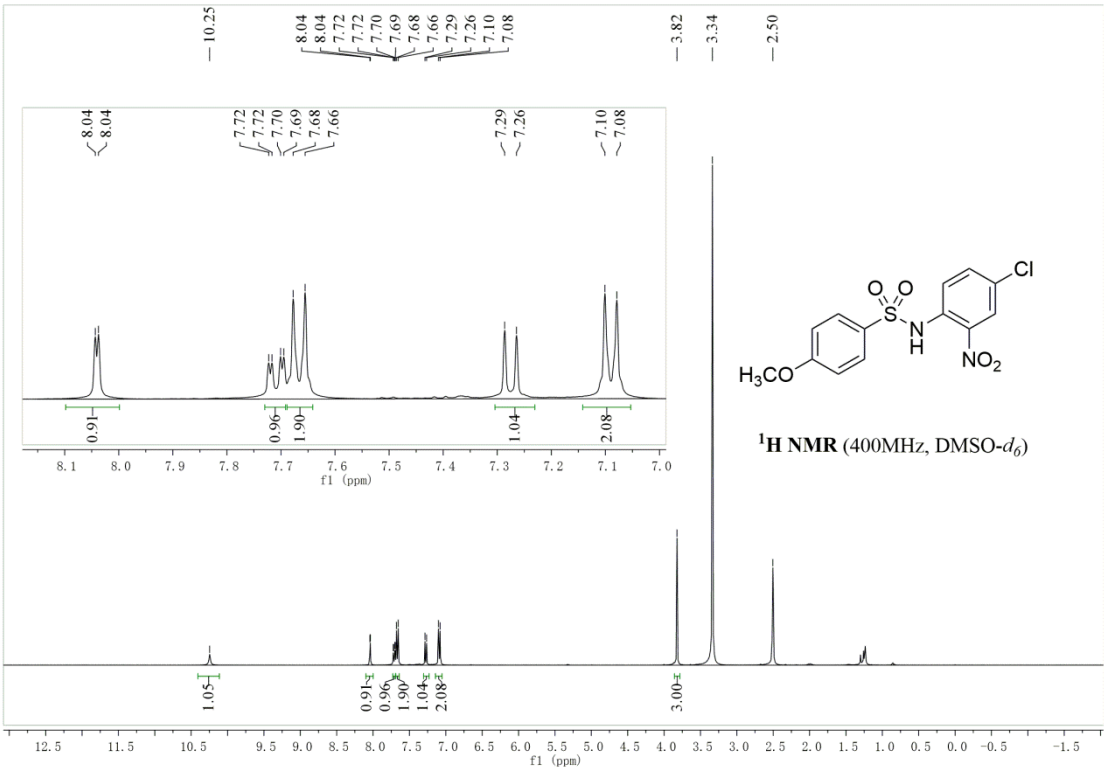


^{13}C NMR (101MHz, DMSO-d_6)

4b $C_{13}H_{11}ClN_2O_4S$, $[M-H]^-$ 325.0050 Found 325.0052.

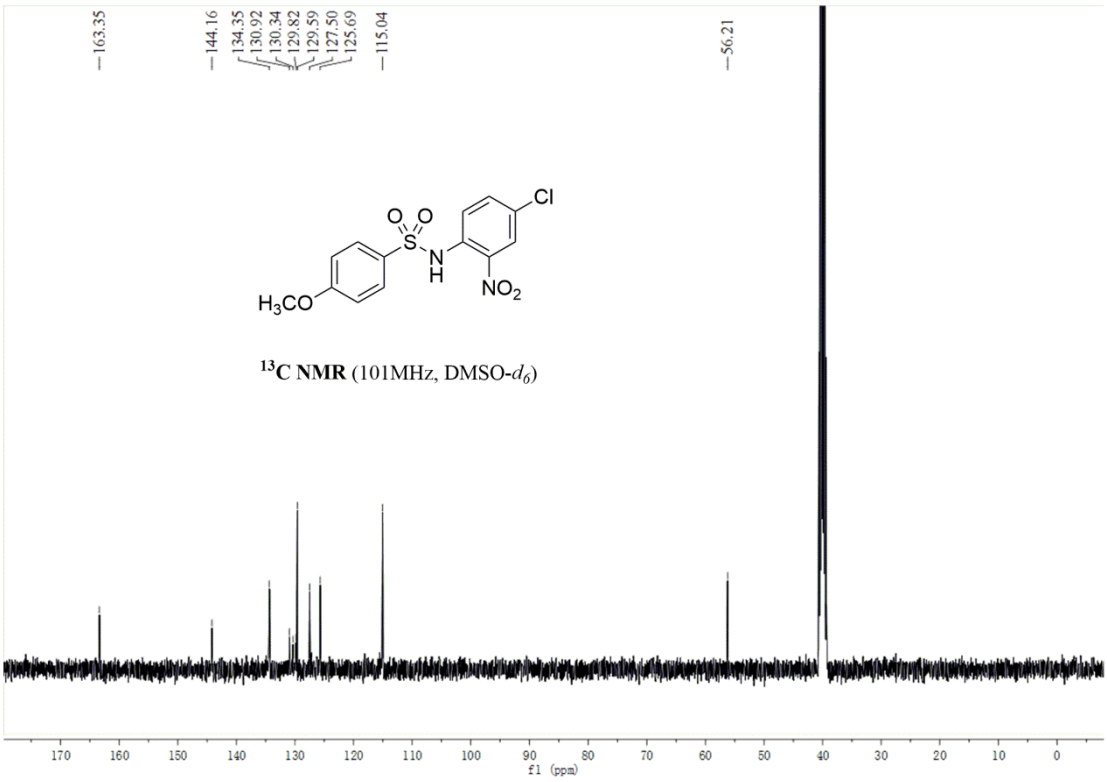


4c ^{1}H NMR



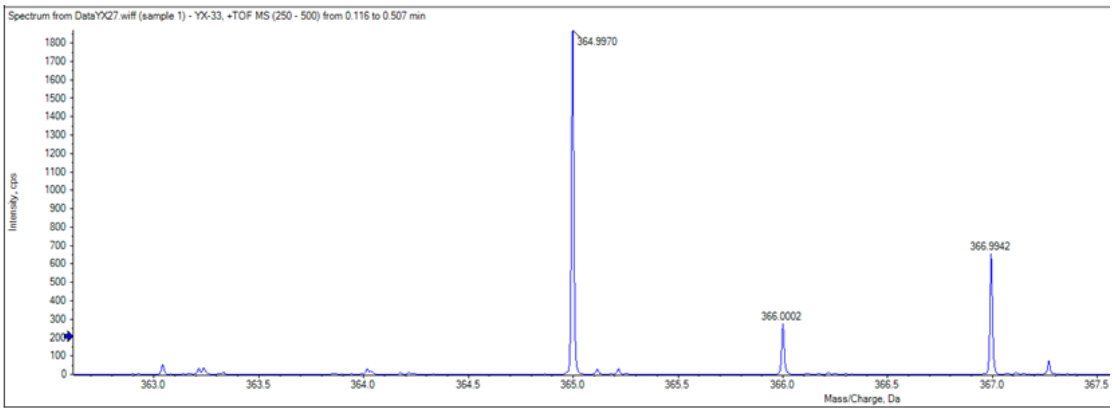
^{1}H NMR (400MHz, DMSO-d_6)

4c ^{13}C NMR

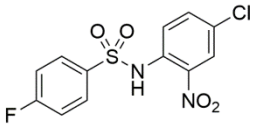


^{13}C NMR (101MHz, DMSO-d_6)

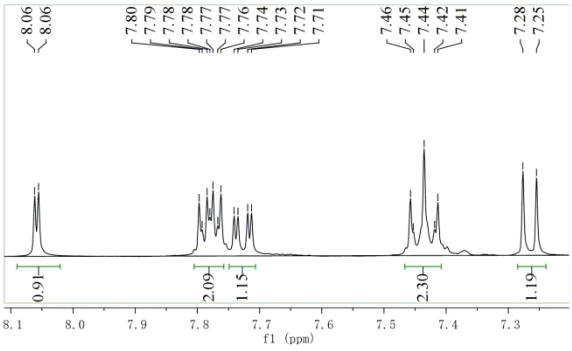
4c $C_{13}H_{11}ClN_2O_5S$, $[M+Na]^+$ 364.9975. Found 364.9970.

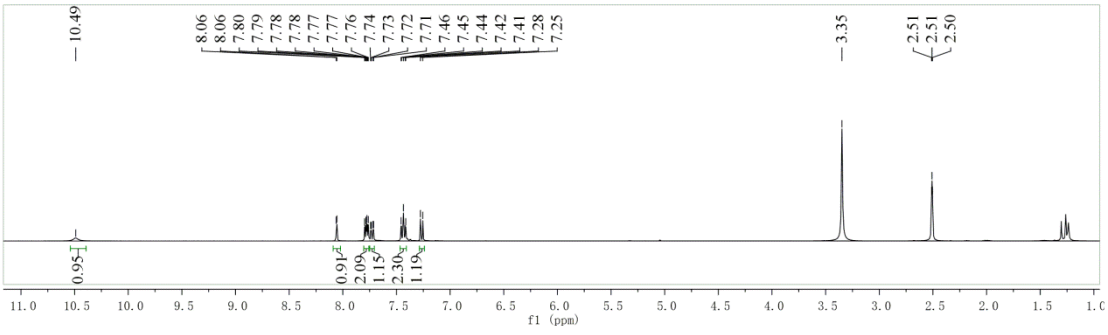


4d ^{1}H NMR

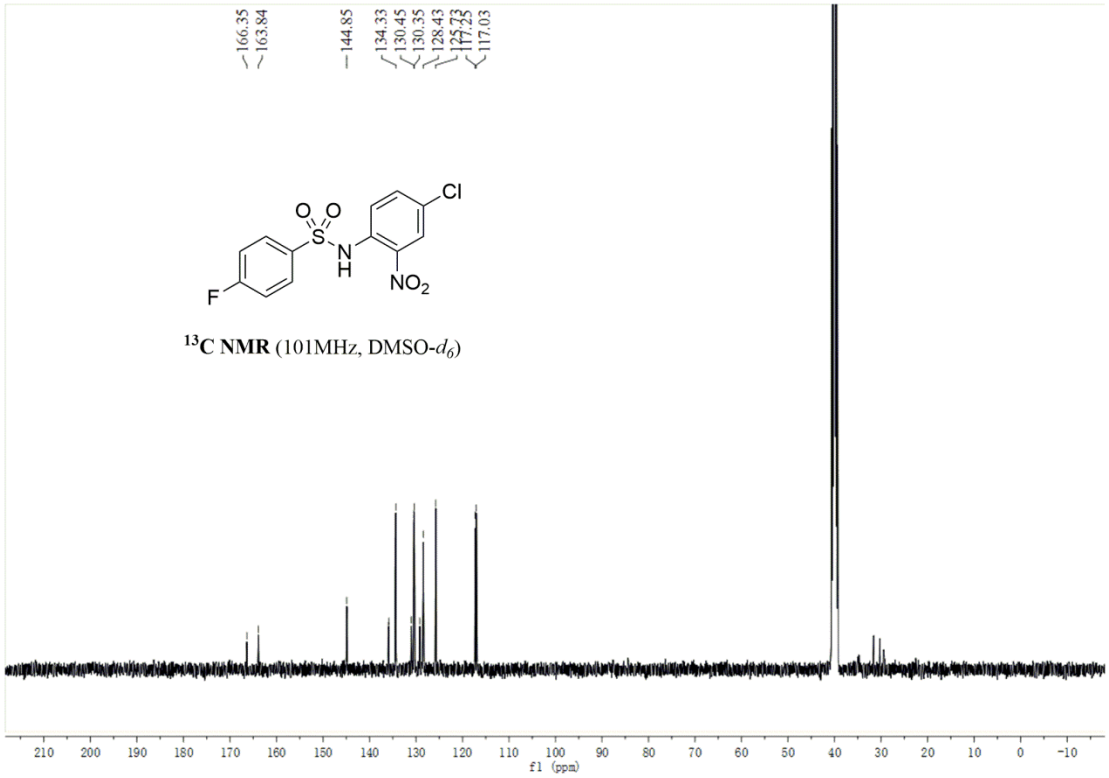


^{1}H NMR (400MHz, DMSO-d_6)



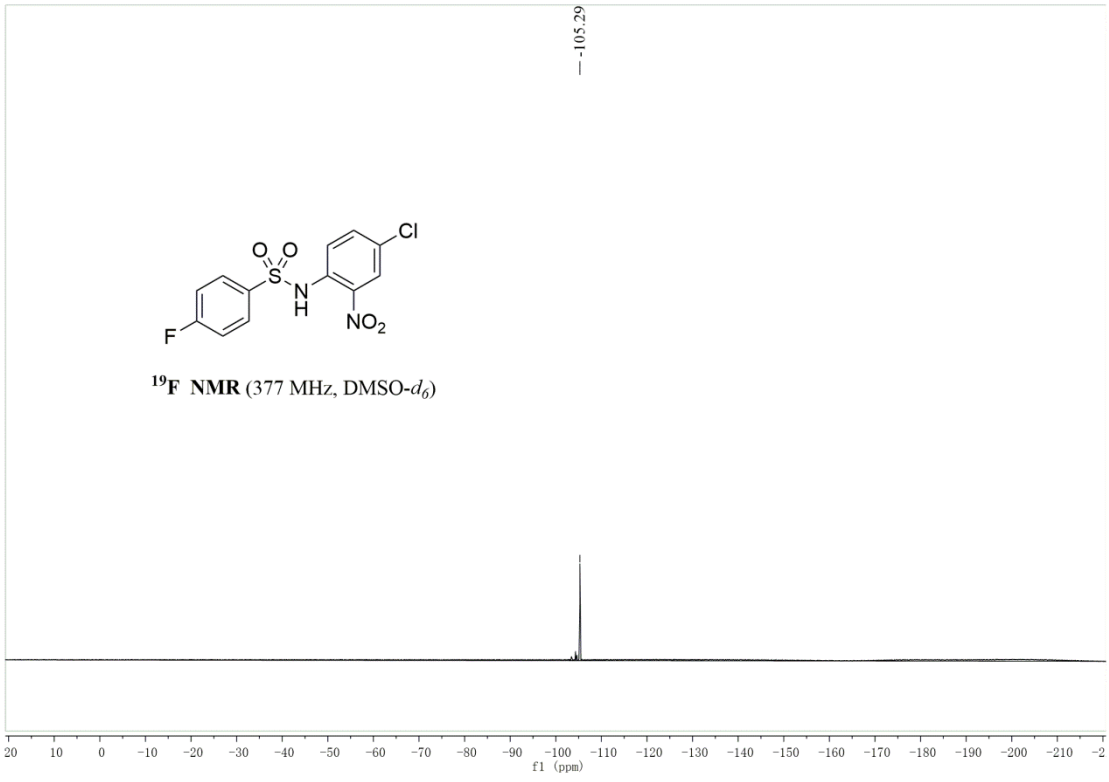


4d ^{13}C NMR



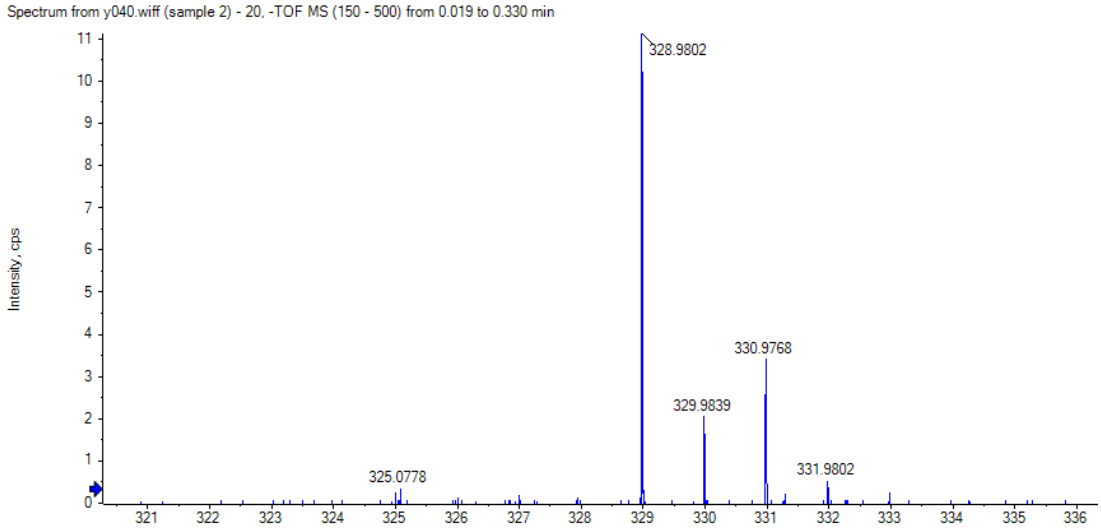
^{13}C NMR (101MHz, DMSO-d_6)

4d ^{19}F NMR

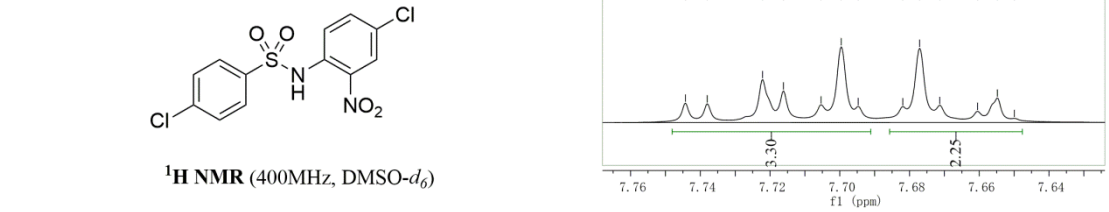


^{19}F NMR (377 MHz, DMSO-d_6)

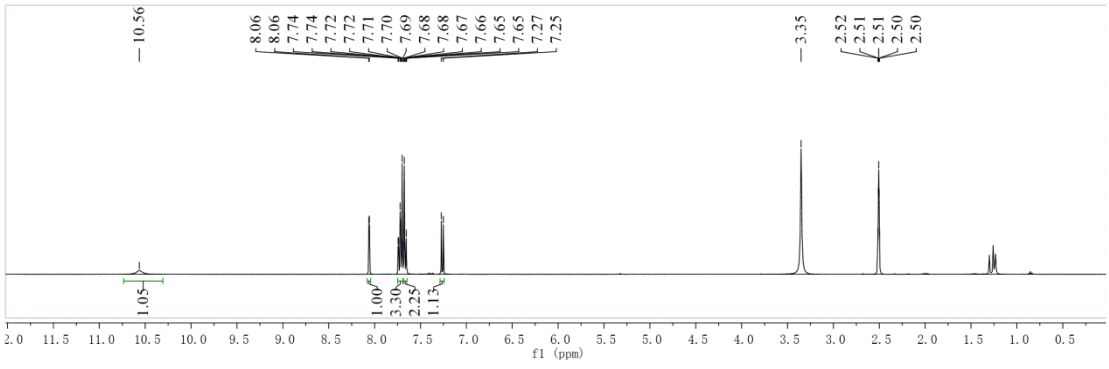
4d $C_{12}H_8ClFN_2O_4S$, $[M-H]^-$ 328.9799. Found 328.9802.



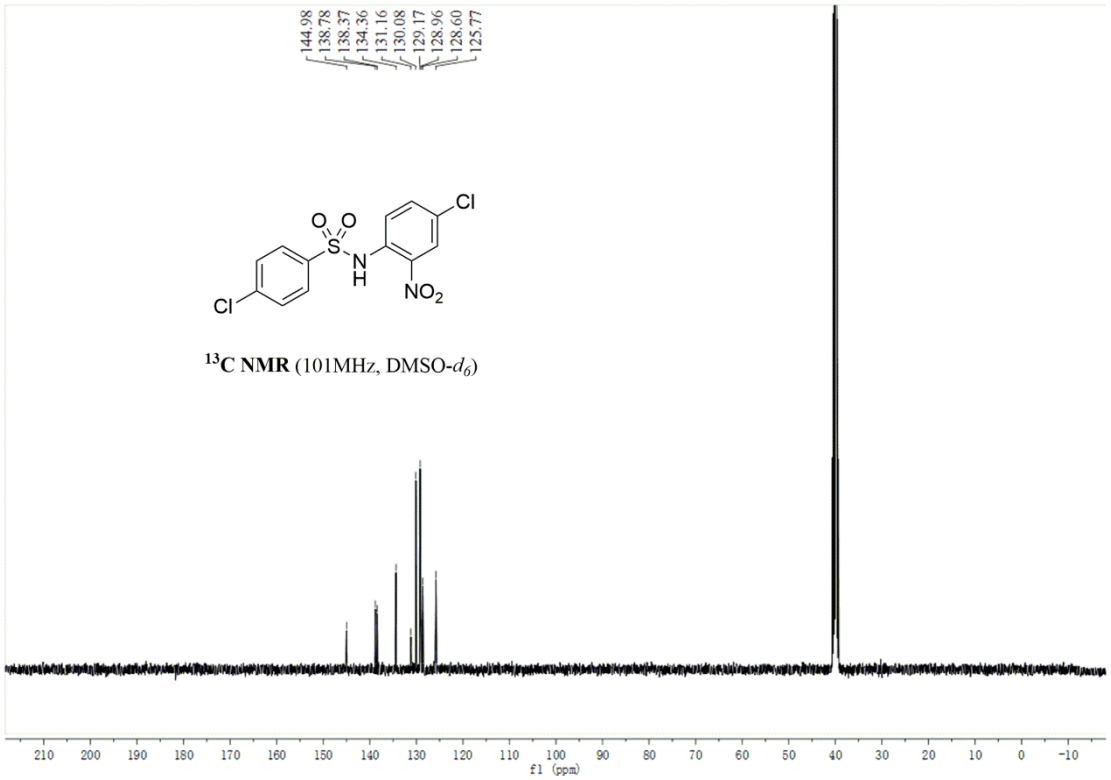
4e ^{1}H NMR



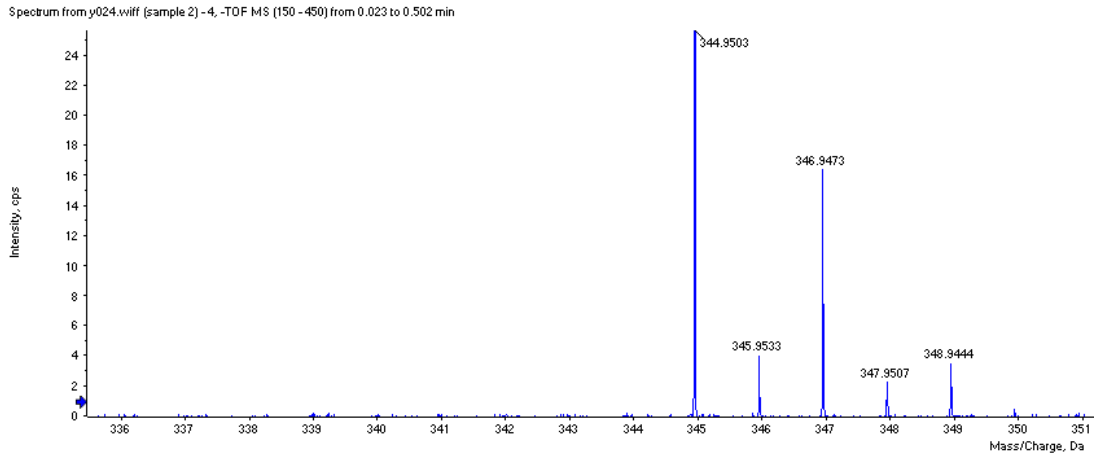
^{1}H NMR (400MHz, DMSO-d_6)



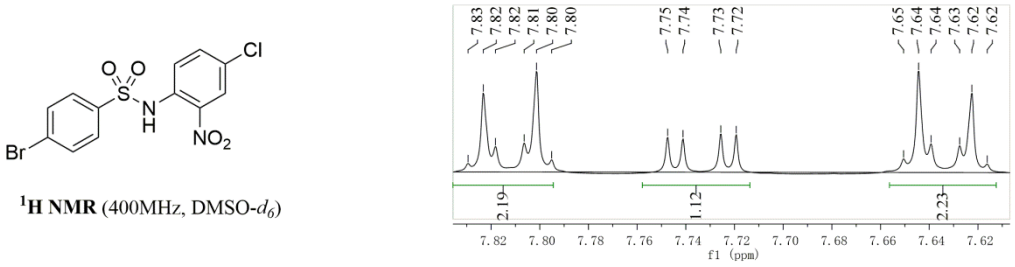
4e ^{13}C NMR



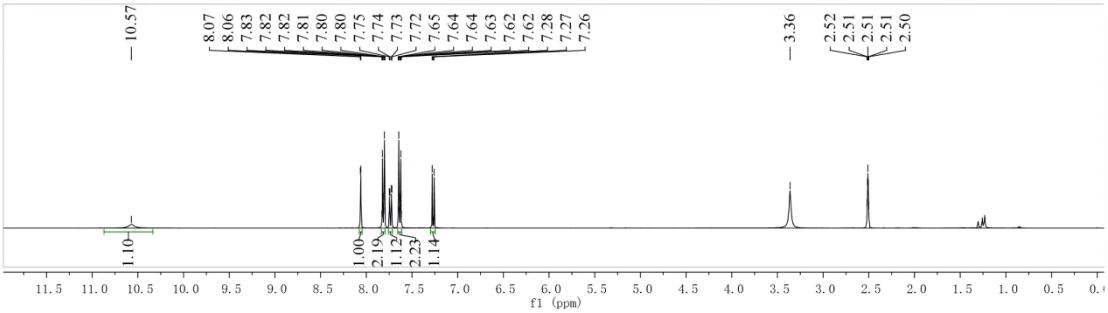
4e $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9503.



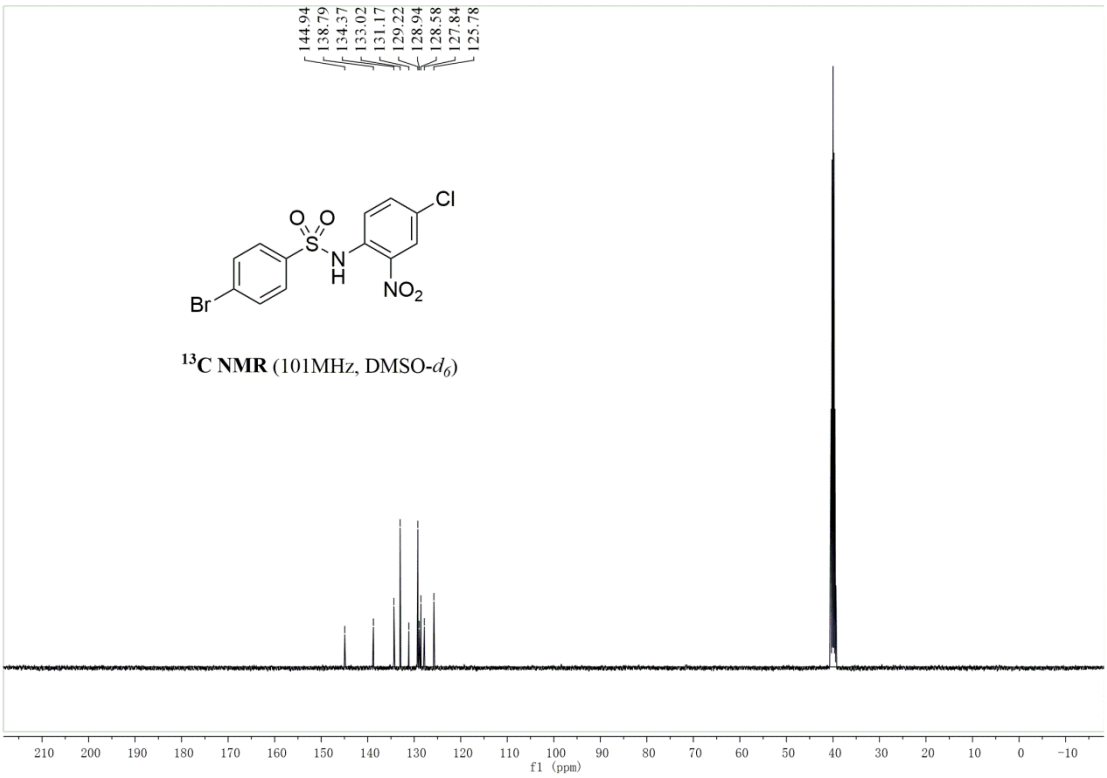
4f ^{1}H NMR



^{1}H NMR (400MHz, DMSO-d_6)

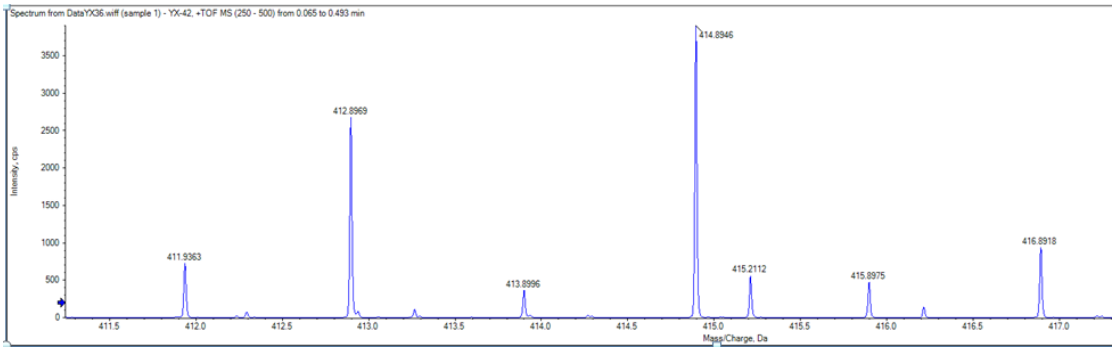


4f ^{13}C NMR

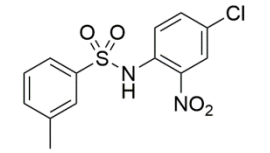


^{13}C NMR (101MHz, DMSO-d_6)

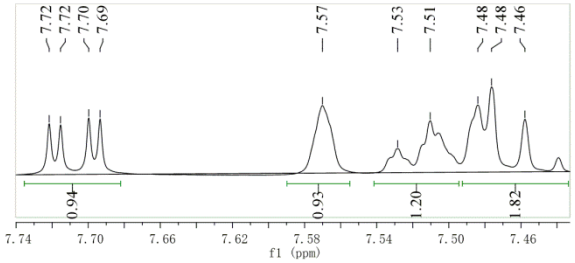
4f $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8969

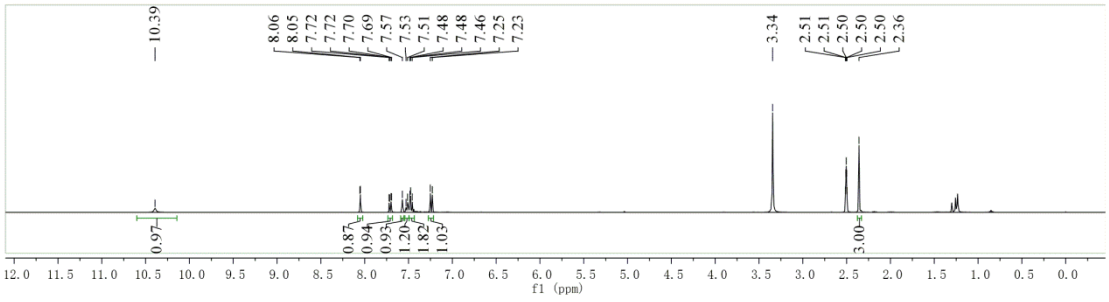


4i ^{1}H NMR

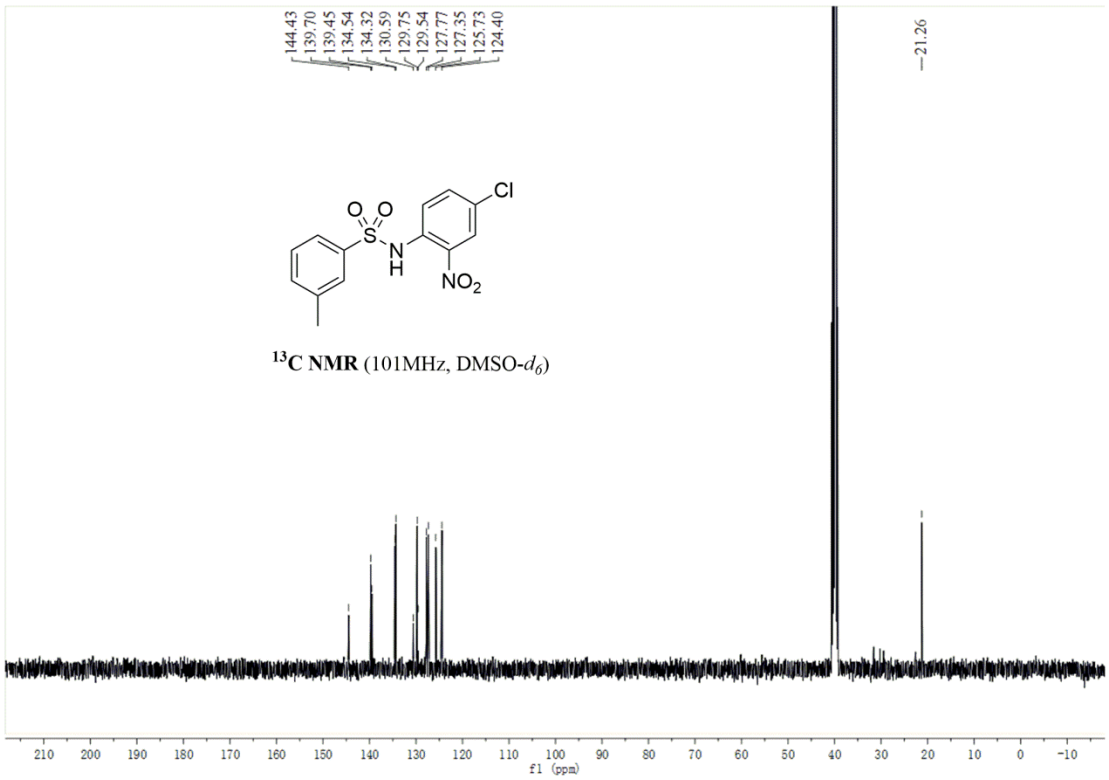


^{1}H NMR (400MHz, DMSO-d_6)



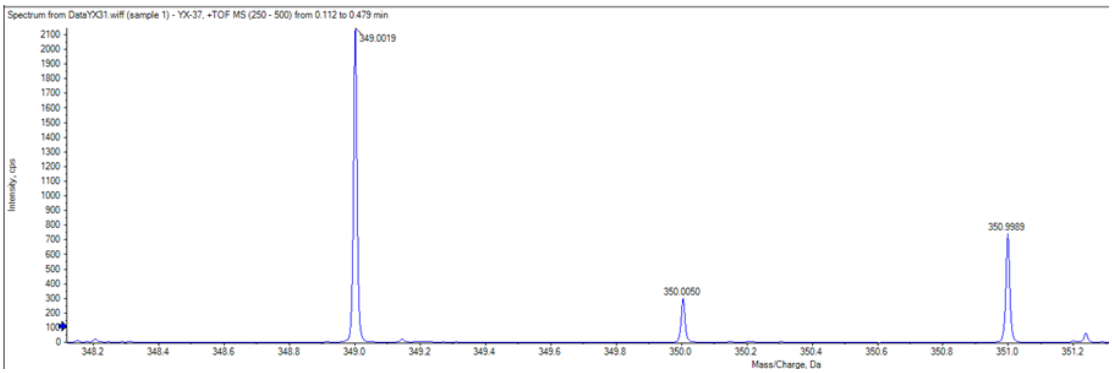


4i ^{13}C NMR

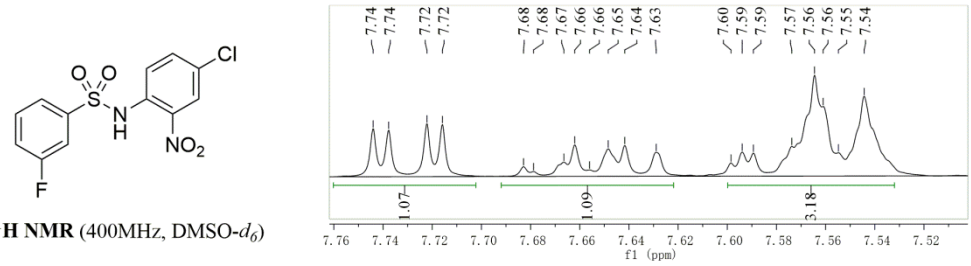


^{13}C NMR (101MHz, DMSO-d_6)

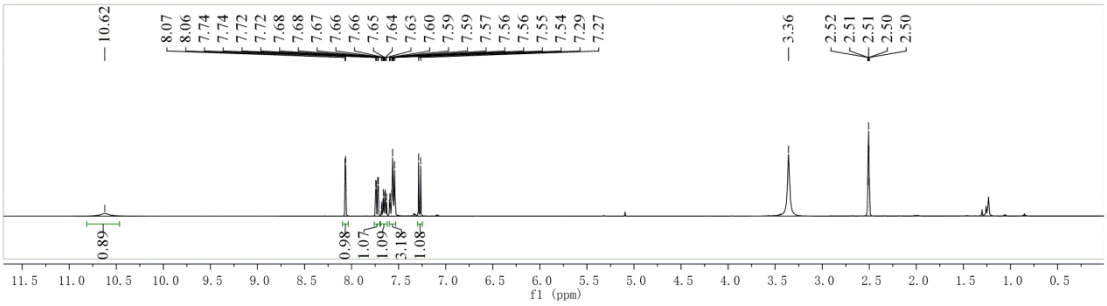
4i $C_{13}H_{11}ClN_2O_4S$, $[M+Na]^+$ 349.0026. Found 349.0019.



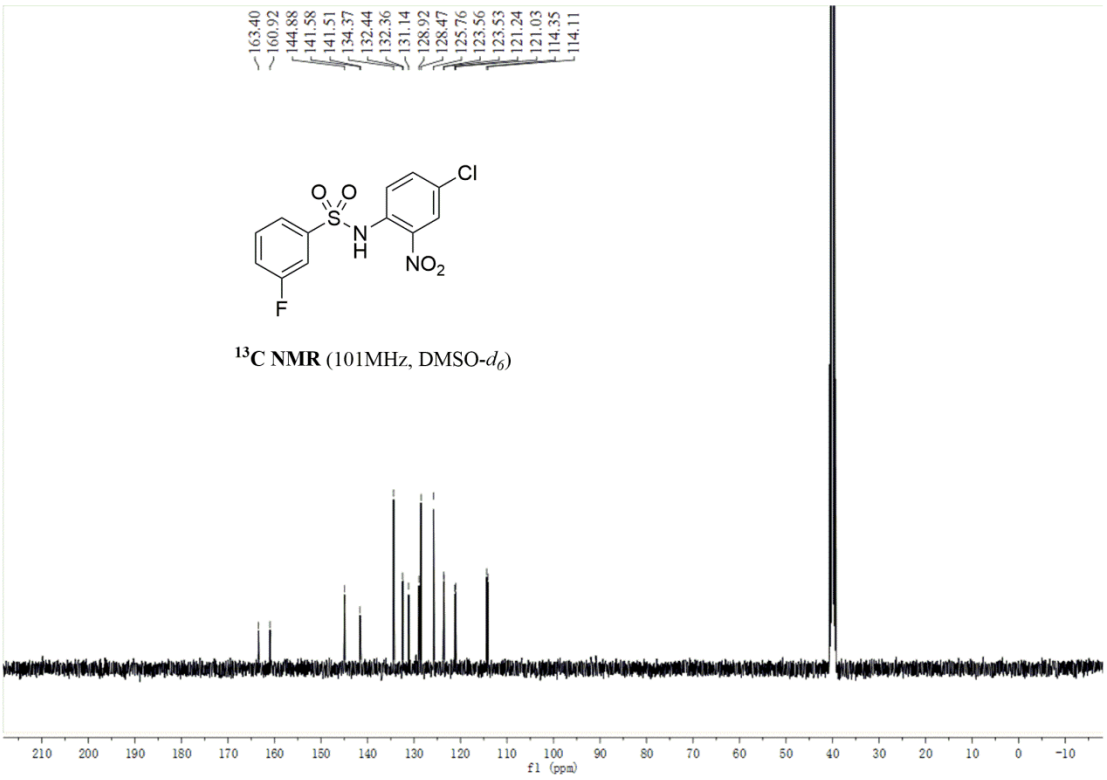
4j ^{1}H NMR



^{1}H NMR (400MHz, DMSO-d_6)

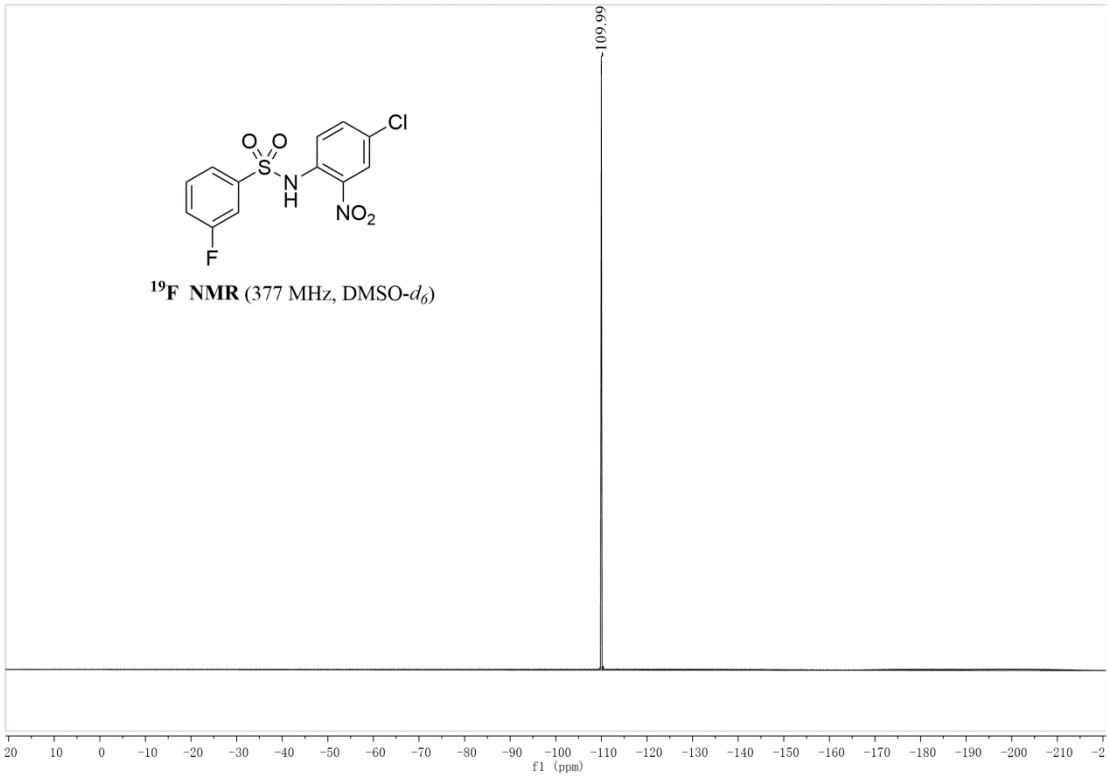


4j ^{13}C NMR



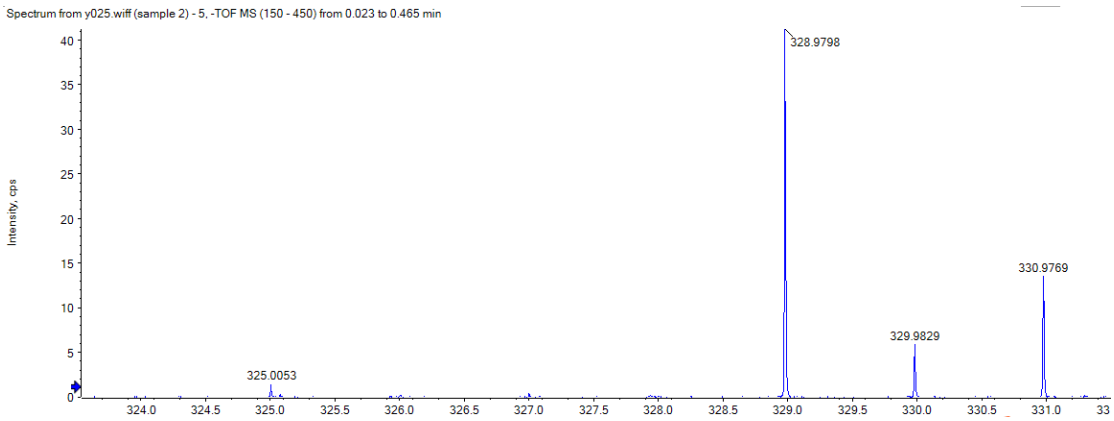
^{13}C NMR (101MHz, DMSO-d_6)

4j ^{19}F NMR

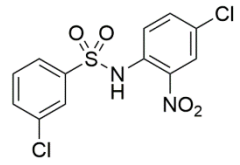


^{19}F NMR (377 MHz, DMSO-d_6)

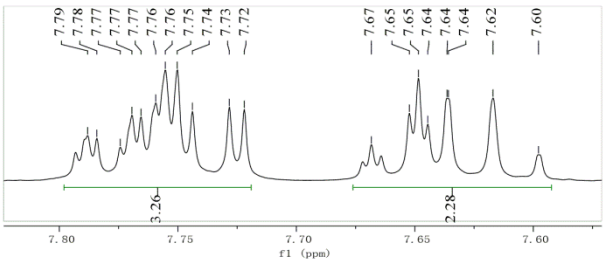
4j $C_{12}H_8ClFN_2O_4S$, $[M-H]^-$ 328.9799. Found 328.9798.

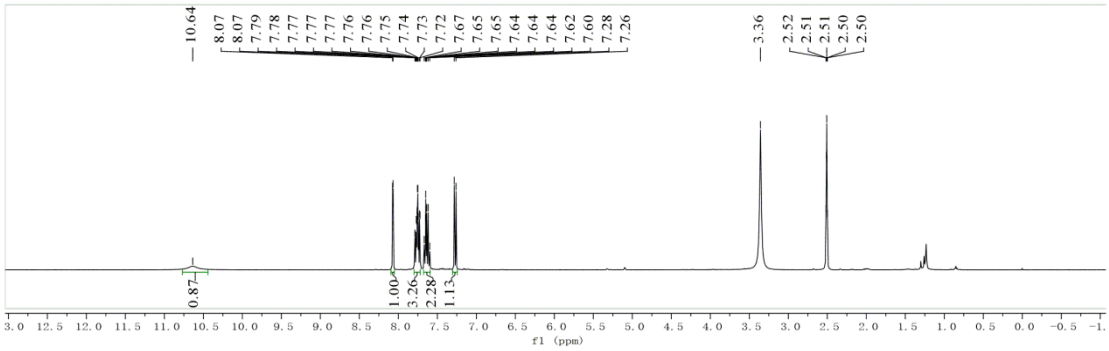


4k ^{1}H NMR

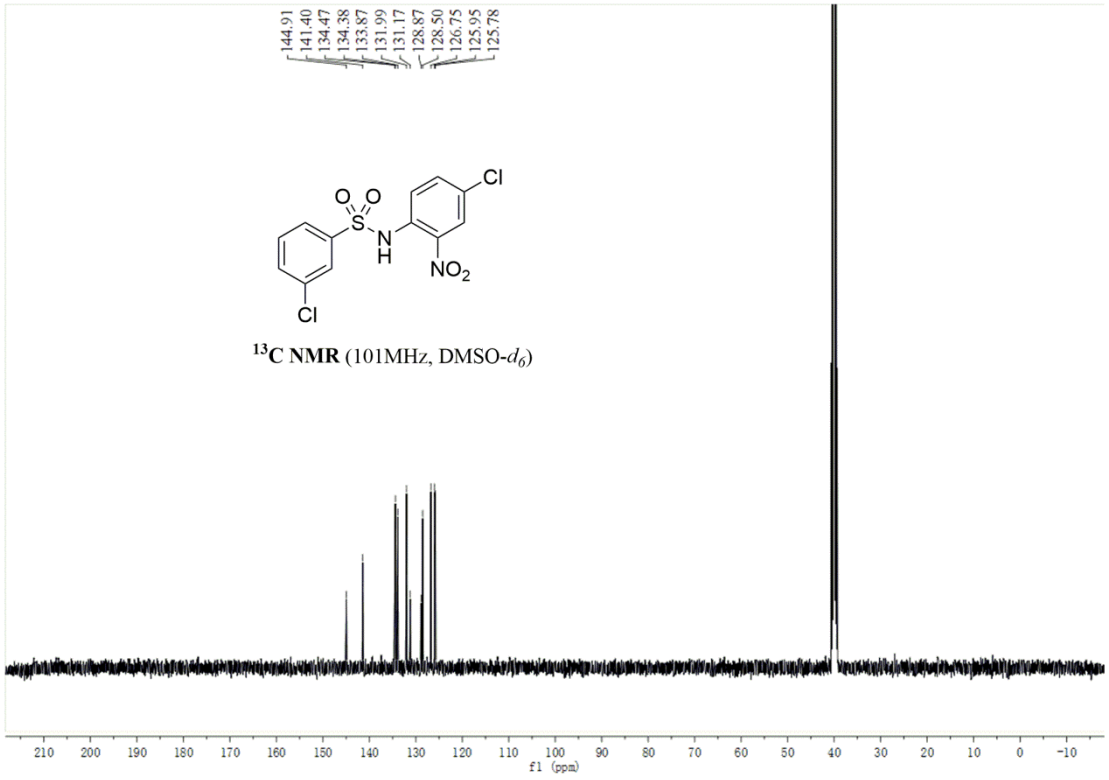


^{1}H NMR (400MHz, DMSO-d_6)



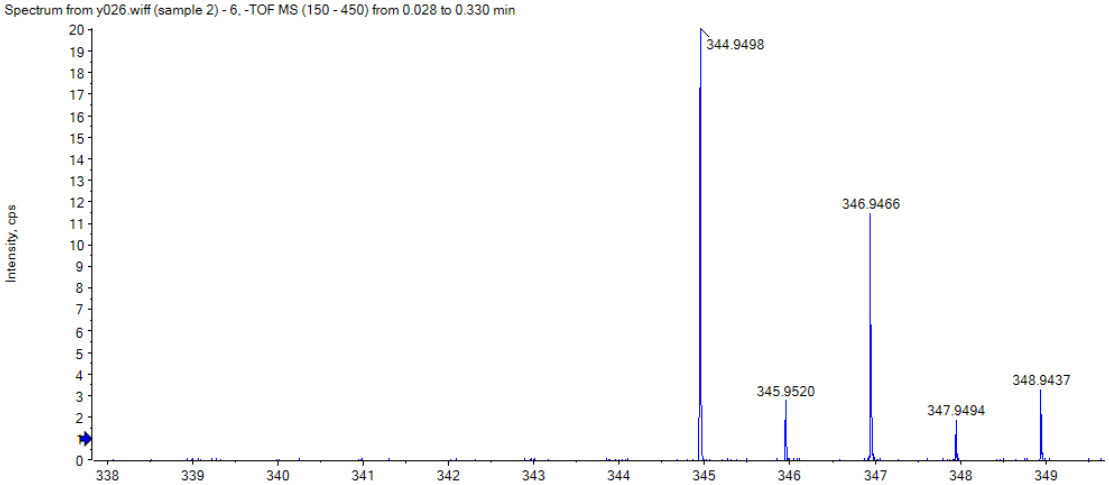


4k ^{13}C NMR

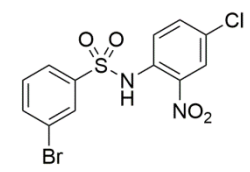


^{13}C NMR (101MHz, DMSO-d_6)

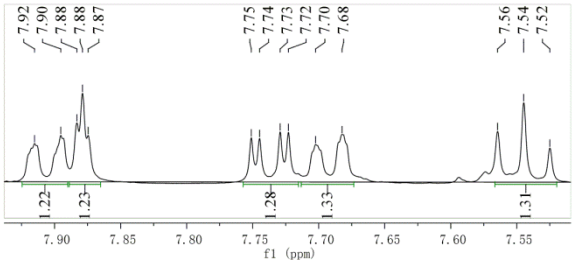
4k $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9498.

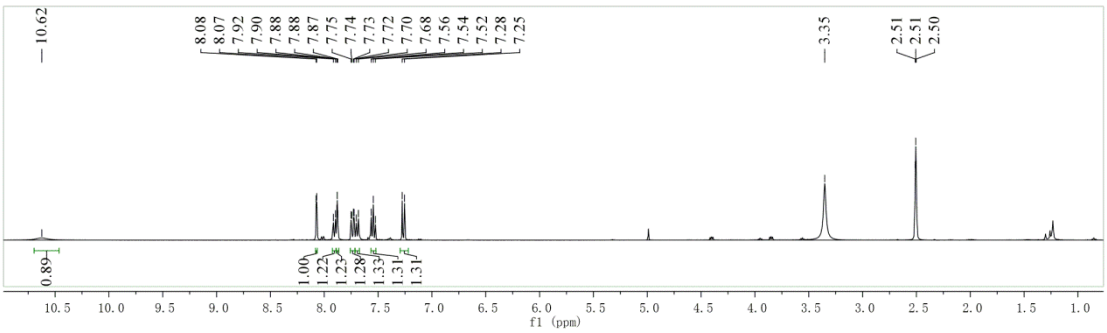


4l ^{1}H NMR

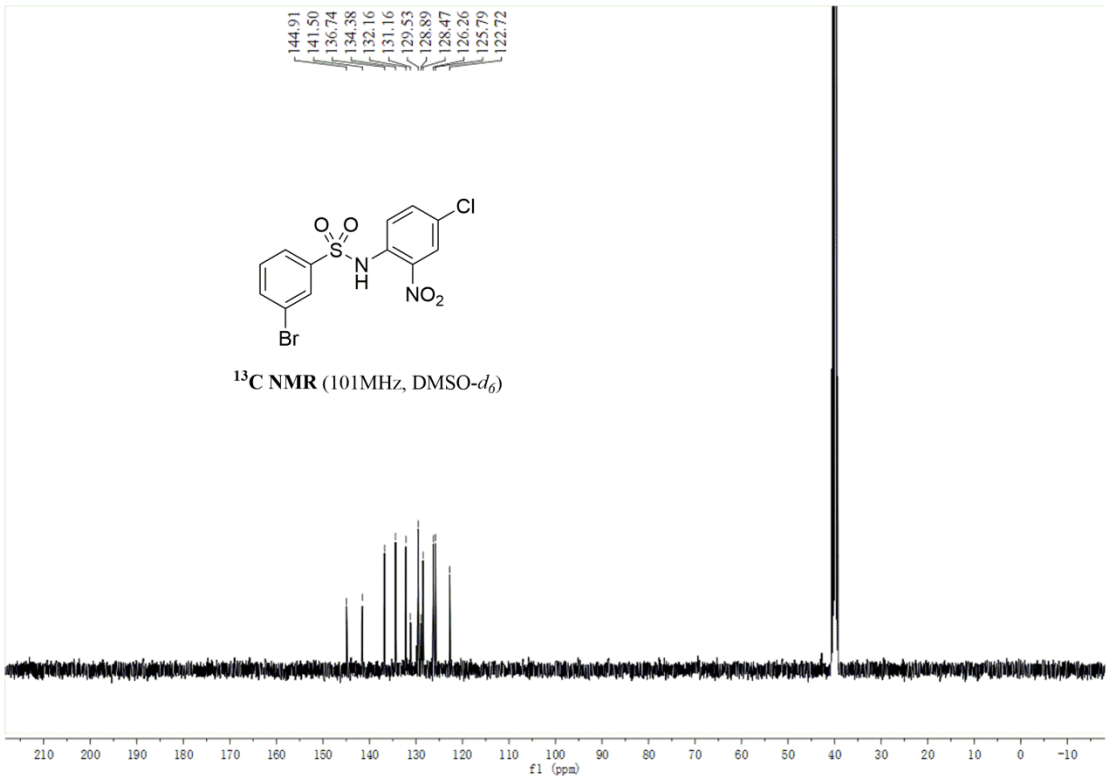


^{1}H NMR (400MHz, DMSO-d_6)

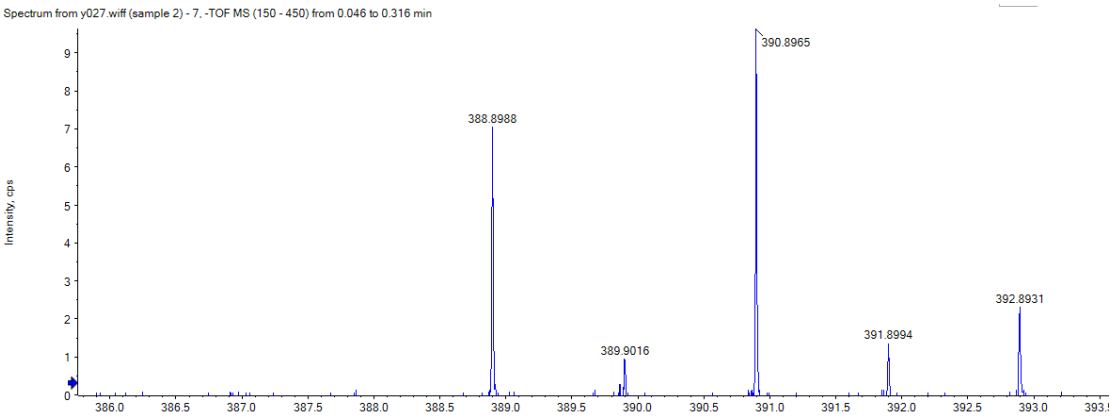




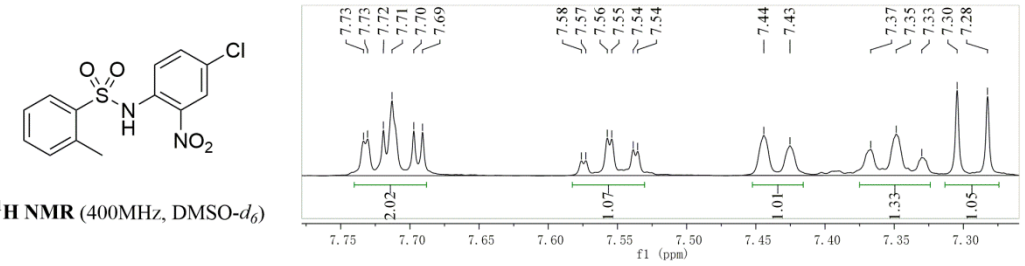
4l ^{13}C NMR



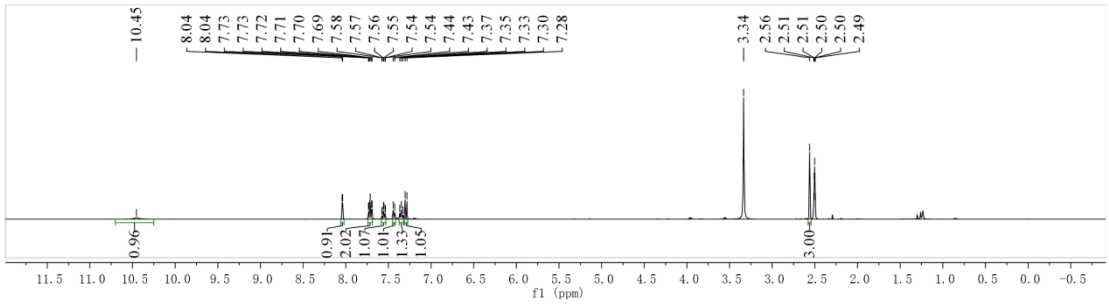
4l $C_{12}H_8BrClN_2O_4S$, $[M-H]^-$ 388.8998. Found 388.8988.



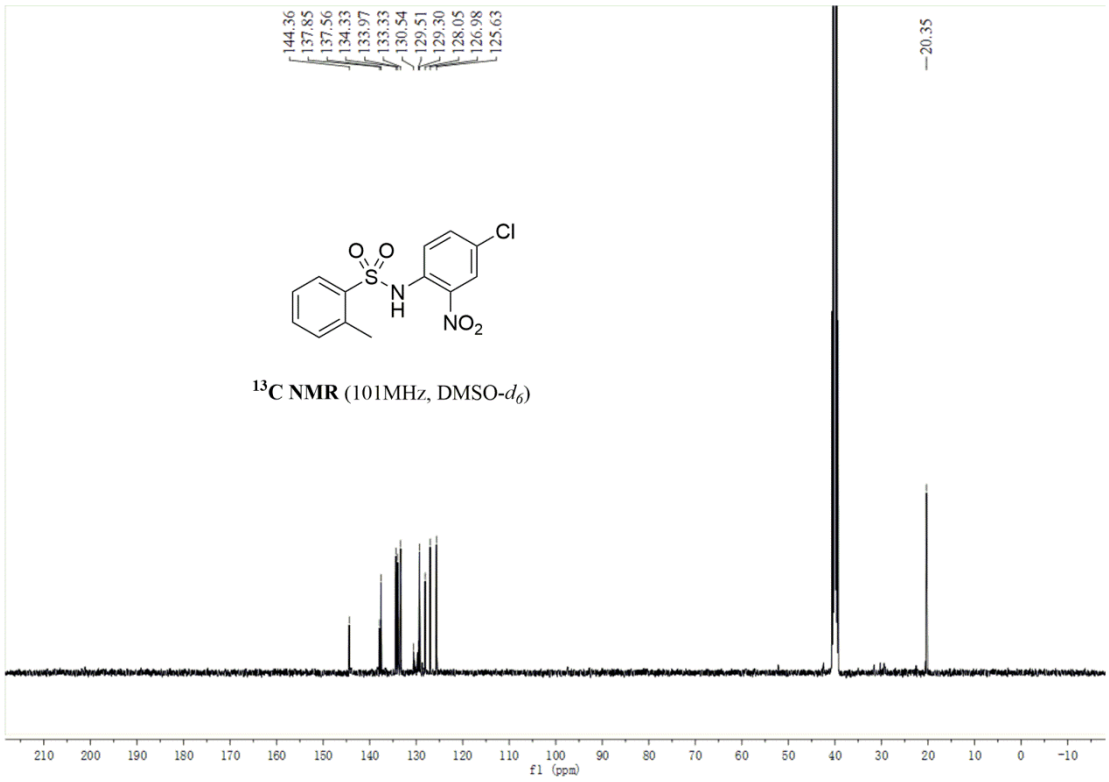
4o ^{1}H NMR



^{1}H NMR (400MHz, DMSO-d_6)

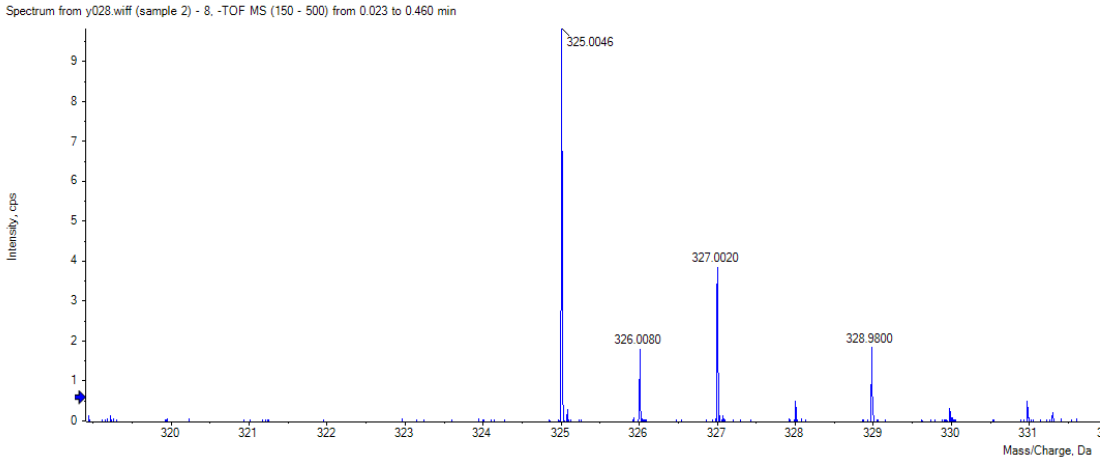


4o ^{13}C NMR

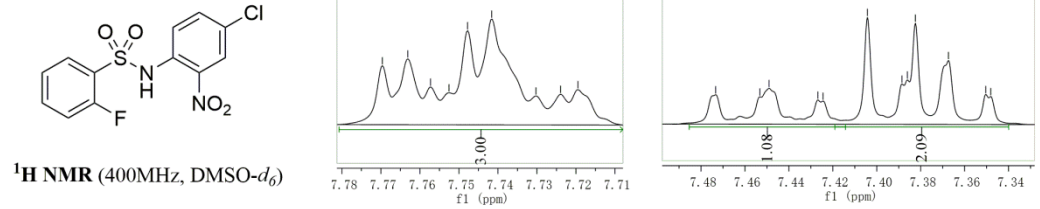


^{13}C NMR (101MHz, DMSO-d_6)

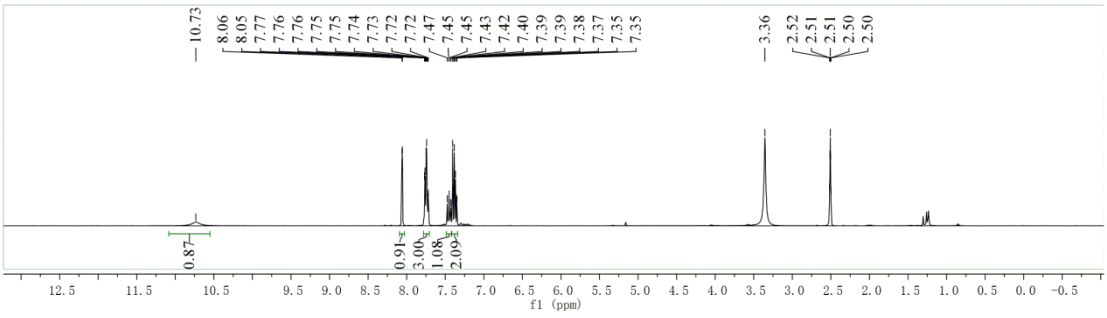
4o $C_{13}H_{11}ClN_2O_4S$, $[M-H]^-$ 325.0050. Found 325.0046.



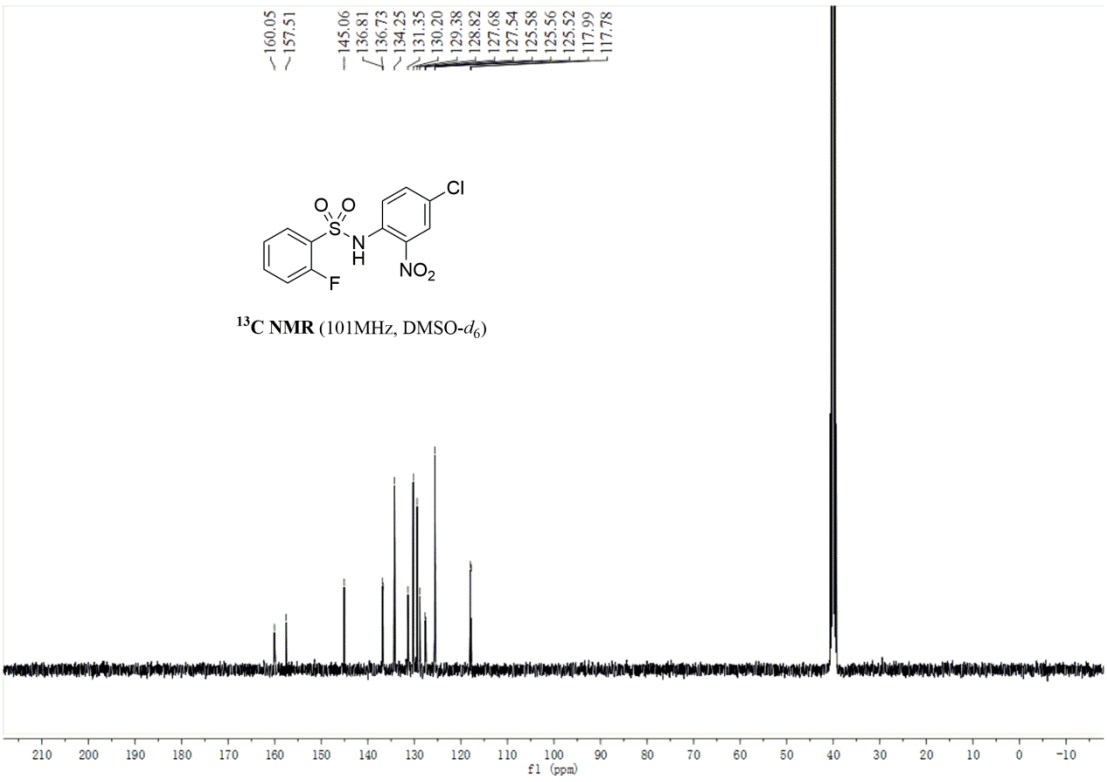
4p ^{1}H NMR



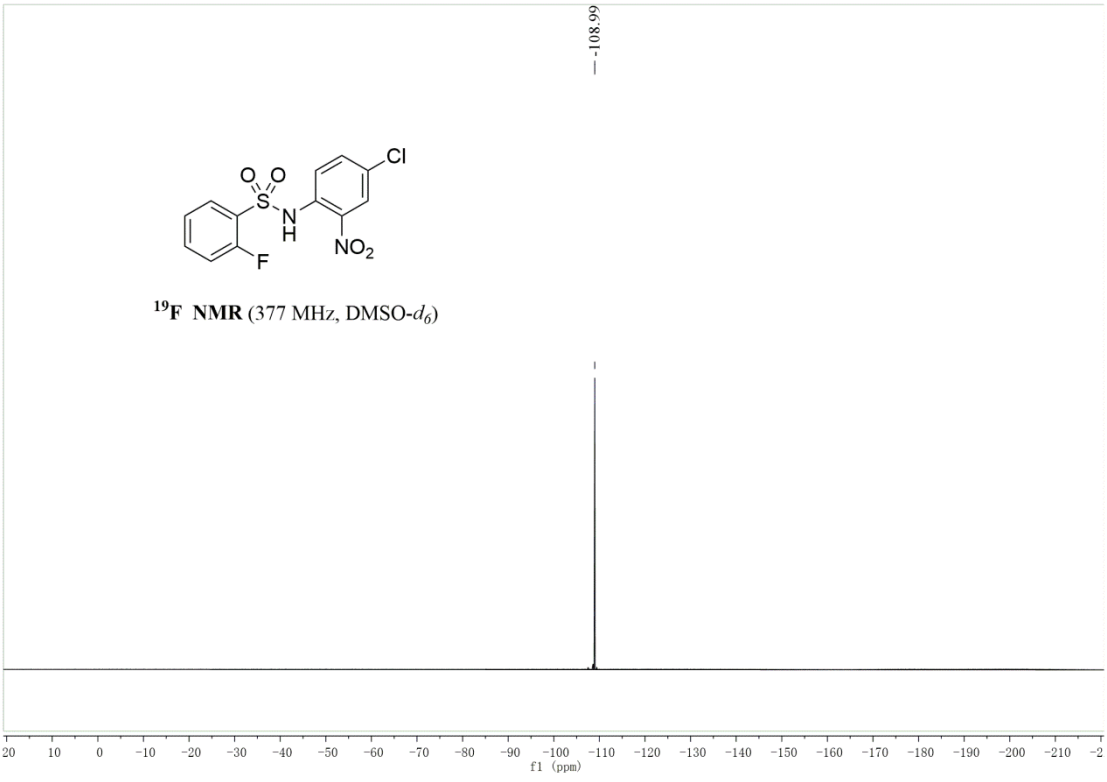
^{1}H NMR (400MHz, DMSO-d_6)



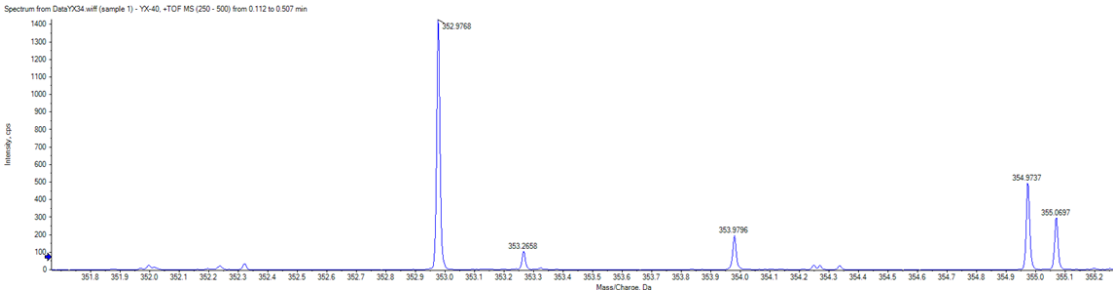
4p ^{13}C NMR



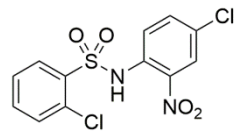
4p ^{19}F NMR



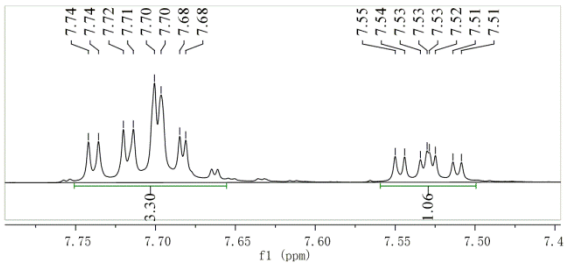
4p $C_{12}H_8ClFN_2O_4S$, $[M+Na]^+$ 352.9775. Found 352.9768.

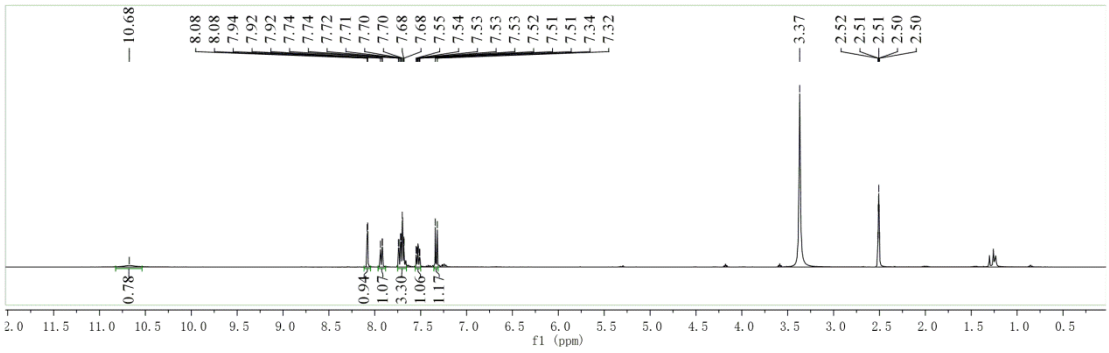


4q ^{1}H NMR

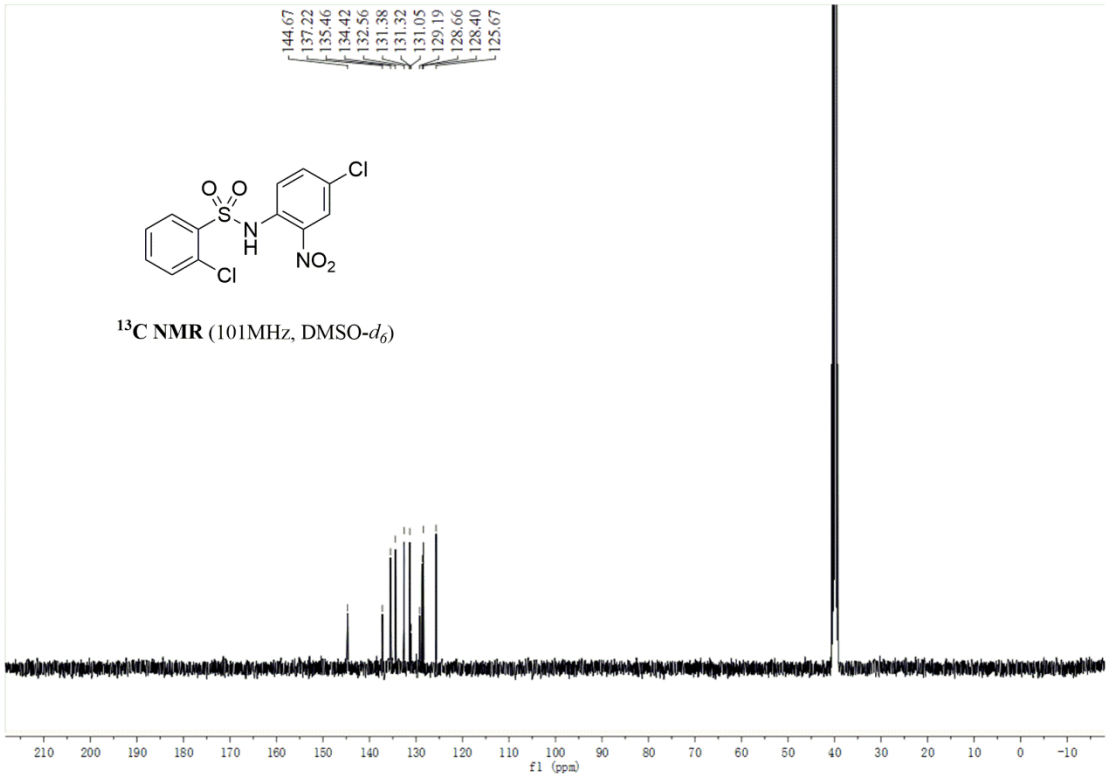


^{1}H NMR (400MHz, DMSO-d_6)

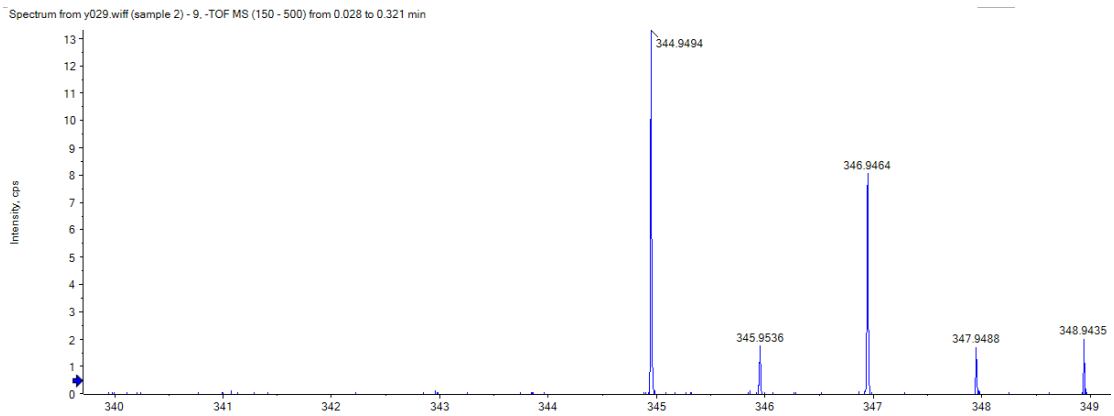




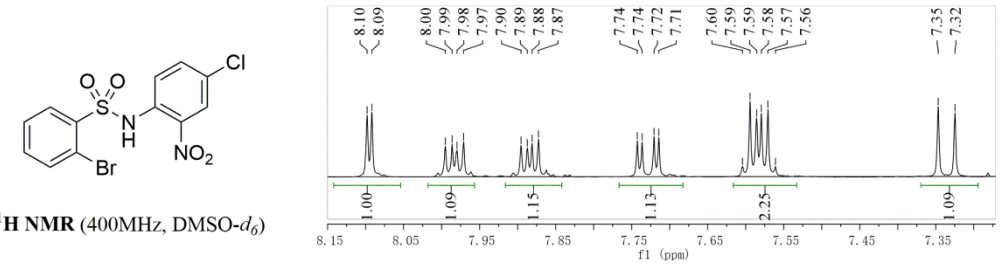
4q ^{13}C NMR



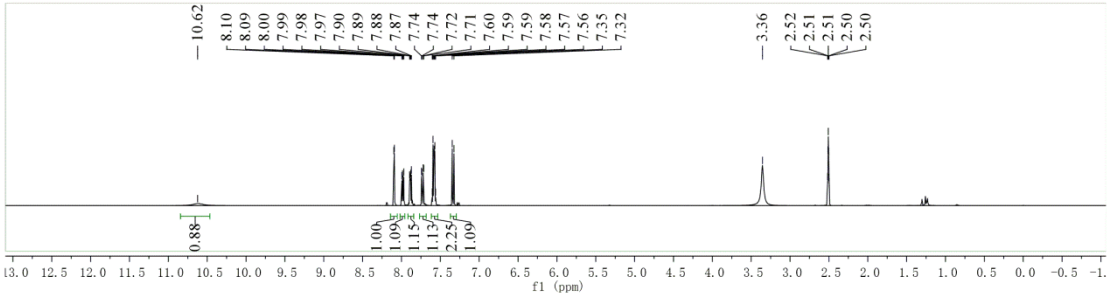
4q $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9494.



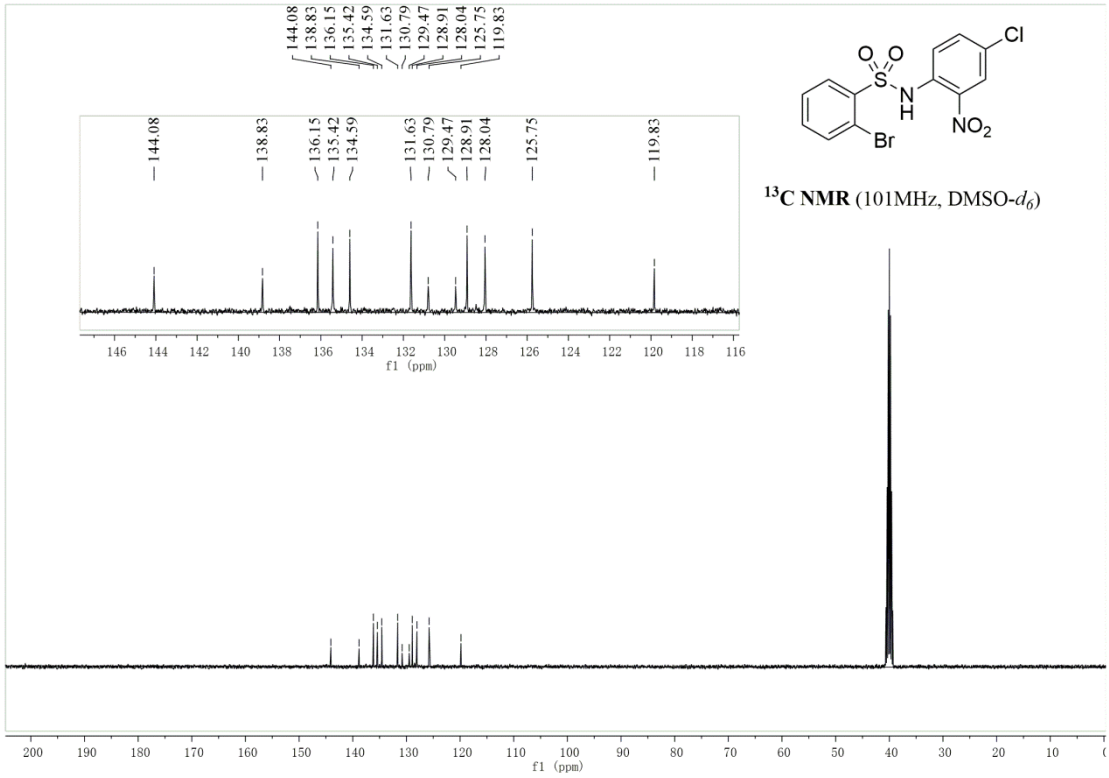
4r ^{1}H NMR



^{1}H NMR (400MHz, DMSO-d_6)

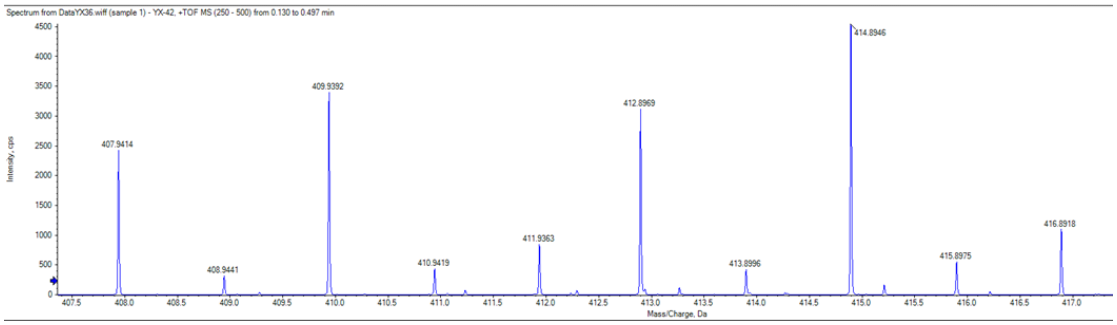


4r ^{13}C NMR

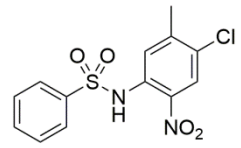


^{13}C NMR (101MHz, DMSO-d_6)

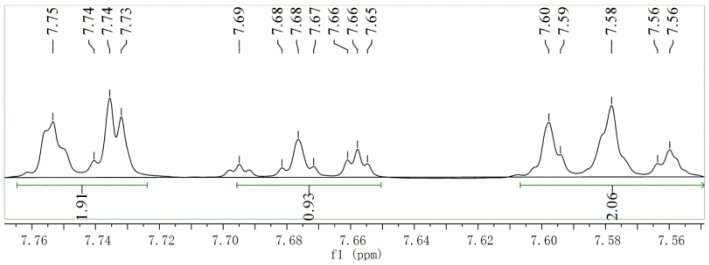
4r $C_{12}H_8BrClN_2O_4S$, $[M+Na]^+$ 412.8974. Found 412.8969.

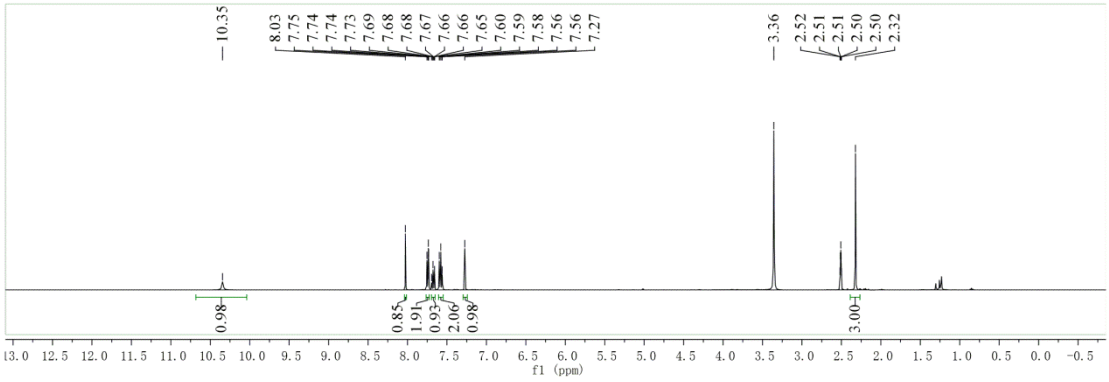


4u ^{1}H NMR

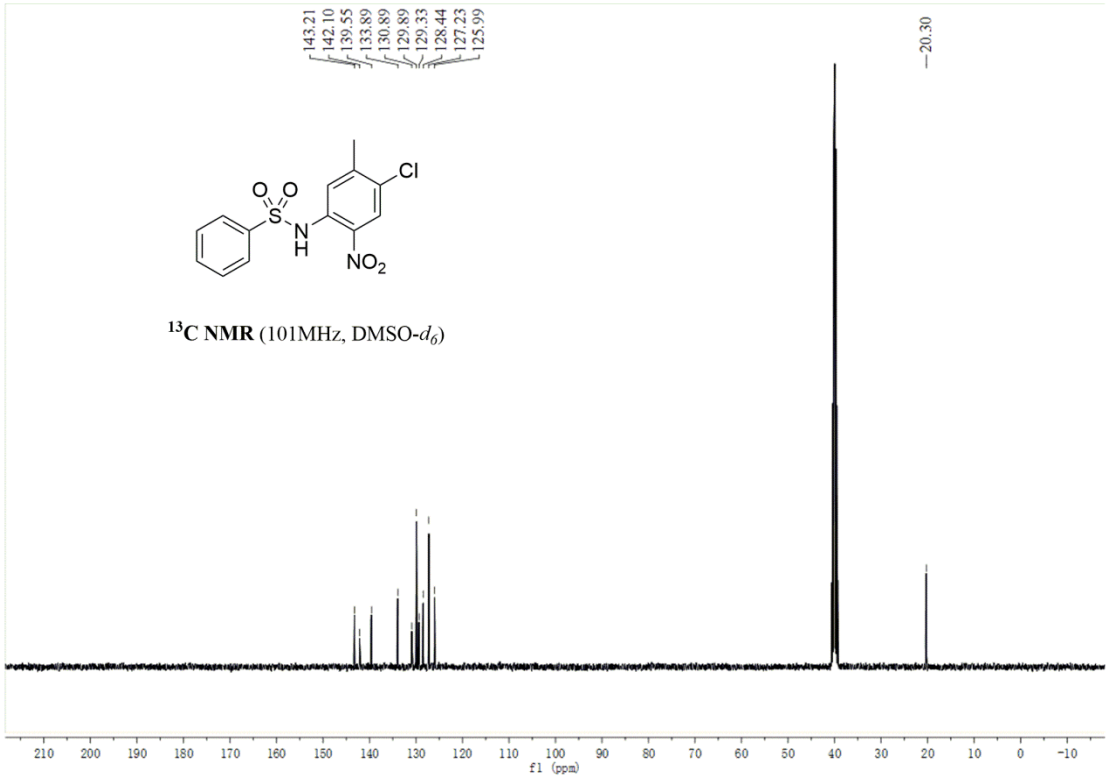


^{1}H NMR (400MHz, DMSO-d_6)



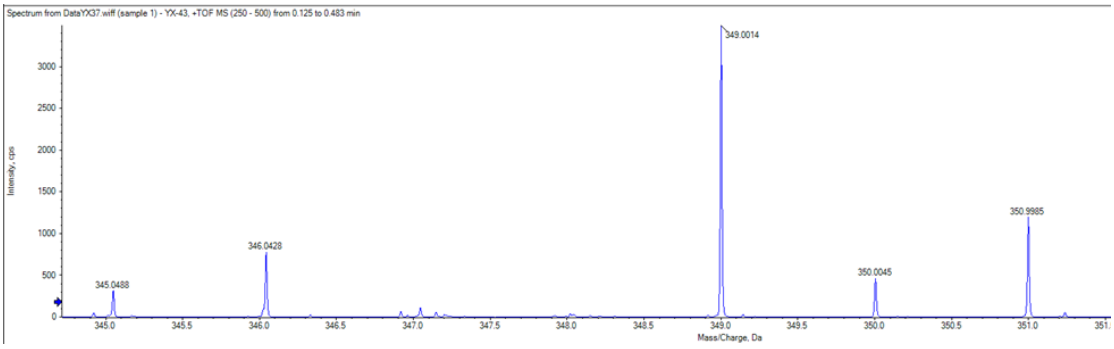


4u ^{13}C NMR

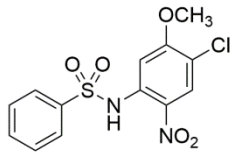


^{13}C NMR (101MHz, DMSO-d_6)

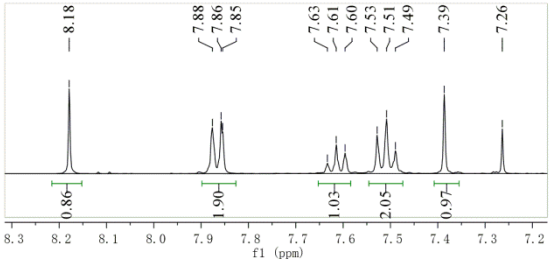
4u $C_{13}H_{11}ClN_2O_4S$, $[M+Na]^+$ 349.0026. Found 349.0014.

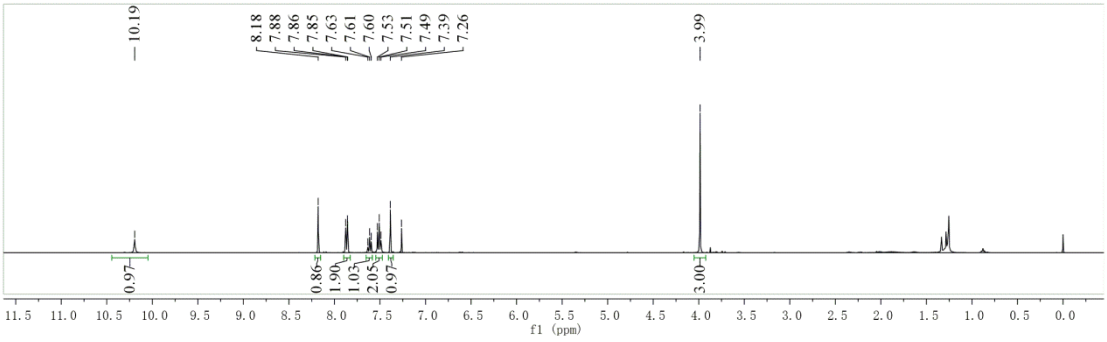


4v ^{1}H NMR

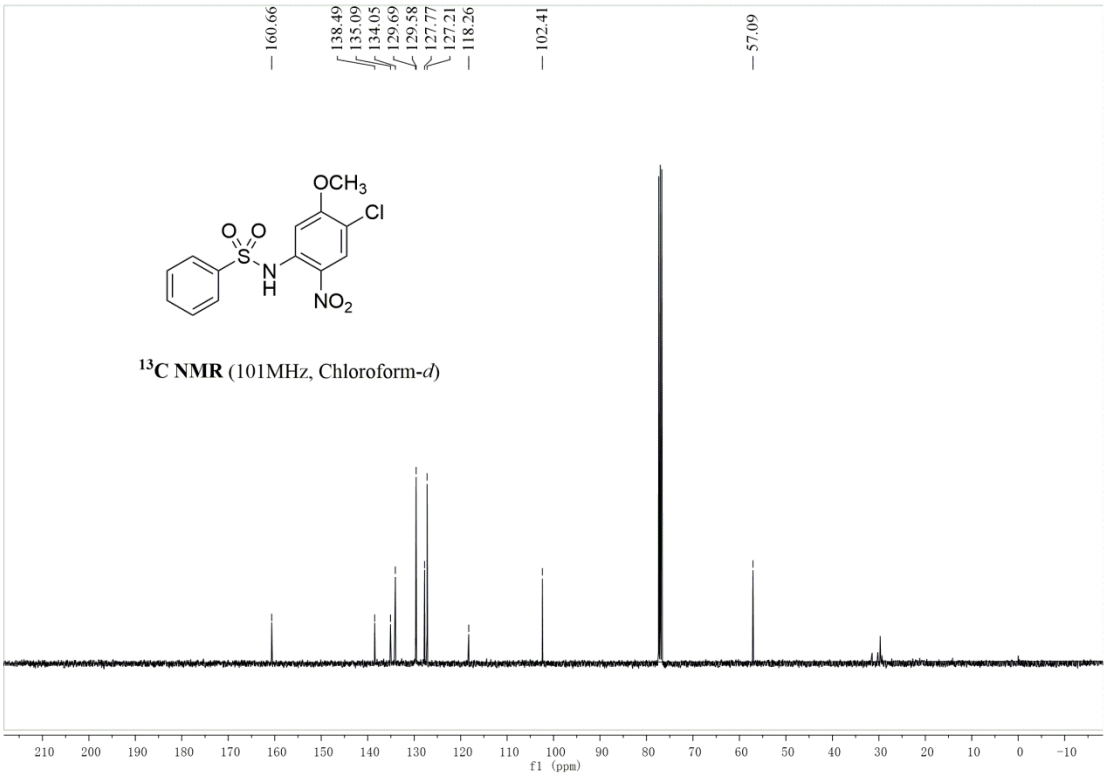


^{1}H NMR (400MHz, Chloroform-*d*)



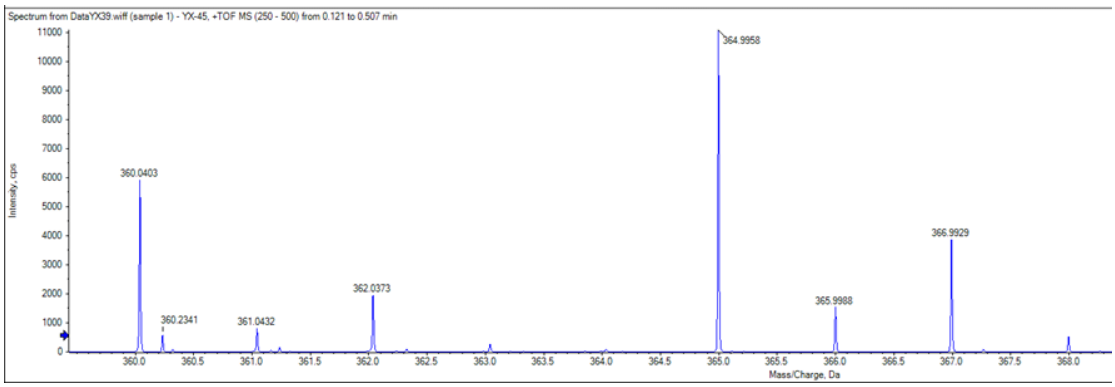


4v ^{13}C NMR

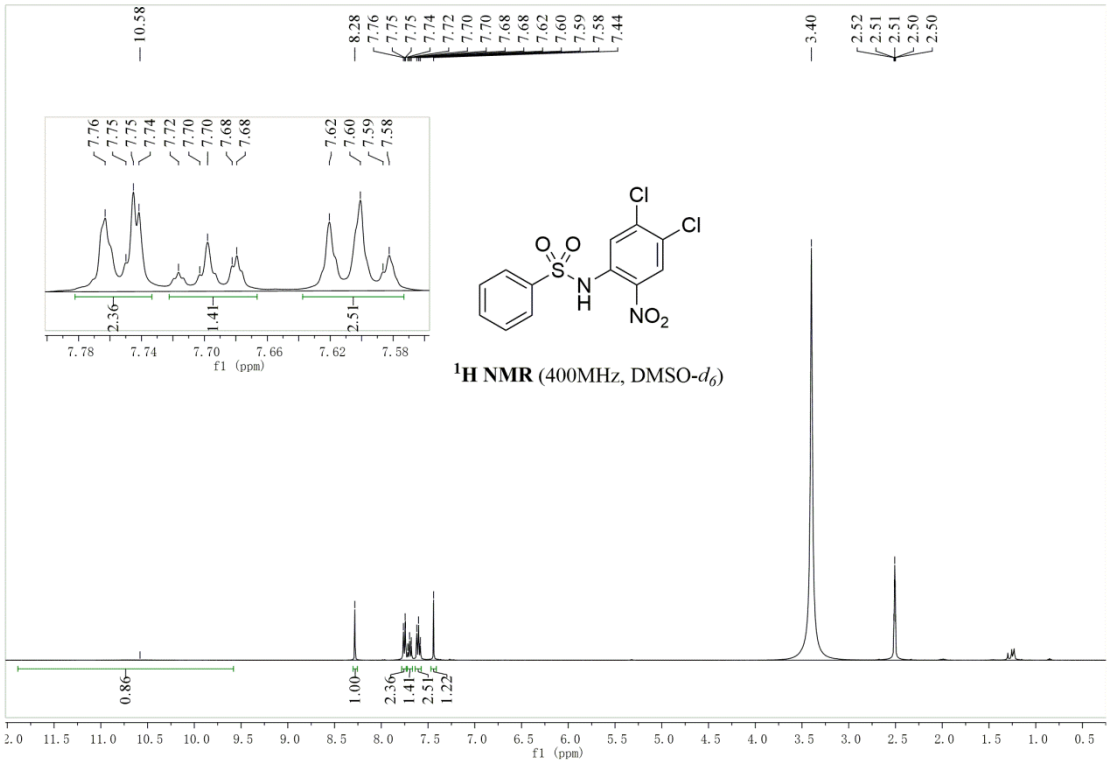


^{13}C NMR (101MHz, Chloroform-*d*)

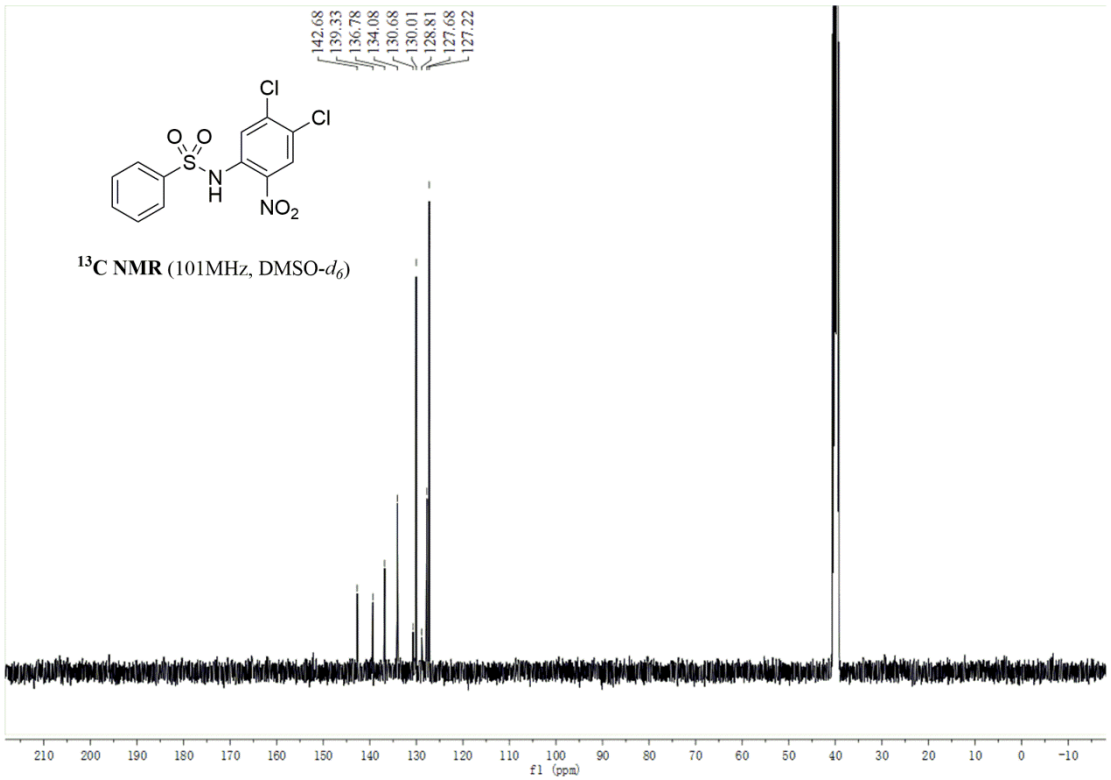
4v $C_{13}H_{11}ClN_2O_5S$, $[M+Na]^+$ 364.9975. Found 364.9958.



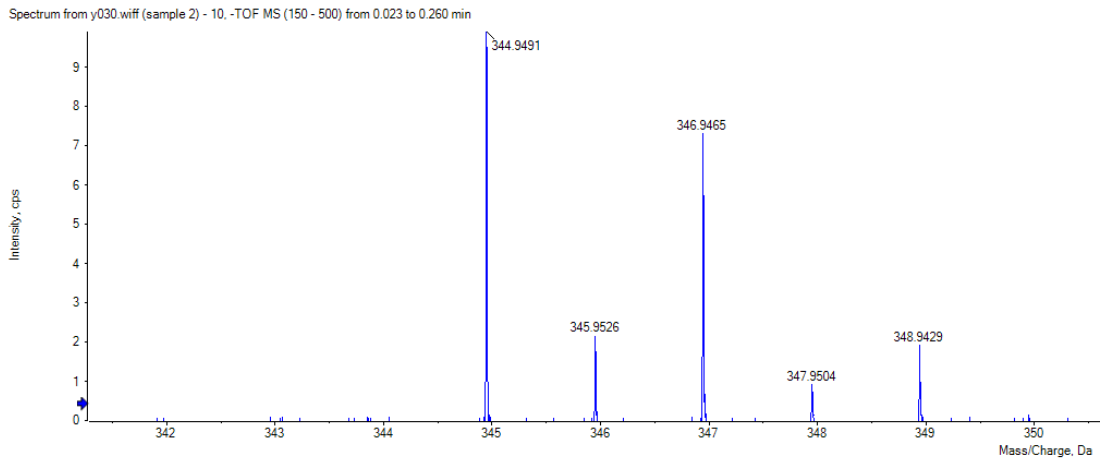
4w ^{1}H NMR



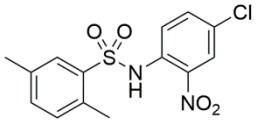
4w ^{13}C NMR



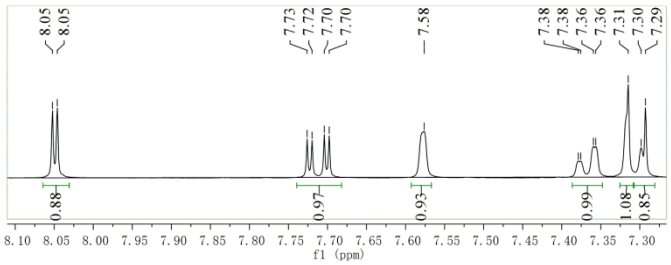
4w $C_{12}H_8Cl_2N_2O_4S$, $[M-H]^-$ 344.9504. Found 344.9491.

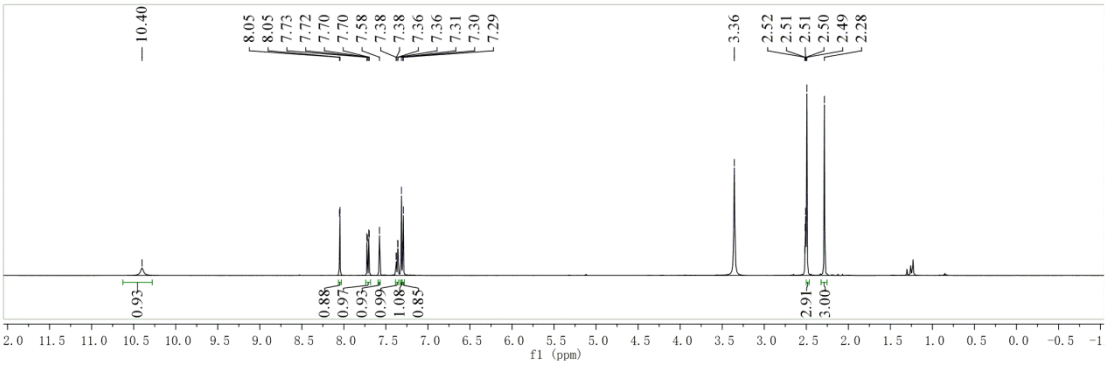


4ab ^{1}H NMR

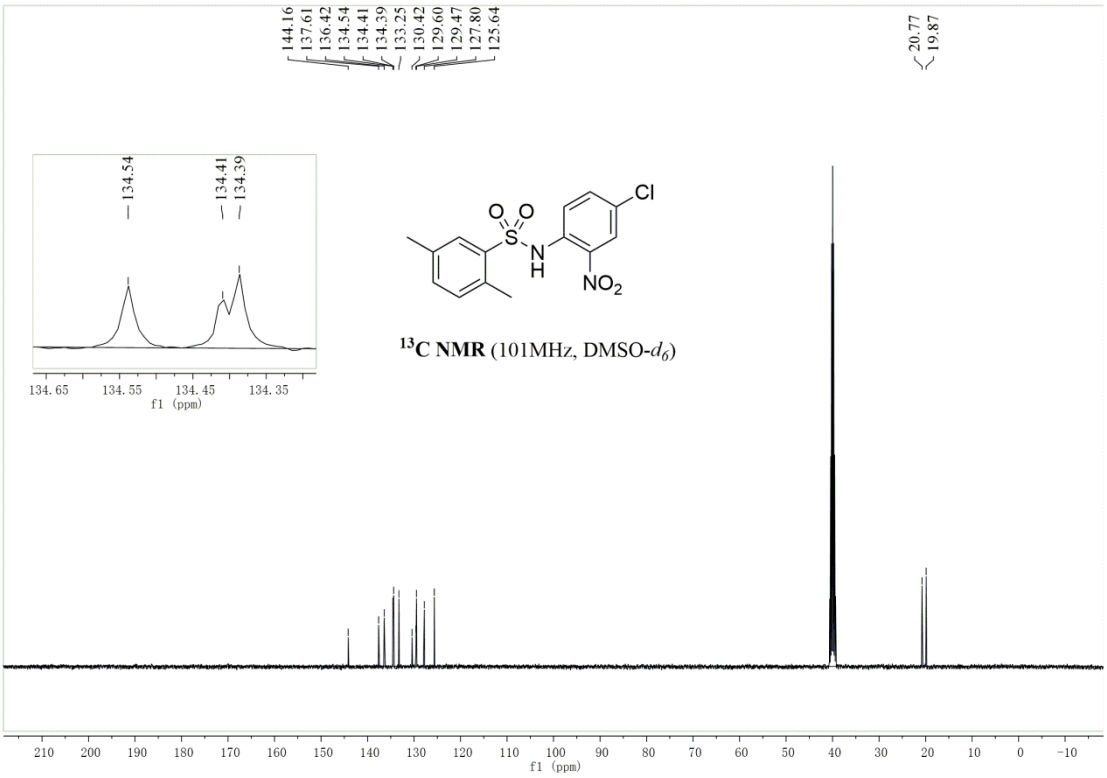


^{1}H NMR (400MHz, DMSO-d_6)



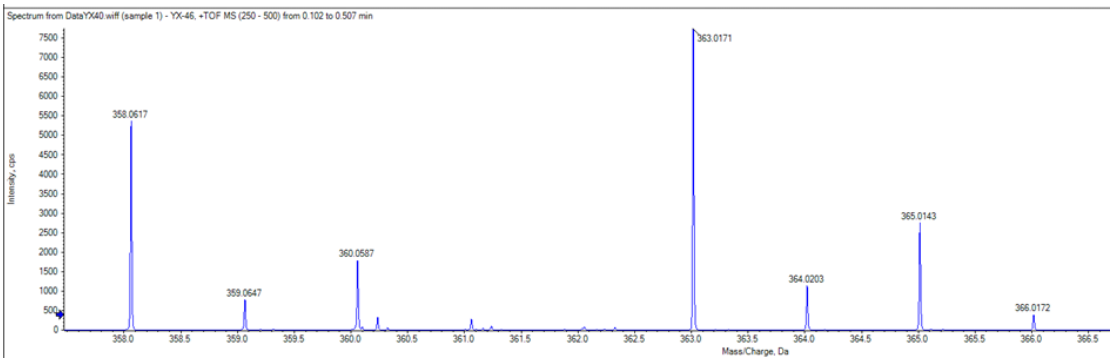


4ab ^{13}C NMR

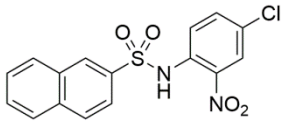


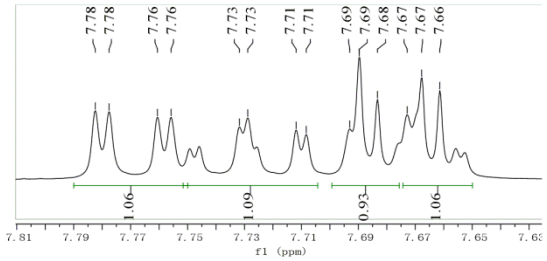
^{13}C NMR (101MHz, DMSO-d_6)

4ab $C_{14}H_{13}ClN_2O_4S$, $[M+Na]^+$ 363.0182. Found 363.0171.

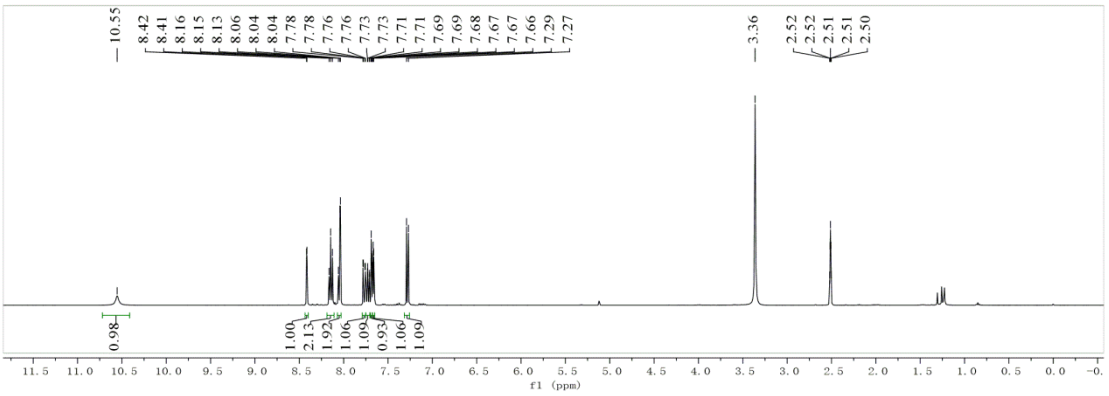


4ac ^{1}H NMR

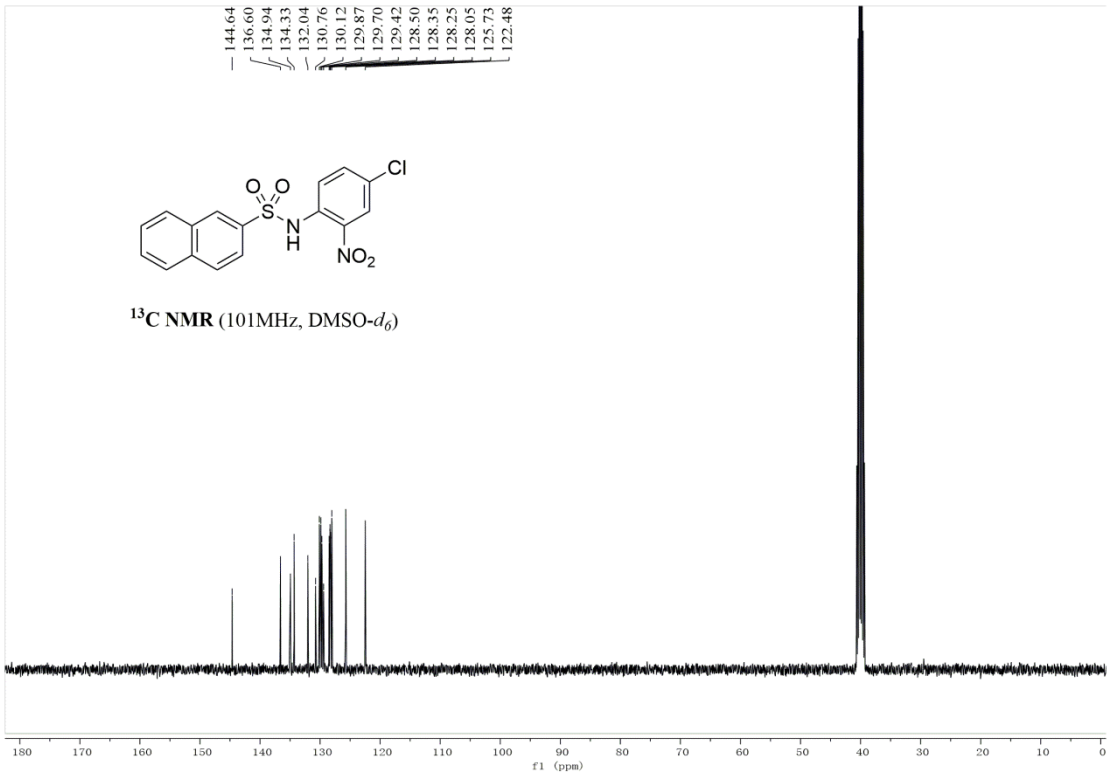




^{1}H NMR (400MHz, DMSO-d_6)

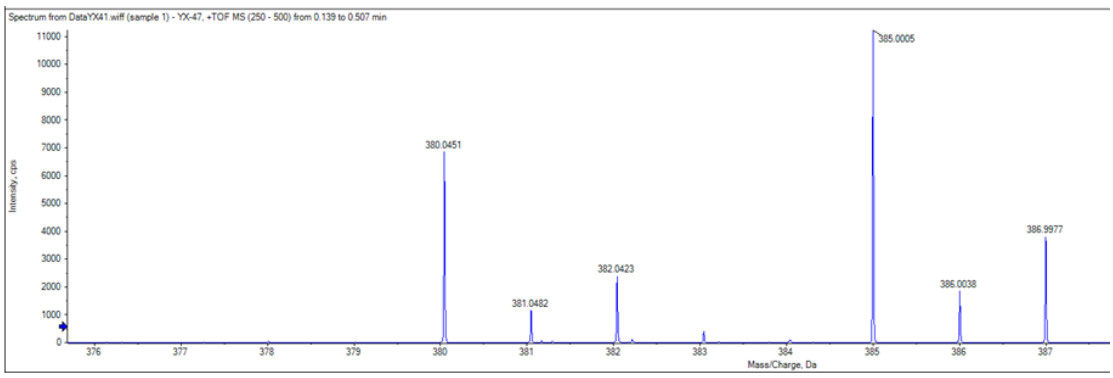


4ac ^{13}C NMR

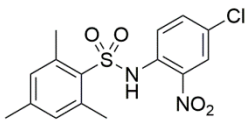


^{13}C NMR (101MHz, DMSO-d_6)

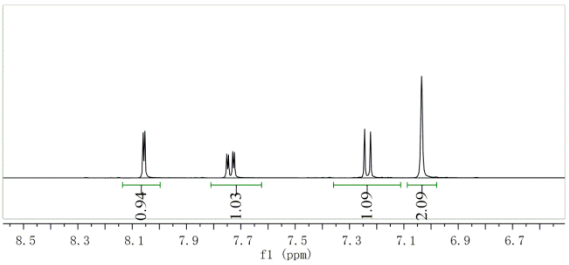
4ac $C_{16}H_{11}ClN_2O_4S$, $[M+Na]^+$ 385.0026. Found 385.0005.

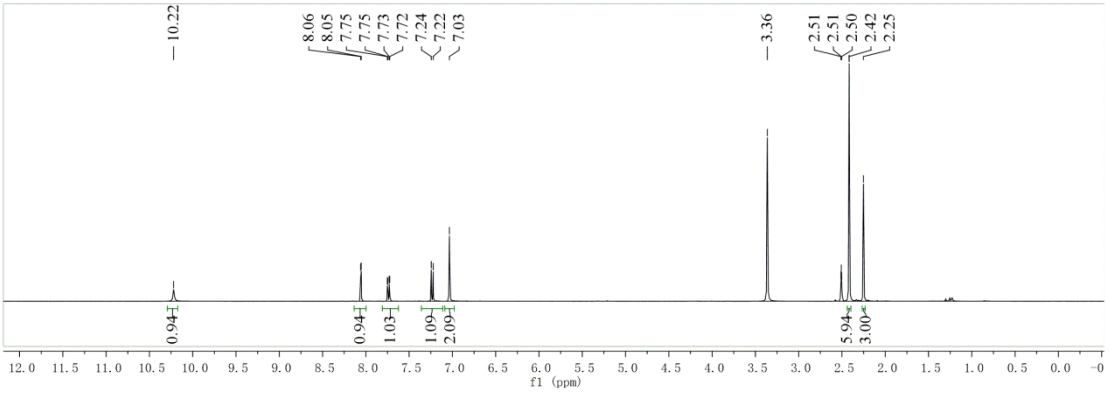


4ad ^{1}H NMR

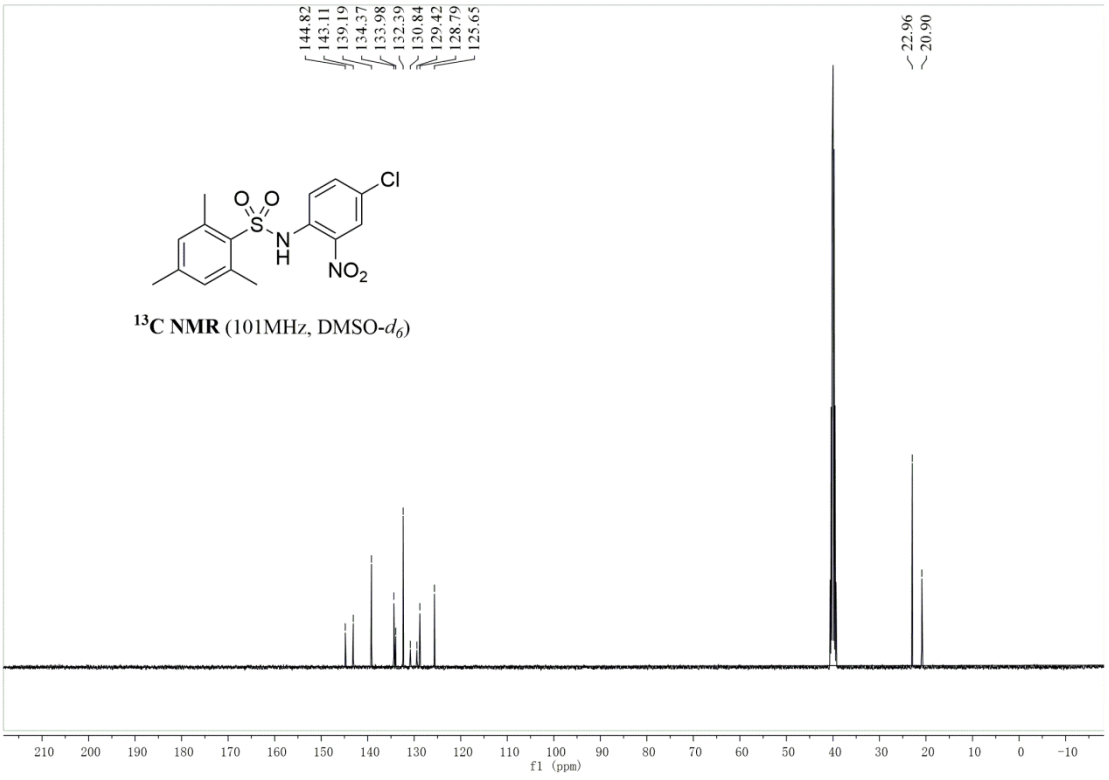


^{1}H NMR (400MHz, DMSO-d_6)



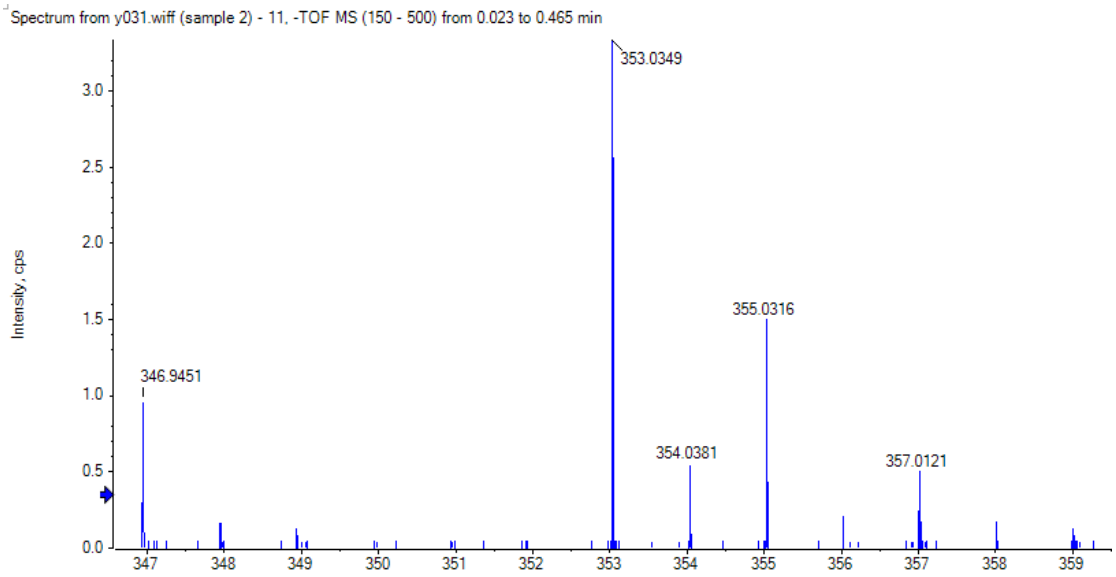


4ad ^{13}C NMR

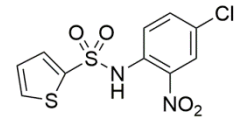


^{13}C NMR (101MHz, DMSO-d_6)

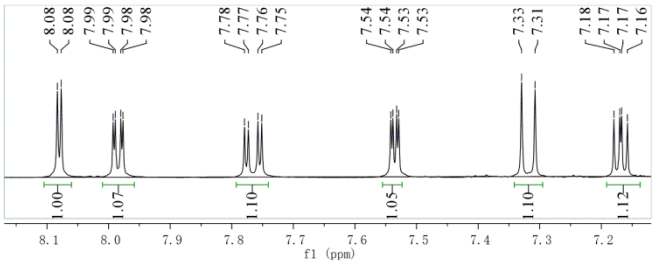
4ad $C_{15}H_{15}ClN_2O_4S$, $[M-H]^-$ 353.0363. Found 353.0349.

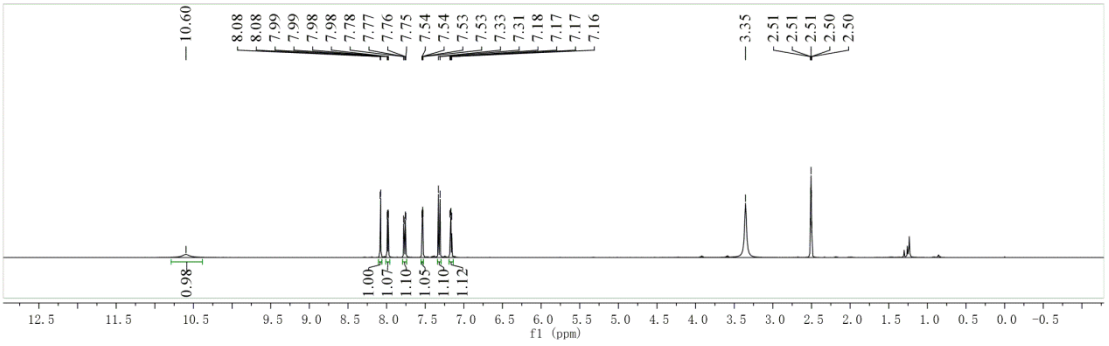


4ag ^{1}H NMR

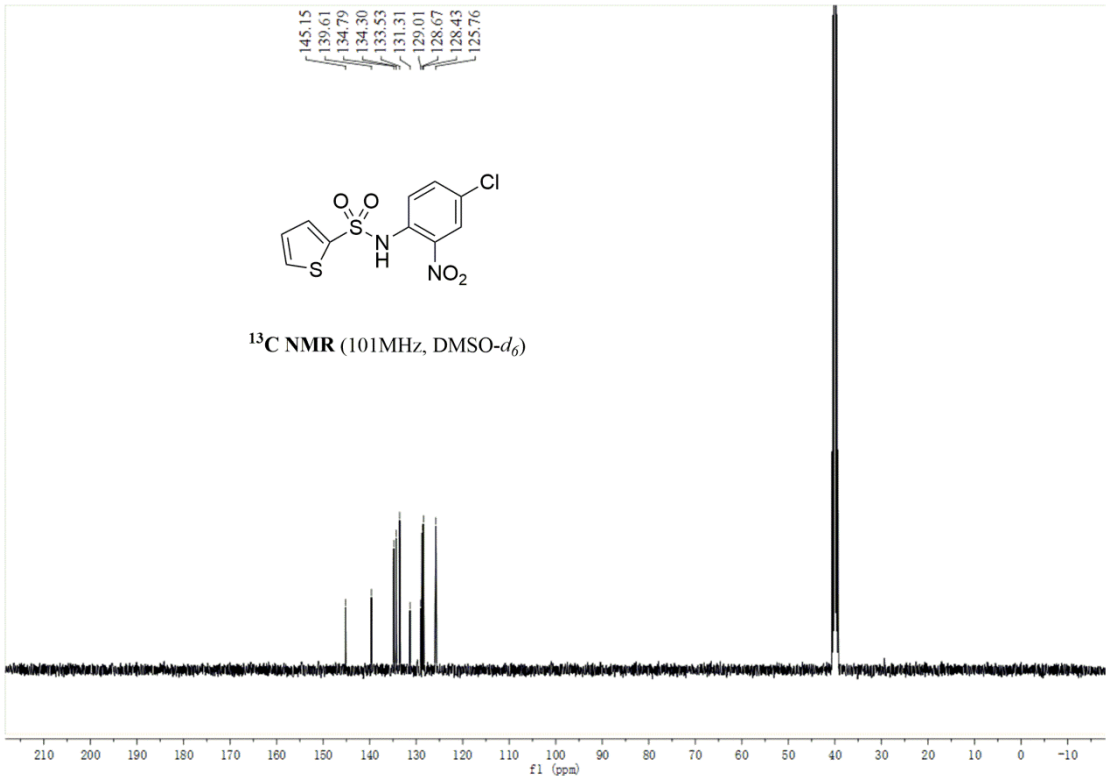


^{1}H NMR (400MHz, DMSO-d_6)

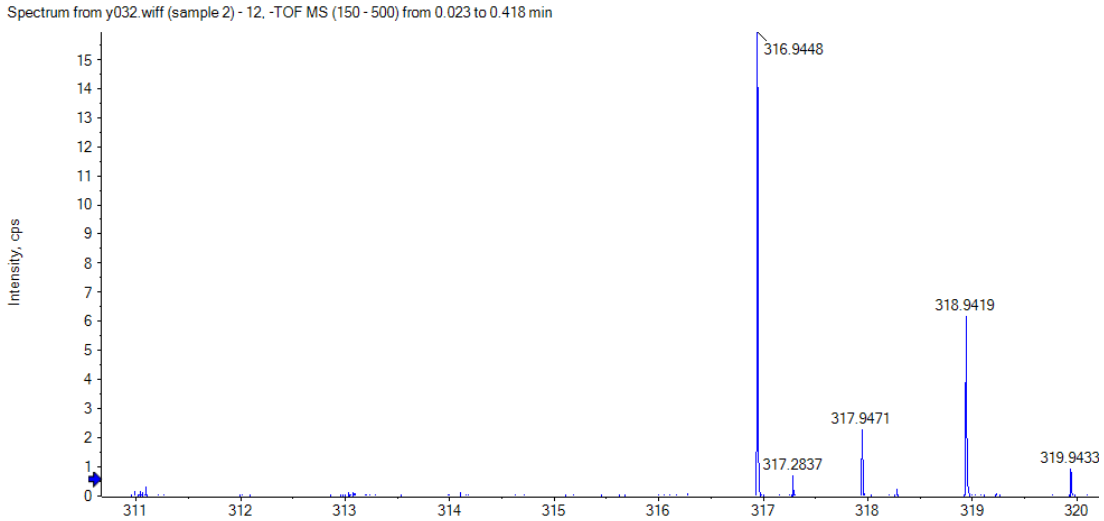




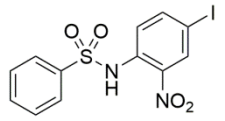
4ag ^{13}C NMR



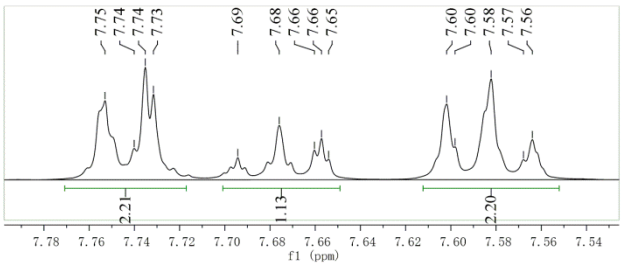
4ag $C_{10}H_7ClN_2O_4S_2$, $[M-H]^-$ 316.9458. Found 316.9448.

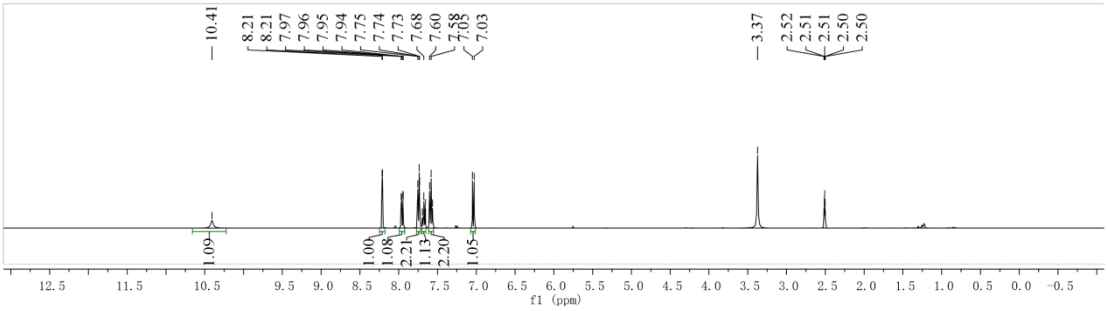


5a ^{1}H NMR

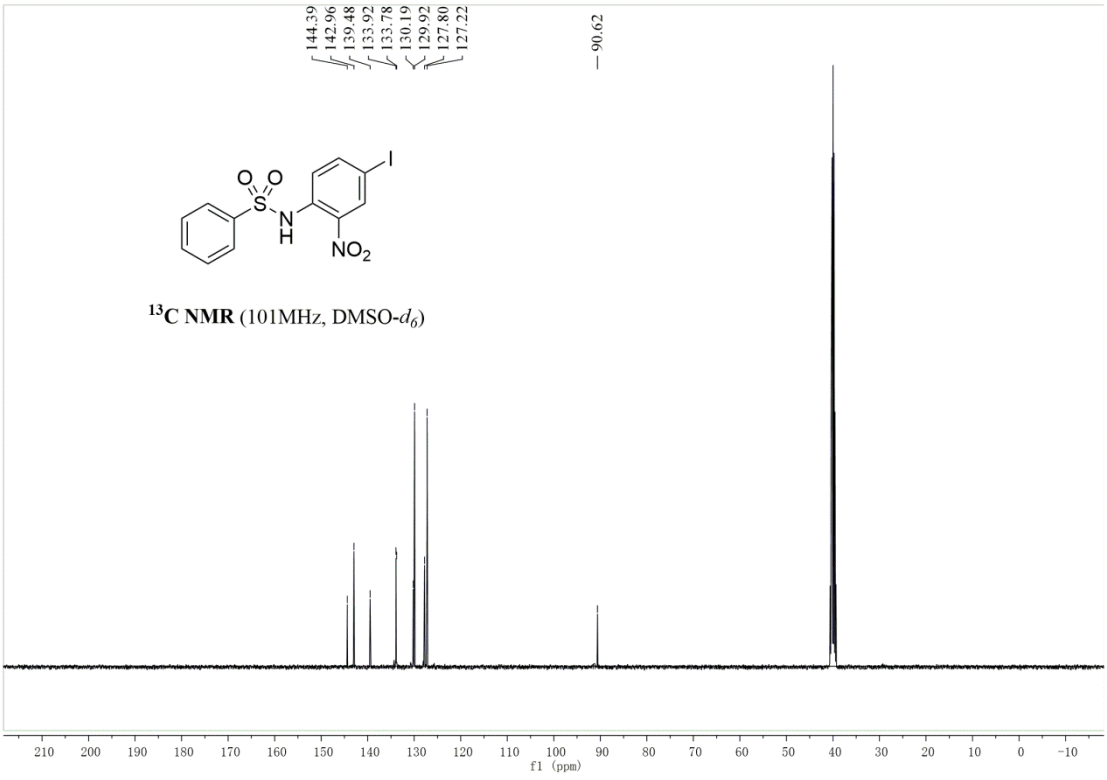


^{1}H NMR (400MHz, DMSO-d_6)



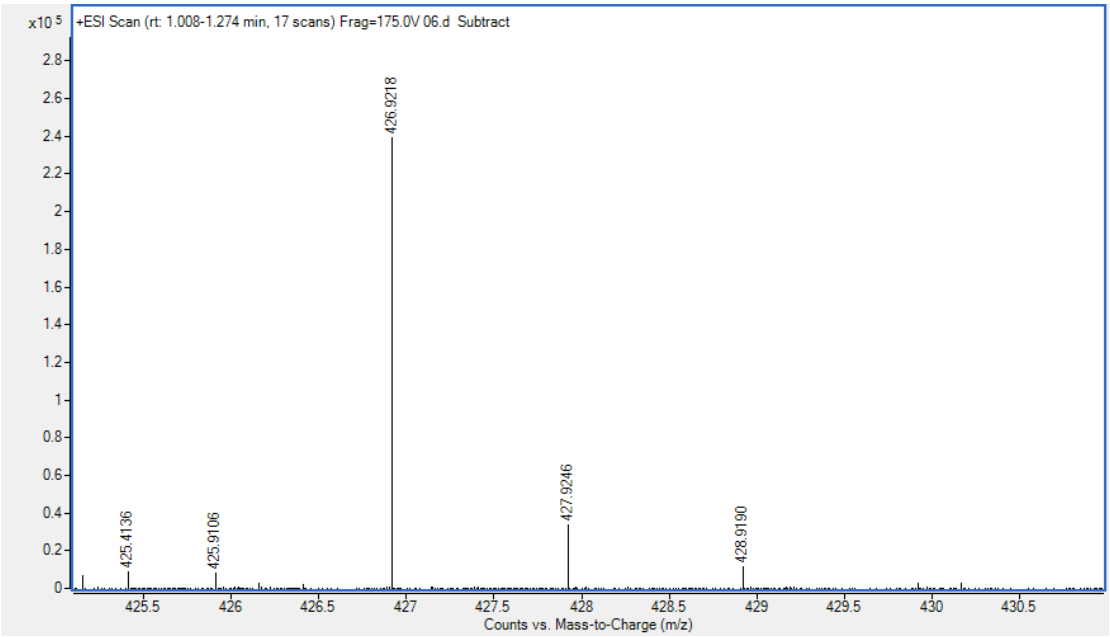


5a ^{13}C NMR

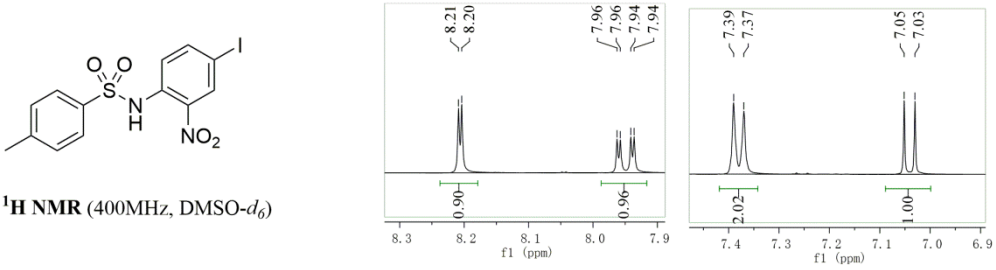


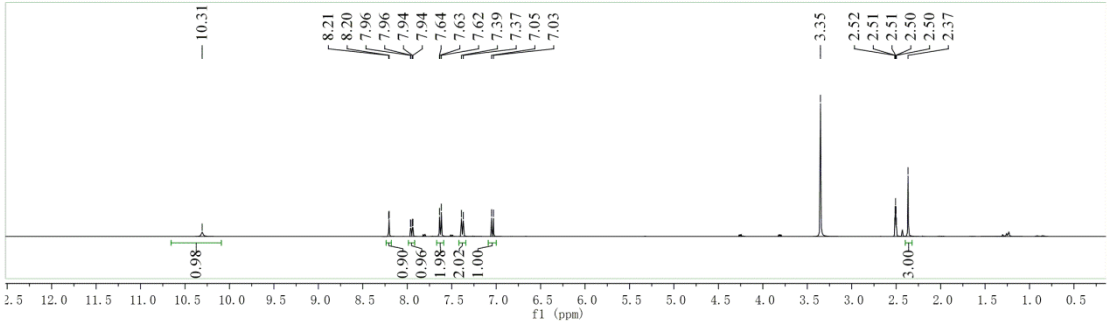
^{13}C NMR (101MHz, DMSO-d_6)

5a $C_{12}H_9IN_2O_4S$, $[M+Na]^+$ 426.9225. Found 426.9218.

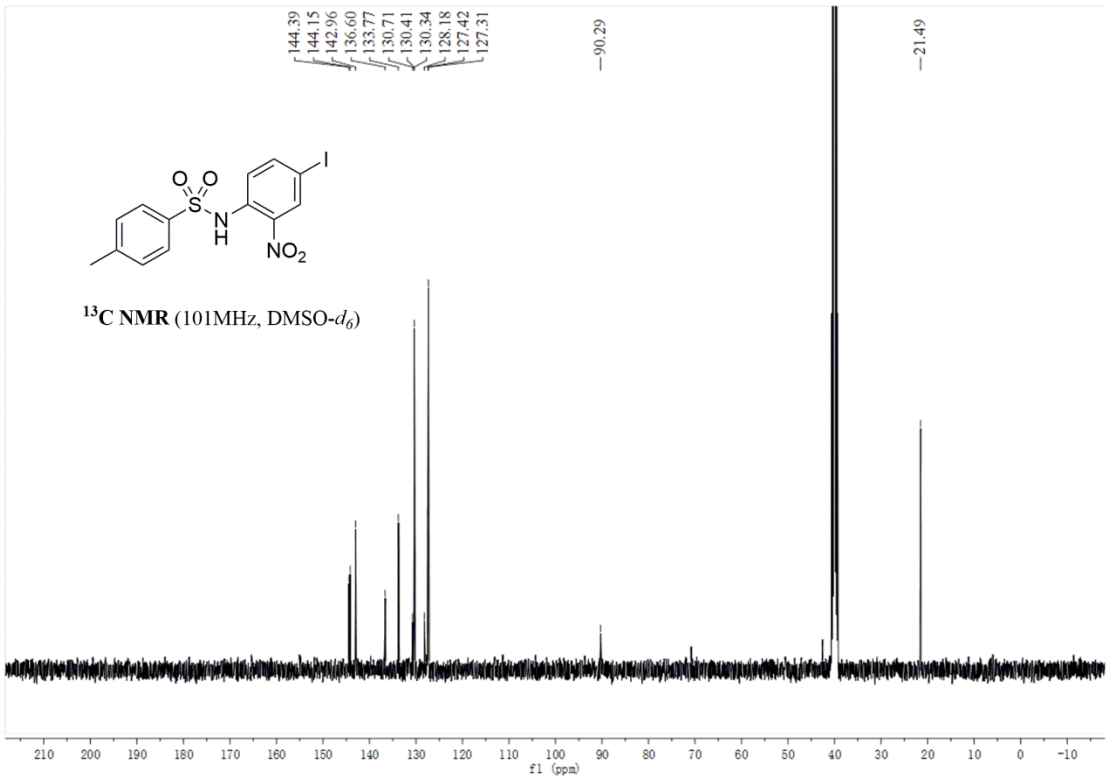


5b ^{1}H NMR

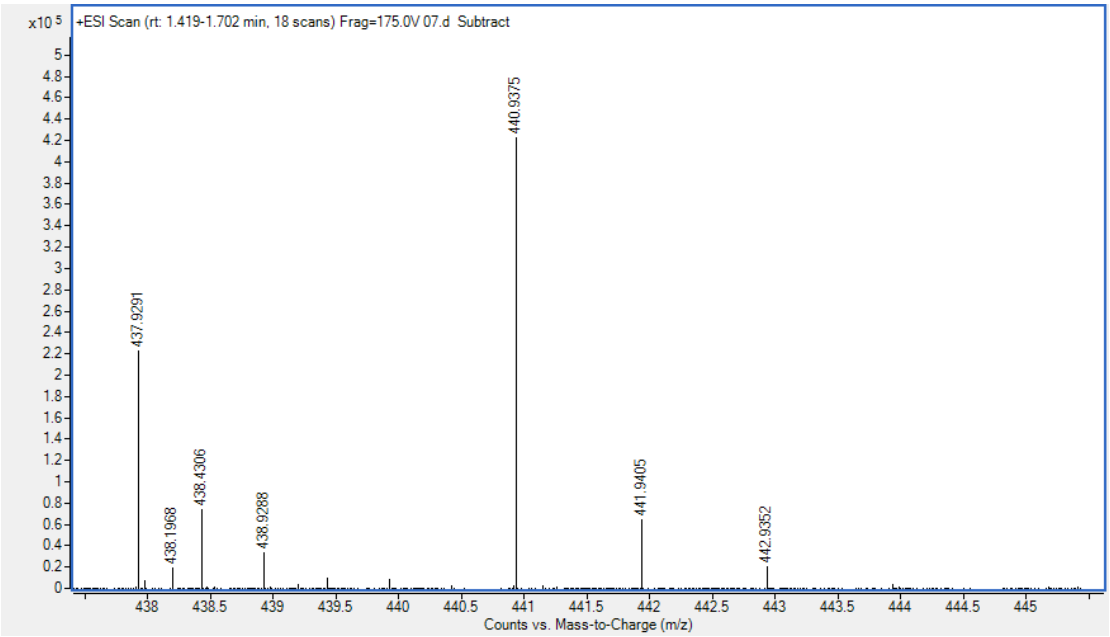




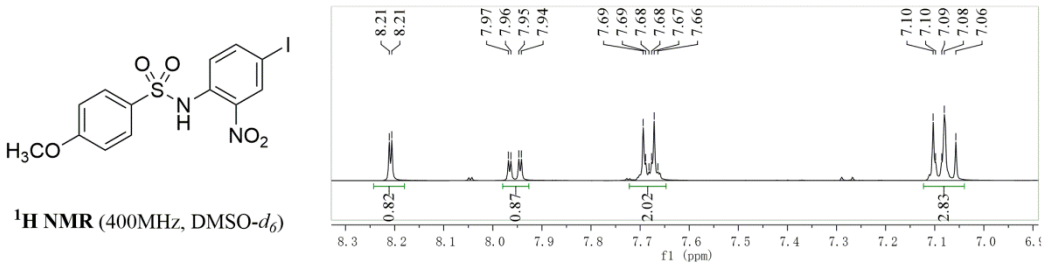
5b ^{1}H NMR



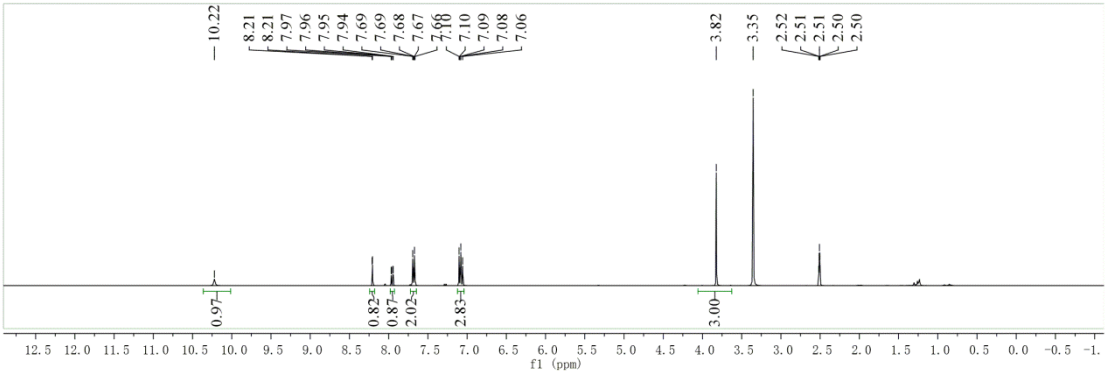
5b $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9375.



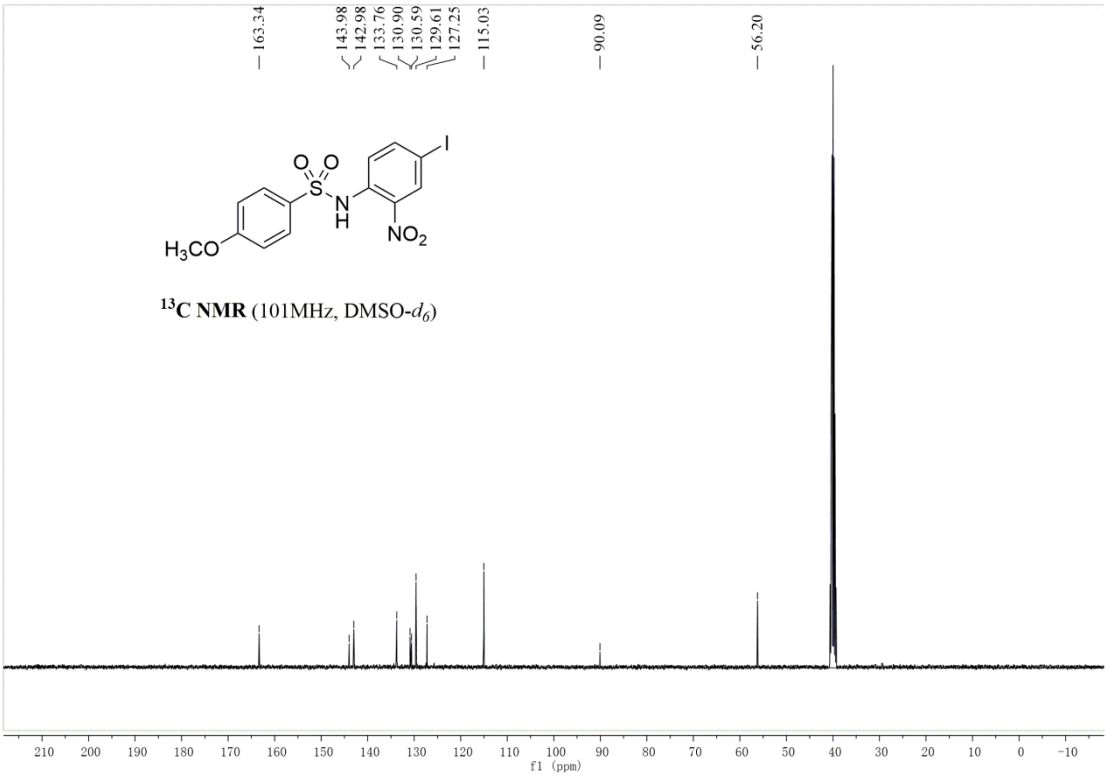
5c ^{1}H NMR



^{1}H NMR (400MHz, DMSO-d_6)

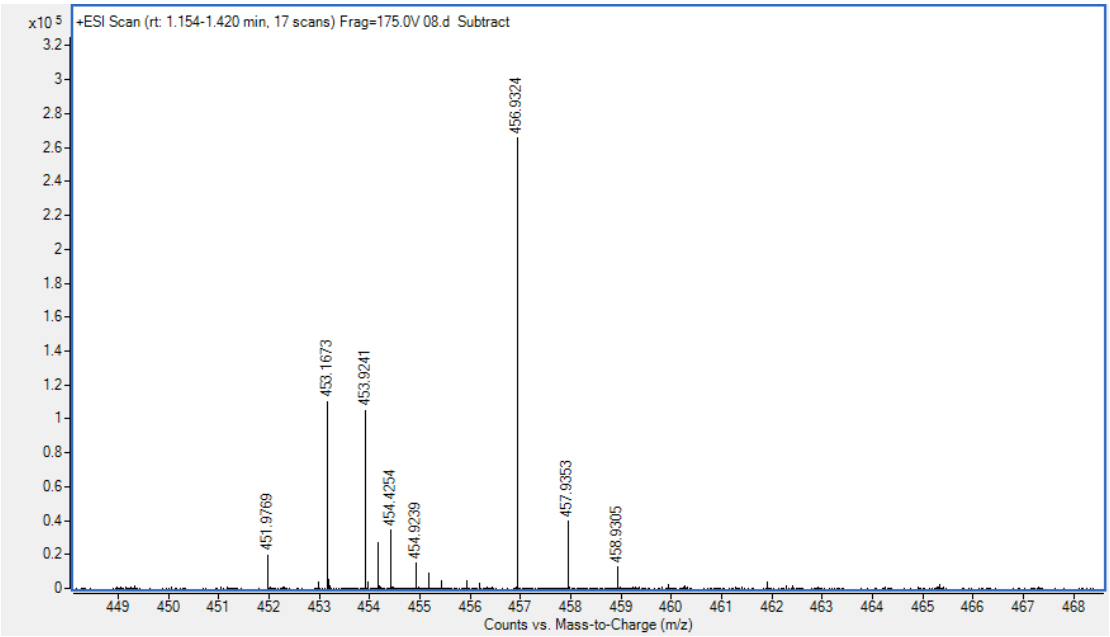


5c ^{13}C NMR

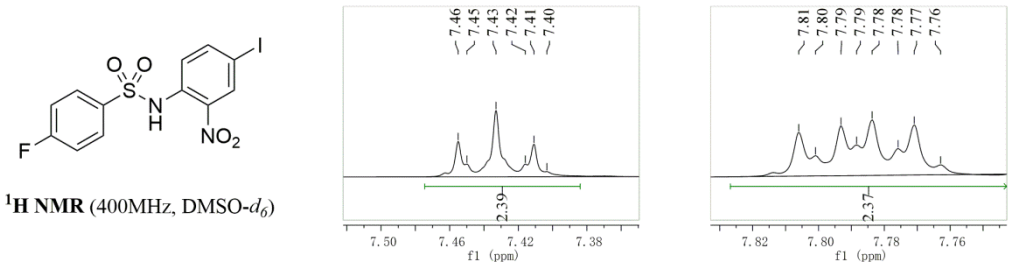


^{13}C NMR (101MHz, DMSO-d_6)

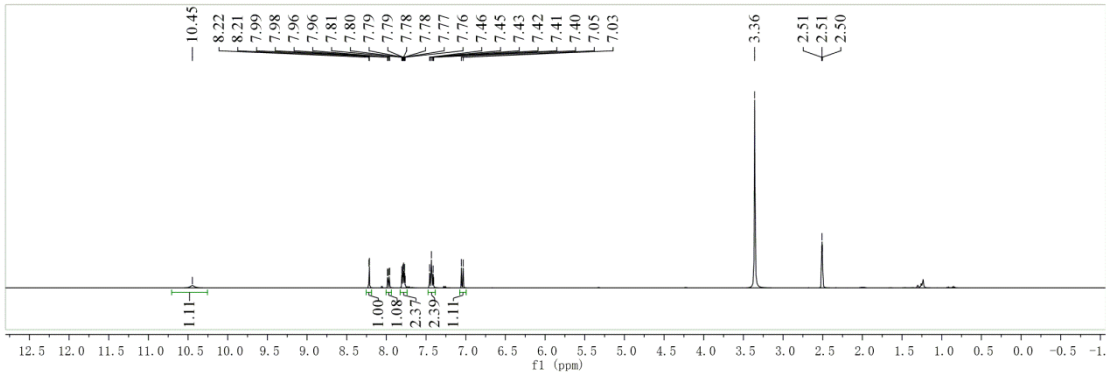
5c $C_{13}H_{11}IN_2O_5S$, $[M+Na]^+$ 456.9331. Found 456.9324.



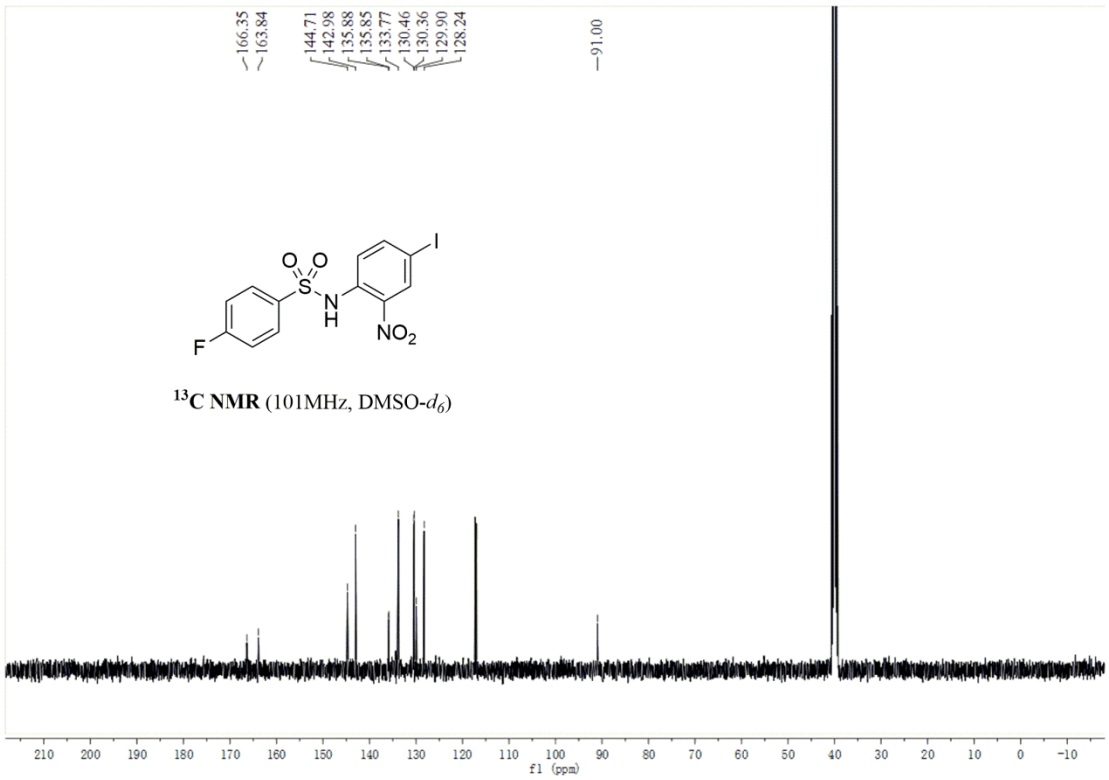
5d ^{1}H NMR



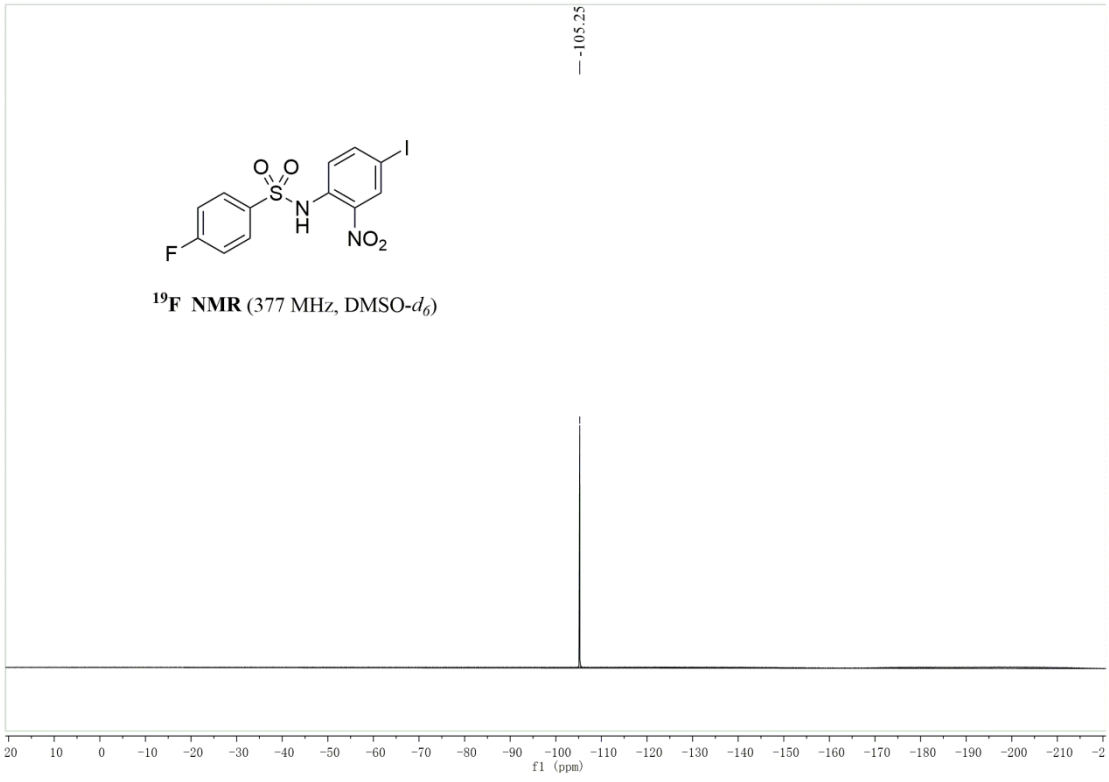
^{1}H NMR (400MHz, DMSO-d_6)



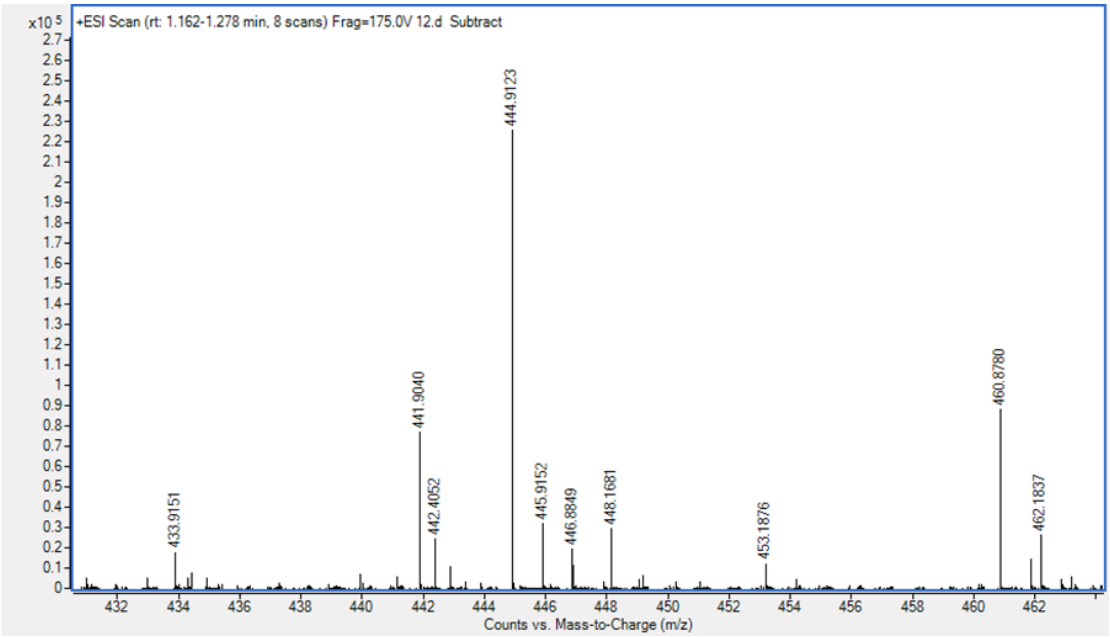
5d ^{13}C NMR



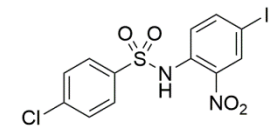
5d ^{19}F NMR



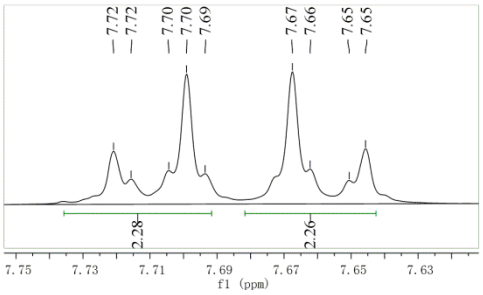
5d $C_{12}H_8FIN_2O_4S$, $[M+Na]^+$ 444.9131. Found 444.9123.

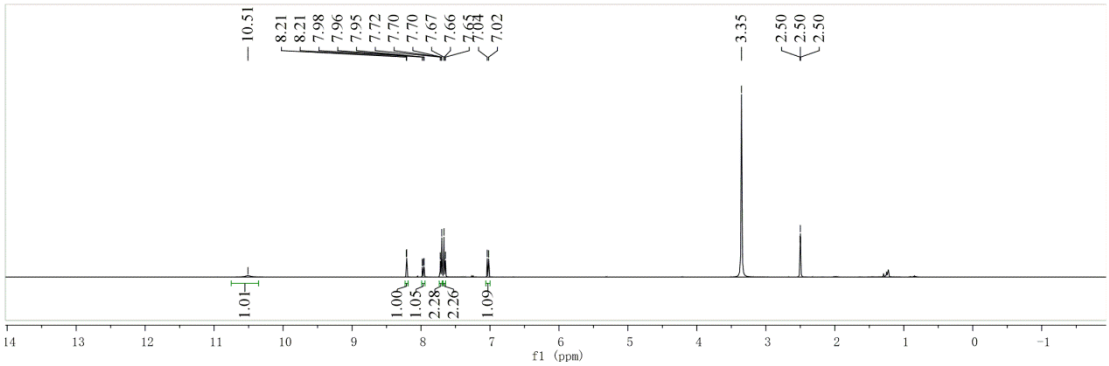


5e ^{1}H NMR

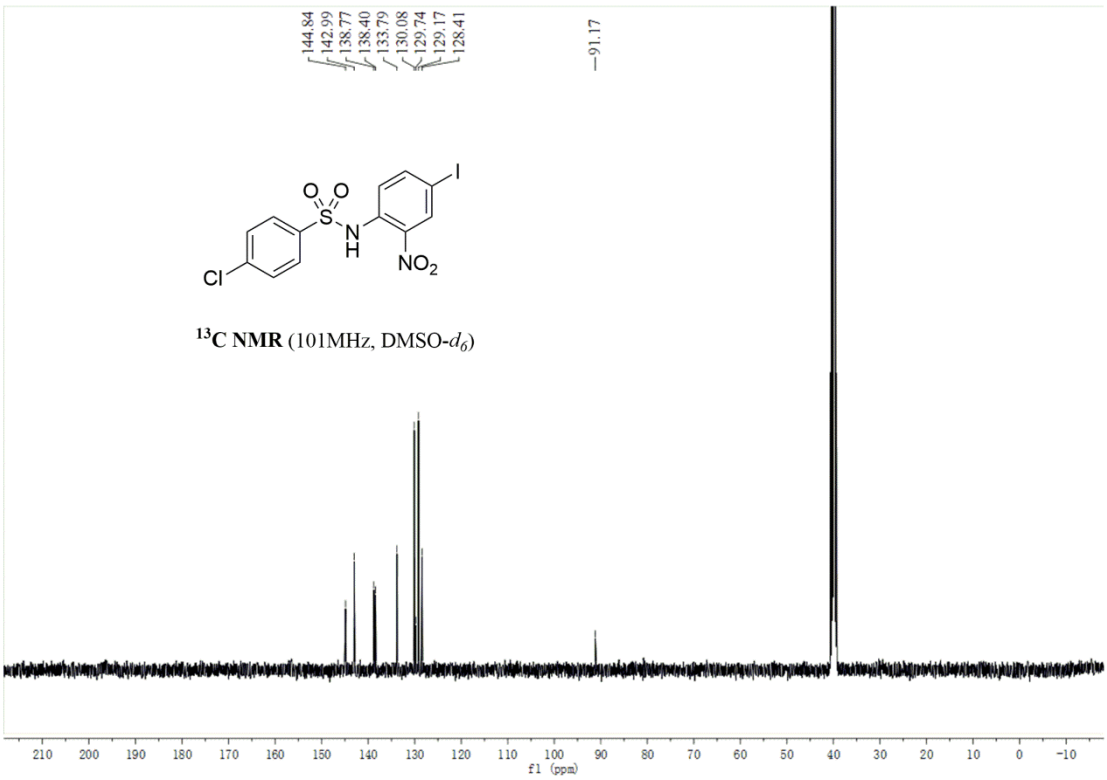


^{1}H NMR (400MHz, DMSO-d_6)

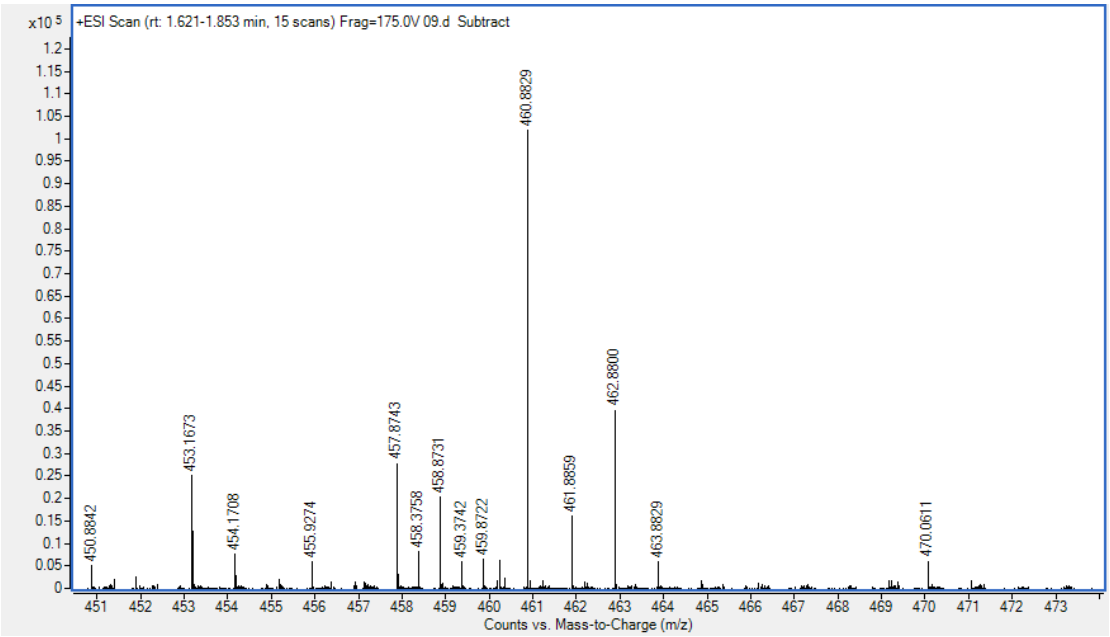




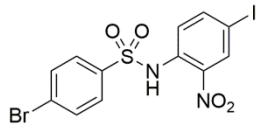
5e ^{13}C NMR



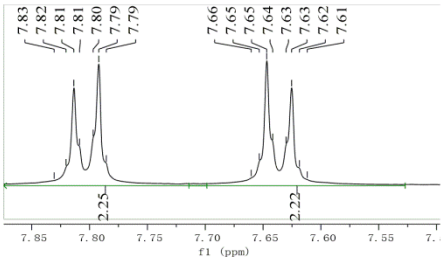
5e $C_{12}H_8ClIN_2O_4S$, $[M+Na]^+$ 460.8836. Found 460.8829.

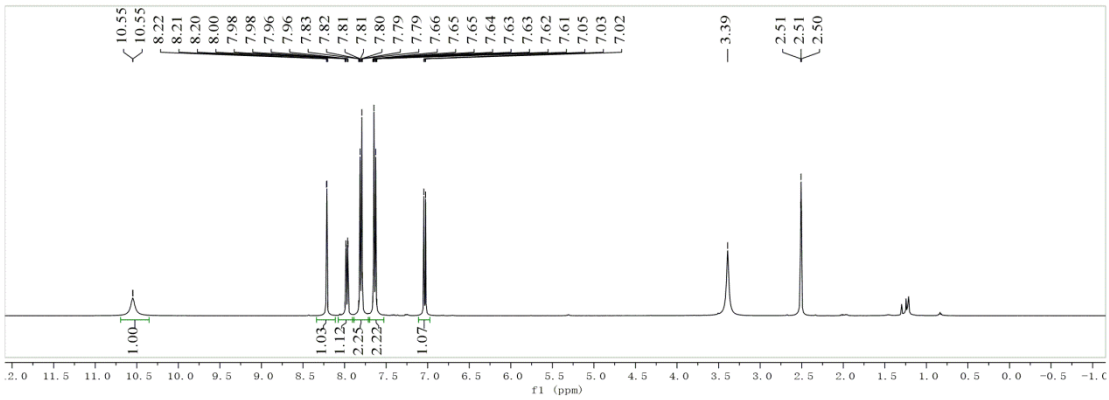


5f ^{1}H NMR

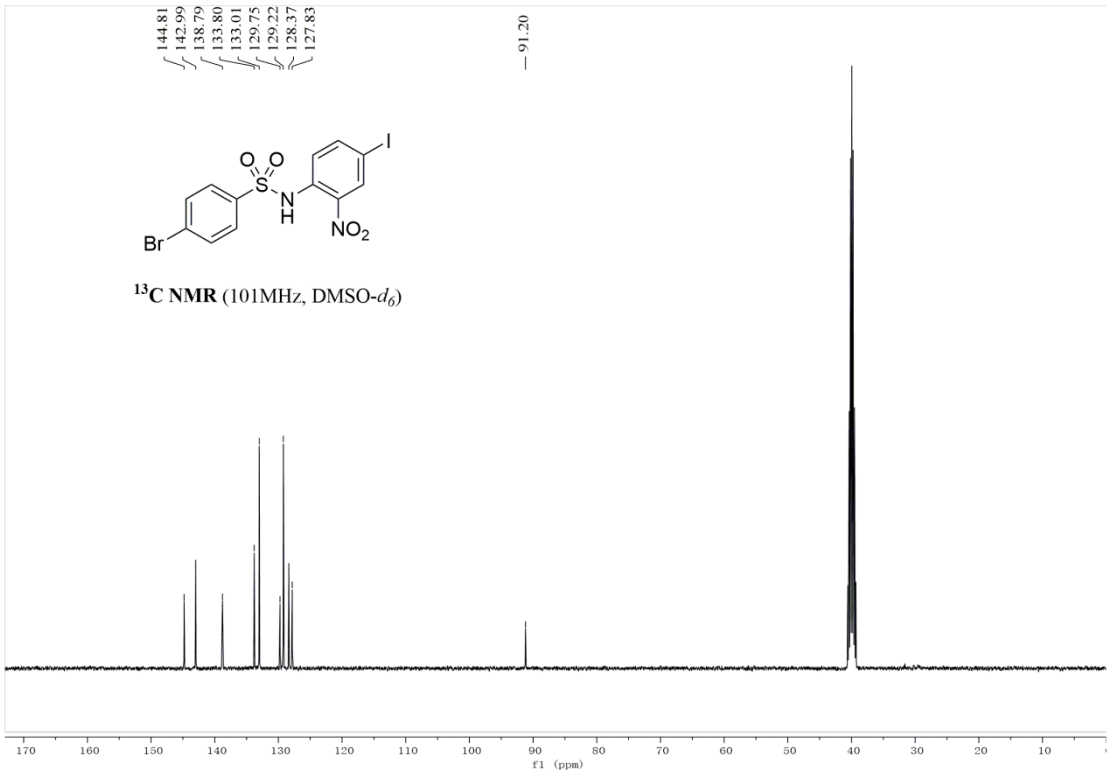


^{1}H NMR (400MHz, DMSO-d_6)



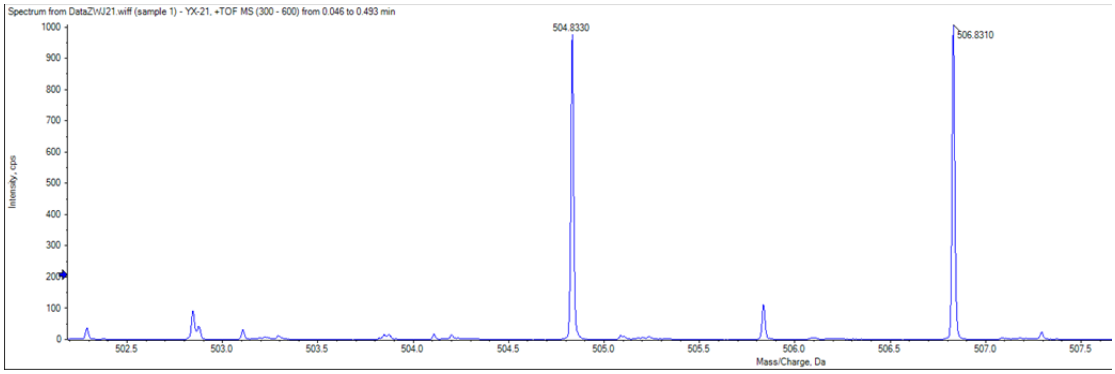


5f ^{13}C NMR

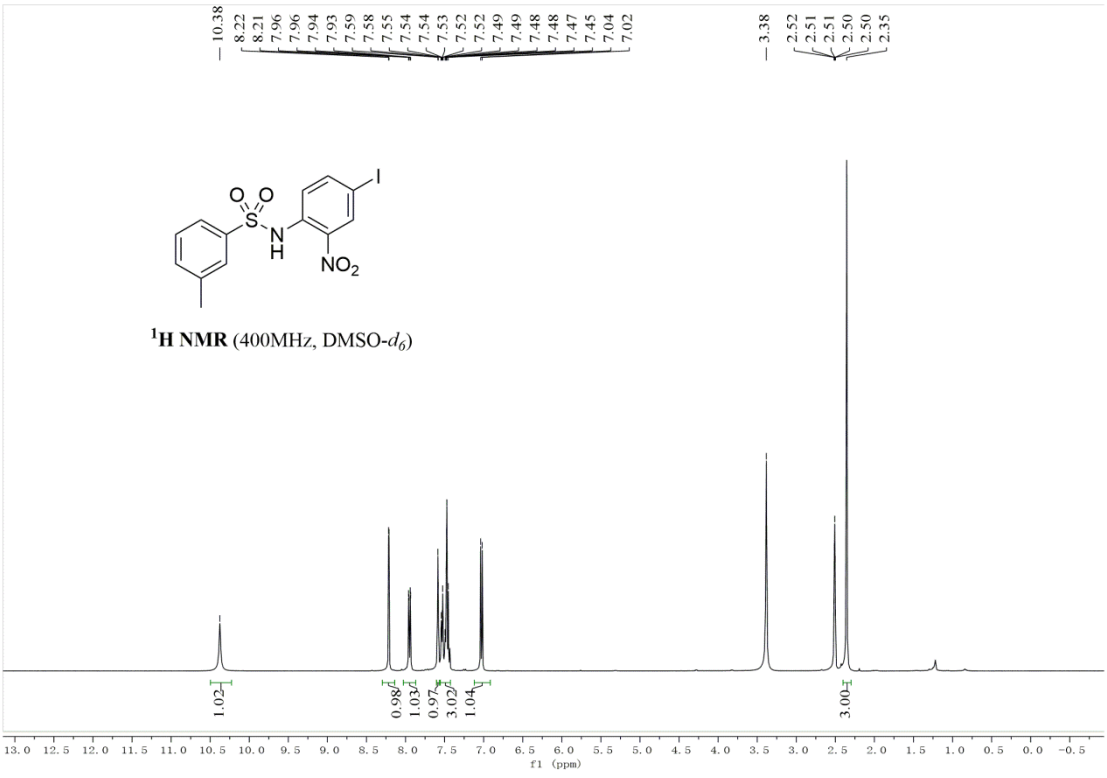


^{13}C NMR (101MHz, DMSO-d_6)

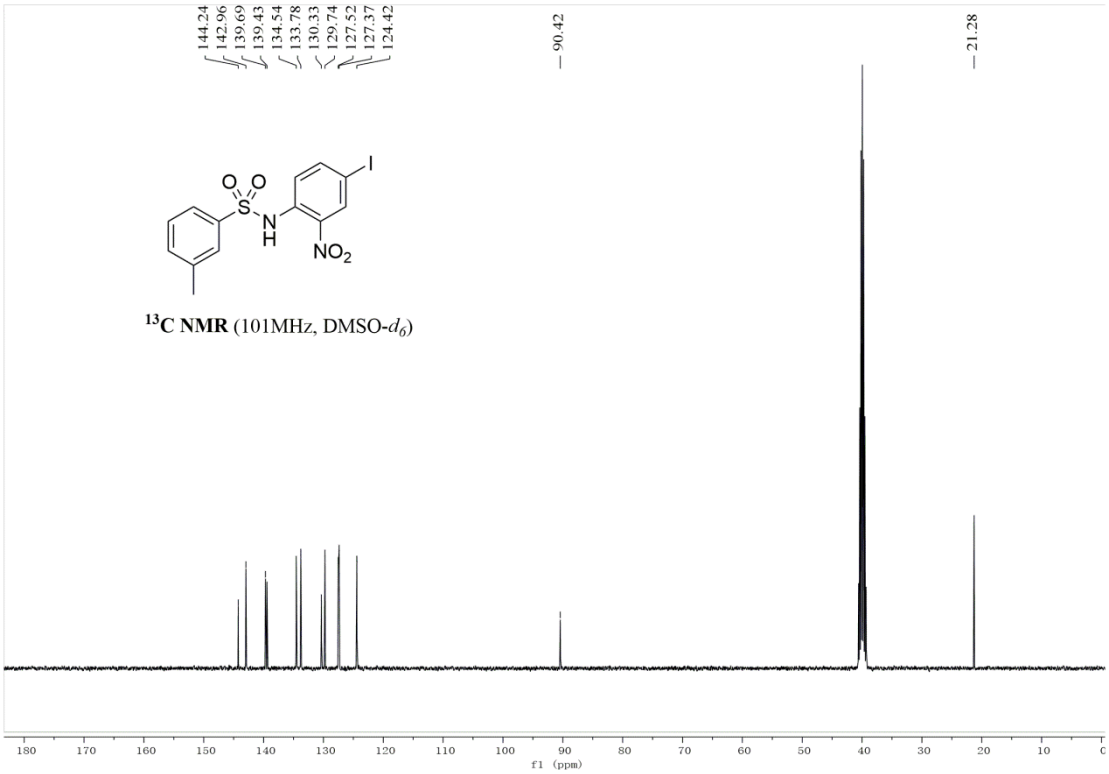
5f $C_{12}H_8BrIN_2O_4S$, $[M+Na]^+$ 504.8331. Found 504.8330.



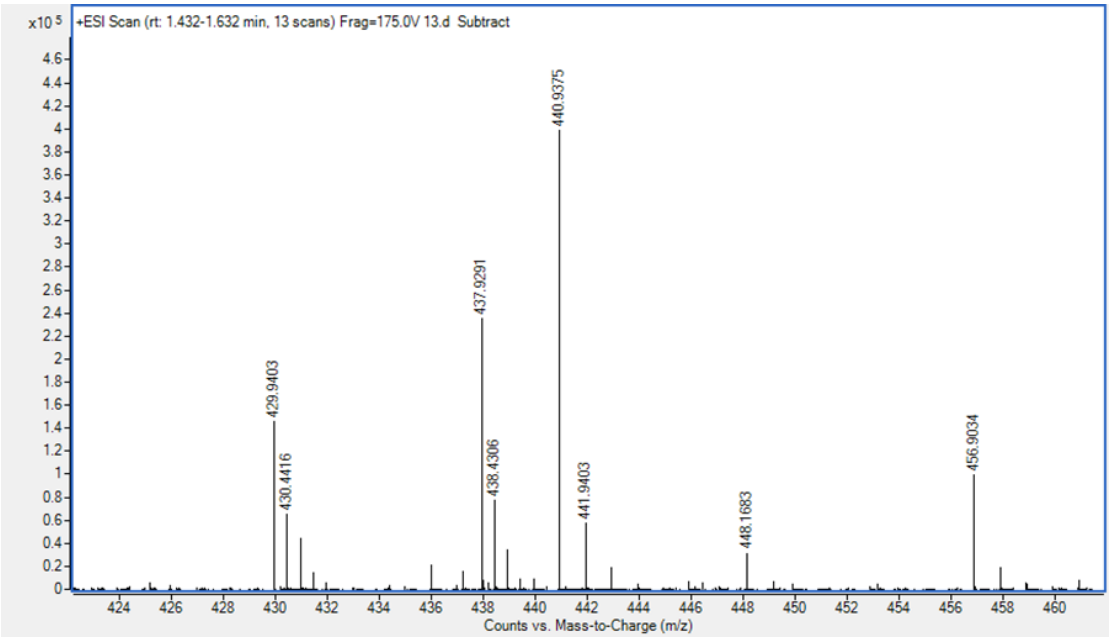
5i ^{1}H NMR



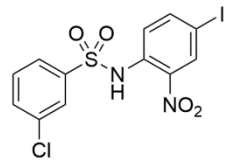
5i ^{13}C NMR



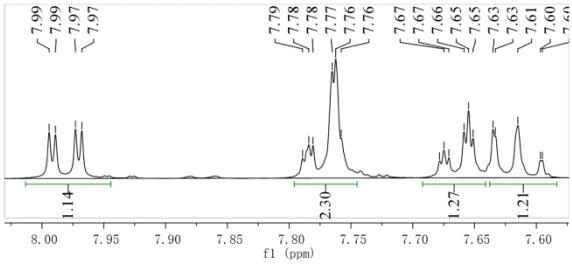
5i $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9375.

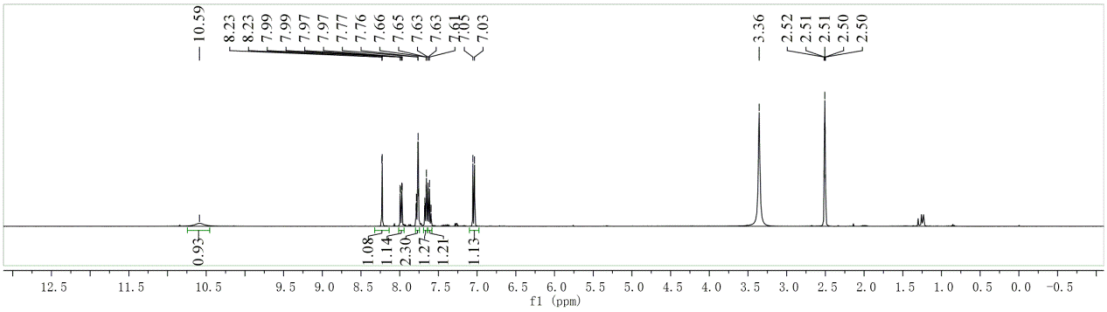


5j ^{1}H NMR

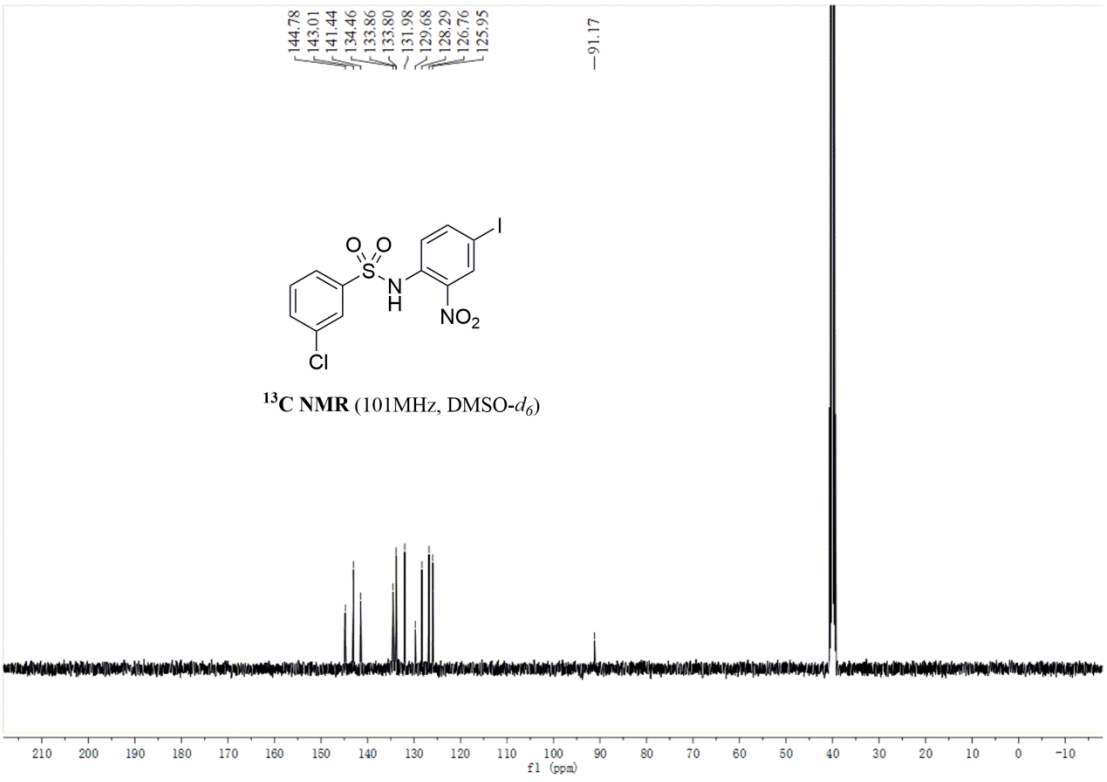


^{1}H NMR (400MHz, DMSO-d_6)



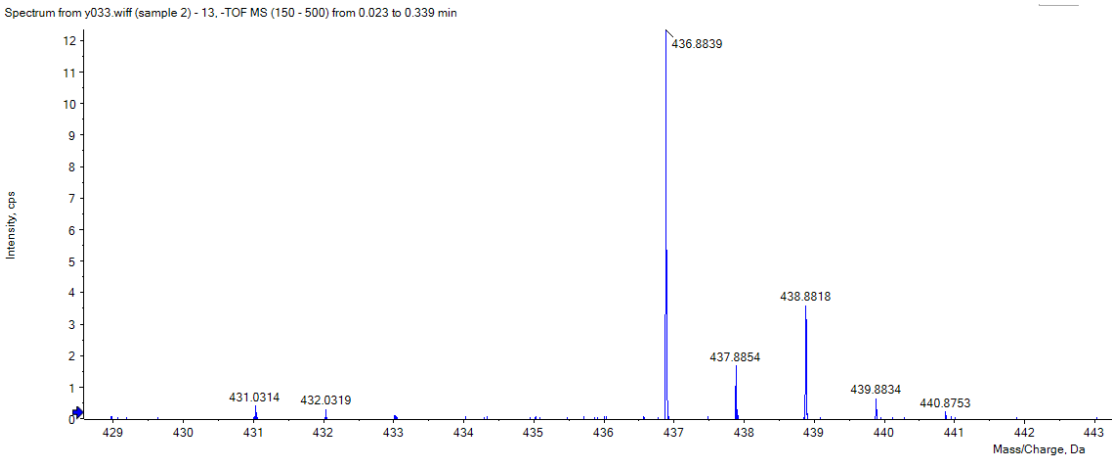


5j ^{13}C NMR

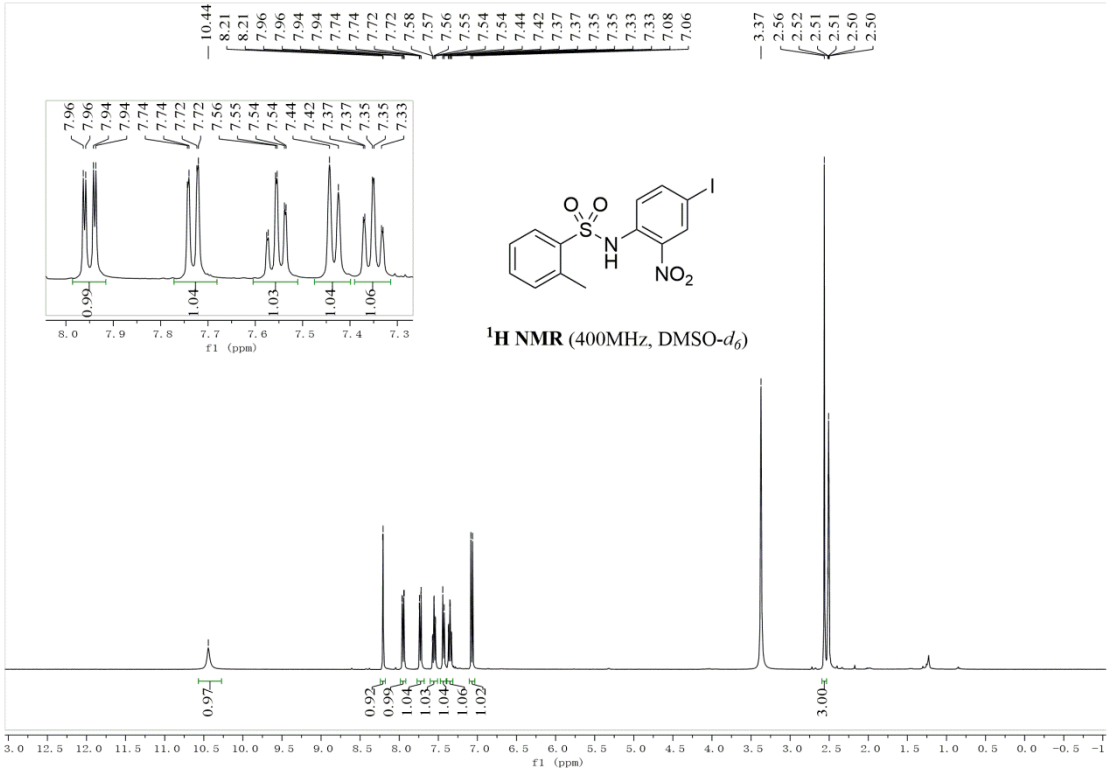


^{13}C NMR (101MHz, DMSO-d_6)

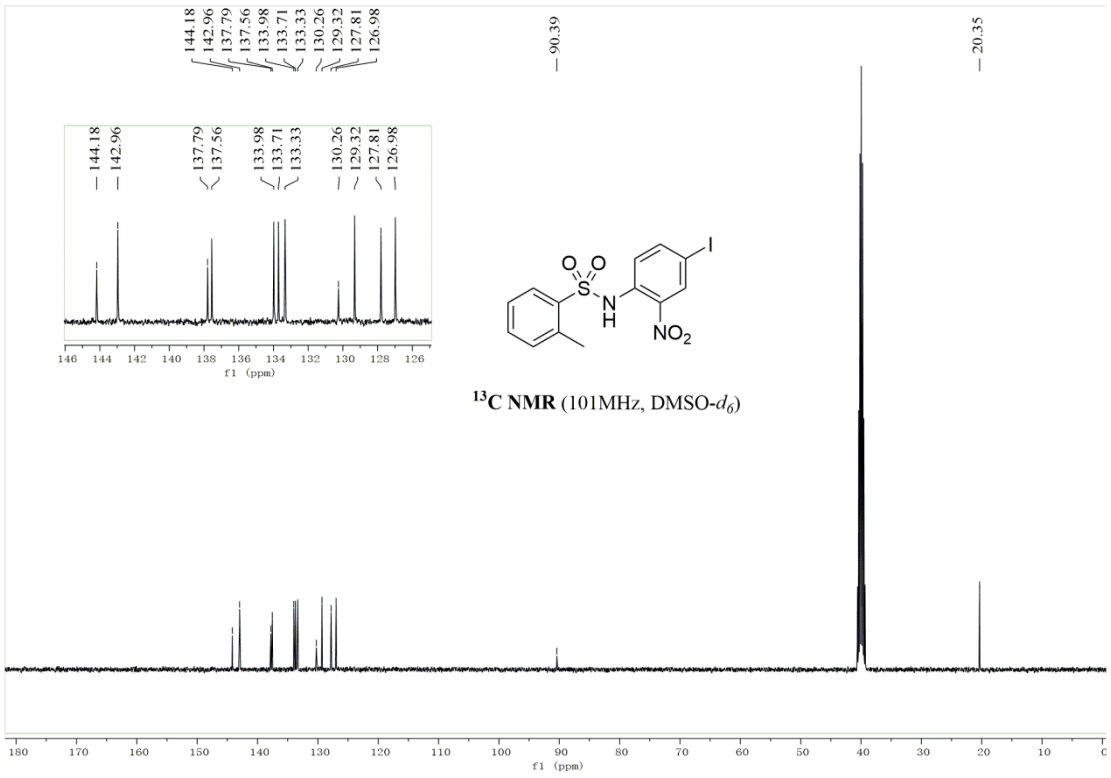
5j Calculated for $C_{12}H_8ClIN_2O_4S$, $[M-H]^-$ 436.8860 Found 436.8839.



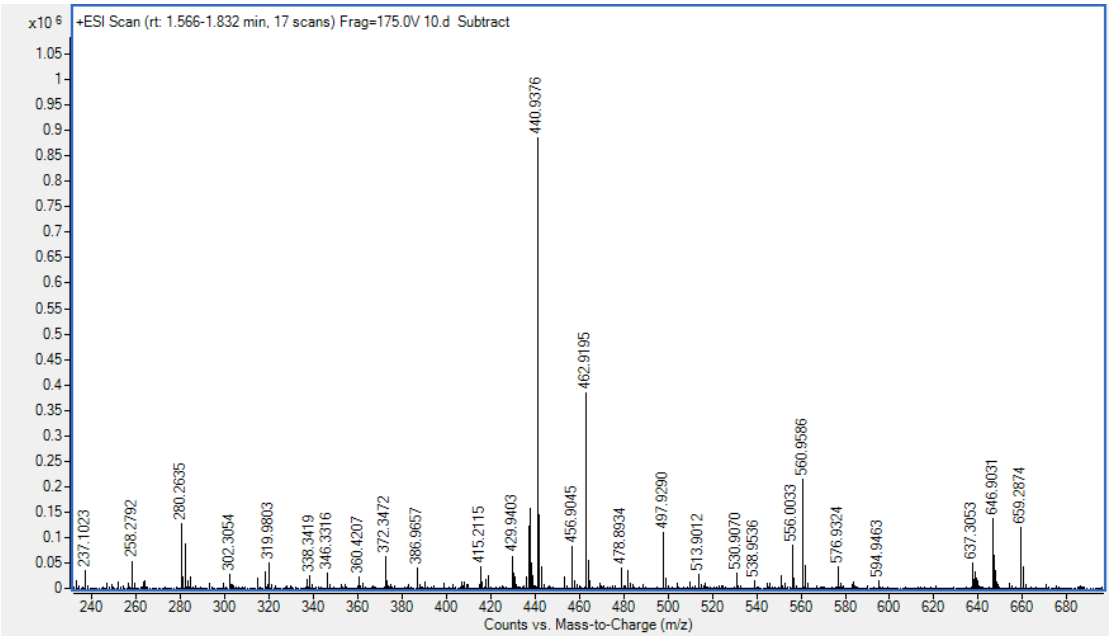
5m ^{1}H NMR



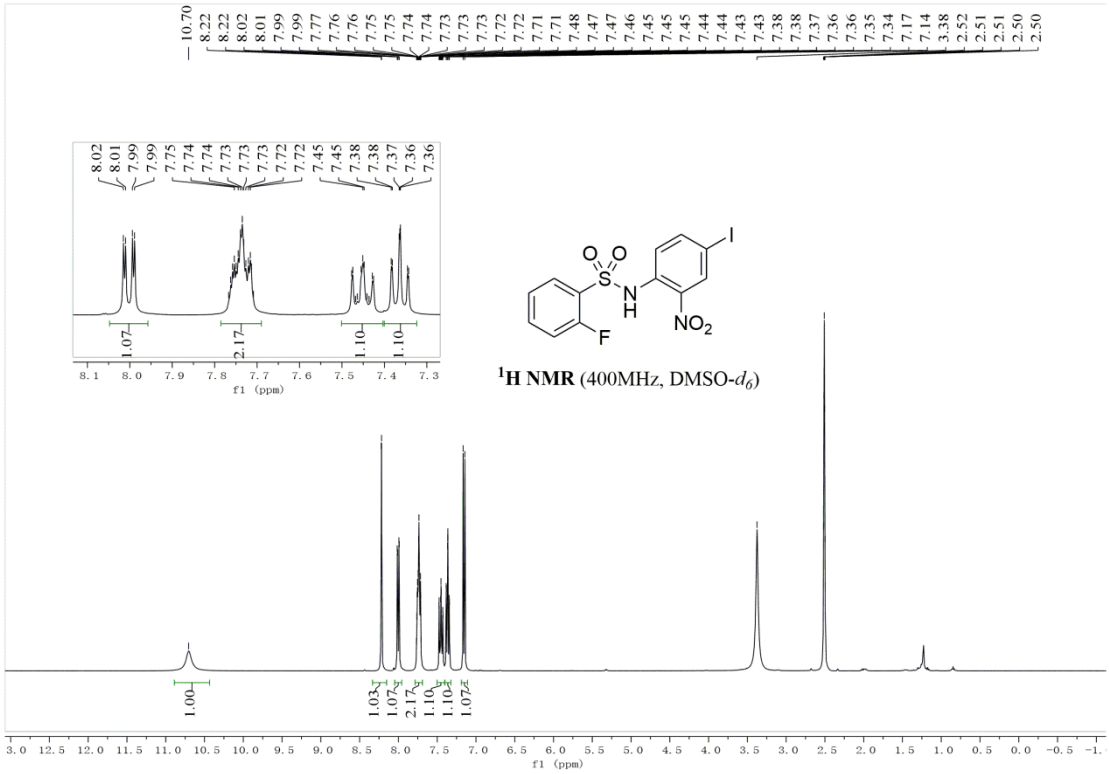
5m ^{13}C NMR



5m $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9376.



5n ^{1}H NMR


10.70
8.22
8.22
8.02
8.01
7.99
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7.77
7.76
7.76
7.75
7.75
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7.73
7.73
7.73
7.72
7.72
7.71
7.71
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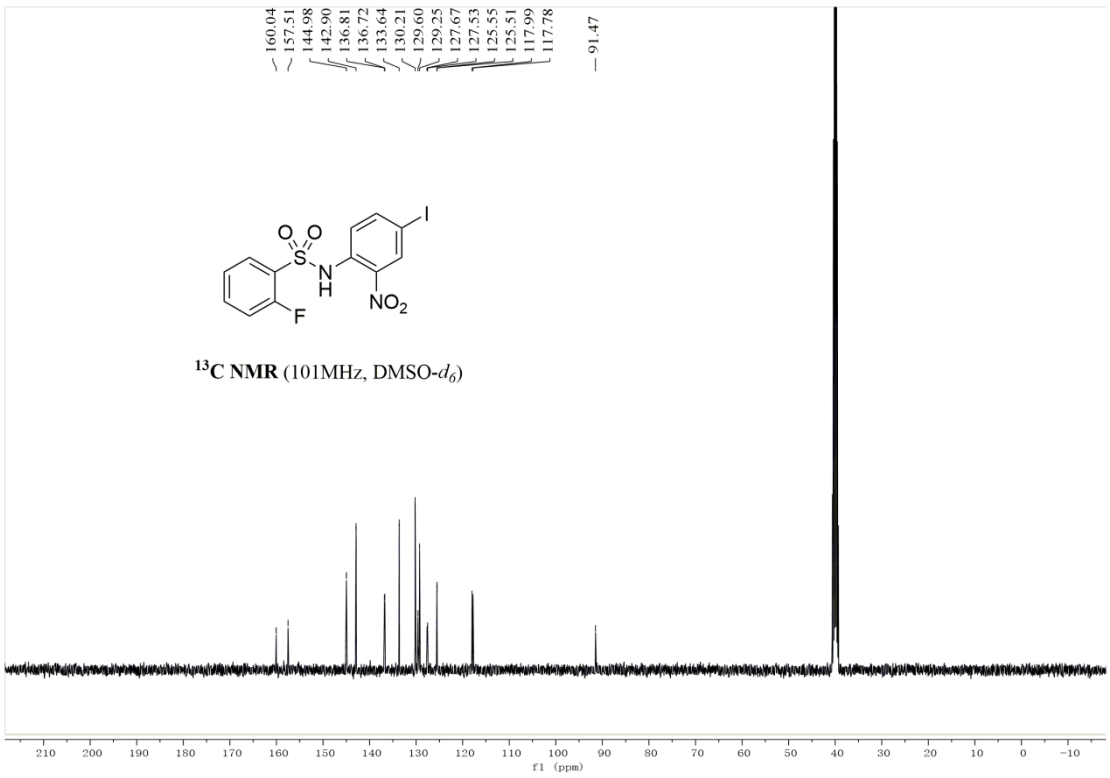
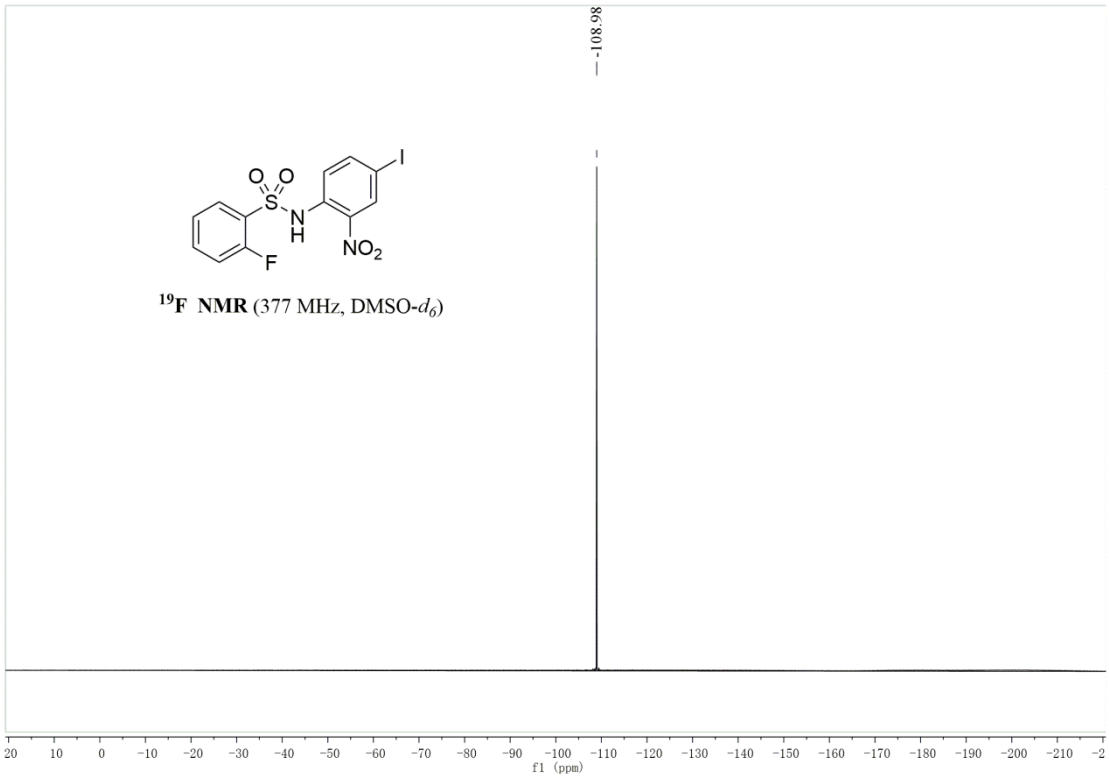
7.47
7.46
7.45
7.45
7.45
7.44
7.44
7.43
7.43
7.38
7.38
7.37
7.36
7.36
7.35
7.34
7.17
7.14
3.38
2.52
2.51
2.51
2.50
2.50
1.07
2.17
1.10
1.10
f1 (ppm)
I
O
O
S
N
H
NO2
F
1H NMR (400MHz, DMSO-d6)
1.00
1.03
1.07
2.17
1.10
1.10
1.07
f1 (ppm)

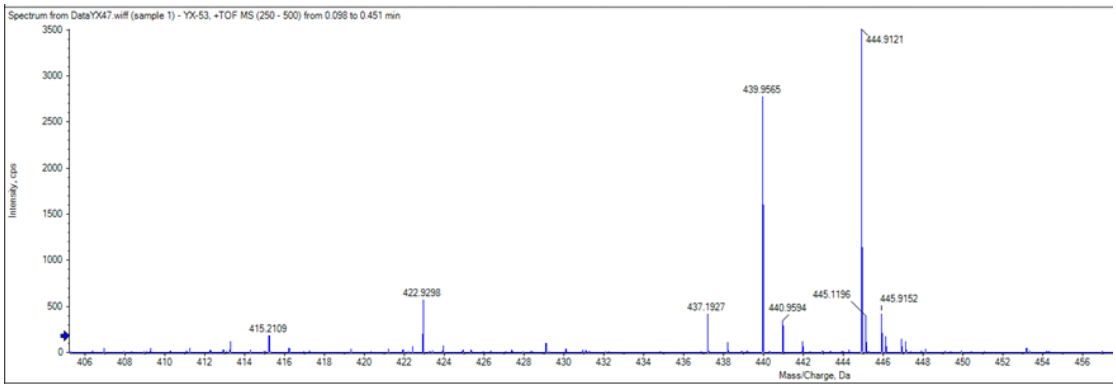
5n ^{13}C NMR


160.04
157.51
144.98
142.90
136.81
136.72
133.64
130.21
129.60
129.25
127.67
127.53
125.55
125.51
117.99
117.78
91.47
I
O
O
S
N
H
NO2
F
13C NMR (101MHz, DMSO-d6)
f1 (ppm)

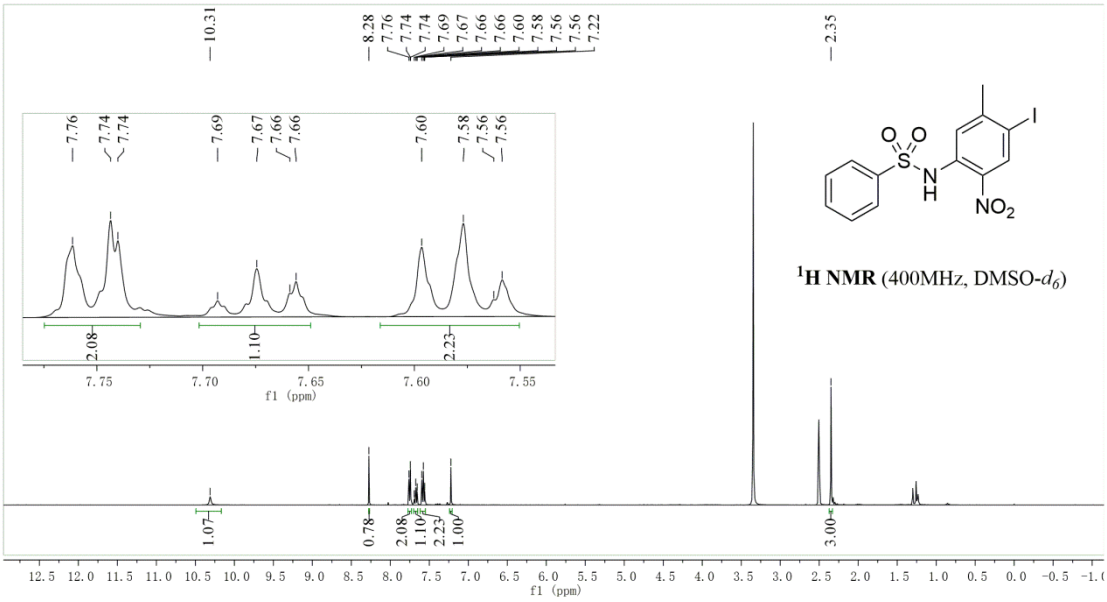
5n ^{19}F NMR



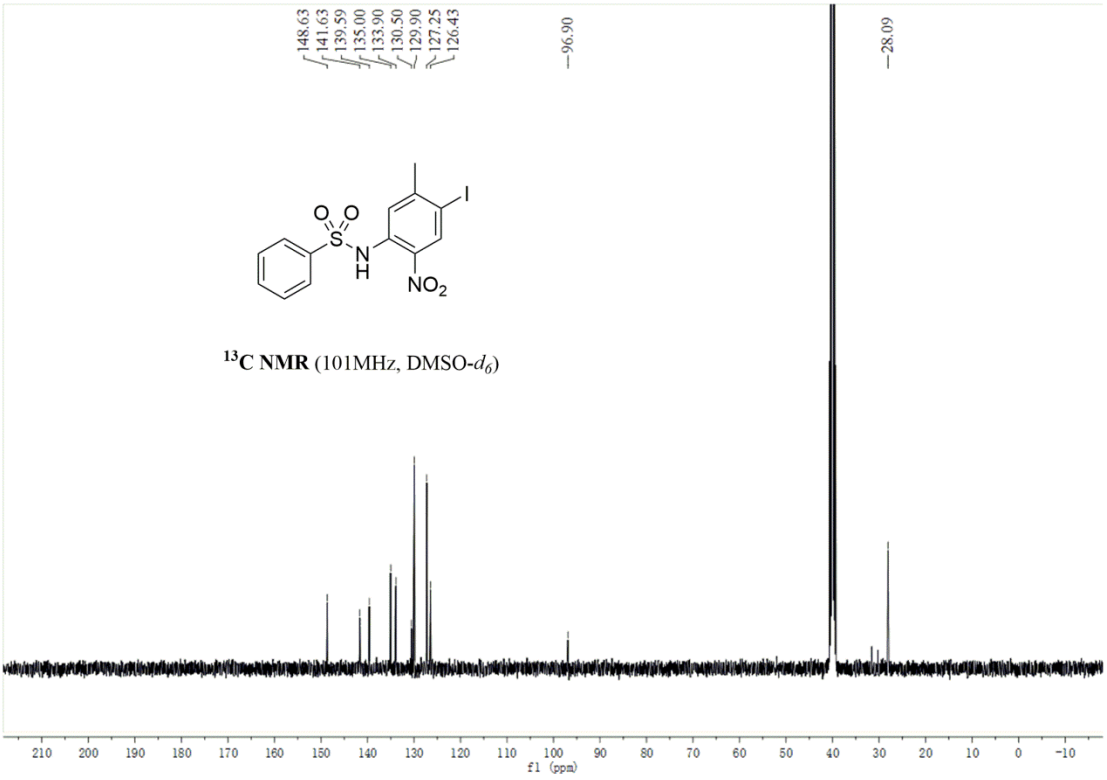
5n $C_{12}H_8FIN_2O_4S$, $[M+Na]^+$ 444.9131. Found 444.9121.



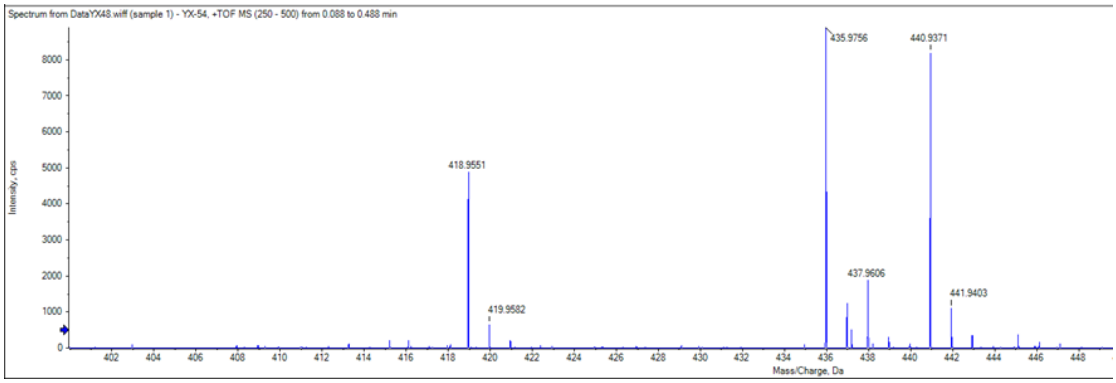
5q ^{1}H NMR



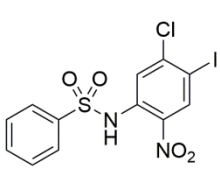
5q ^{13}C NMR



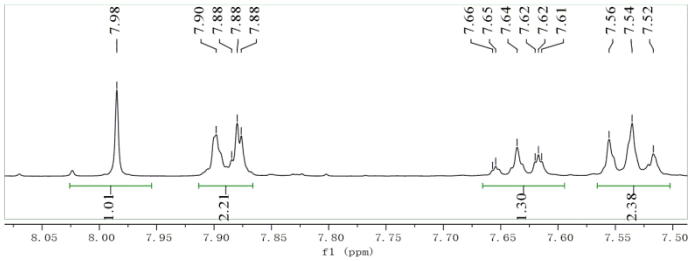
5q $C_{13}H_{11}IN_2O_4S$, $[M+Na]^+$ 440.9382. Found 440.9371.

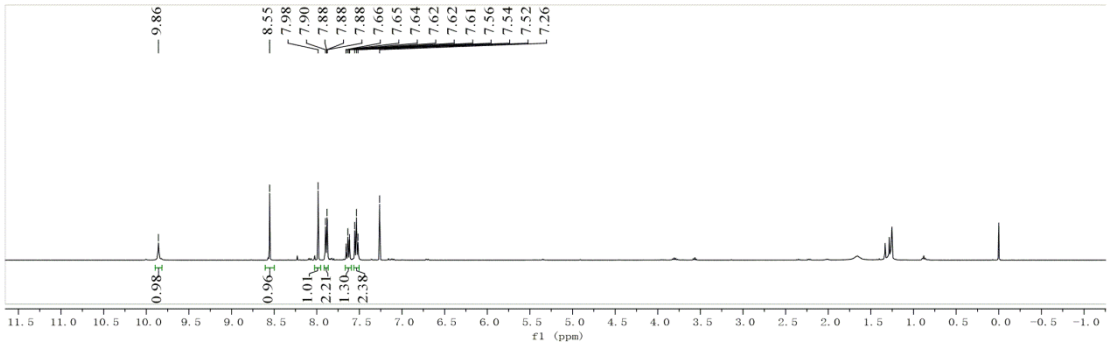


5r ^{1}H NMR

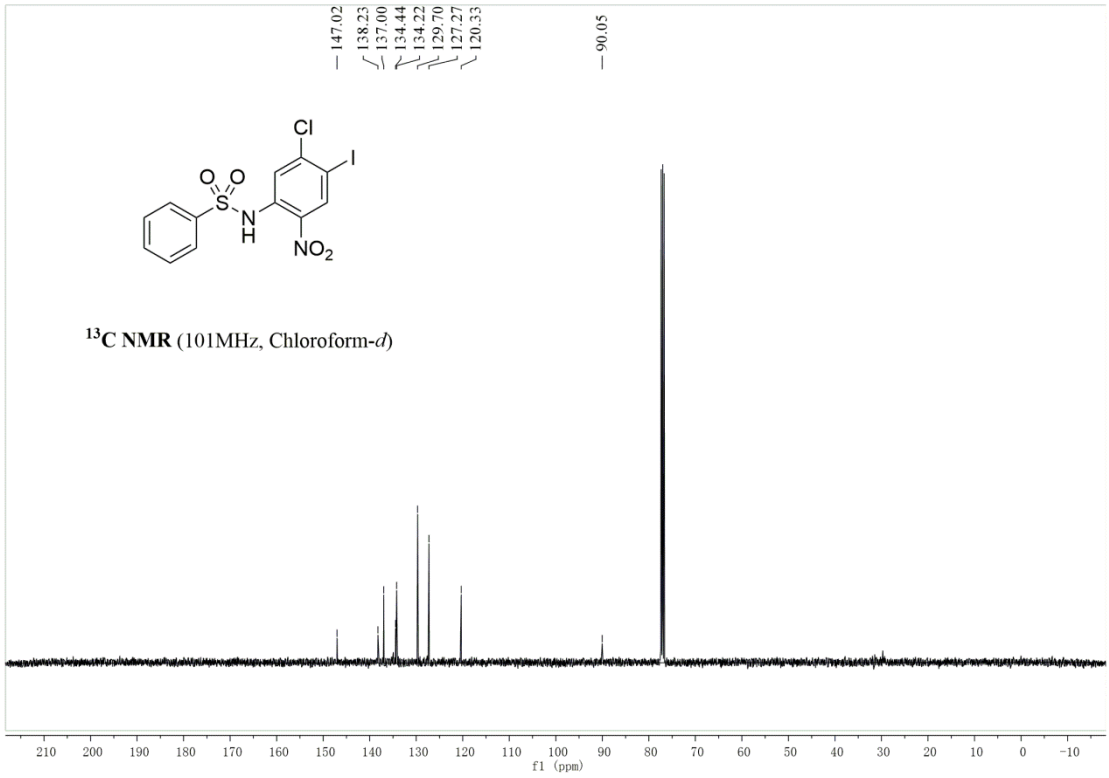


^{1}H NMR (400MHz, Chloroform-*d*)

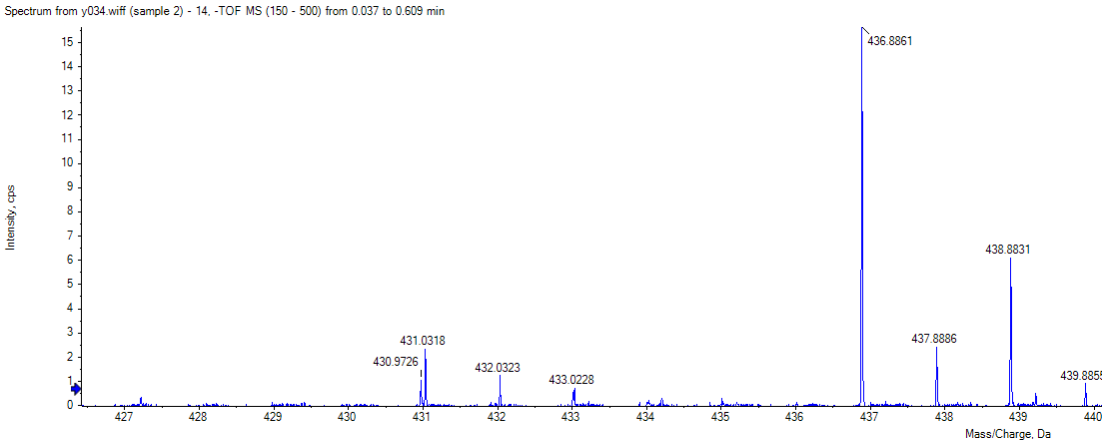




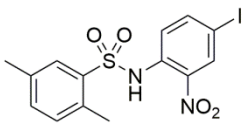
5r ^{13}C NMR



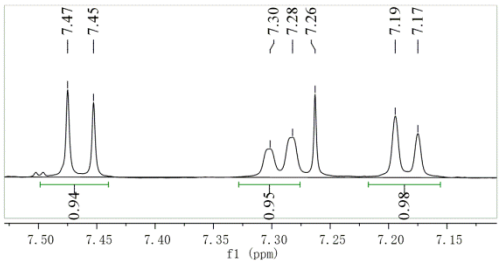
5r Calculated for $C_{12}H_8ClIN_2O_4S$, $[M-H]^-$ 436.8860. Found 436.8861.

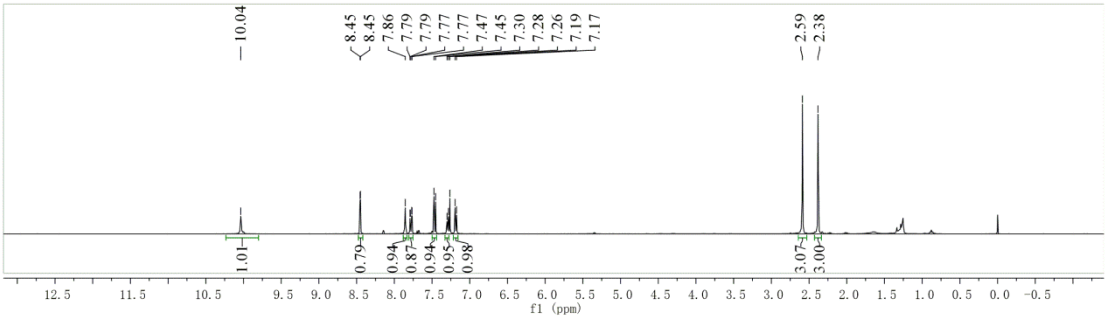


5w ^{1}H NMR

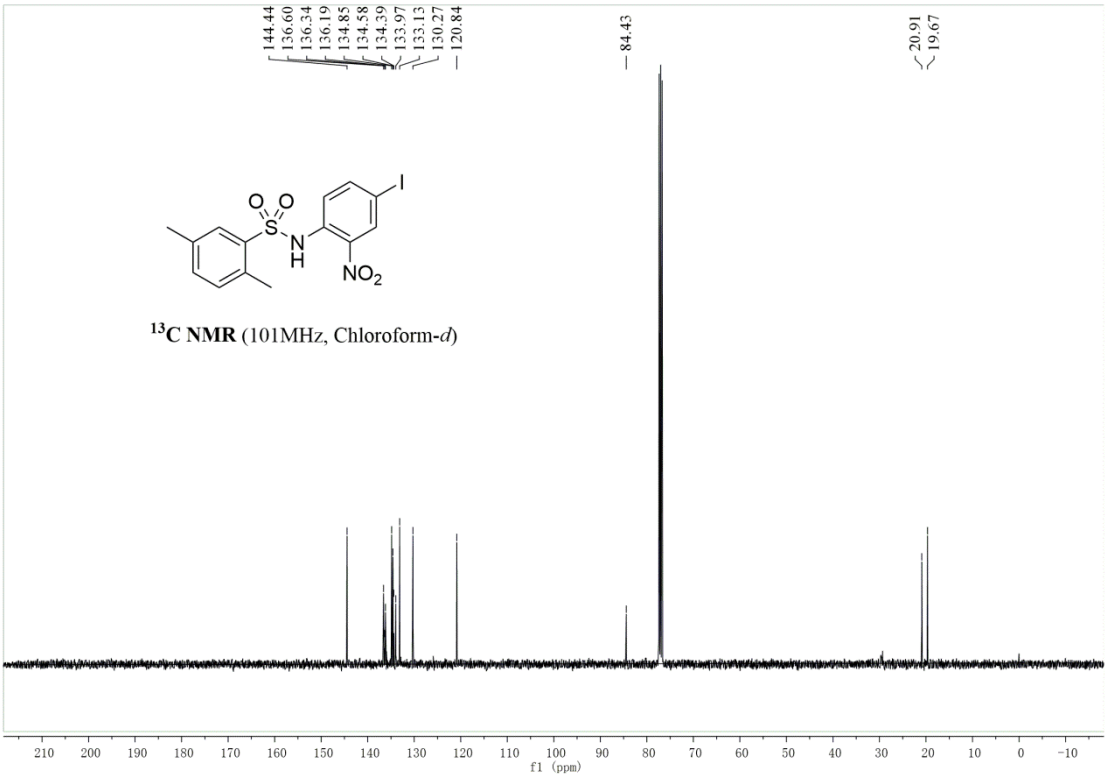


^{1}H NMR (400MHz, Chloroform-*d*)



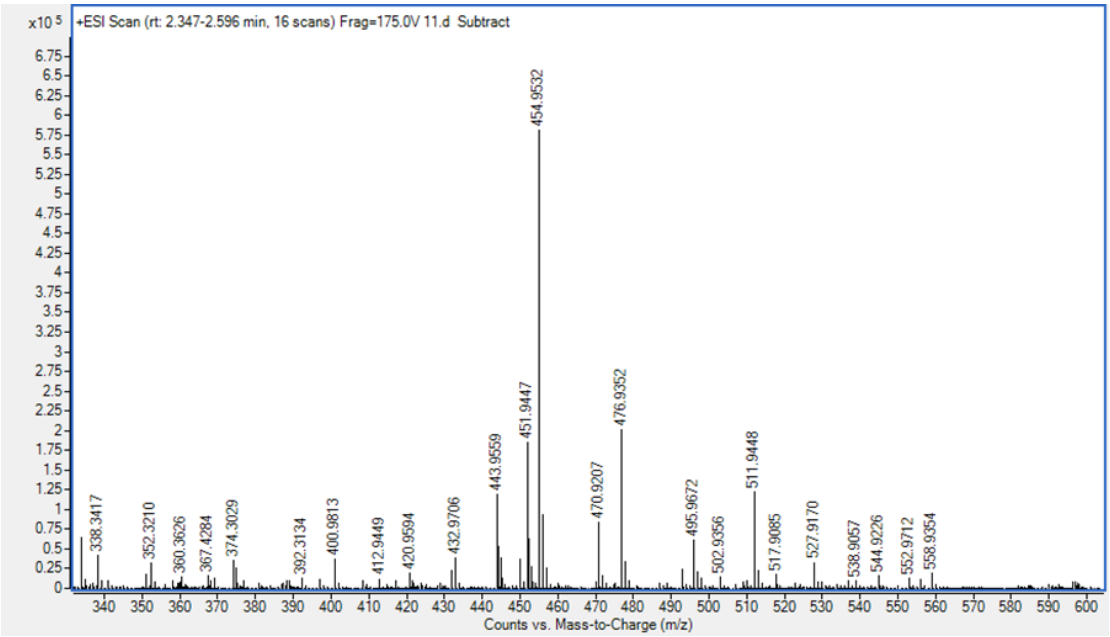


5w ^{13}C NMR

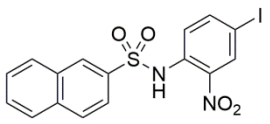


^{13}C NMR (101MHz, Chloroform-*d*)

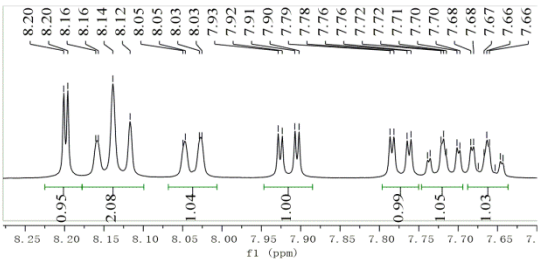
5w $C_{14}H_{13}IN_2O_4S$, $[M+Na]^+$ 454.9538. Found 454.9532.

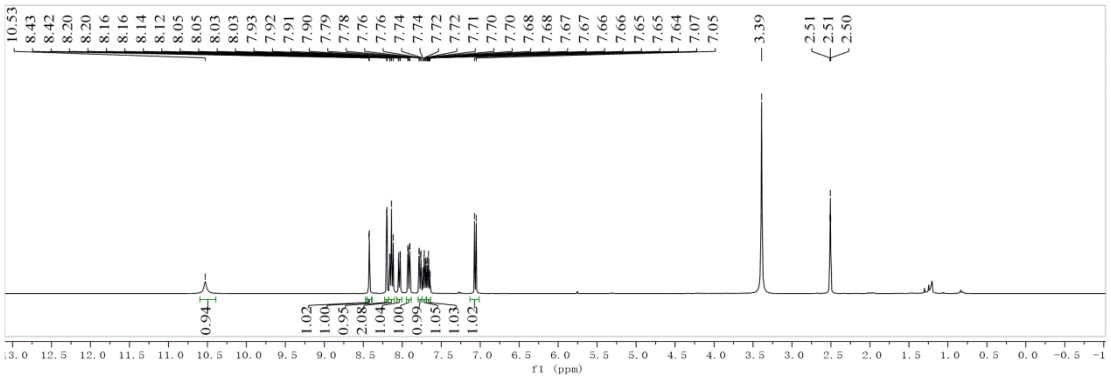


5x ^{1}H NMR

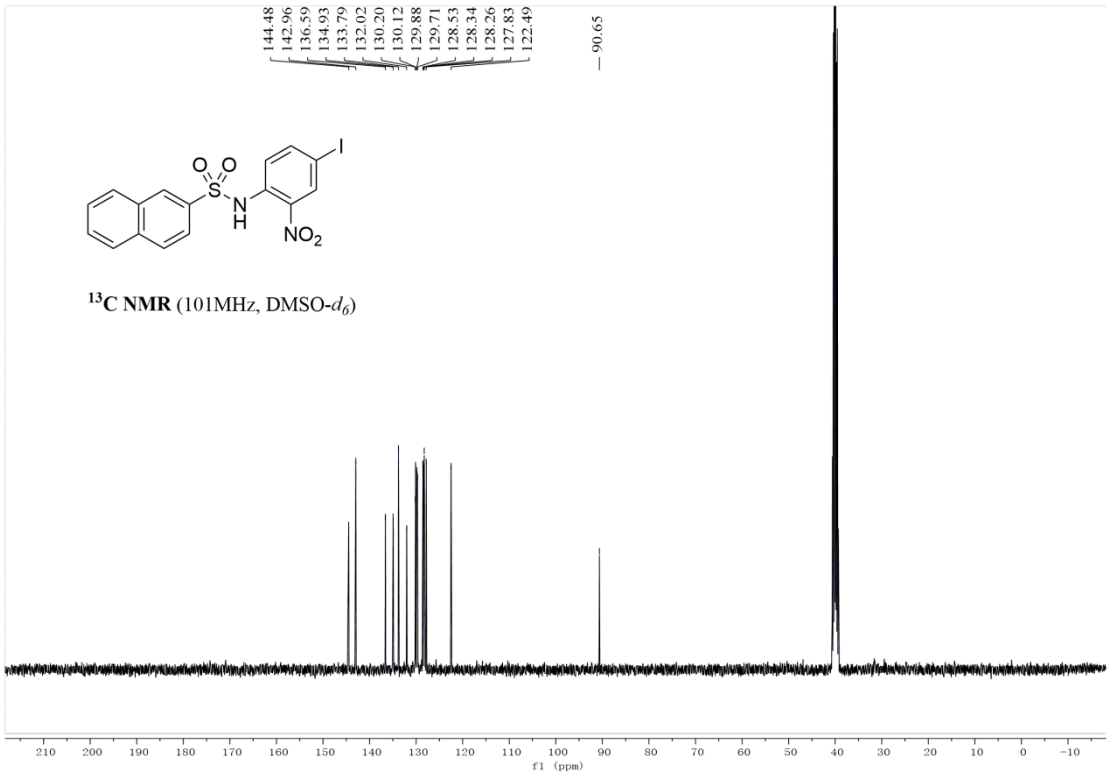


^{1}H NMR (400MHz, DMSO-d_6)

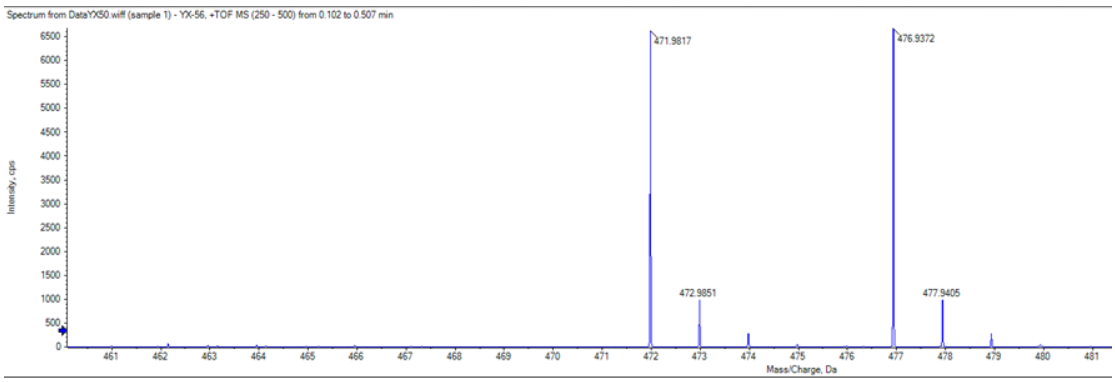




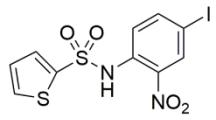
5x ^{13}C NMR



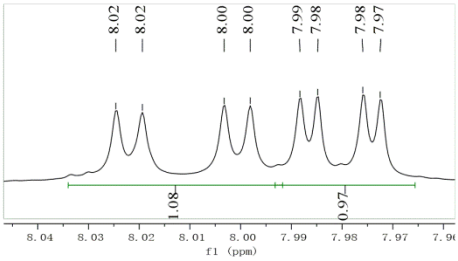
5x $C_{16}H_{11}IN_2O_4S$, $[M+Na]^+$ 476.9382. Found 476.9372.

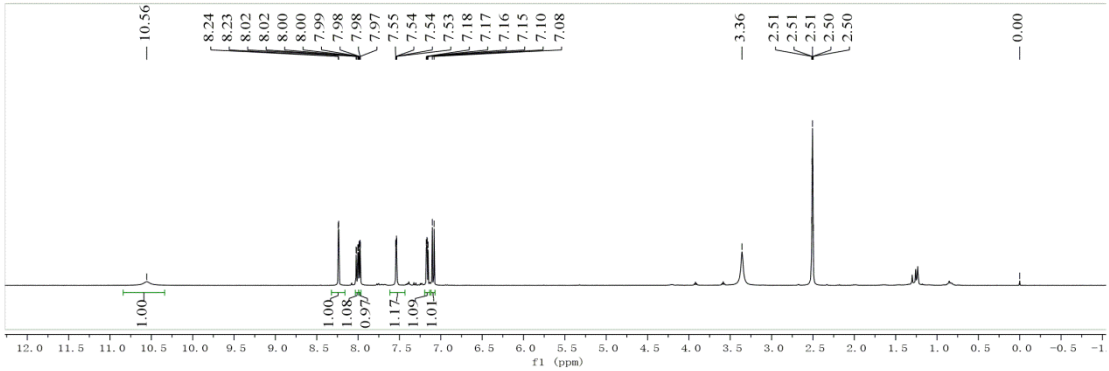


5aa ^{1}H NMR

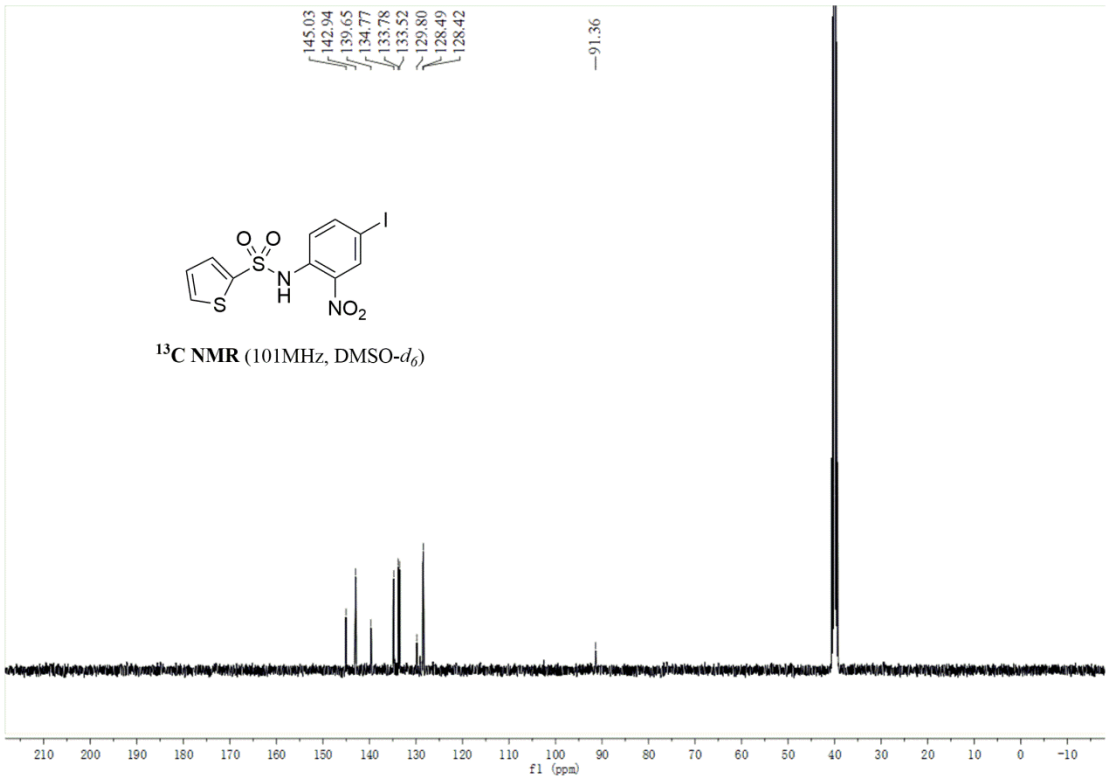


^{1}H NMR (400MHz, DMSO-d_6)



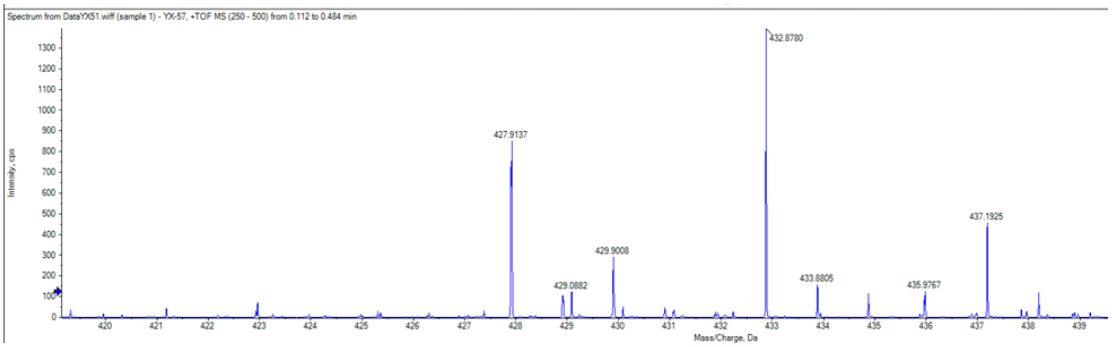


5aa ^{13}C NMR

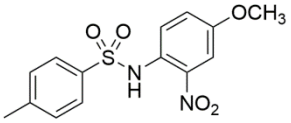


^{13}C NMR (101MHz, DMSO-d_6)

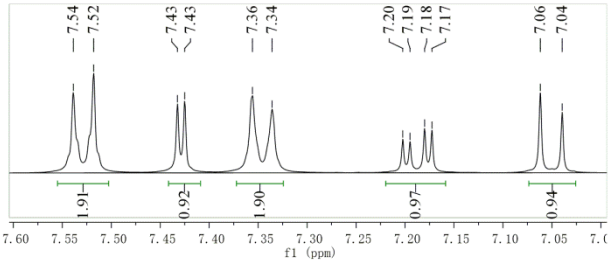
5aa $C_{10}H_7IN_2O_4S_2$, $[M+Na]^+$ 432.8790. Found 432.8780.

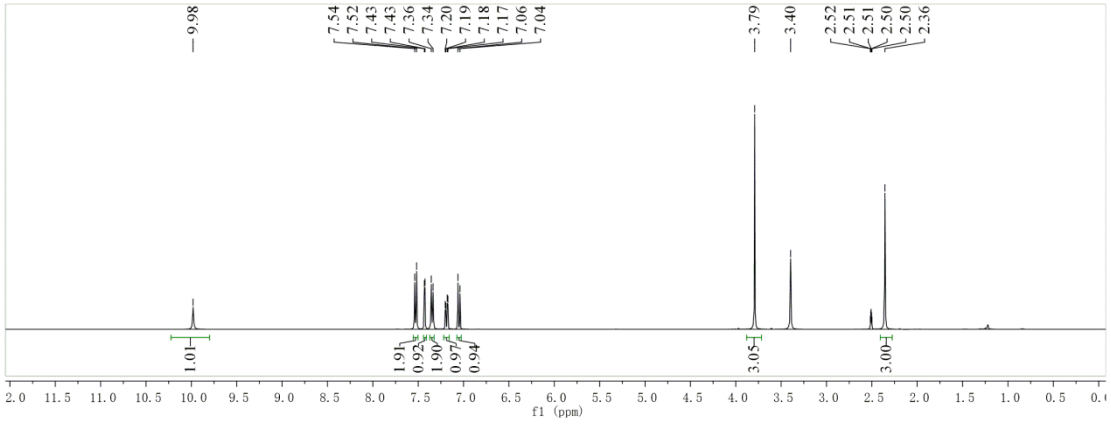


7a ^{1}H NMR

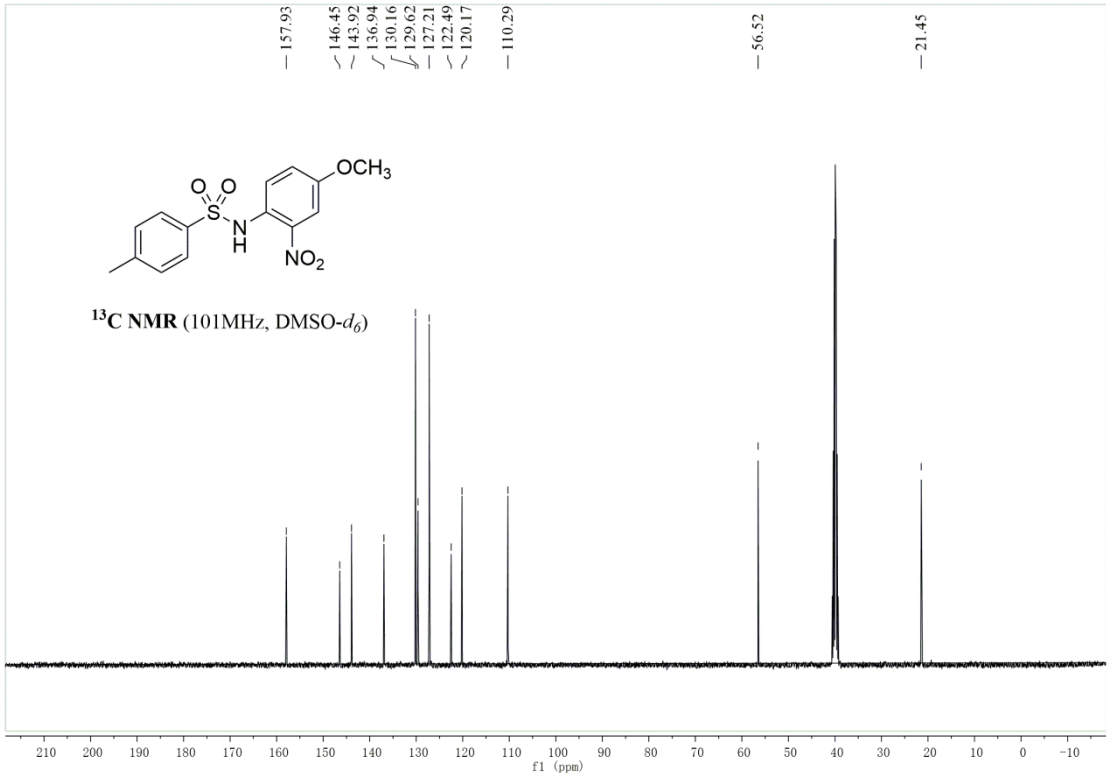


^{1}H NMR (400MHz, DMSO-d_6)

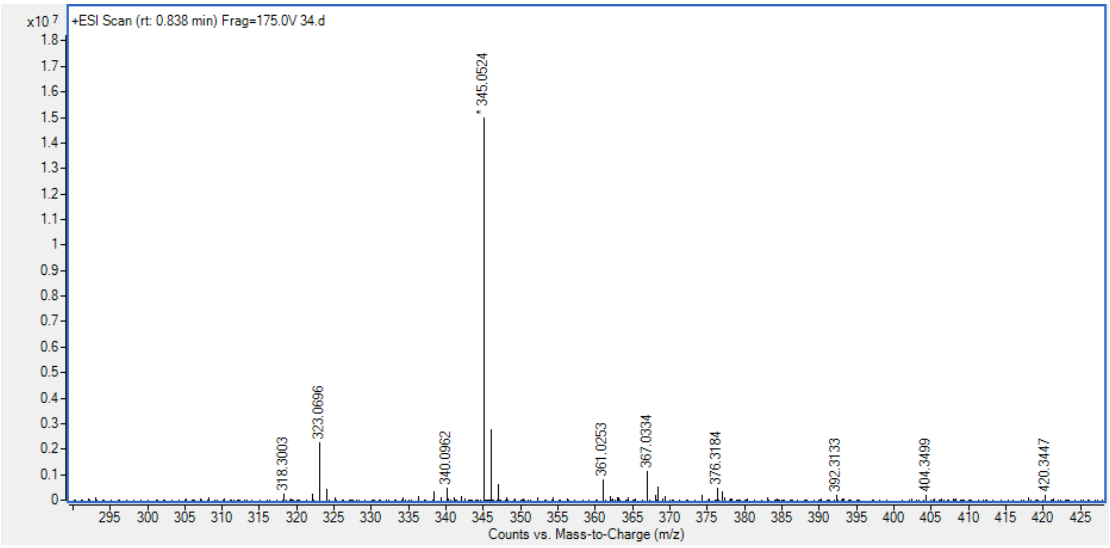




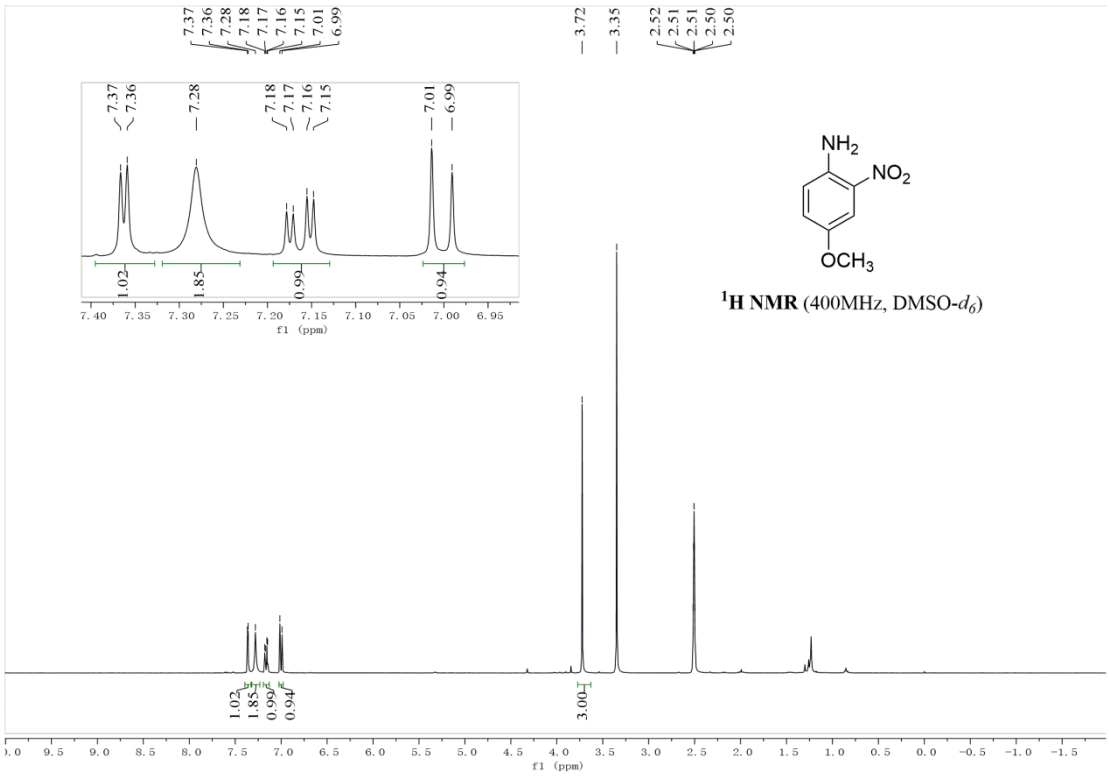
7a ^{13}C NMR



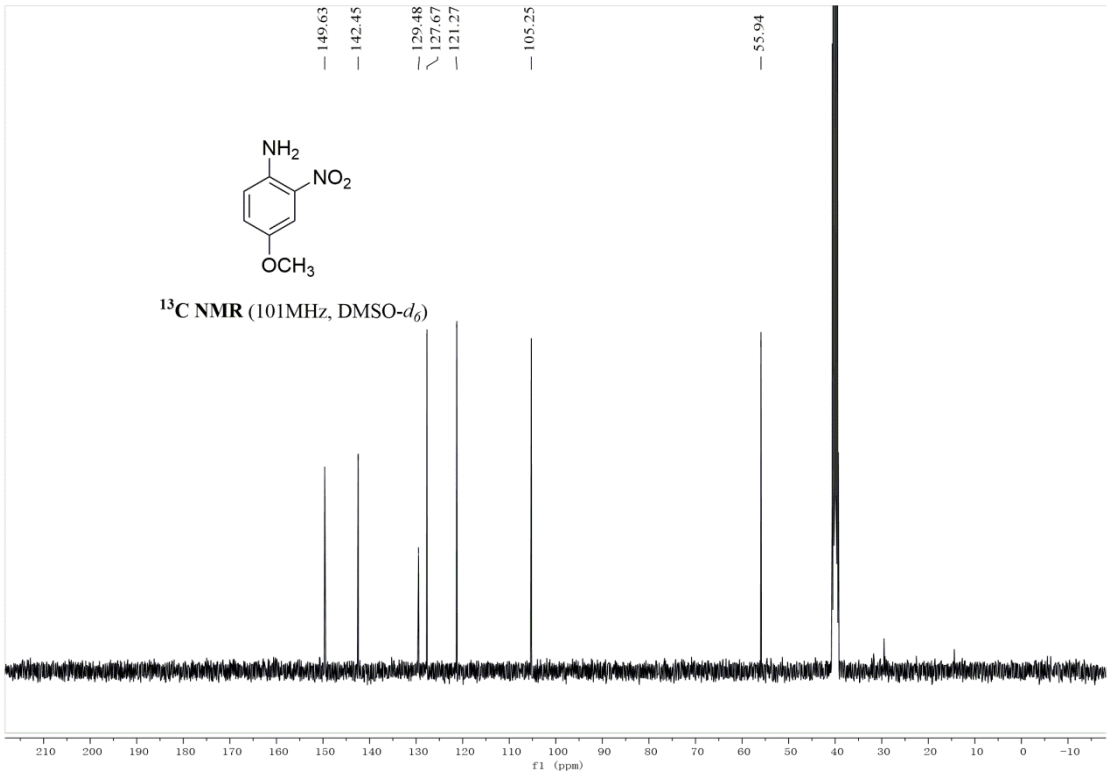
7a $C_{14}H_{14}N_2O_5S$, $[M+Na]^+$ 345.0521. Found 345.0524.



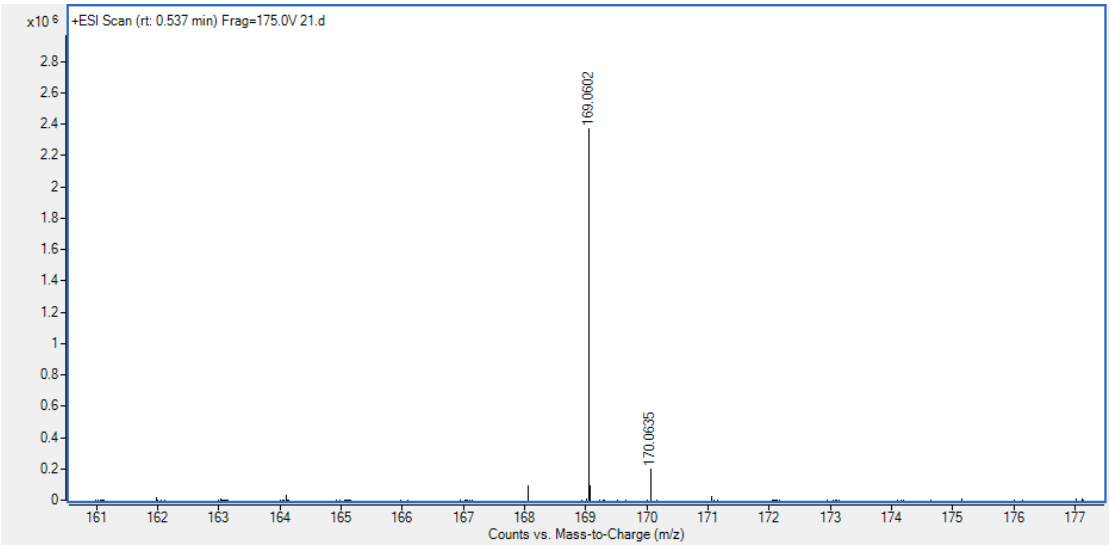
8a ^{1}H NMR


7.37
7.36
7.28
7.18
7.17
7.16
7.15
7.01
6.99
3.72
3.35
2.52
2.51
2.51
2.50
2.50
1.02
1.85
0.99
0.94
3.00
NH2
NO2
OCH3
1H NMR (400MHz, DMSO-d6)
f1 (ppm)

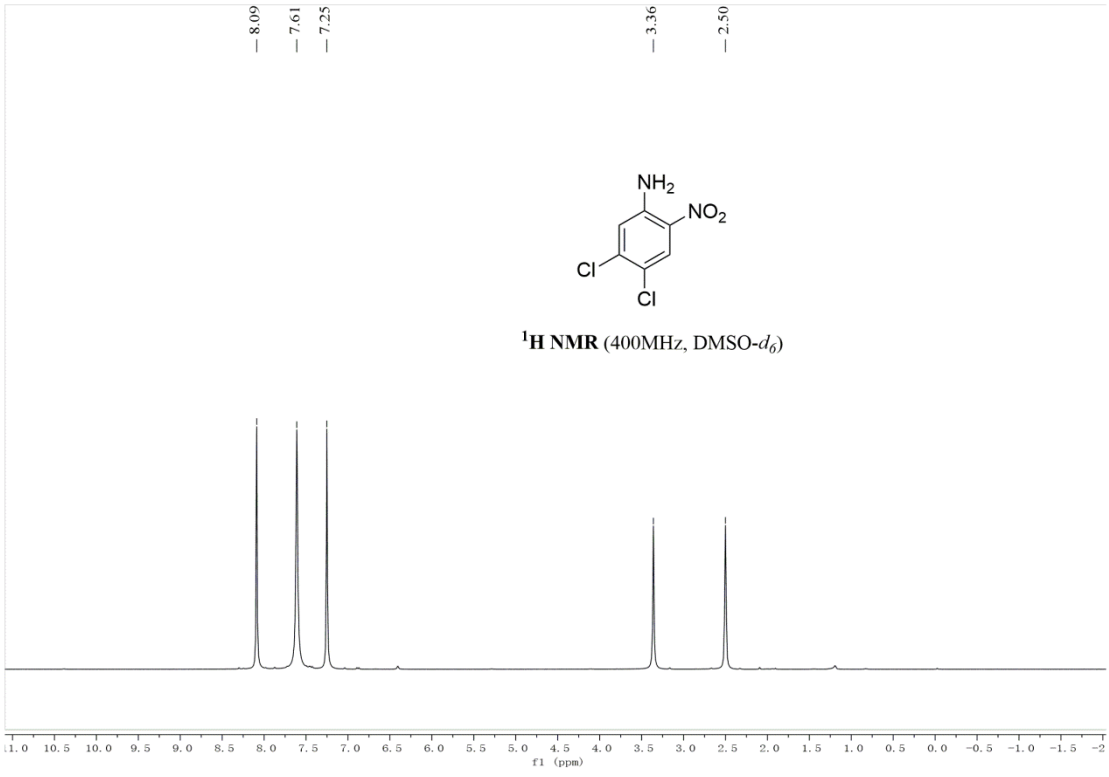
8a ^{13}C NMR


149.63
142.45
129.48
127.67
121.27
105.25
55.94
NH2
NO2
OCH3
13C NMR (101MHz, DMSO-d6)
f1 (ppm)

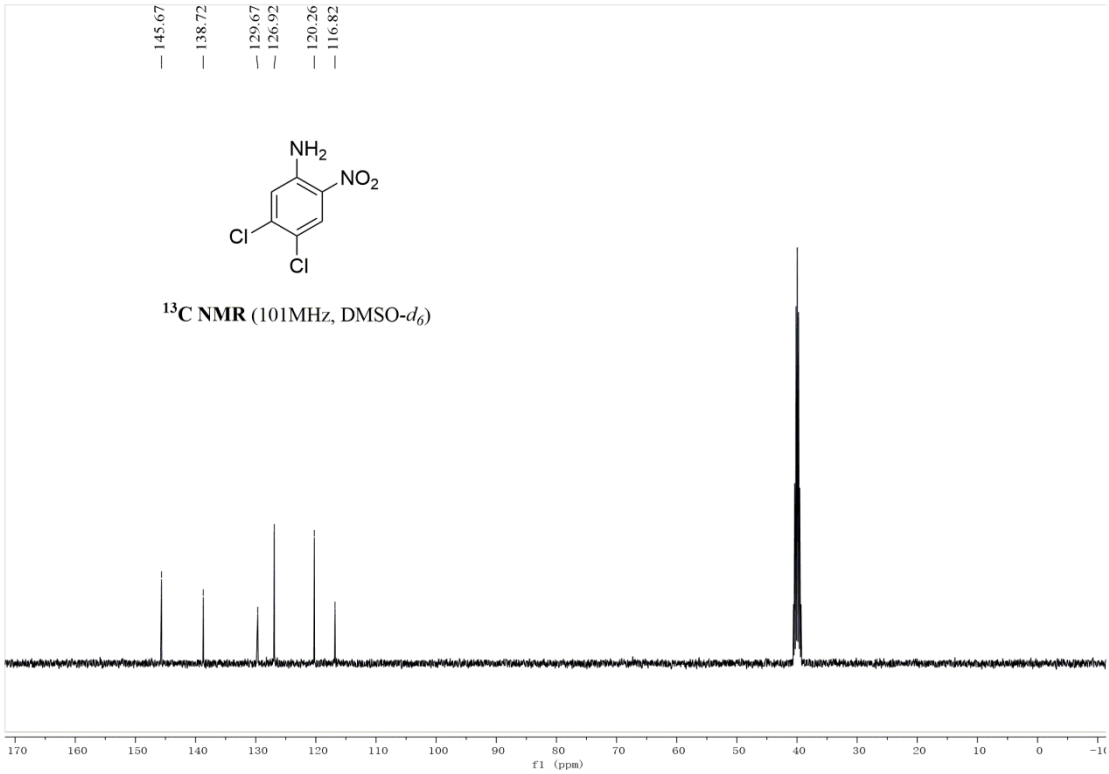
8a $C_7H_8N_2O_3$ $[M+H]^+$ 169.0613. Found 169.0602.



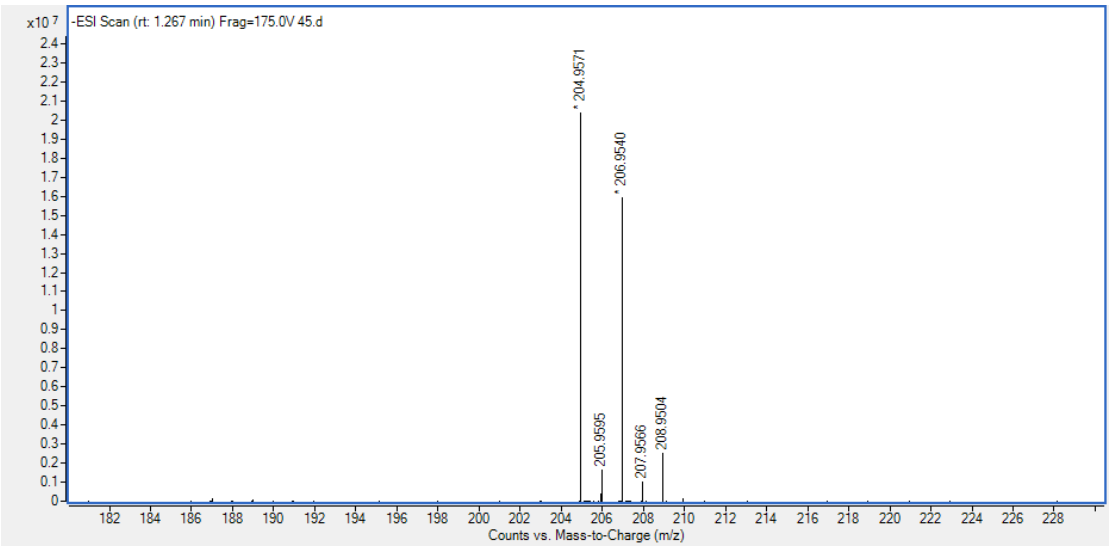
8b ^{1}H NMR



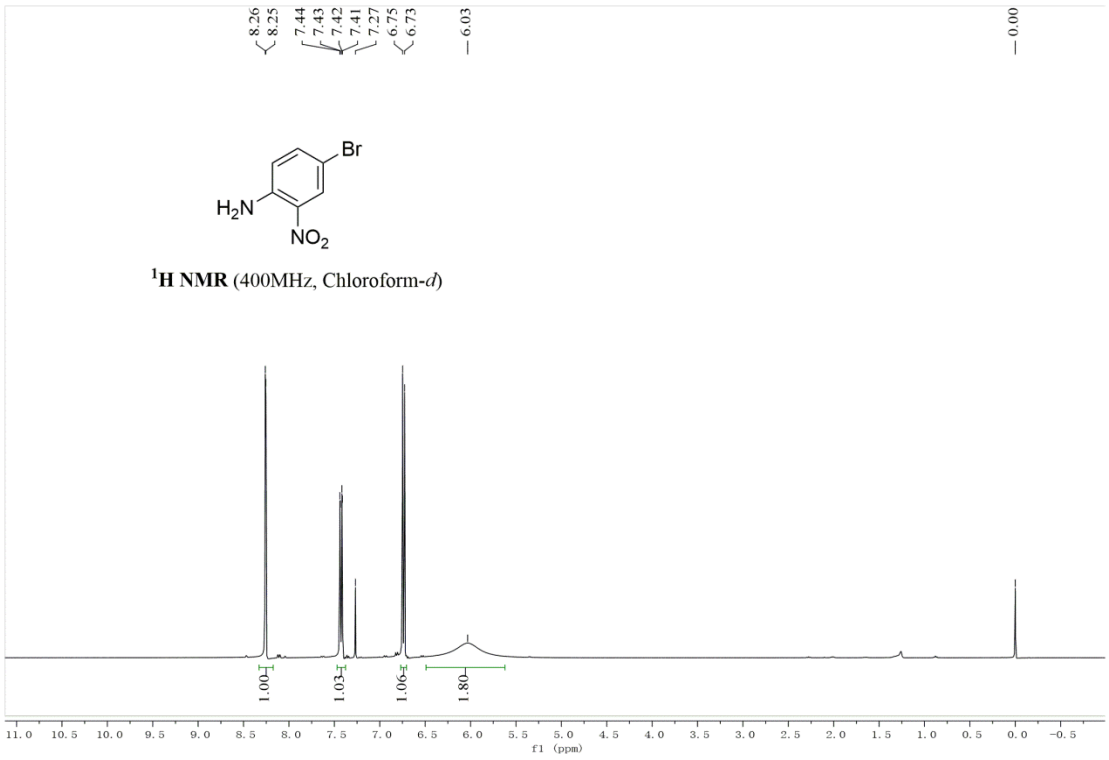
8b ^{13}C NMR



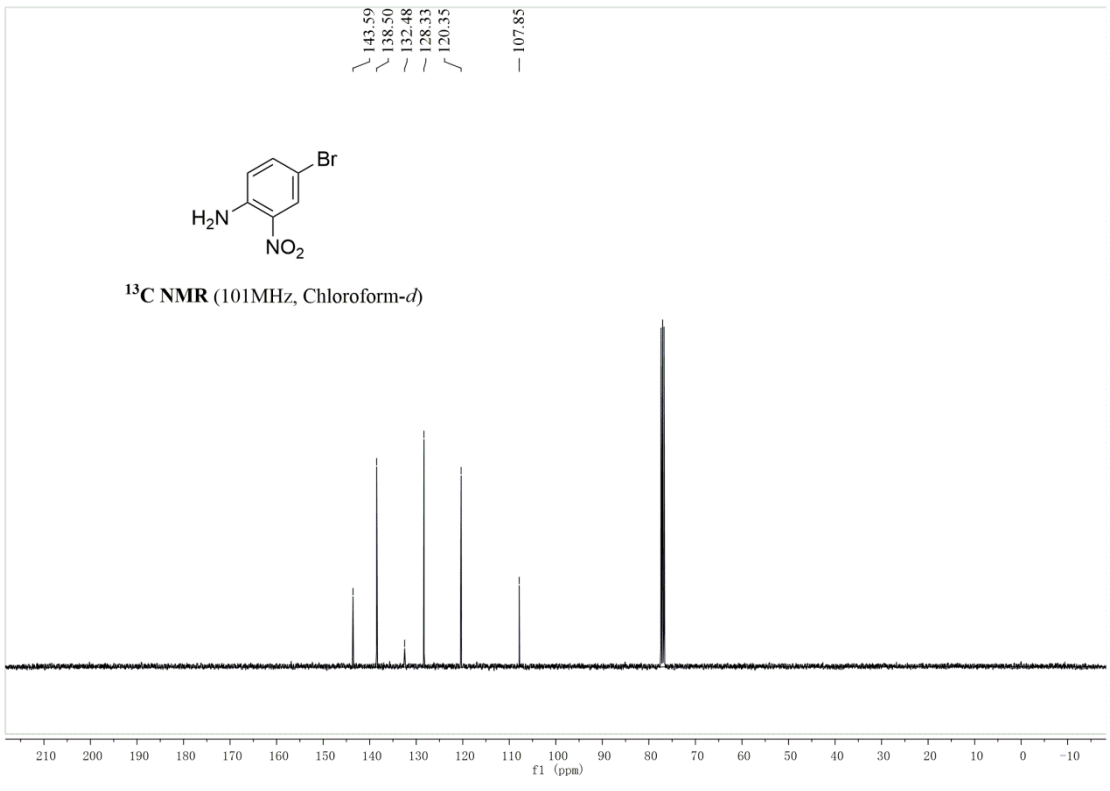
8b Calculated for $C_6H_4Cl_2N_2O_2$, $[M-H]^-$ 204.9572. Found 204.9571.



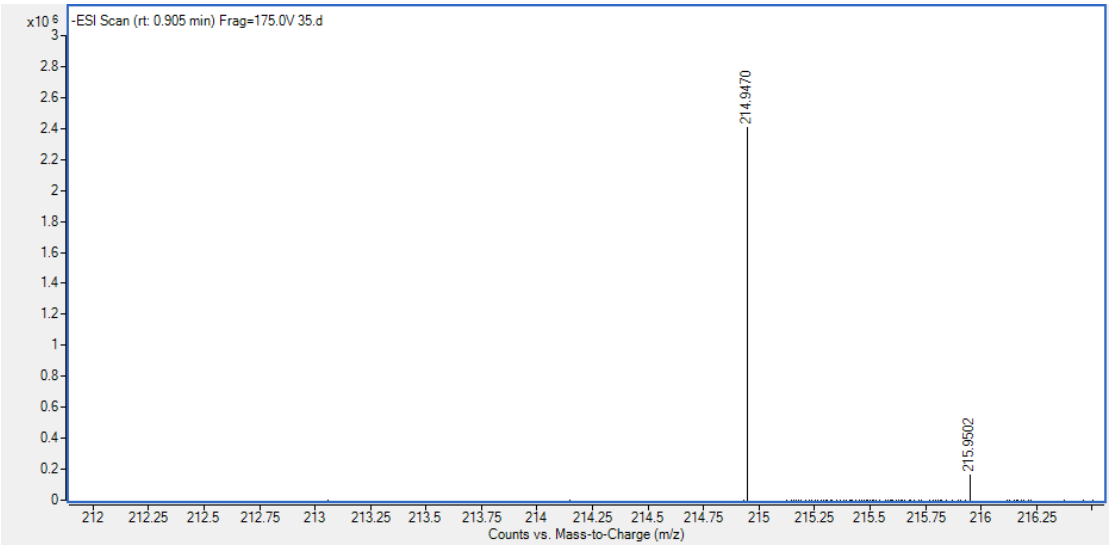
8c ^{1}H NMR


8.26
8.25
7.44
7.43
7.42
7.41
7.27
6.75
6.73
6.03
0.00
Br
H2N
NO2
1H NMR (400MHz, Chloroform-d)
1.00
1.03
1.06
1.80
f1 (ppm)

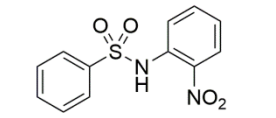
8c ^{13}C NMR


143.59
138.50
132.48
128.33
120.35
107.85
Br
H2N
NO2
13C NMR (101MHz, Chloroform-d)
f1 (ppm)

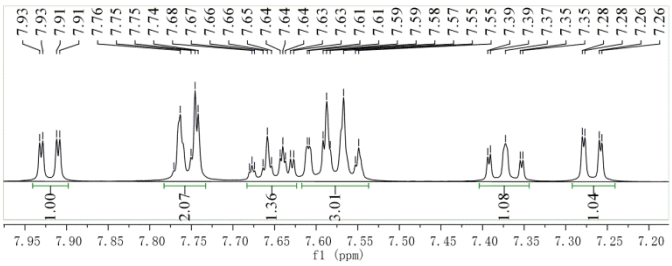
8c $C_6H_5BrN_2O_2$, $[M-H]^-$ 214.9456. Found 214.9470.

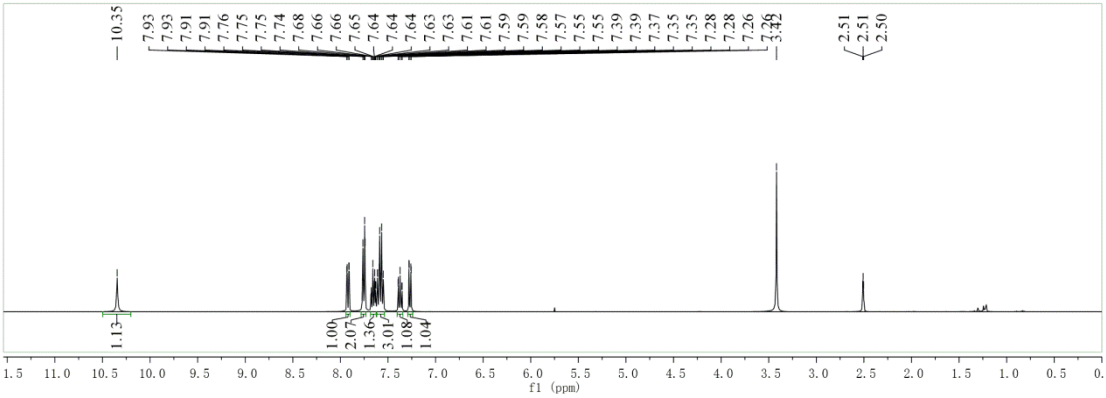


11 ^{1}H NMR

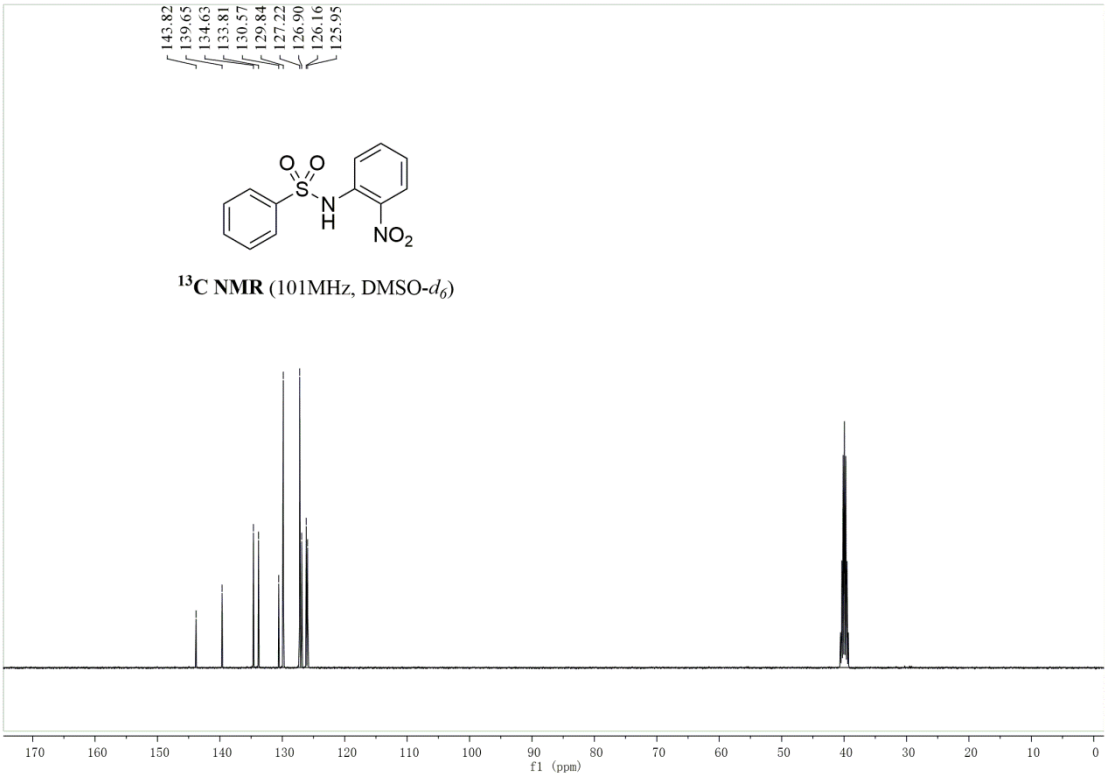


^{1}H NMR (400MHz, DMSO-d_6)

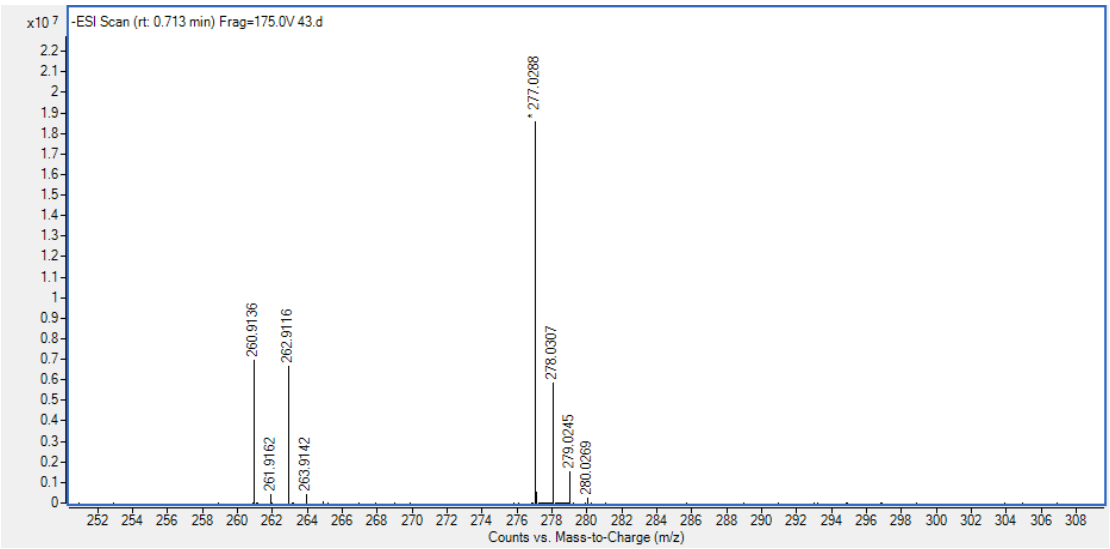




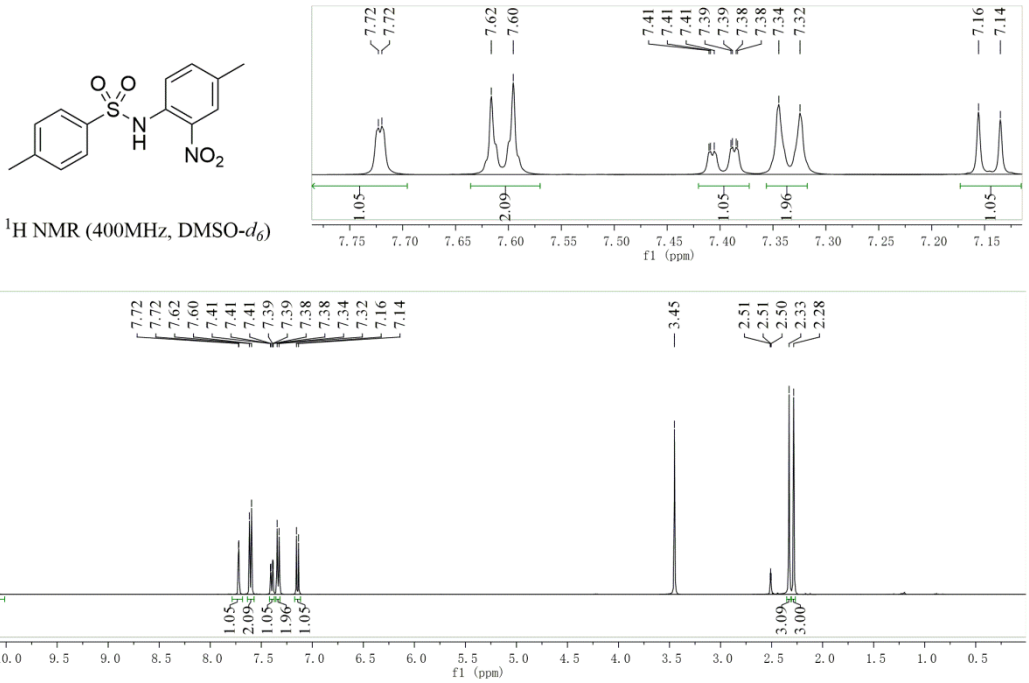
11 ^{13}C NMR



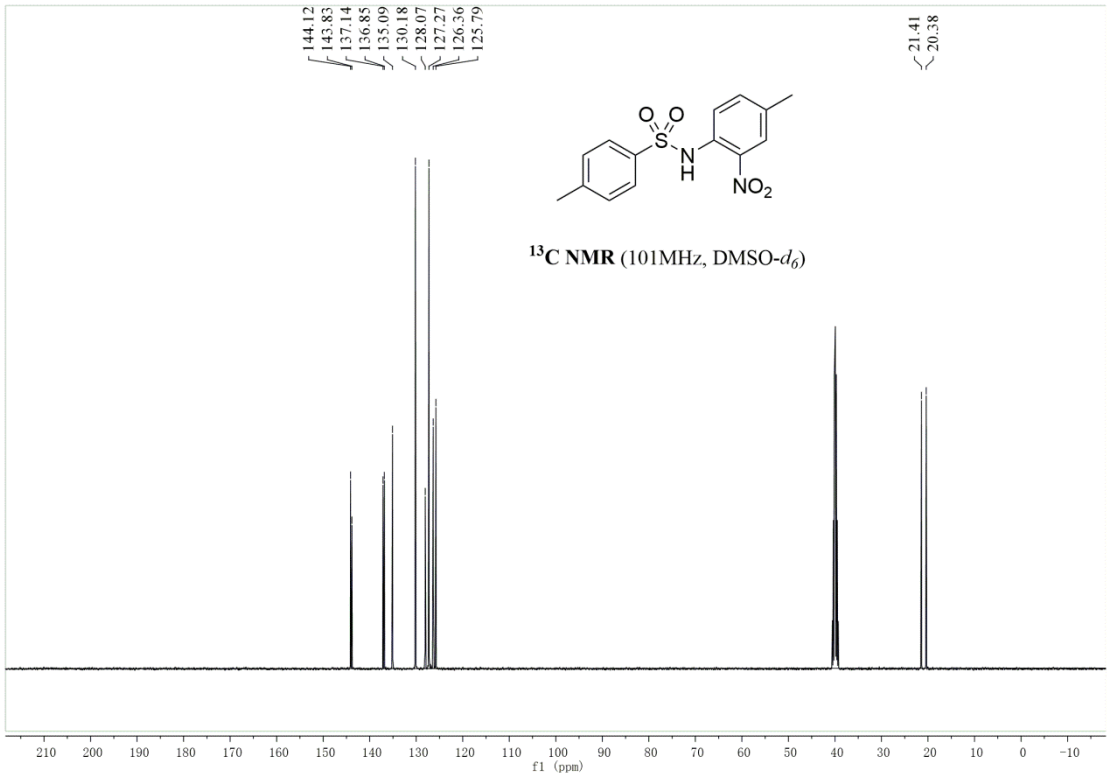
11 $C_{12}H_{10}N_2O_4S$, $[M-H]^-$ 277.0283. Found 277.0288.



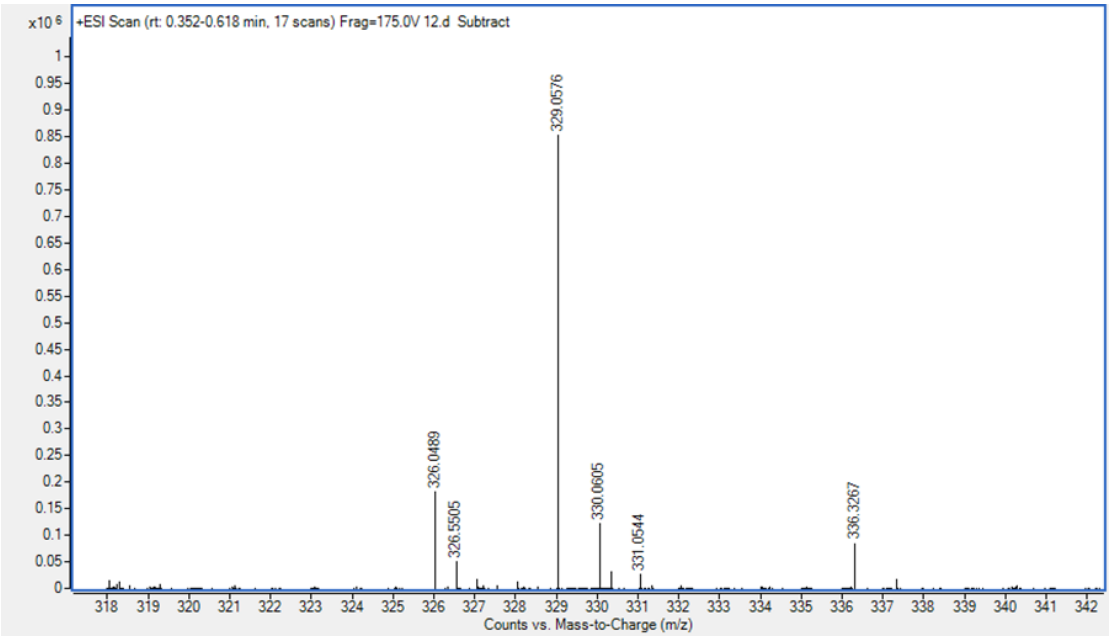
13 ^{1}H NMR



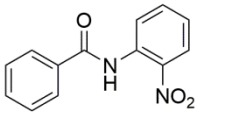
13 ^{13}C NMR



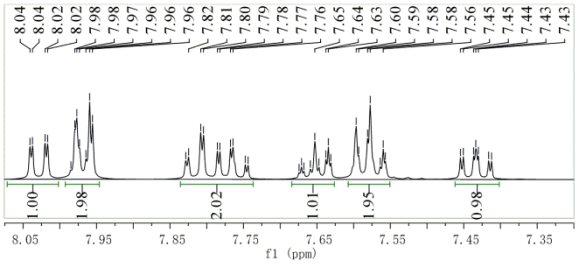
13 $C_{14}H_{14}N_2O_4S$, $[M+Na]^+$ 329.0572. Found 329.0576.

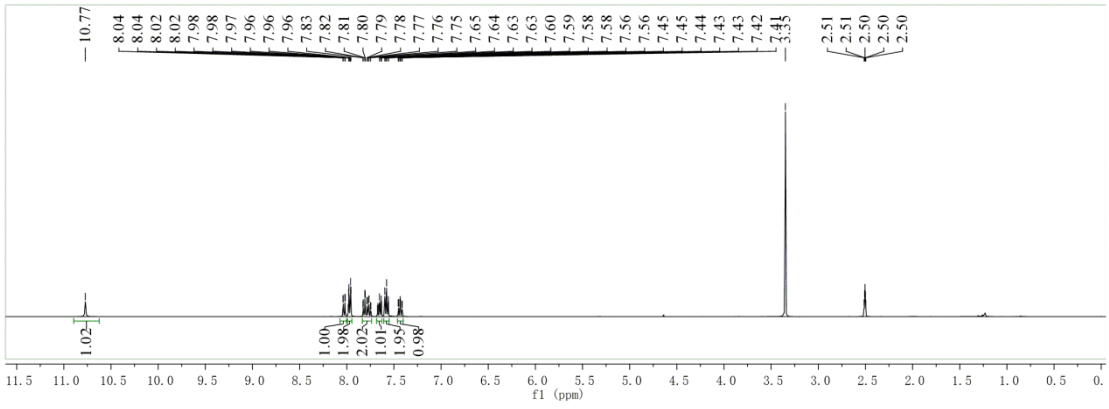


18 ^{1}H NMR

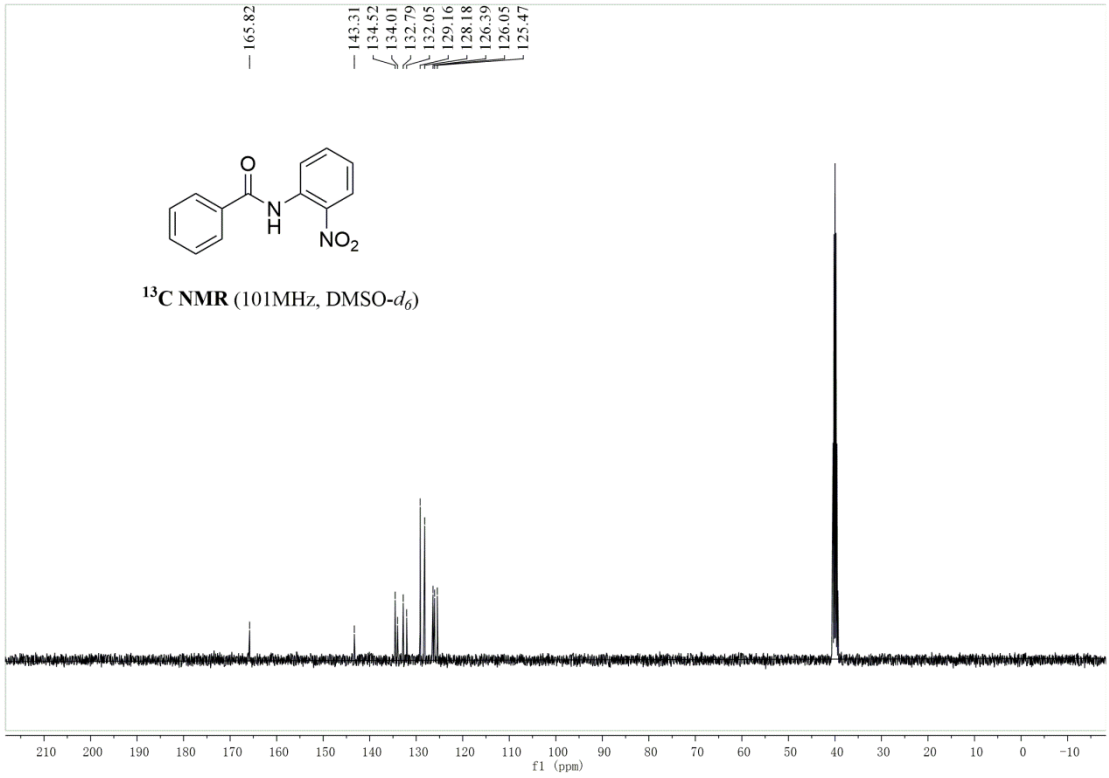


^{1}H NMR (400MHz, DMSO-d_6)

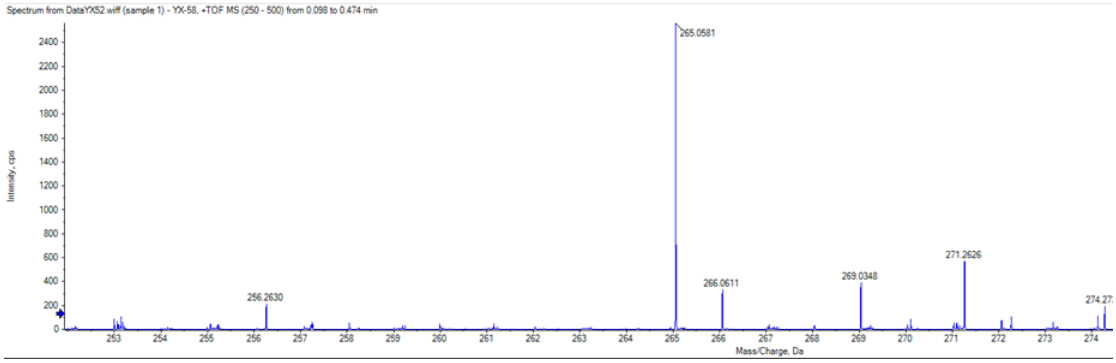




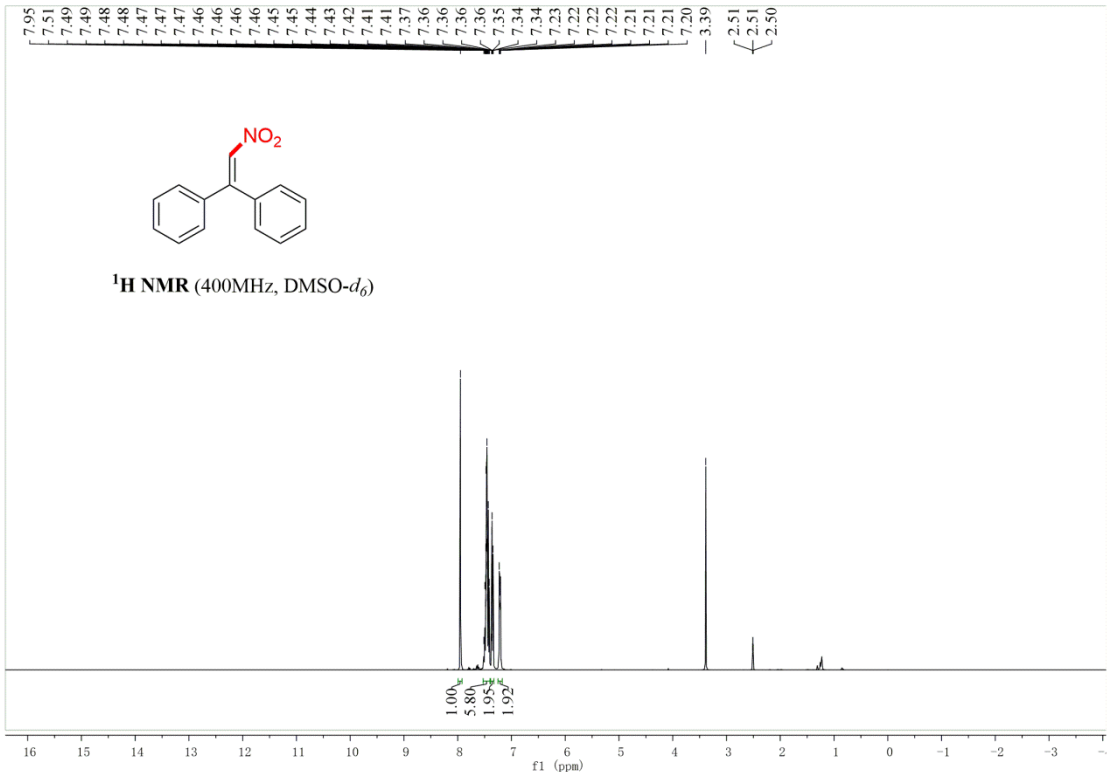
18 ^{13}C NMR



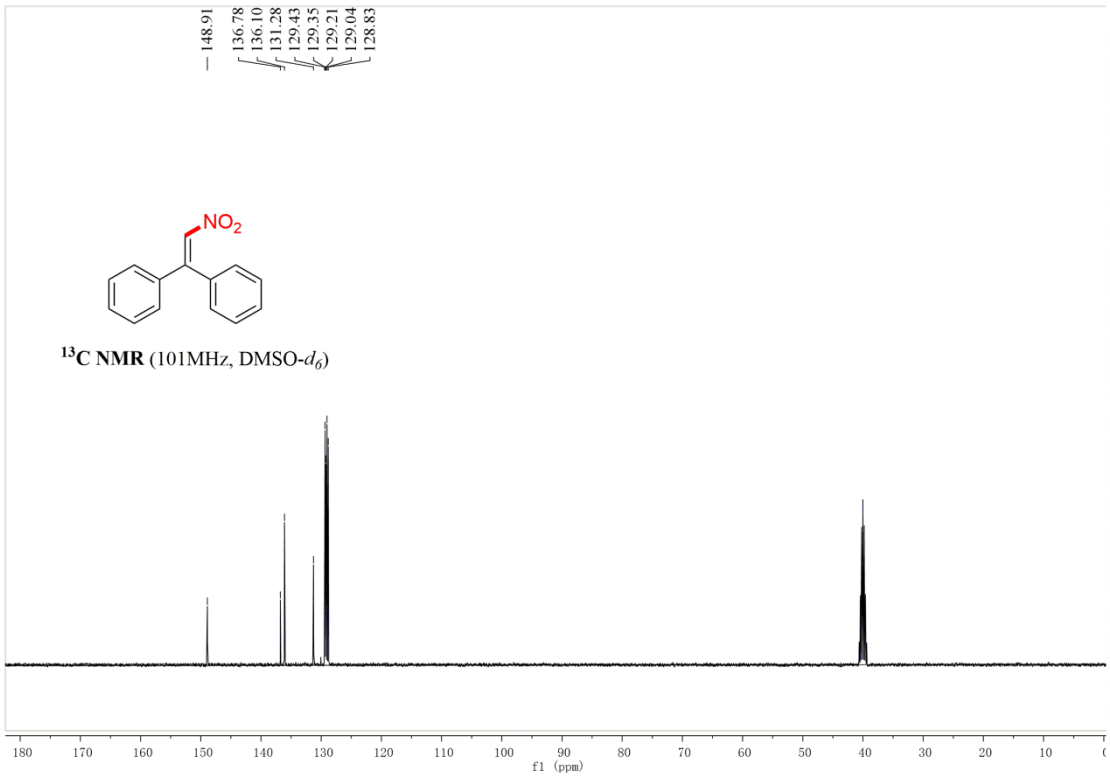
18 $C_{13}H_{10}N_2O_3$, $[M+Na]^+$ 265.0589. Found 265.0581.



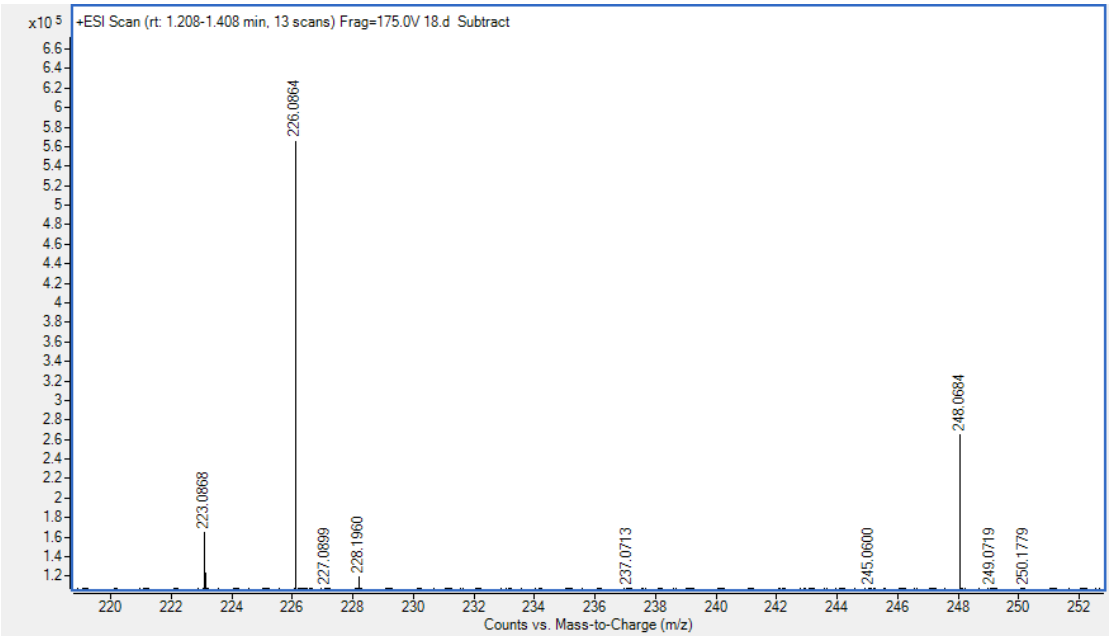
21 ^{1}H NMR


7.95
7.51
7.49
7.49
7.48
7.48
7.47
7.47
7.47
7.46
7.46
7.46
7.46
7.45
7.45
7.44
7.43
7.42
7.41
7.41
7.37
7.36
7.36
7.36
7.35
7.34
7.34
7.23
7.22
7.22
7.22
7.21
7.21
7.21
7.20
3.39
2.51
2.51
2.50
NO2
1H NMR (400MHz, DMSO-d6)
1.00
5.80
1.95
1.92
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

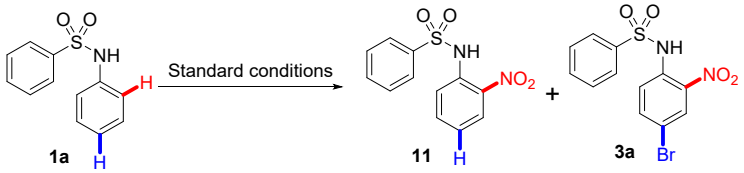
21 ^{13}C NMR


148.91
136.78
136.10
131.28
129.43
129.35
129.21
129.04
128.83
NO2
13C NMR (101MHz, DMSO-d6)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

21 $C_{14}H_{11}NO_2$, $[M+H]^+$ 226.0868. Found 226.0864.



Reaction solution for two hours:



11 $C_{12}H_{10}N_2O_4S$, $[M-H]^-$ 277.0283. Found 277.0285.

3a $C_{12}H_9BrN_2O_4S$, $[M-H]^-$ 354.9388. Found 354.9400.