Supporting Information

Surfactant-controlled Switchable Oxygenation of Sulfides to Sulfoxides or Sulfones under Visible-light Irradiation

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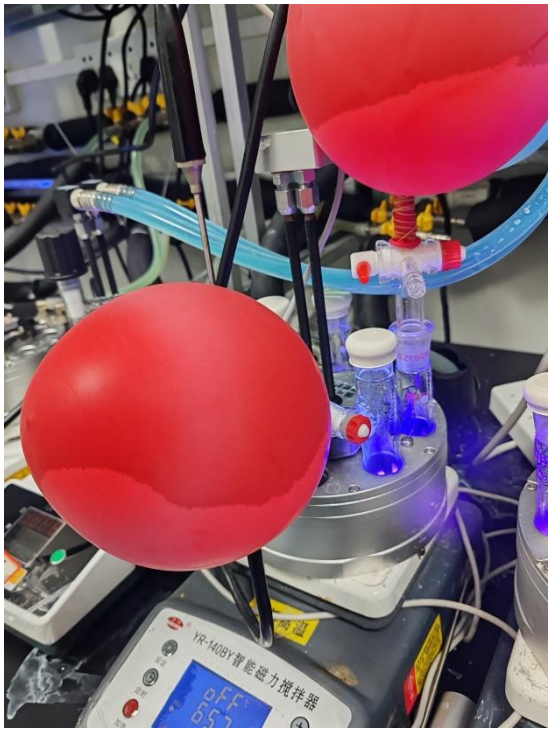
1. General Information

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel. ^{1}H NMR spectra were recorded at 500 MHz, ^{13}C NMR spectra were recorded at 126 MHz by using a Bruker Avance 500 spectrometer. Chemical shifts were calibrated using residual undeuterated solvent as an internal reference (^{1}H NMR: $CDCl_3$ 7.26 ppm, ^{13}C NMR: $CDCl_3$ 77.0 ppm), the chemical shifts (δ) were expressed in ppm, and J values were given in Hz. HRMS were performed on a spectrometer operating on ESI-TOF.

2. Information for the photoreactor



LED Test Report

Product Mark

Model: 2A494000-415nm（415.7）　　Manufacture: Beijing rogertech Ltd

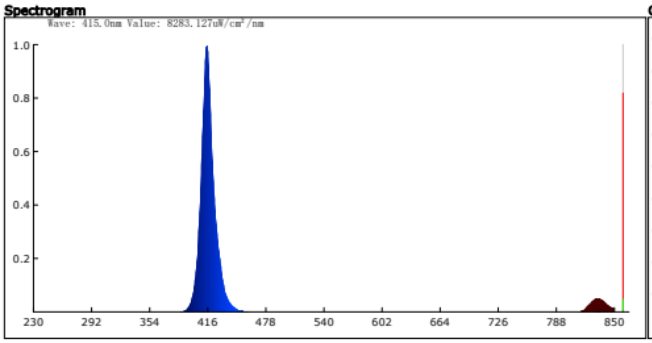
Temperature: 25°C　　Humidity: 65%

Tester: admin　　Test Date: 2023-10-26,11:30:08

Parameter

Name	Value	Name	Value	Name	Value	Name	Value
ESuv(mW/cm²)	0.0001	SDCM	100.00	Peak Signal	53636		
Euvc(mW/cm²)	0.0000	Ra	-82.8	Dark Signal	3124		
Euvb(mW/cm²)	0.0000	Ee(mW/cm²)	144.57433	Compensate level	2904		
Euva(mW/cm²)	1.7754	S/P	51.306				
Euv(mW/cm²)	1.78	Dominant(nm)	426.10				
Eb(mW/cm²)	134.03	Purity(%)	99.9				
Eg(mW/cm²)	0.00	HalfWidth(nm)	13.5				
Er(mW/cm²)	0.00	Peak(nm)	415.7				
Eir(mW/cm²)	9.30	Center(nm)	416.1				
E(lx)	4025.03	Centroid(nm)	444.2				
Candle E(fc)	373.93	Color Ratio(RGB)	0.0,0.0,100.0				
CCT(K)	100000	CIE1931 X	161929.688				
Duv	-0.12865	CIE1931 Y	5893.156				
CIE x,y	0.1701,0.0062	CIE1931 Z	784093.125				
CIE u,v	0.2489,0.0136	TLCI-2012	0				
CIE u',v'	0.2489,0.0204	Integral Time(ms)	0.1				

Spectrogram



CIE1931

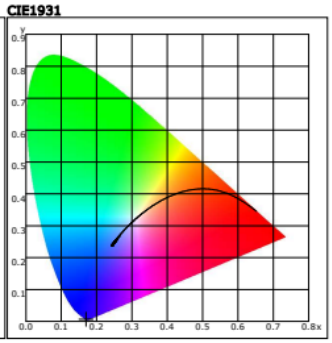
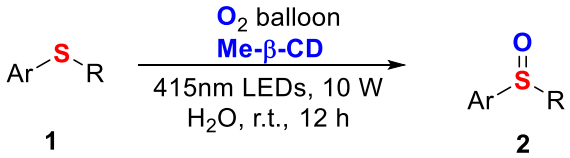


Figure S1. The visible-light irradiation instrument and the spectrum of our lamp

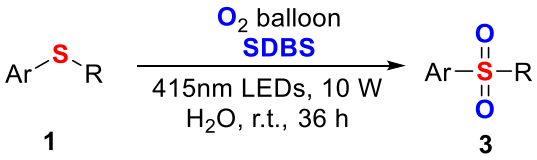
3. Experimental Section

3.1 General experimental procedures for sulfoxides 2



In a 10 mL Schlenk with a stirring bar, sulfides **1** (0.2 mmol, 0.2 mmol/mL) and Me-β-CD (0.1 g/mL) were dissolved in H_2O (1 mL). The mixture was stirred at 25 ℃ with 10 W LED (415 nm) irradiation for 12 h. After the reaction was completed, the reaction mixture was diluted and extracted by ethyl acetate (10 mL x 3). The combined organic layer was dried over Na_2SO_4 AND evaporated under vacuum. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to afford the desired sulfoxides **2**.

3.2 General experimental procedures for sulfones 3



In a 10 mL Schlenk with a stirring bar, sulfides **1** (0.2 mmol, 0.2 mmol/mL) and SDBS (0.1 g/mL) were dissolved in H_2O (1 mL). The mixture was stirred at 25 ℃ with 10 W LED (415 nm) irradiation for 36 h. After the reaction was completed, the reaction mixture was diluted and extracted by ethyl acetate (10 mL x 3). The combined organic layer was dried over Na_2SO_4 AND evaporated under vacuum. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to afford the desired sulfones **3**.

3.3 Control Experiments.

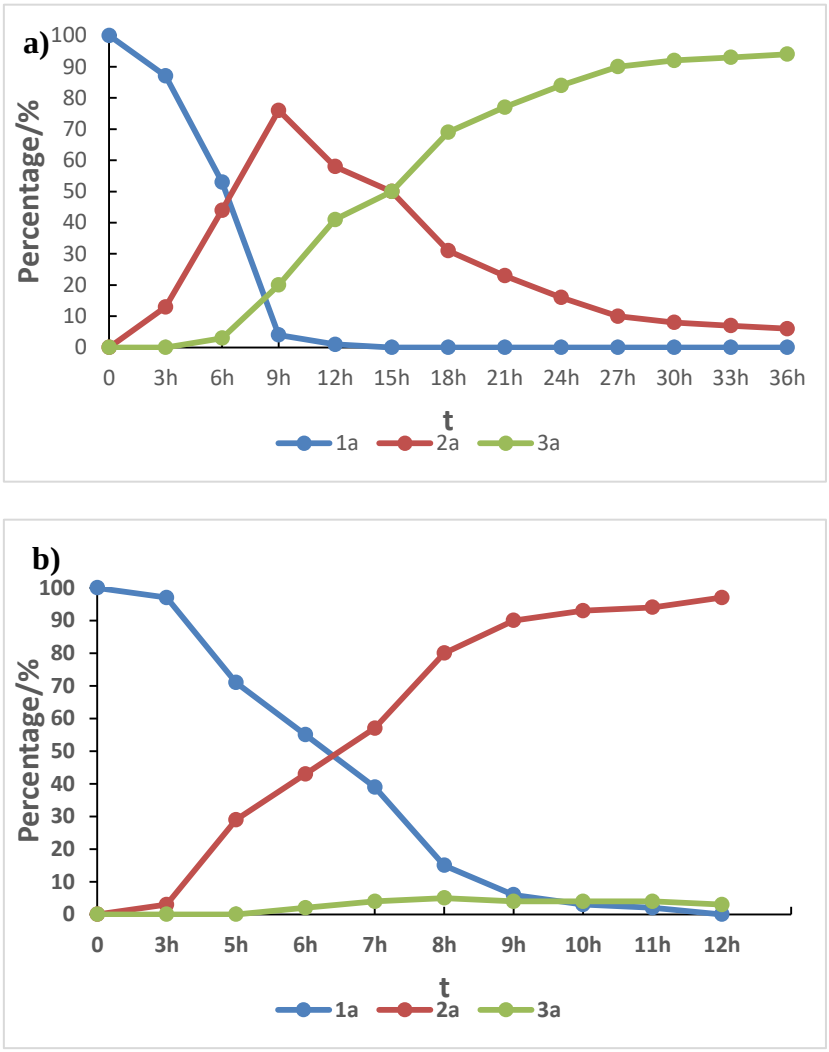
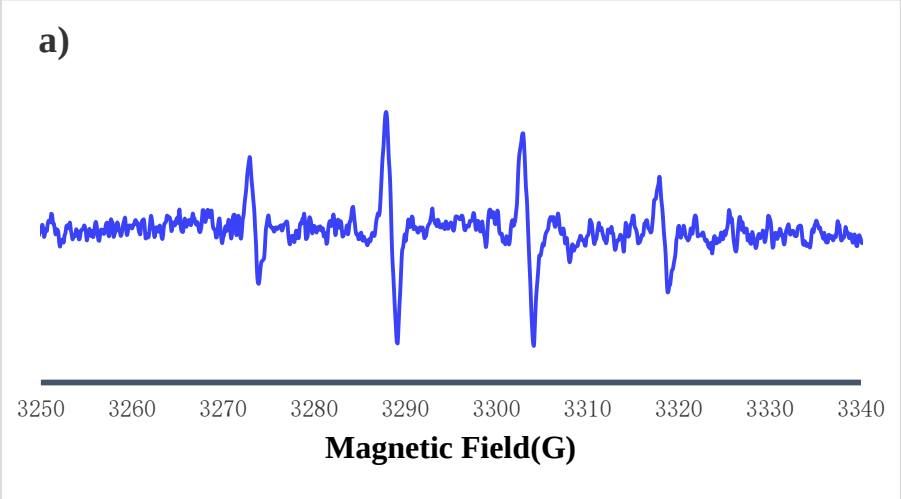
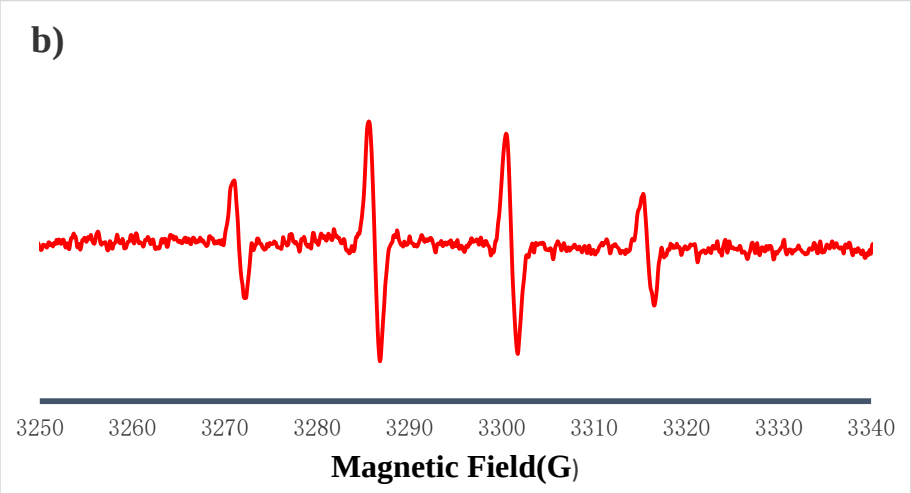
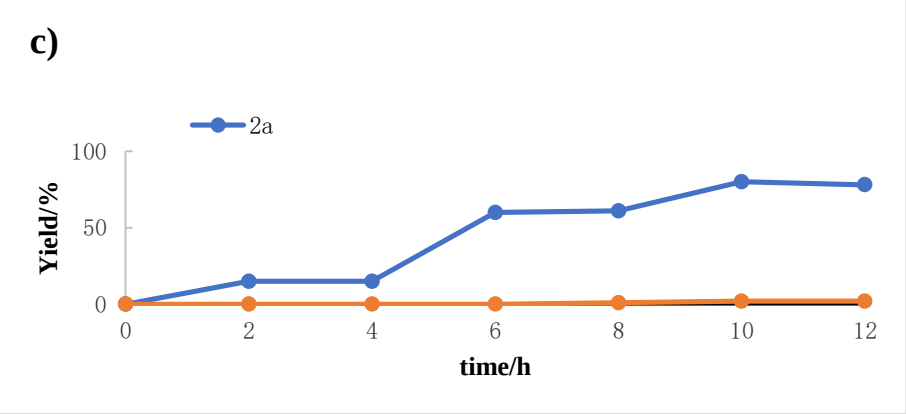


Figure S2. Time course for the conversion of methylphenyl sulfide **1a.**


a)
3250
3260
3270
3280
3290
3300
3310
3320
3330
3340
Magnetic Field(G)


b)
3250
3260
3270
3280
3290
3300
3310
3320
3330
3340
Magnetic Field(G)


c)
2a
100
50
0
Yield/%
0
2
4
6
8
10
12
time/h

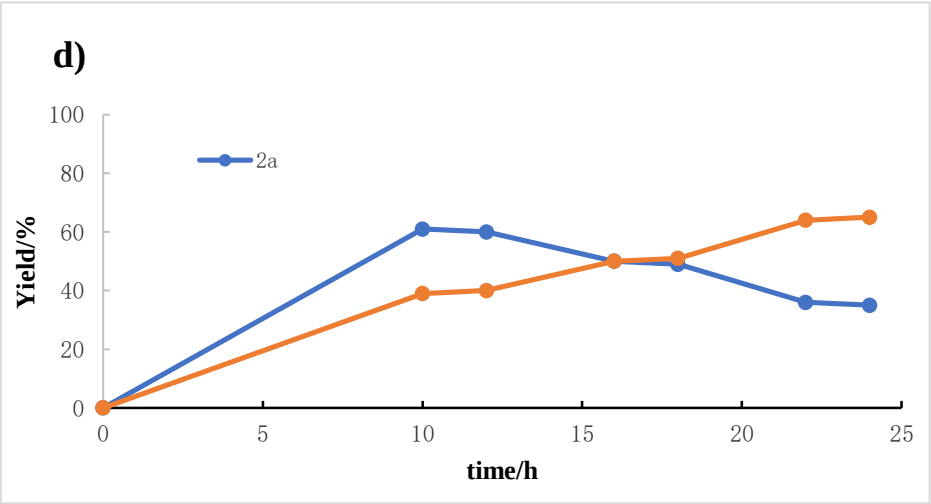


Figure S3. a) EPR Experiment for sulfoxides **2a**; b) EPR Experiment for sulfones **3a;** c) On-off Experiment for sulfoxides **2a**; d) On-off Experiment for sulfones **3a**.

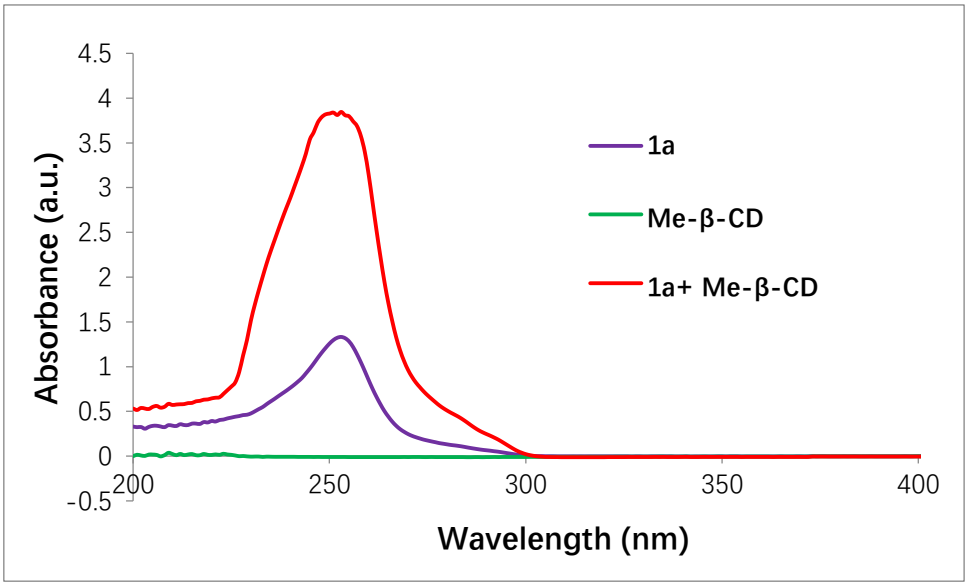
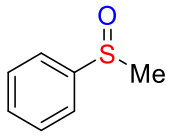
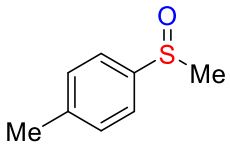


Figure S4. The UV-vis absorption spectra of **1a,** Me-β-CD or the mixture of **1a** and Me-β-CD in ethanol (0.01 M).

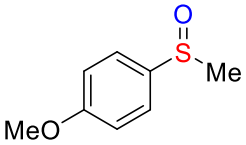
4. Characterization data of sulfoxides 2 and sulfones 3



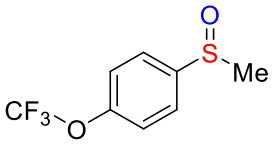
(methylsulfinyl)benzene (**2a**)[1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 7.6 Hz, 2H), 7.53-7.45 (m, 3H), 2.69 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 145.69, 131.04, 129.36, 123.49, 43.95.



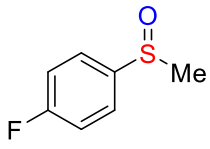
1-methyl-4-(methylsulfinyl)benzene (**2b**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 2.71 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 142.53, 141.56, 130.07, 123.58, 44.08, 21.43.



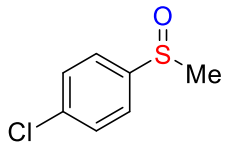
1-methoxy-4-(methylsulfinyl)benzene (**2c**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 8.6 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H), 2.70 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 161.99, 136.63, 125.48, 114.87, 55.56, 44.04.



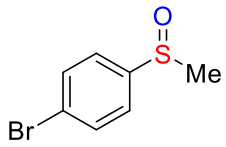
1-(methylsulfinyl)-4-(trifluoromethoxy)benzene (**2d**)[2]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.3 Hz, 2H), 2.73 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 151.10 (d, *J* = 1.83 Hz), 144.15, 125.43, 121.77, 120.32 (q, *J* = 257.5 Hz), 44.07.



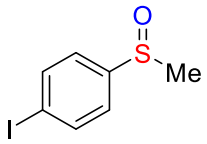
1-fluoro-4-(methylsulfinyl)benzene (**2e**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.66 (dd, *J* = 8.5, 5.1 Hz, 2H), 7.24 (dd, *J* = 15.0, 6.6 Hz, 2H), 2.72 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.47 (d, *J* = 250 Hz), 141.46, 125.99 (d, *J* = 8.75 Hz), 116.86 (d, *J* = 21.25 Hz), 44.39.



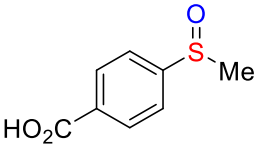
1-chloro-4-(methylsulfinyl)benzene (**2f**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 2.52 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.28, 137.28, 129.69, 124.99, 44.12.



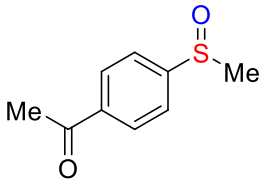
1-bromo-4-(methylsulfinyl)benzene (**2g**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.5 Hz, 2H), 7.31 (d, *J* = 8.5 Hz, 2H), 2.51 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.87, 132.61, 125.49, 125.16, 44.02.



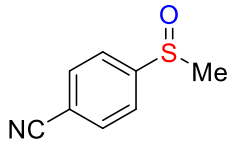
1-iodo-4-(methylsulfinyl)benzene (**2h**)[3]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 7.2 Hz, 2H), 7.38 (d, *J* = 7.0 Hz, 2H), 2.72 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 145.71, 138.49, 125.16, 97.40, 43.99.



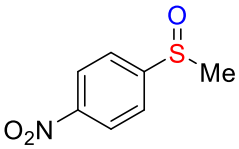
4-(methylsulfinyl)benzoic acid (**2i**) [4]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.00 (d, *J* = 8.6 Hz, 2H), 7.28 (d, *J* = 8.9 Hz, 2H), 2.53 (s, 3H), 1.25 (s, 1H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 171.41, 146.89, 130.61, 125.34, 125.01, 14.89.



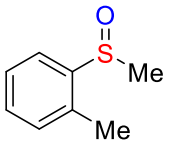
1-(4-(methylsulfinyl)phenyl)ethan-1-one (**2j**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.11 (d, *J* = 8.2 Hz, 2H), 7.75 (d, *J* = 8.3 Hz, 2H), 2.76 (s, 3H), 2.66 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 197.08, 150.92, 139.09, 129.18, 123.77, 43.84, 26.83.



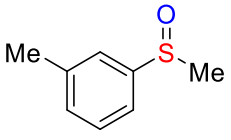
4-(methylsulfinyl)benzonitrile (**2k**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.1 Hz, 2H), 7.76 (d, *J* = 8.1 Hz, 2H), 2.76 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 151.53, 133.14, 124.44, 117.83, 114.96, 43.92.



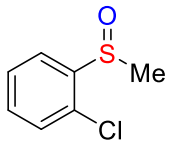
1-(methylsulfinyl)-4-nitrobenzene (**2l**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.40 (d, *J* = 8.8 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 2.79 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 153.25, 149.52, 124.68, 124.53, 43.91.



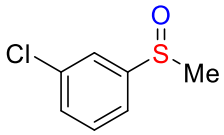
1-methyl-2-(methylsulfinyl)benzene (**2m**) [5]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 7.7 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.4 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 1H), 2.69 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 143.97, 133.95, 130.77, 130.66, 127.46, 123.00, 42.08, 18.07.



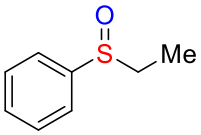
1-methyl-3-(methylsulfinyl)benzene (**2n**) [5]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.47 (s, 1H), 7.41 -7.37 (m, 2H), 7.29 (dt, *J* = 3.6, 2.2 Hz, 1H), 2.70 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 145.60, 139.72, 131.95, 129.25, 123.85, 120.69, 44.03, 21.53.



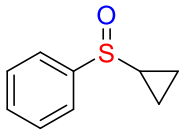
1-chloro-2-(methylsulfinyl)benzene (**2o**) [4]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.38 (d, *J* = 6.8 Hz, 1H), 2.80 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 143.61, 131.99, 129.78, 128.17, 125.32, 125.05, 41.66.



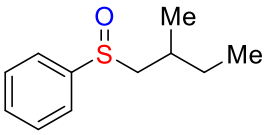
1-chloro-3-(methylsulfinyl)benzene (**2p**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.63 (s, 1H), 7.51 -7.41 (m, 3H), 2.71 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 147.87, 135.71, 131.19, 130.60, 123.63, 121.62, 44.03.



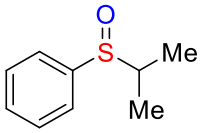
(ethylsulfinyl)benzene (**2q**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 7.3 Hz, 2H), 7.52-7.46 (m, 3H), 2.92-2.85 (m, 1H), 2.79-2.71 (m, 1H), 1.18 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 143.38, 131.02, 129.23, 124.27, 50.38, 6.05.



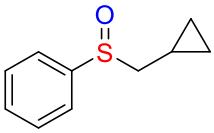
(cyclopropylsulfinyl)benzene (**2r**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.66 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.56-7.47 (m, 3H), 2.29-2.24 (m, 1H), 1.27-1.22 (m, 1H), 1.07-1.00 (m, 1H), 1.00-0.90 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.99, 131.07, 129.30, 124.15, 33.96, 3.55, 2.98.



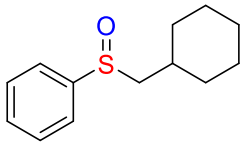
((2-methylbutyl)sulfinyl)benzene (**2s**)[1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 5.6 Hz, 2H), 7.54-7.45 (m, 3H), 2.88 (dd, *J* = 13.0, 4.0 Hz, 0.5H), 2.78 (dd, *J* = 13.1, 5.9 Hz, 0.5H), 2.60 (dd, *J* = 13.1, 7.9 Hz, 0.5H), 2.44-2.37 (m, 1H), 2.08-1.93 (m, 1H), 1.68 (dt, *J* = 13.3, 6.3 Hz, 1H), 1.43 (dq, *J* = 14.1, 7.0 Hz, 0.5H), 1.38-1.27 (m, 1H), 1.15 (d, *J* = 6.6 Hz, 1.5H), 1.04 (d, *J* = 6.8 Hz, 1.5H), 0.90 (q, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.94, 144.86, 131.08, 130.98, 129.37, 124.10, 123.97, 66.23, 65.97, 30.38, 30.22, 29.76, 28.59, 19.51, 18.70, 11.14, 10.91.



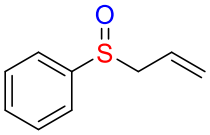
(isopropylsulfinyl)benzene (**2t**) [6]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.58 (dd, *J* = 7.6, 2.1 Hz, 2H), 7.54-7.45 (m, 3H), 2.82 (hept, *J* = 6.9 Hz, 1H), 1.22 (d, *J* = 6.9 Hz, 3H), 1.13 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 141.76, 130.97, 128.88, 125.01, 54.55, 15.87, 13.94.



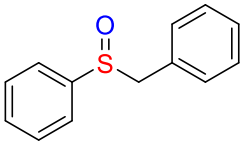
((cyclopropylmethyl)sulfinyl)benzene (**2u**) [7]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 5.7 Hz, 2H), 7.54-7.50 (m, 3H), 2.86 (dd, *J* = 13.2, 7.0 Hz, 1H), 2.68 (t, *J* = 10.5 Hz, 1H), 1.01-0.96 (m, 1H), 0.63 (d, *J* = 8.3 Hz, 2H), 0.27 (dd, *J* = 9.9, 4.9 Hz, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.00, 131.13, 129.22, 124.32, 63.38, 5.27, 4.94, 4.80.



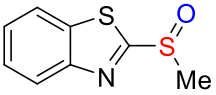
((cyclohexylmethyl)sulfinyl)benzene (**2v**) [8]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.65-7.60 (m, 2H), 7.54-7.45 (m, 3H), 2.79 (dd, *J* = 13.0, 4.7 Hz, 1H), 2.48 (dd, *J* = 13.1, 9.3 Hz, 1H), 2.10 (dt, *J* = 13.0, 3.1 Hz, 1H), 1.99-1.90 (m, 1H), 1.77-1.65 (m, 4H), 1.36-1.25 (m, 2H), 1.21-1.15 (m, 1H), 1.12-1.04 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.72, 130.88, 129.23, 123.85, 66.26, 33.40, 33.00, 32.22, 26.00, 25.91, 25.60.



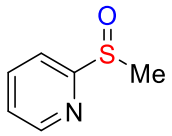
(allylsulfinyl)benzene (**2w**) [9]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.43-7.37 (m, 2H), 7.34-7.28 (m, 3H), 5.48-5.40 (m, 1H), 5.13 (d, *J* = 10.1 Hz, 1H), 4.99 (dd, *J* = 17.0, 1.4 Hz, 1H), 3.40-3.28 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 143.00, 131.26, 129.19, 125.36, 124.49, 124.07, 60.98.



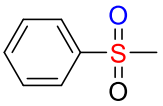
(benzylsulfinyl)benzene (**2x**) [9]: ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.56-7.48 (m, 5H), 7.31-7.23 (m, 3H), 7.11-7.05 (m, 2H), 4.25 (d, *J* = 12.8 Hz, 1H), 4.06 (d, *J* = 12.8 Hz, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 143.38, 130.89, 130.41, 130.40, 128.92, 128.12, 127.84, 124.31, 61.59.



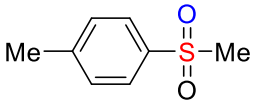
2-(methylsulfinyl)benzo[d]thiazole (**2y**) [10]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.58 (t, *J* = 7.7 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 3.09 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 178.44, 153.81, 136.04, 127.03, 126.31, 124.02, 122.37, 43.21.



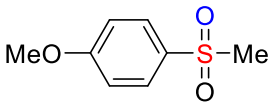
2-(methylsulfinyl)pyridine (**2z**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.59 (d, *J* = 4.0 Hz, 1H), 8.00 (d, *J* = 8.1 Hz, 1H), 7.94-7.91 (m, 1H), 7.40-7.33 (m, 1H), 2.82 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.86, 149.56, 138.16, 124.64, 119.26, 41.28.



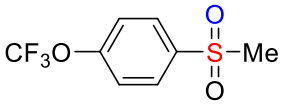
(methylsulfonyl)benzene (**3a**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 6.9 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.57 (t, *J* = 7.7 Hz, 2H), 3.05 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.70, 133.83, 129.49, 127.46, 44.61.



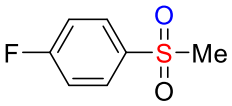
1-methyl-4-(methylsulfonyl)benzene (**3b**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 3.03 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.79, 137.84, 130.07, 127.49, 44.73, 21.73.



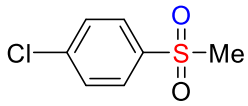
1-methoxy-4-(methylsulfonyl)benzene (**3c**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.64 (d, *J* = 8.6 Hz, 2H), 6.80 (d, *J* = 8.6 Hz, 2H), 3.66 (d, *J* = 1.2 Hz, 3H), 2.80 (d, *J* = 1.2 Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.79, 132.37, 129.62, 114.60, 55.80, 44.93.



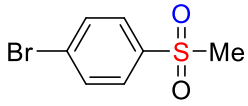
1-(methylsulfonyl)-4-(trifluoromethoxy)benzene (**3d**)[2]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.8 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 3.07 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 153.01 (d, *J* = 2.5 Hz), 138.82, 129.76, 121.20, 120.20 (q, *J* = 257.5 Hz), 44.56.



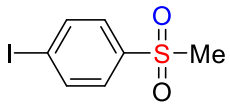
1-fluoro-4-(methylsulfonyl)benzene (**3e**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 8.5, 5.1 Hz, 2H), 7.25 (t, *J* = 8.5 Hz, 2H), 3.05 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.80 (d, *J* = 256.4 Hz), 136.68 (d, *J* = 3.2 Hz), 130.30 (d, *J* = 9.6 Hz), 116.69 (d, *J* = 22.6 Hz), 44.67.



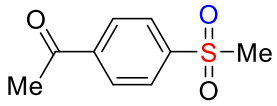
1-chloro-4-(methylsulfonyl)benzene (**3f**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 3.05 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.55, 139.09, 129.81, 129.02, 44.63.



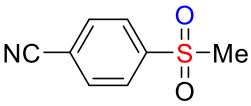
1-bromo-4-(methylsulfonyl)benzene (**3g**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 8.4 Hz, 2H), 8.10 (d, *J* = 8.4 Hz, 2H), 3.06 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.98, 146.05, 129.10, 124.77, 44.41.



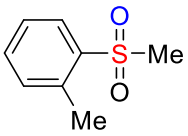
1-iodo-4-(methylsulfonyl)benzene (**3h**) [3]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 7.3 Hz, 2H), 7.65 (d, *J* = 8.6 Hz, 2H), 3.04 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.25, 138.77, 128.87, 101.70, 44.57.



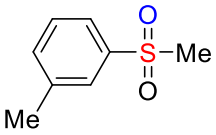
1-(4-(methylsulfonyl)phenyl)ethan-1-one (**3j**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 8.1 Hz, 2H), 8.04 (d, *J* = 8.3 Hz, 2H), 3.08 (s, 3H), 2.66 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 196.79, 144.31, 141.04, 129.27, 127.94, 44.44, 27.06.



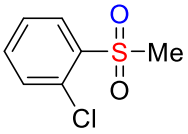
4-(methylsulfonyl)benzonitrile (**3k**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 7.9 Hz, 2H), 7.89 (d, *J* = 7.9 Hz, 2H), 3.09 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.56, 133.33, 128.32, 117.71, 117.17, 44.34.



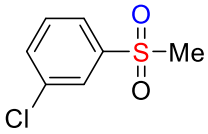
1-methyl-2-(methylsulfonyl)benzene (**3m**) [5]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 7.9 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 3.29 (s, 3H), 2.93 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.83, 137.67, 133.81, 132.84, 129.37, 126.86, 43.79, 20.39.



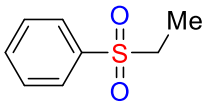
1-methyl-3-(methylsulfonyl)benzene (**3n**) [5]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.93-7.86 (m, 2H), 7.64-7.57 (m, 2H), 3.20 (s, 3H), 2.59 (d, *J* = 3.4 Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.37, 139.64, 134.47, 129.24, 127.57, 124.35, 44.42, 21.28.



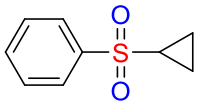
1-chloro-2-(methylsulfonyl)benzene (**3o**) [4]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.34 (d, *J* = 7.9 Hz, 1H), 7.82-7.73 (m, 2H), 7.69-7.66 (m, 1H), 3.47 (s, 3H);^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.98, 134.90, 132.55, 131.96, 130.83, 127.60, 42.79.



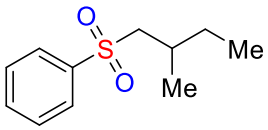
1-chloro-3-(methylsulfonyl)benzene (**3p**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 (s, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.43 (t, *J* = 7.9 Hz, 1H), 2.98 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 142.22, 135.68, 133.97, 130.80, 127.65, 125.57, 44.50.



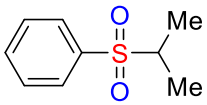
(ethylsulfonyl)benzene (**3q**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 2H), 3.10 (q, *J* = 7.4 Hz, 2H), 1.25 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.49, 133.70, 129.27, 128.18, 50.58, 7.43.



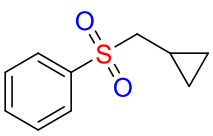
(cyclopropylsulfonyl)benzene (**3r**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.10 (d, *J* = 7.7 Hz, 2H), 7.84 (t, *J* = 7.4 Hz, 1H), 7.75 (t, *J* = 7.6 Hz, 2H), 2.66 (tt, *J* = 8.5, 4.9 Hz, 1H), 1.58-1.51 (m, 2H), 1.26-1.19 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.81, 133.48, 129.34, 127.66, 33.02, 6.08.



((2-methylbutyl)sulfonyl)benzene (**3s**) [1]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 7.7 Hz, 2H), 7.67-7.60 (m, 1H), 7.55 (t, *J* = 7.2 Hz, 2H), 3.07 (dd, *J* = 14.1, 4.7 Hz, 1H), 2.91 (dd, *J* = 14.2, 7.8, 1H), 2.07-1.96 (m, 1H), 1.51-1.39 (m, 1H), 1.28 (dp, *J* = 14.7, 7.5 Hz, 1H), 1.04 (dd, *J* = 6.7, 1.6 Hz, 3H), 0.82 (td, *J* = 7.3, 1.5 Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.21, 133.53, 129.27, 127.83, 62.26, 30.03, 29.40, 19.38, 10.71.

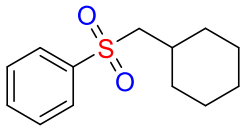


(isopropylsulfonyl)benzene (**3t**) [6]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 7.8 Hz, 2H), 7.64-7.59 (m, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 3.16 (p, *J* = 6.8 Hz, 1H), 1.24 (dd, *J* = 7.0, 1.6 Hz, 6H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 136.85, 133.59, 129.02, 128.89, 55.42, 15.58.

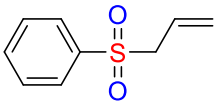


((cyclopropylmethyl)sulfonyl)benzene (**3u**) [7]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.92-7.83 (m, 2H), 7.60 (dd, *J* = 8.4, 6.5 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 2.97 (d, *J* = 7.3 Hz, 2H), 0.93-0.89 (m,

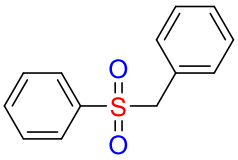
1H), 0.56-0.42 (m, 2H), 0.11-0.02 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.22, 133.65, 129.12, 128.33, 61.25, 4.80, 4.32.



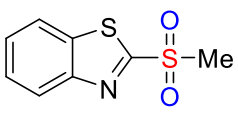
((cyclohexylmethyl)sulfonyl)benzene (**3v**) [11]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 7.8 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 2H), 2.98 (d, *J* = 6.2 Hz, 2H), 2.02-1.95 (m, 1H), 1.86 (dd, *J* = 13.3, 3.8 Hz, 2H), 1.70-1.60 (m, 3H), 1.31-1.21 (m, 2H), 1.18-1.11 (m, 1H), 1.10-1.01 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.51, 133.63, 129.39, 127.89, 63.05, 33.28, 32.93, 25.90, 25.85.



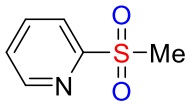
(allylsulfonyl)benzene (**3w**) [9]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.91-7.82 (m, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 2H), 5.85-5.72 (m, 1H), 5.32 (d, *J* = 10.1 Hz, 1H), 5.14 (d, *J* = 17.1 Hz, 1H), 3.80 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.35, 133.89, 129.17, 128.59, 124.87, 124.72, 60.97.



(benzylsulfonyl)benzene (**3x**) [9]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.63 (dd, *J* = 16.4, 7.7 Hz, 3H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.28 (d, *J* = 6.5 Hz, 2H), 7.09 (d, *J* = 7.5 Hz, 2H), 4.33 (s, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.94, 133.85, 130.95, 129.01, 128.91, 128.78, 128.72, 128.22, 63.02.



2-(methylsulfonyl)benzo[d]thiazole (**3y**) [12]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 8.2 Hz, 1H), 8.06-8.00 (m, 1H), 7.68-7.58 (m, 2H), 3.42 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.36, 152.44, 136.60, 128.12, 127.73, 125.41, 122.40, 42.44.



2-(methylsulfonyl)pyridine (**3z**) [13]: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.72 (d, *J* = 3.1 Hz, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 7.97 (t, *J* = 7.8 Hz, 1H), 7.59-7.53 (m, 1H), 3.22 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 158.13, 150.18, 138.40, 127.57, 121.18, 40.12.

5. References

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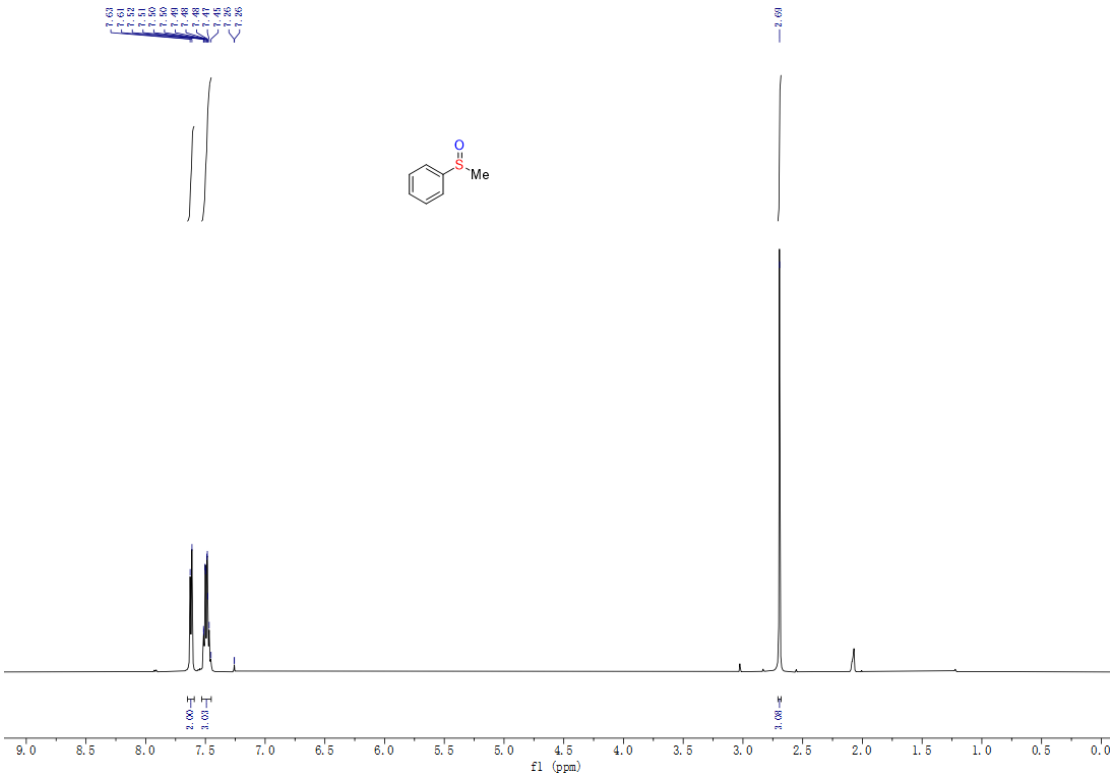
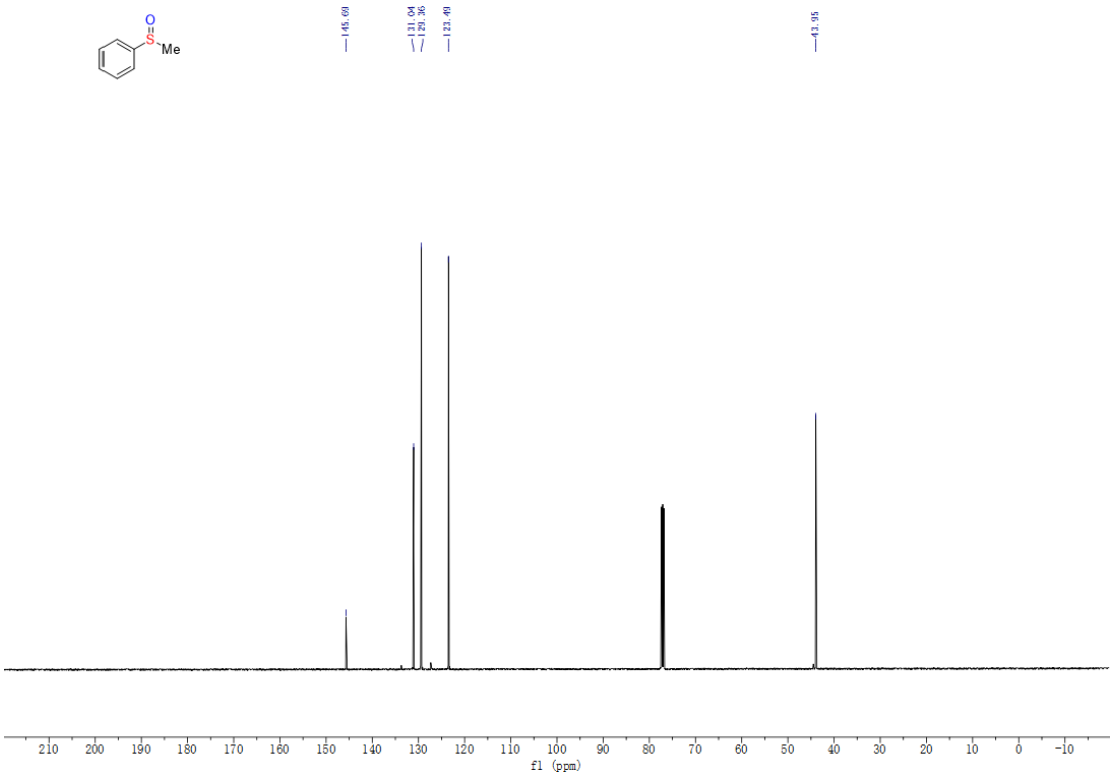
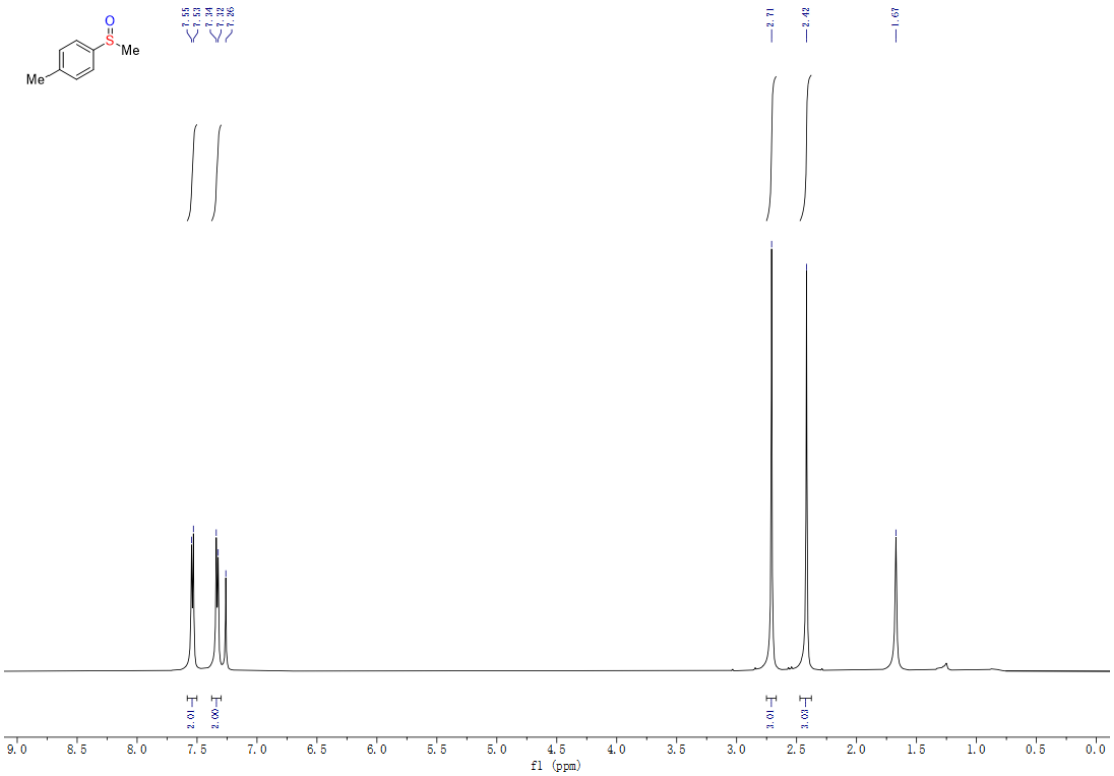
6. ^{1}H and ^{13}C NMR spectra of sulfoxides 2 and sulfones 3



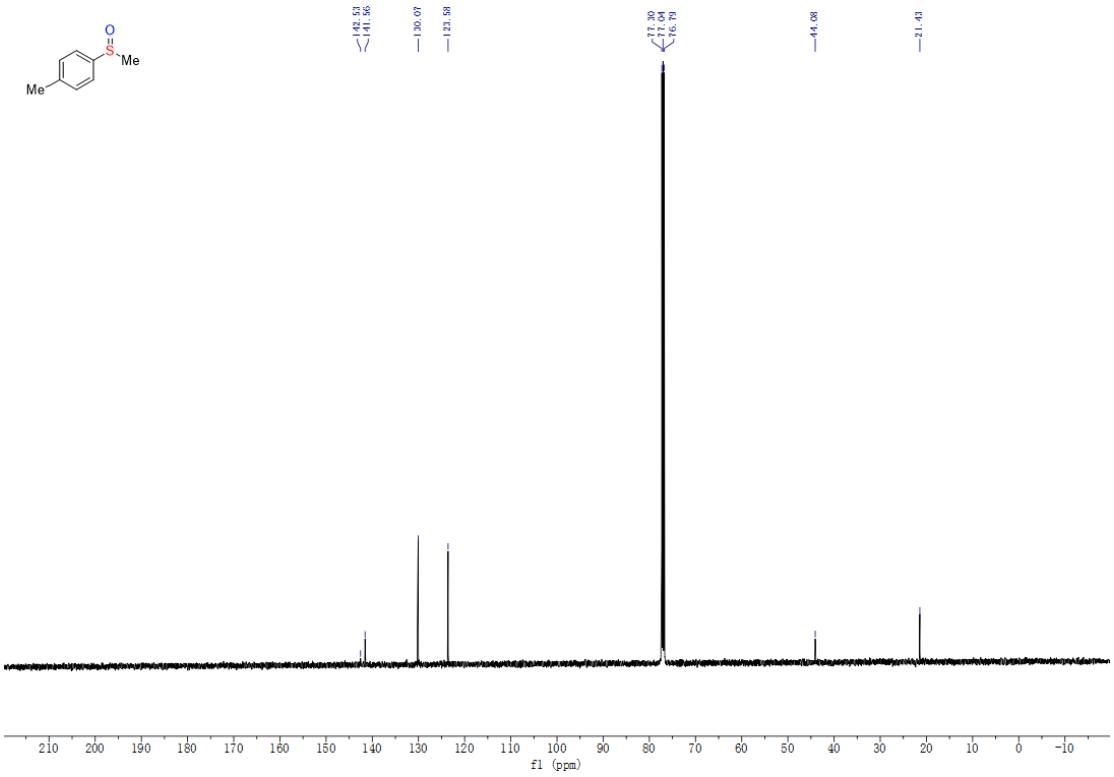
^{1}H NMR of compound **2a**



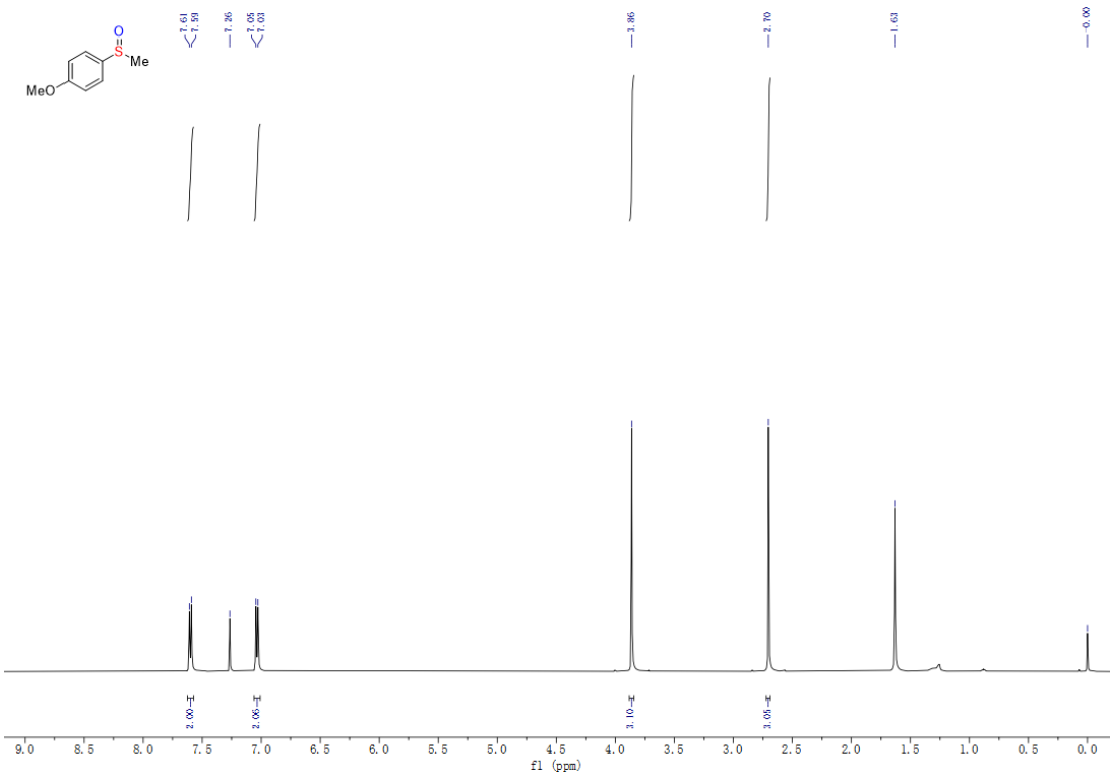
^{13}C NMR of compound **2a**



^{1}H NMR of compound **2b**



^{13}C NMR of compound **2b**



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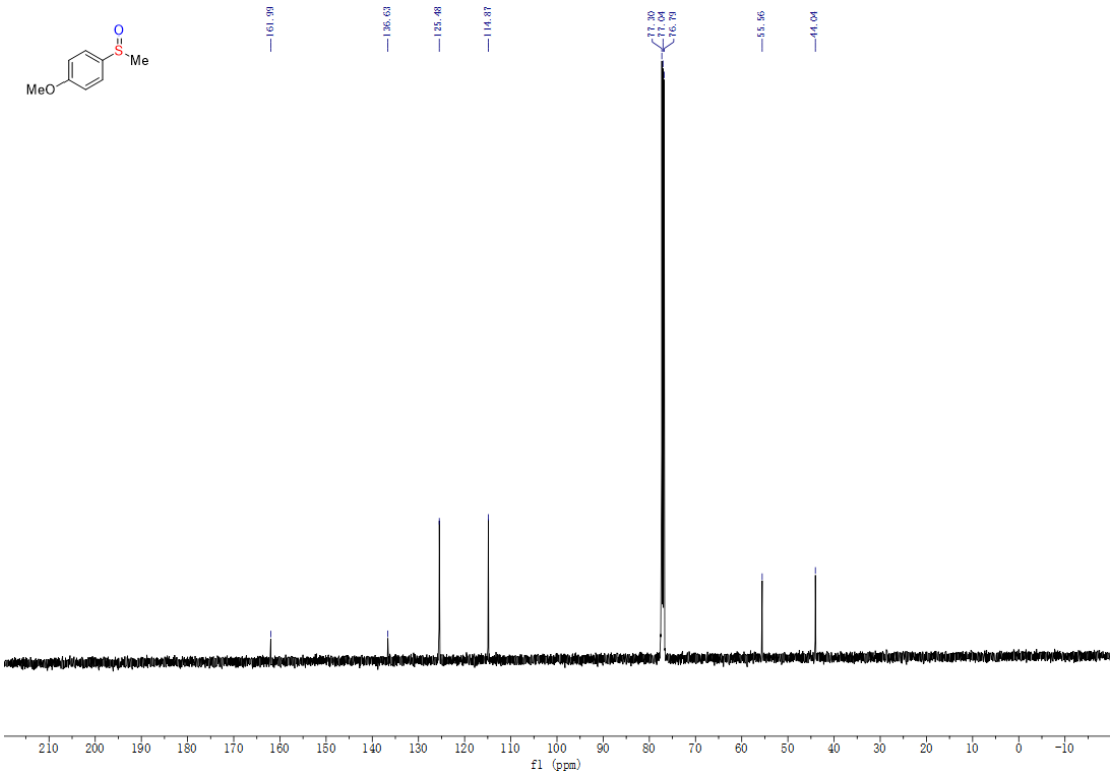

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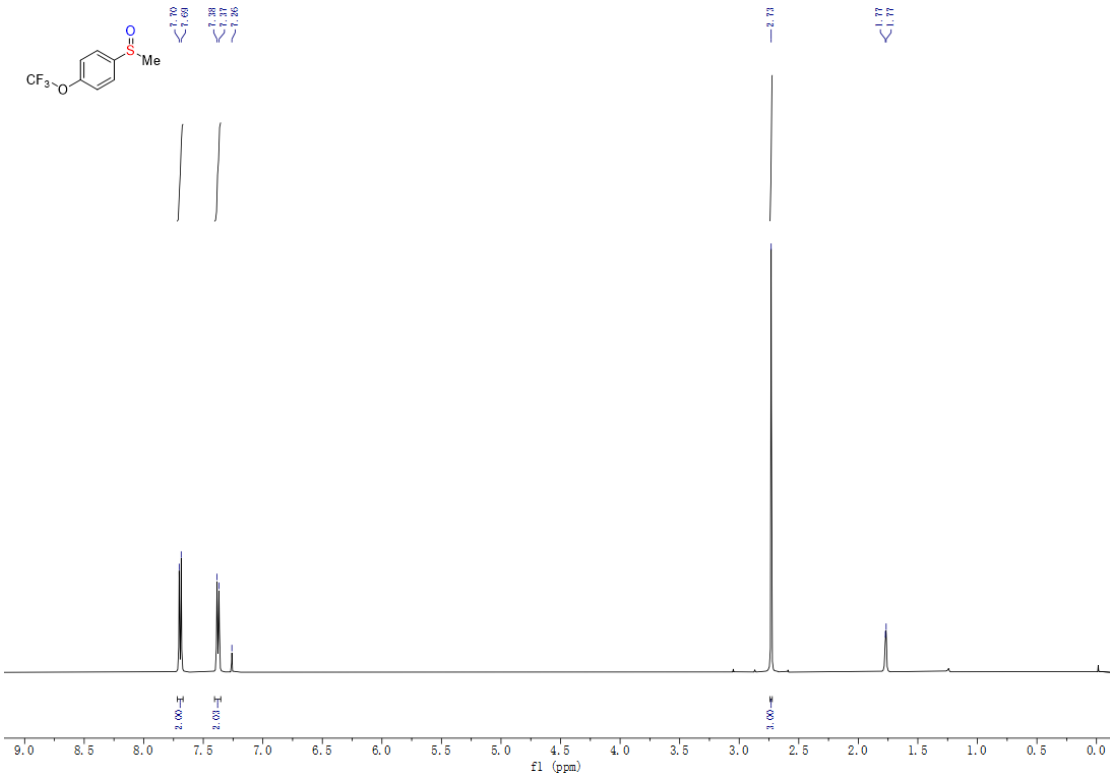

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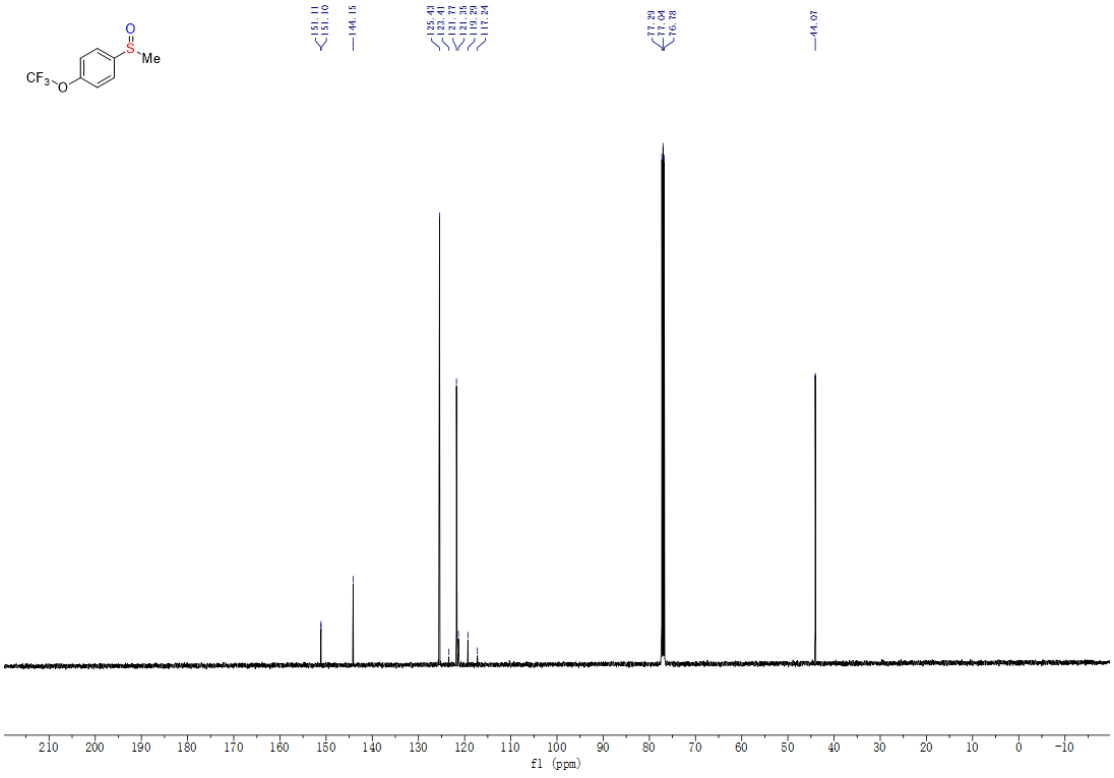

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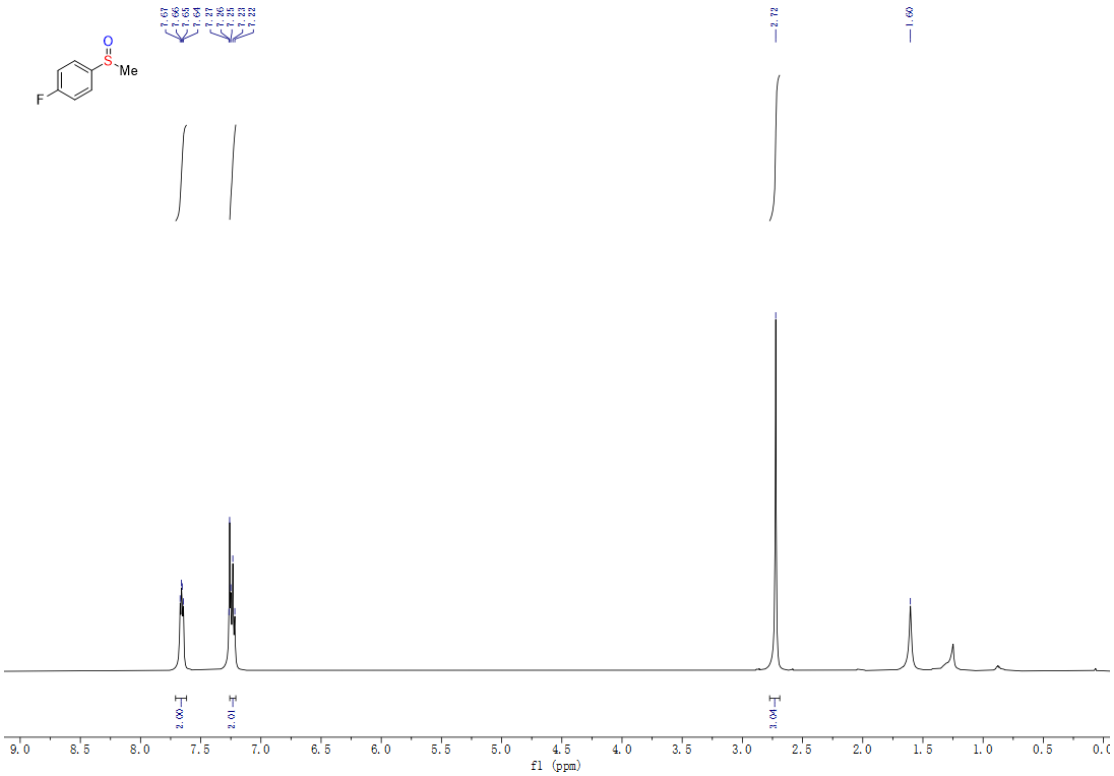

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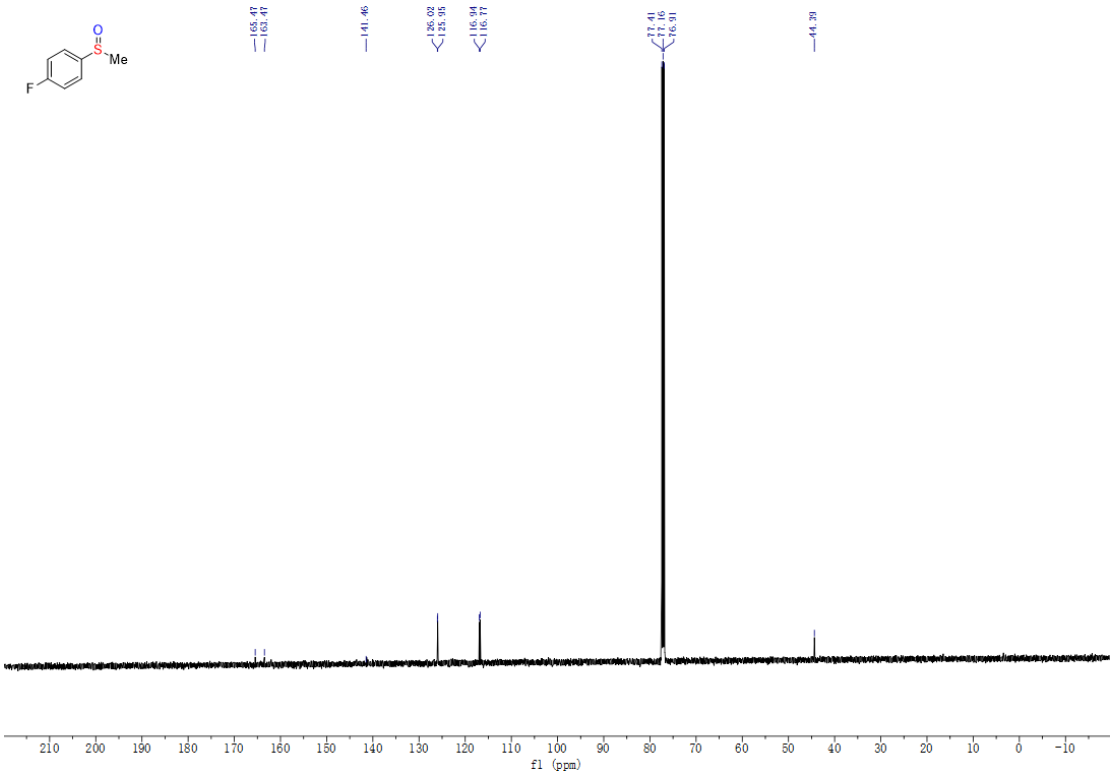

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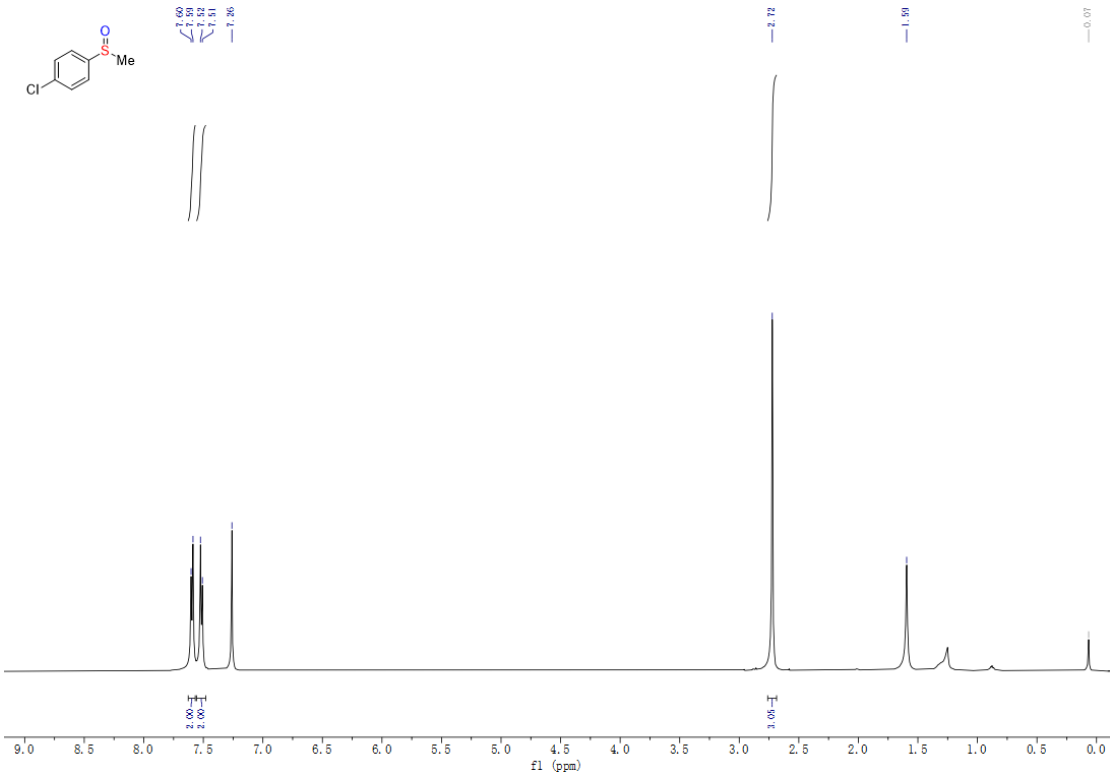
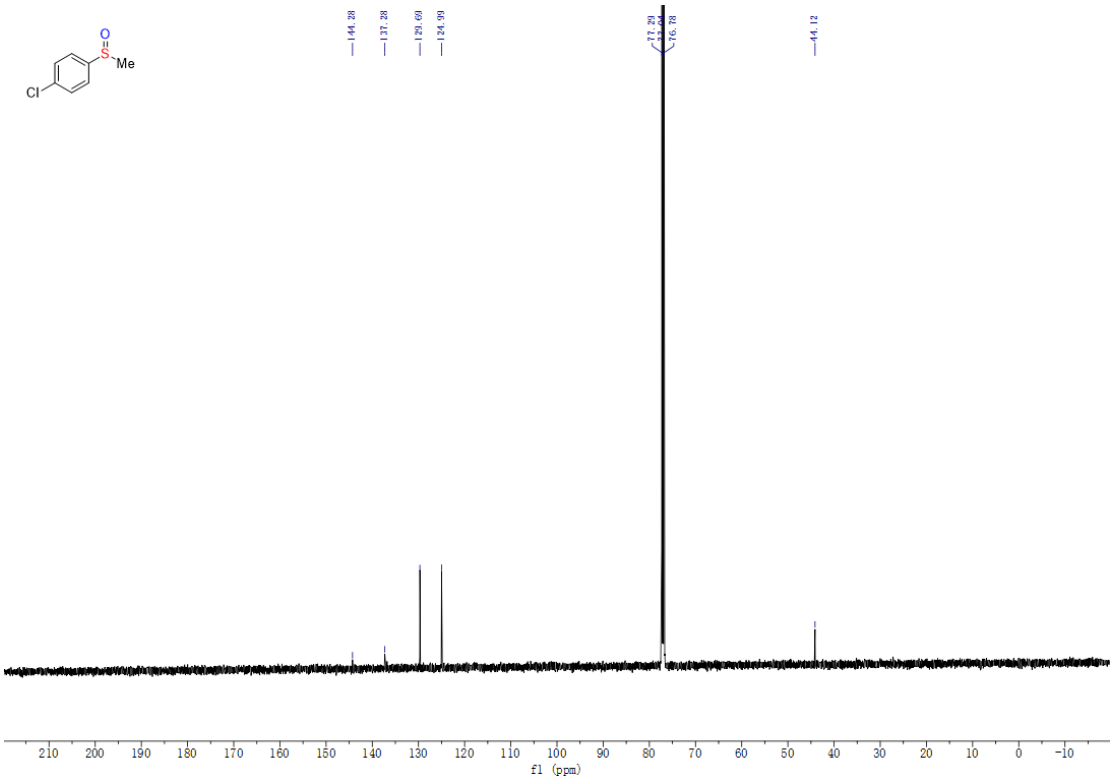


^{1}H NMR of compound **2f**



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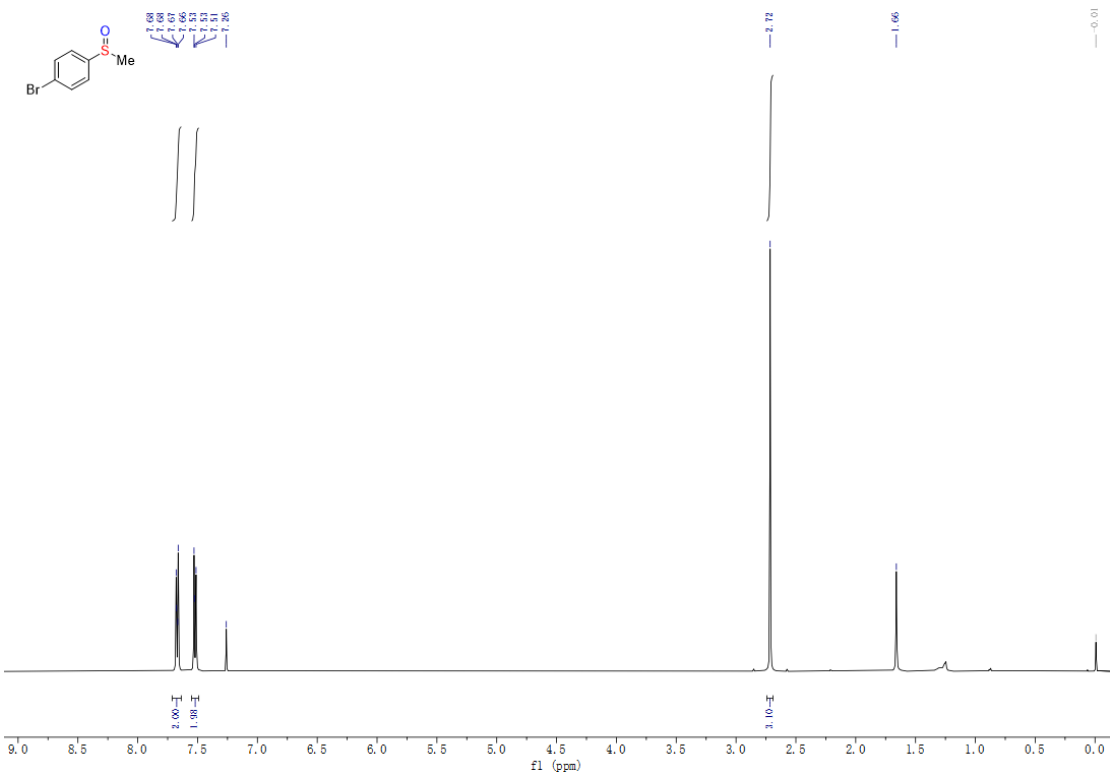

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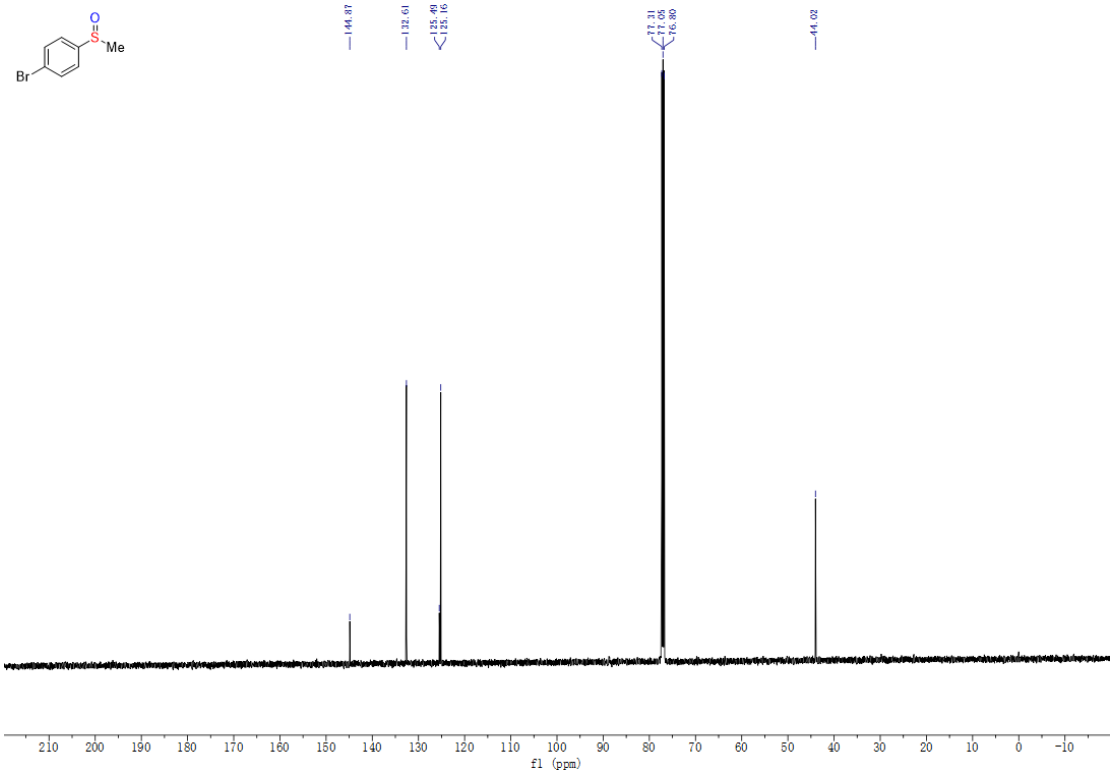

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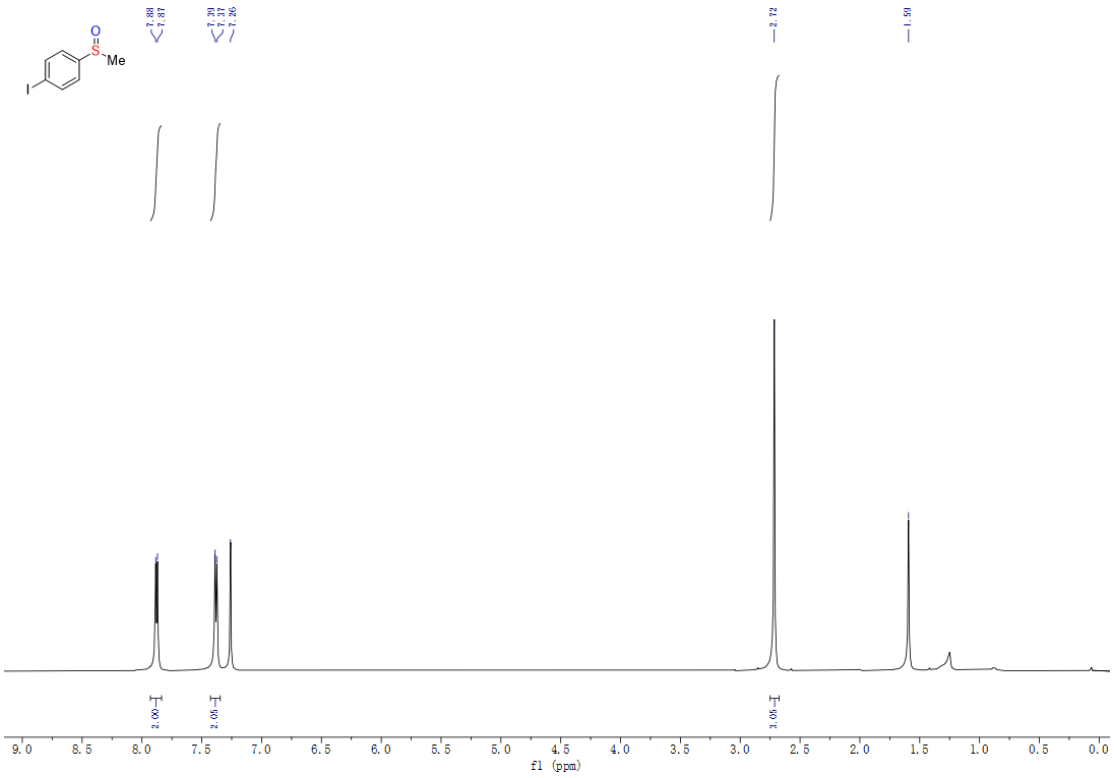

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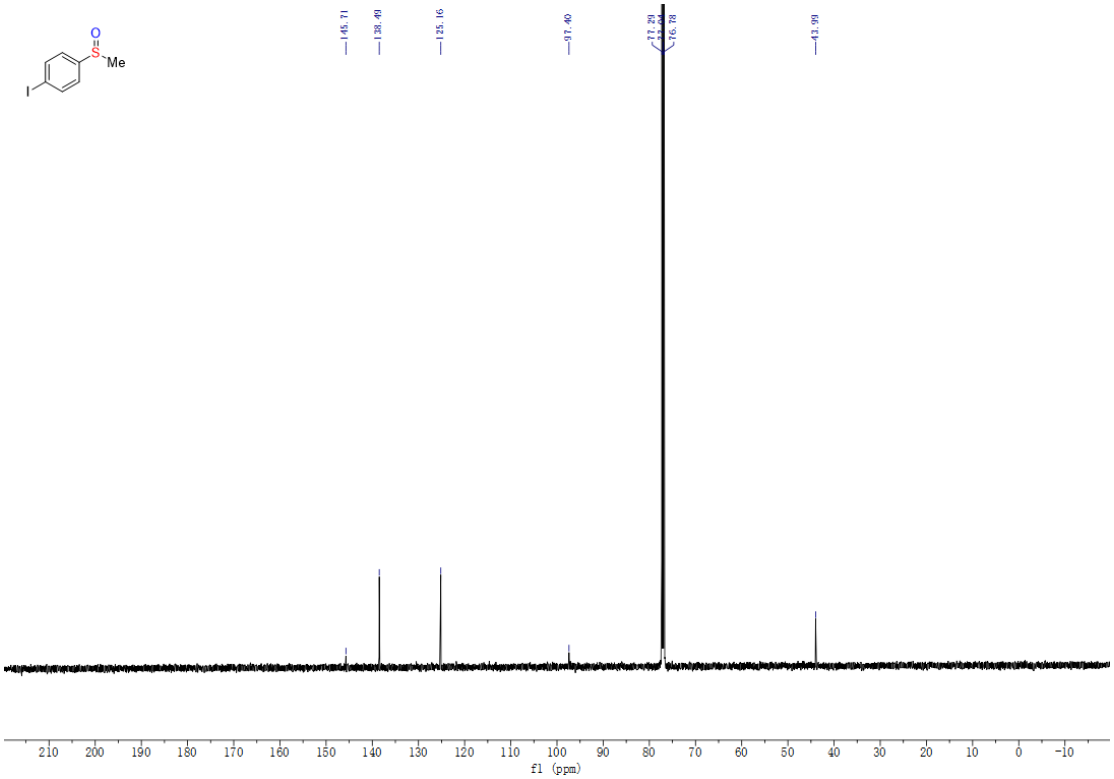

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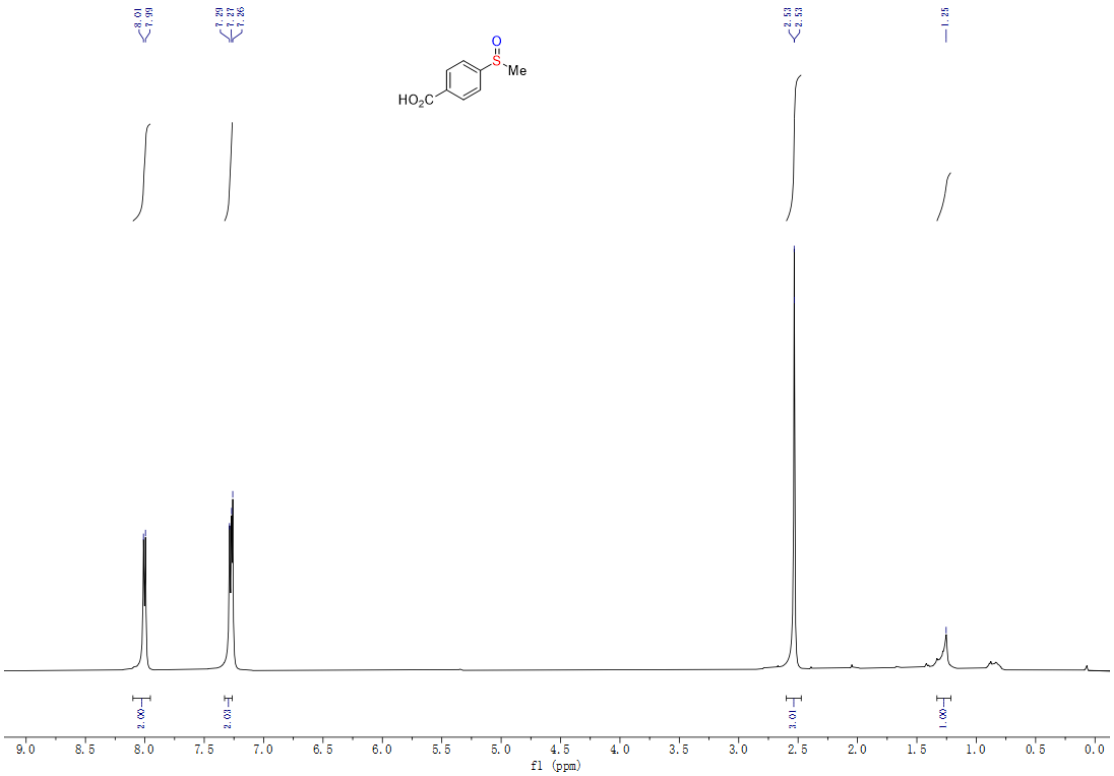
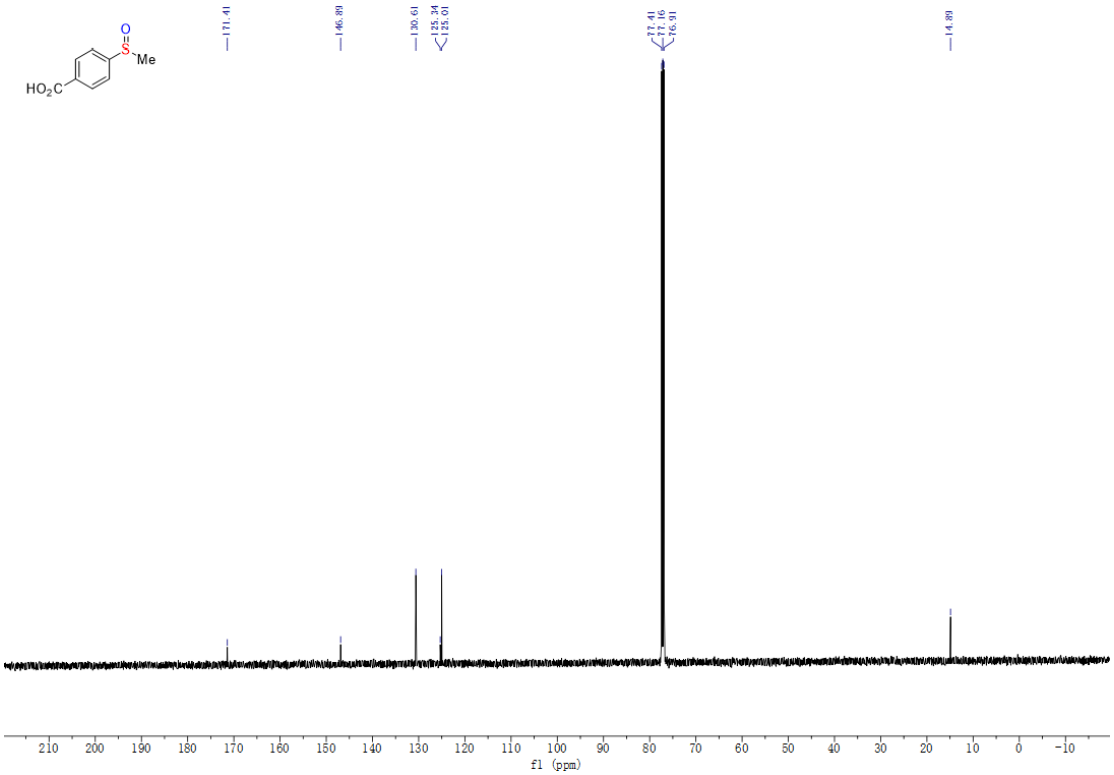


^{1}H NMR of compound **2i**



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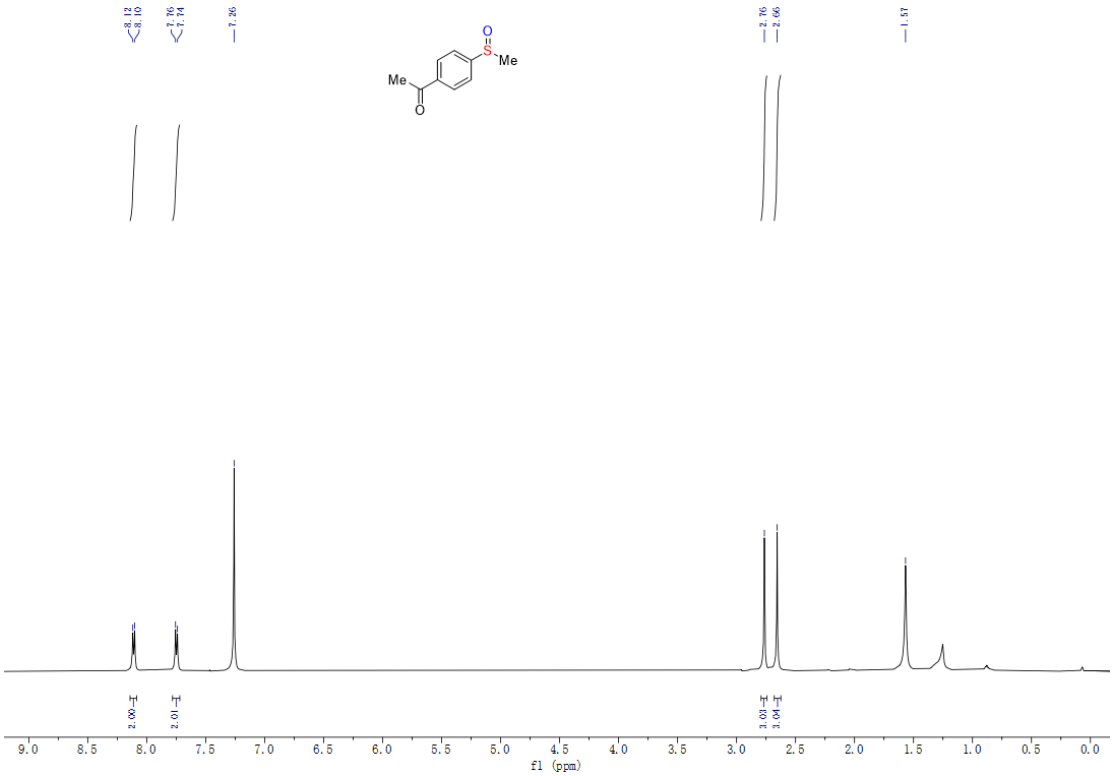

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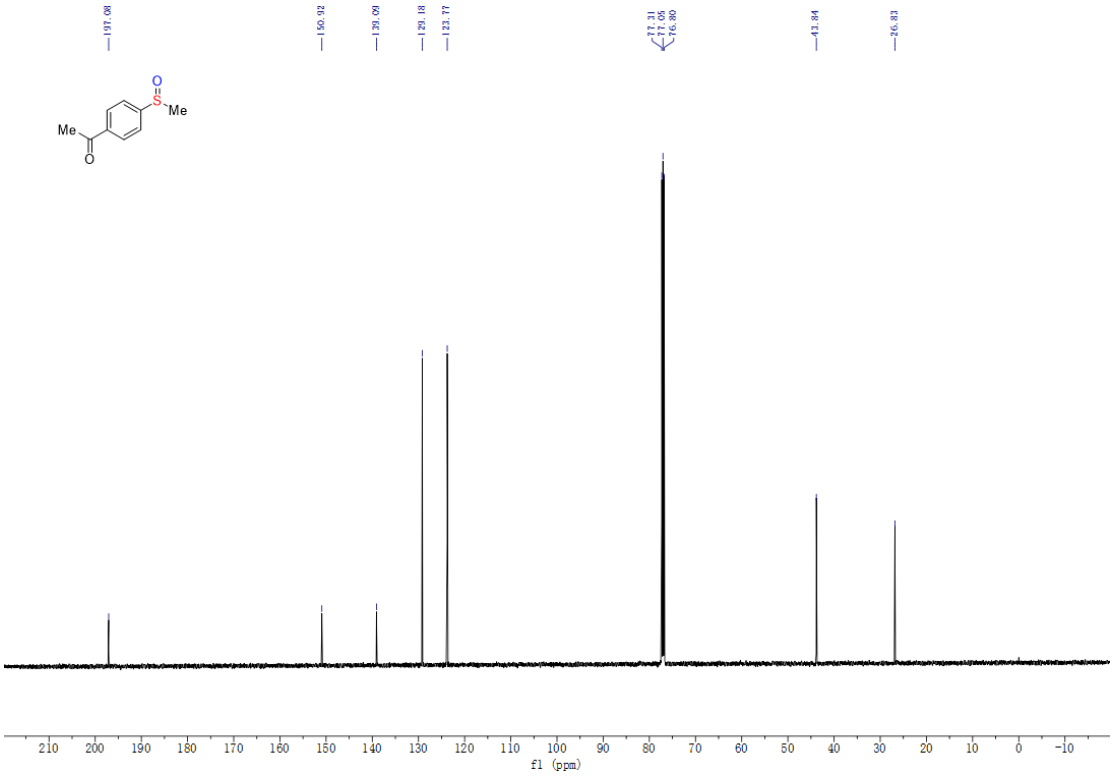

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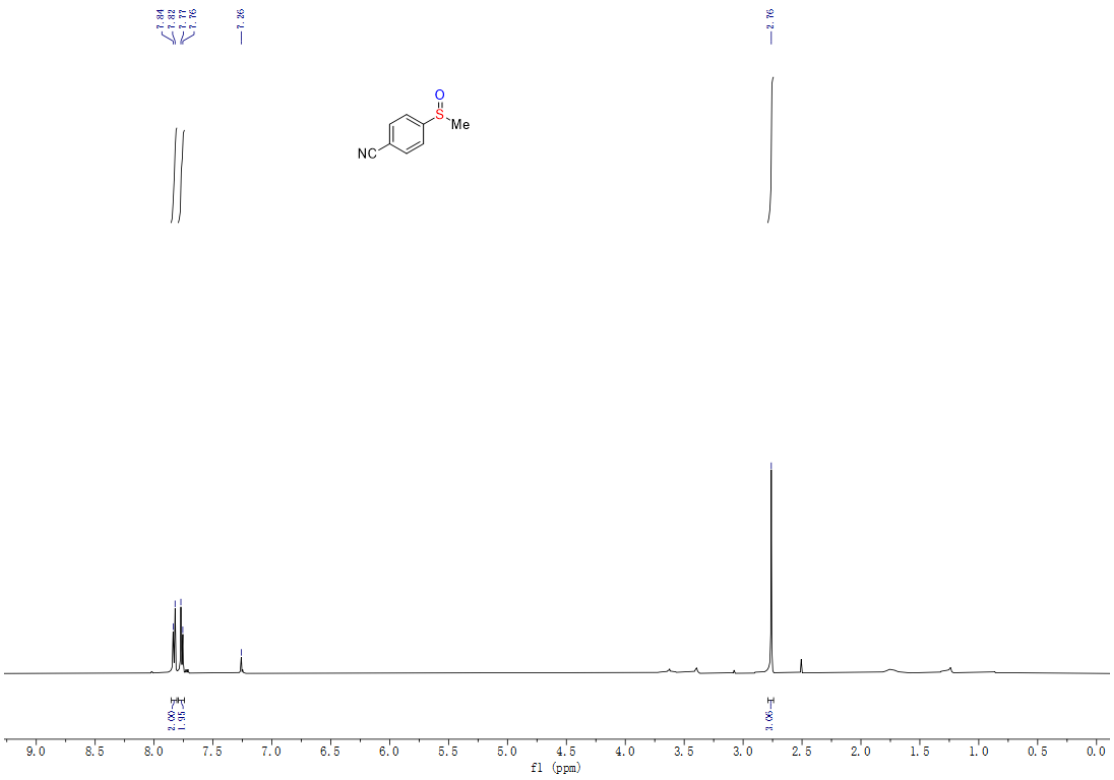

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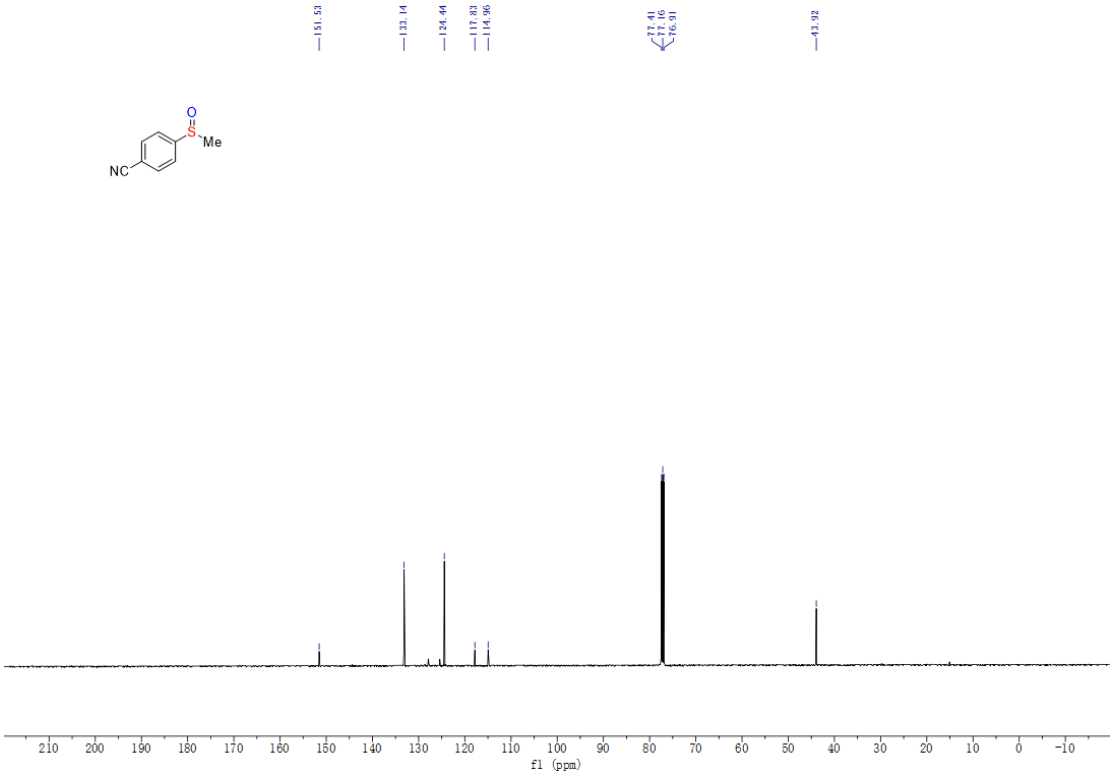

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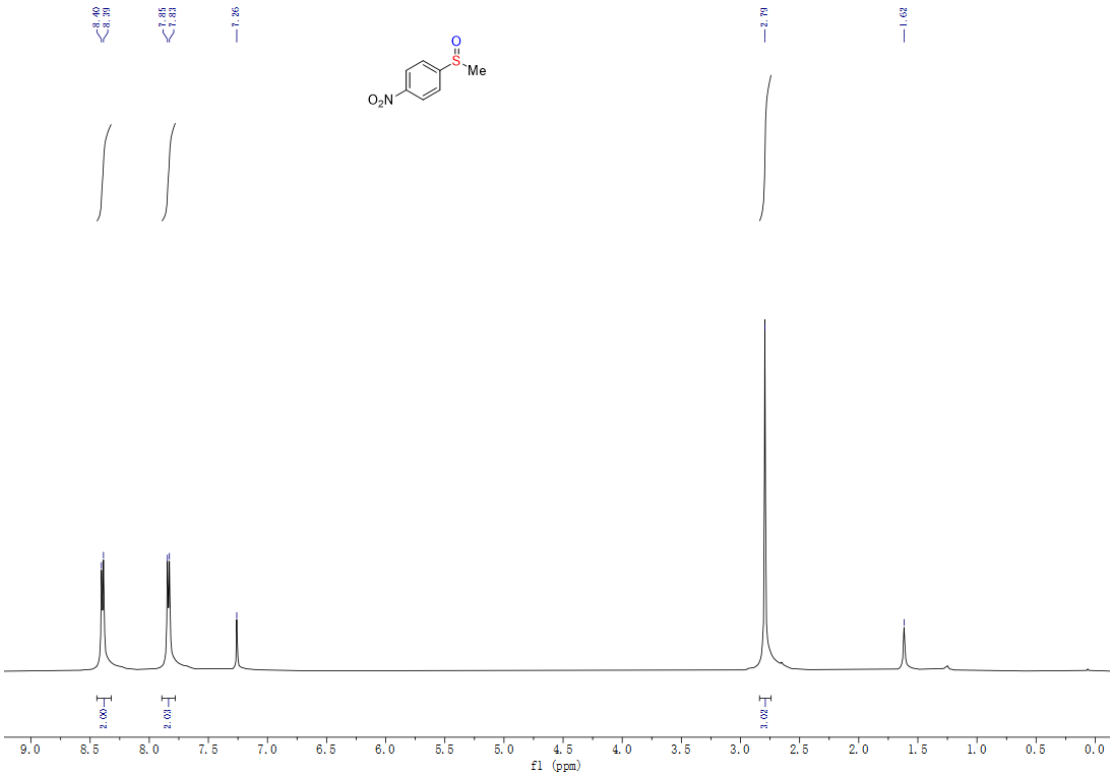

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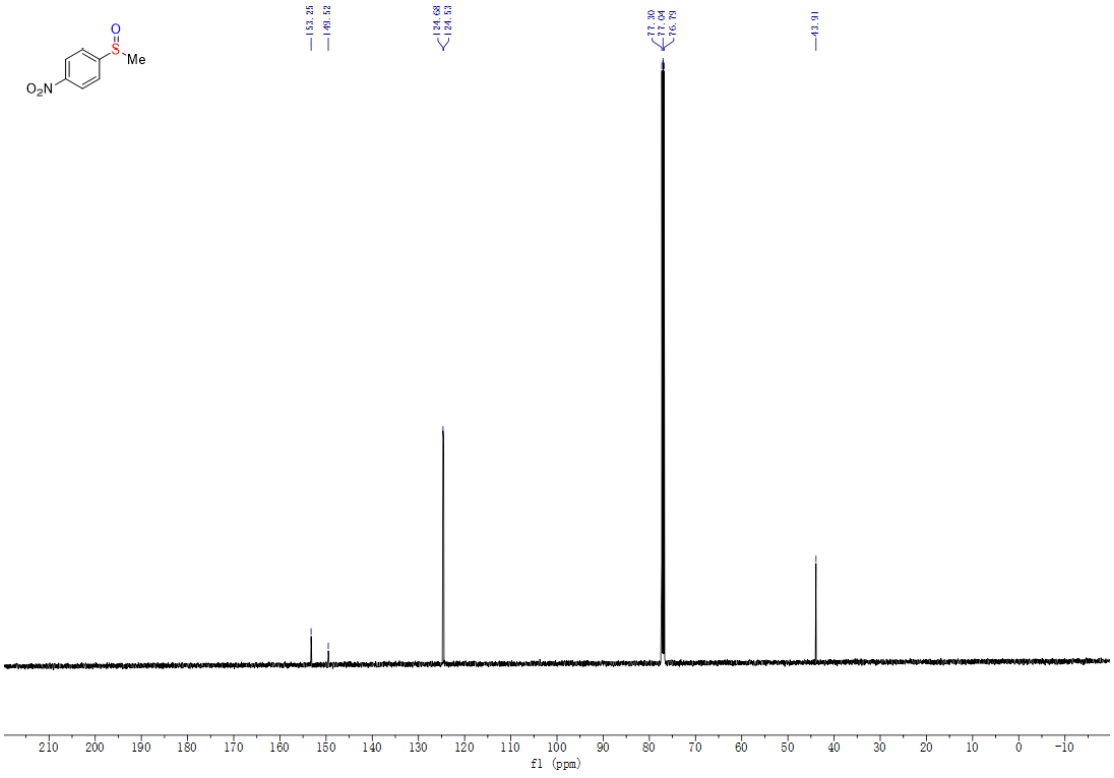

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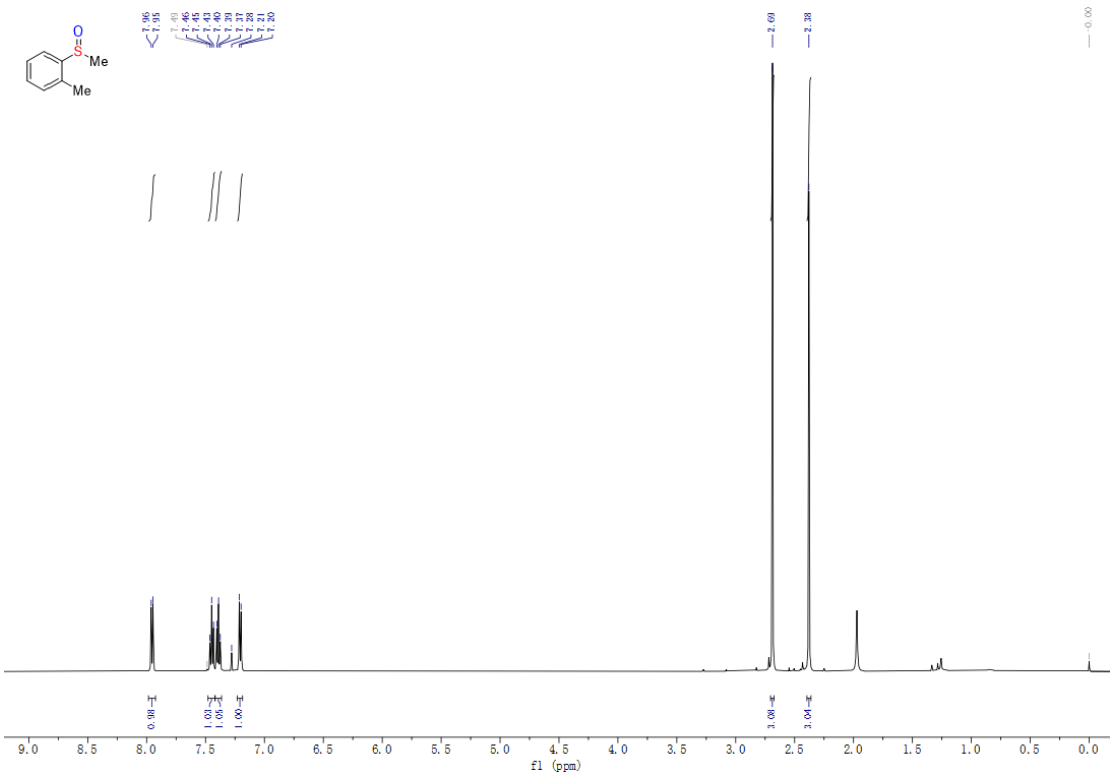

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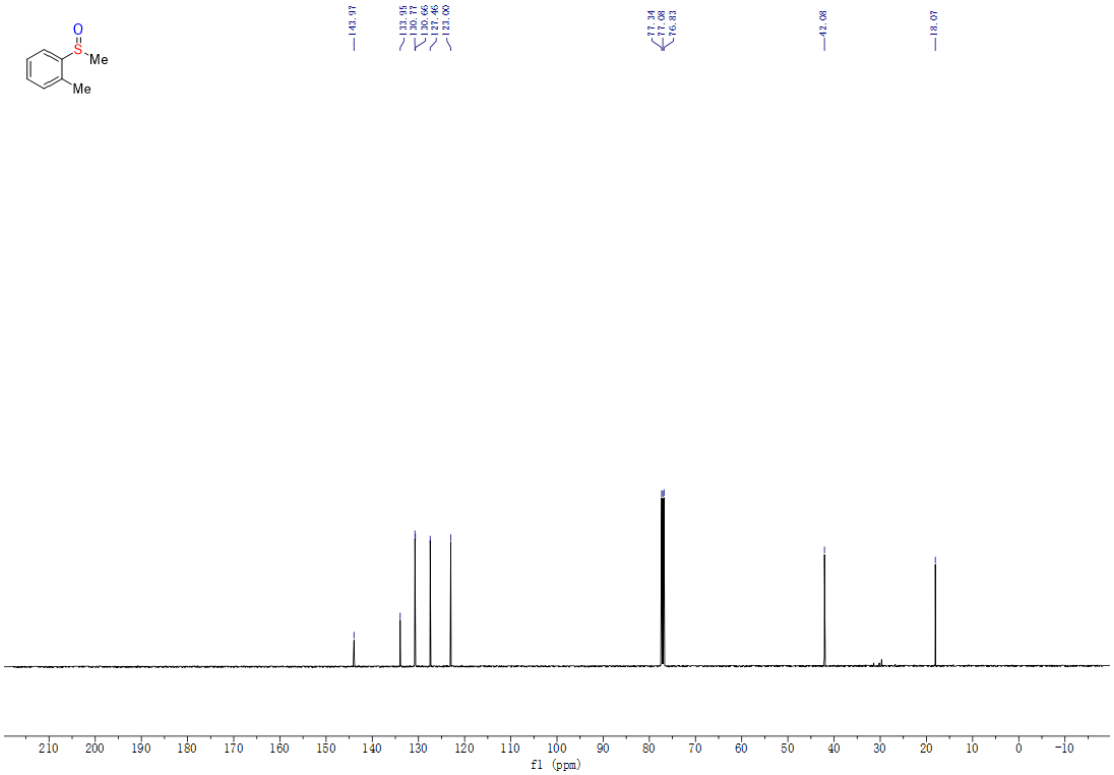

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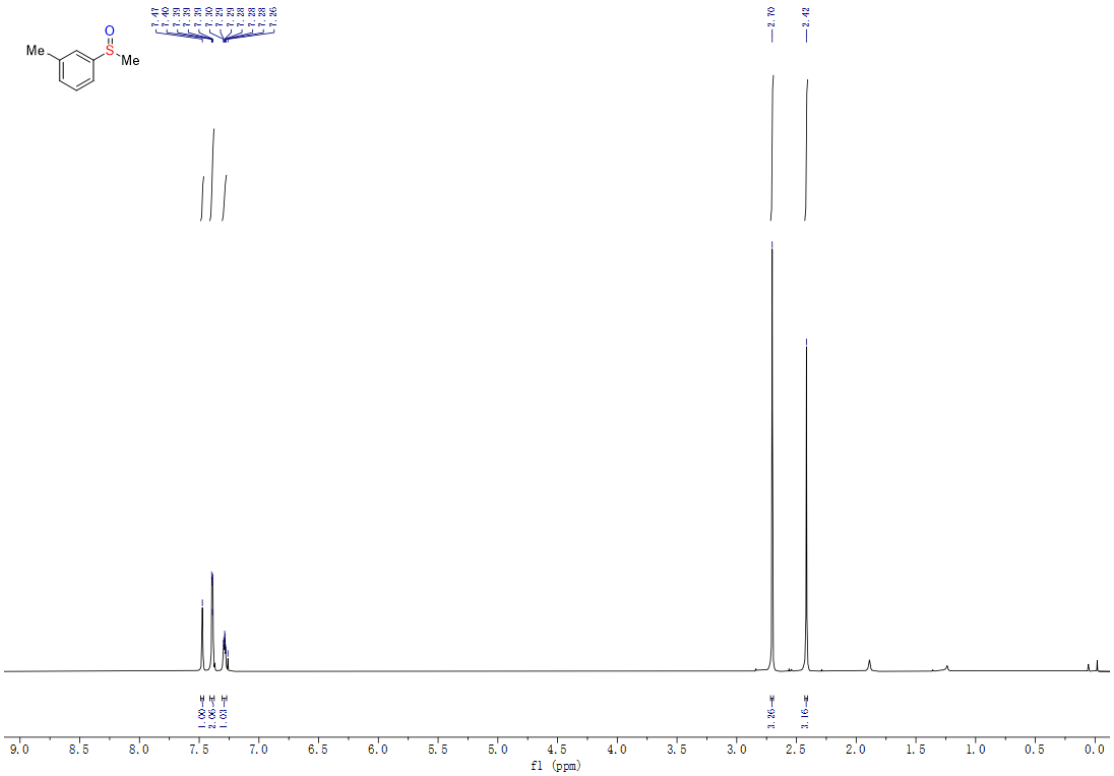

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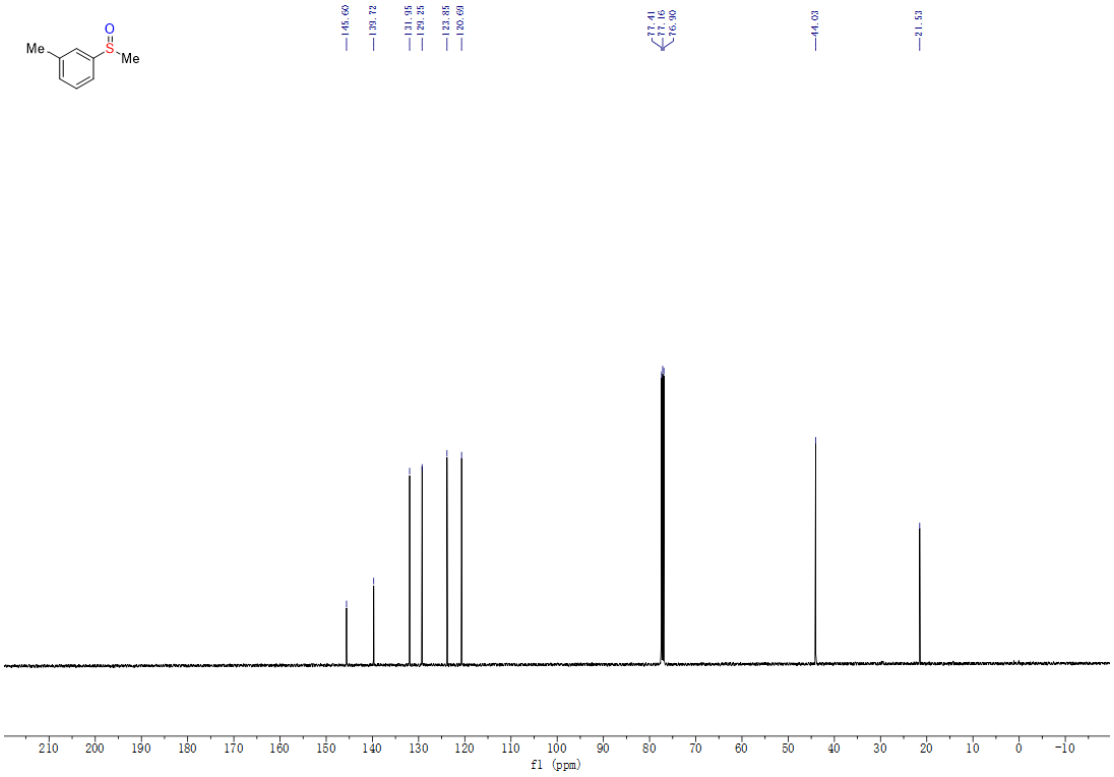

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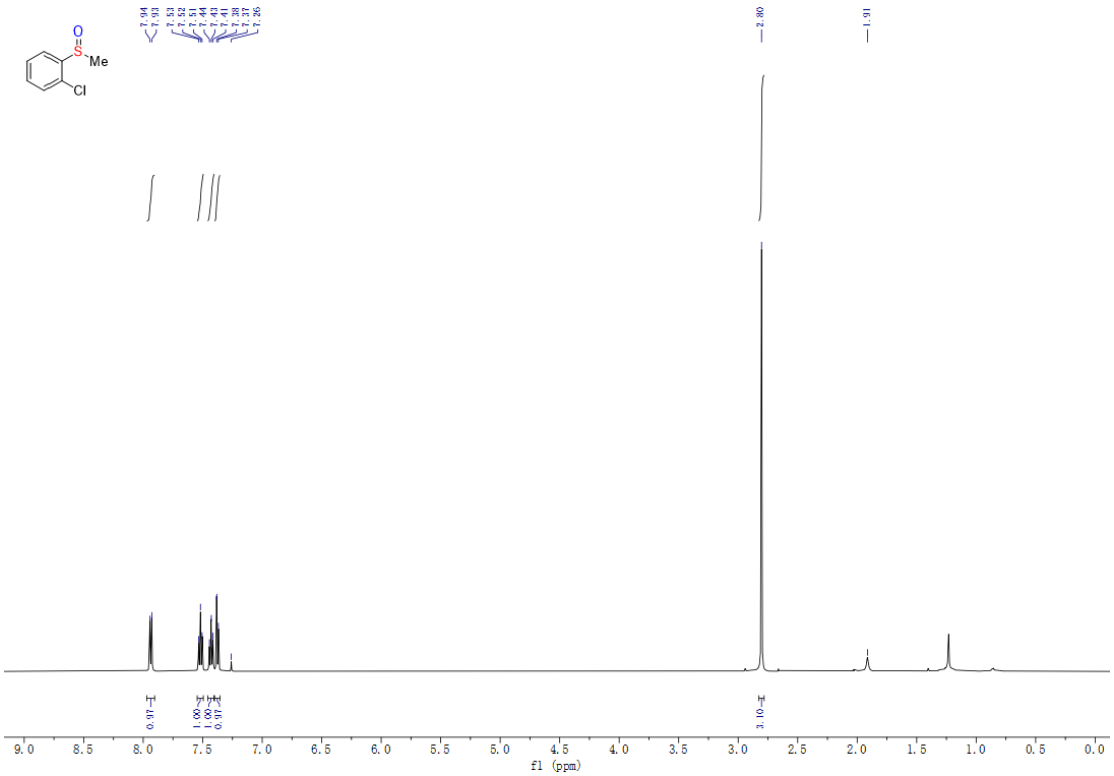

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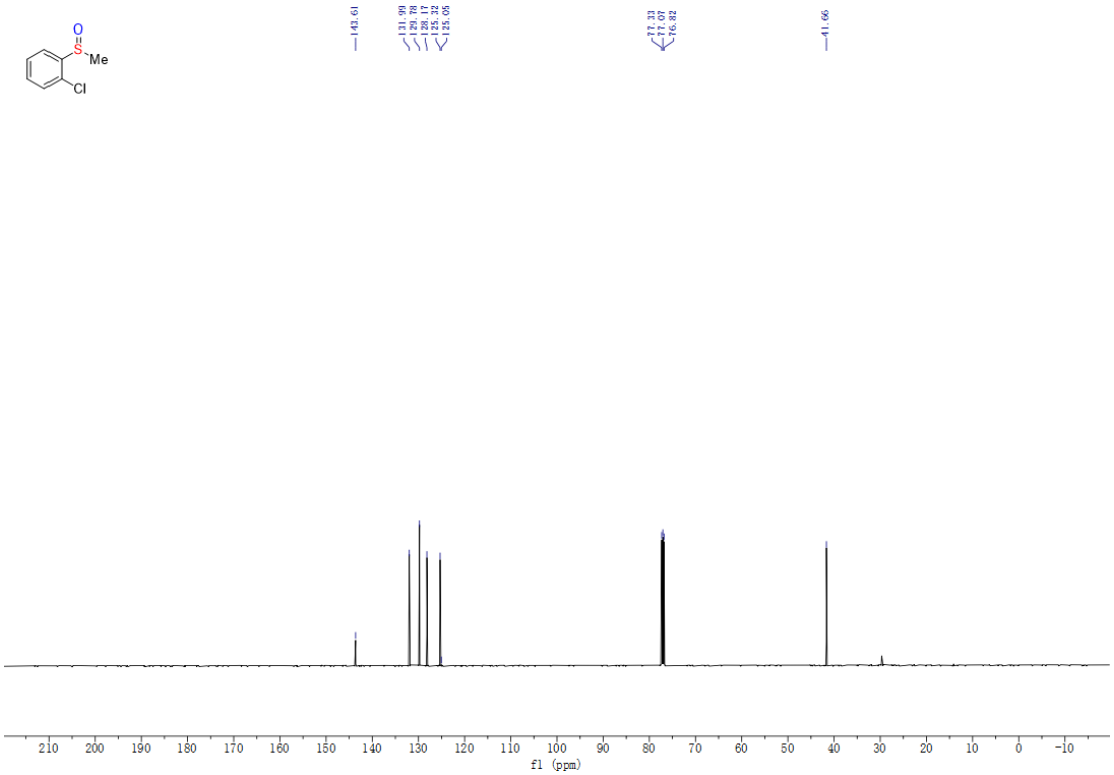

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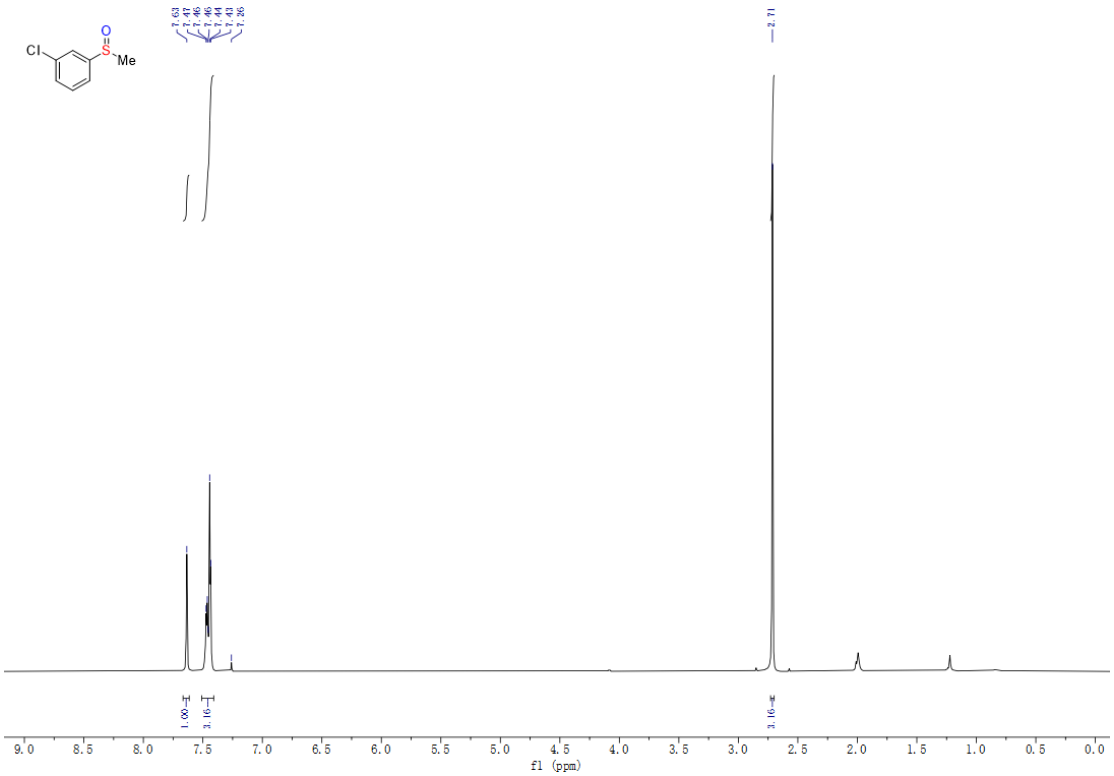

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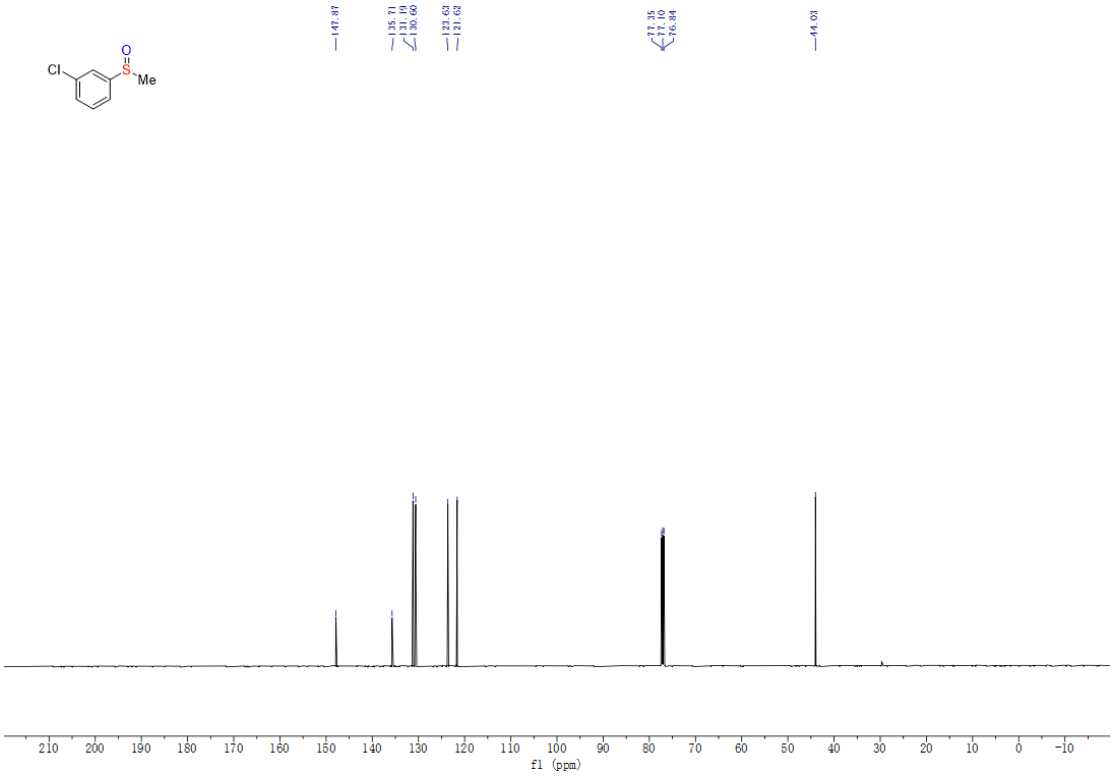

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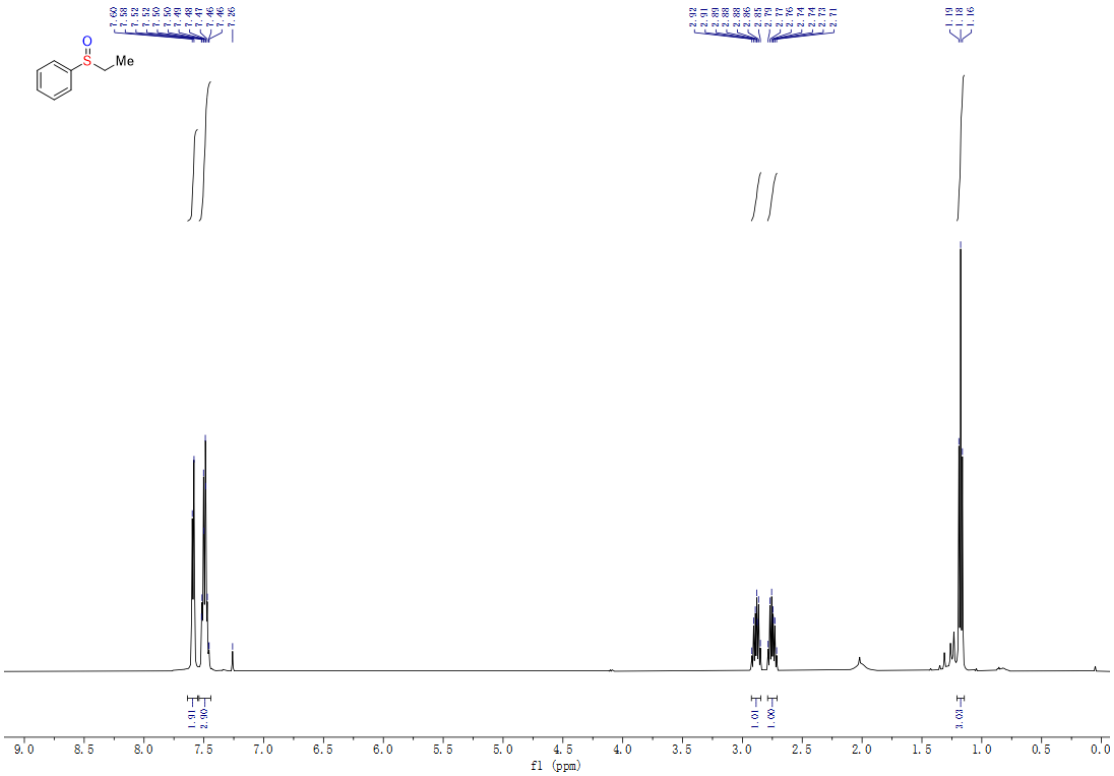

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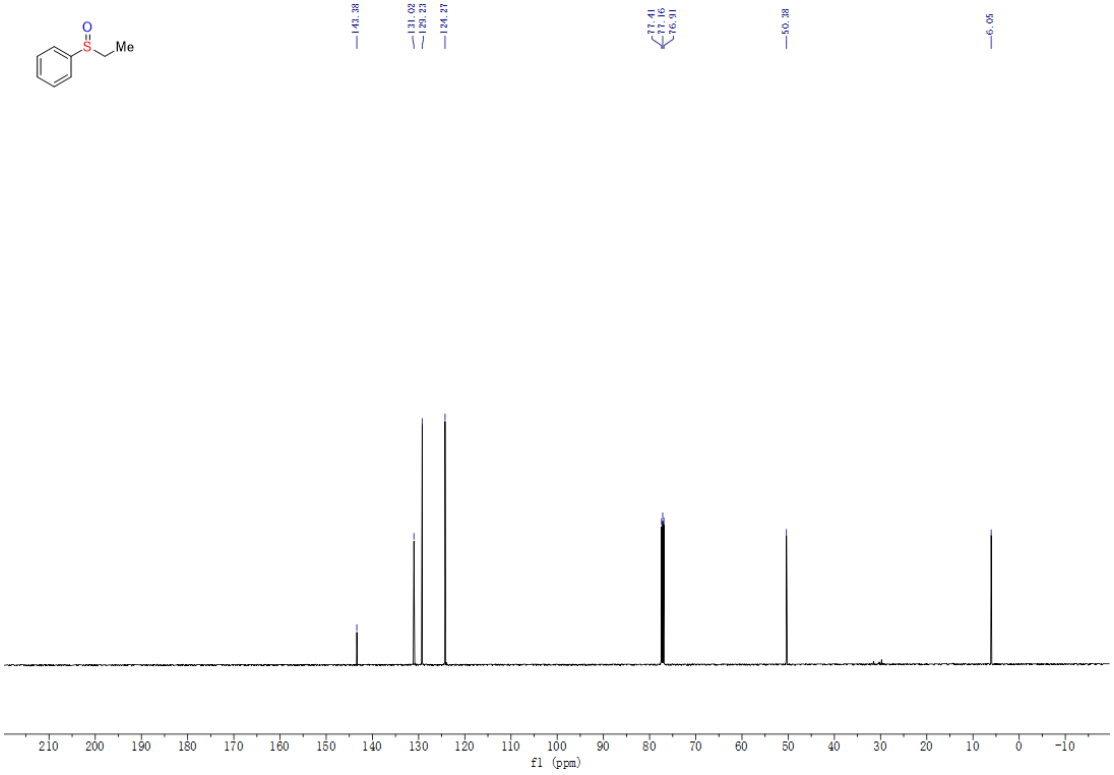

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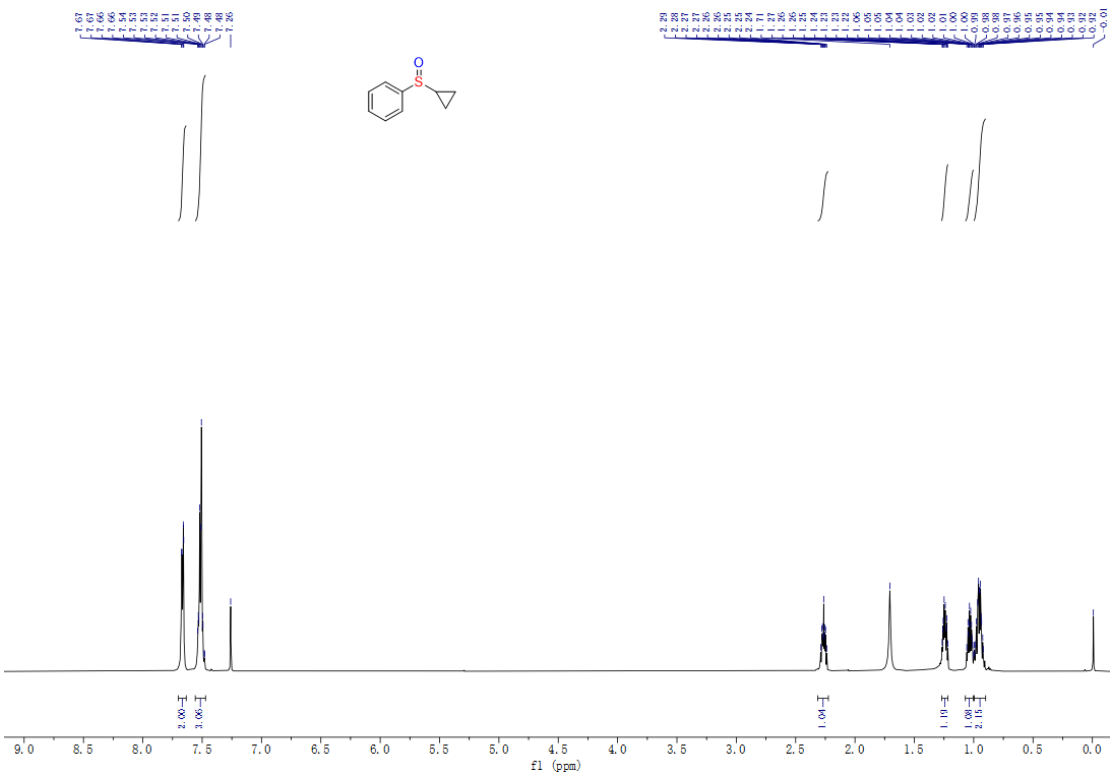

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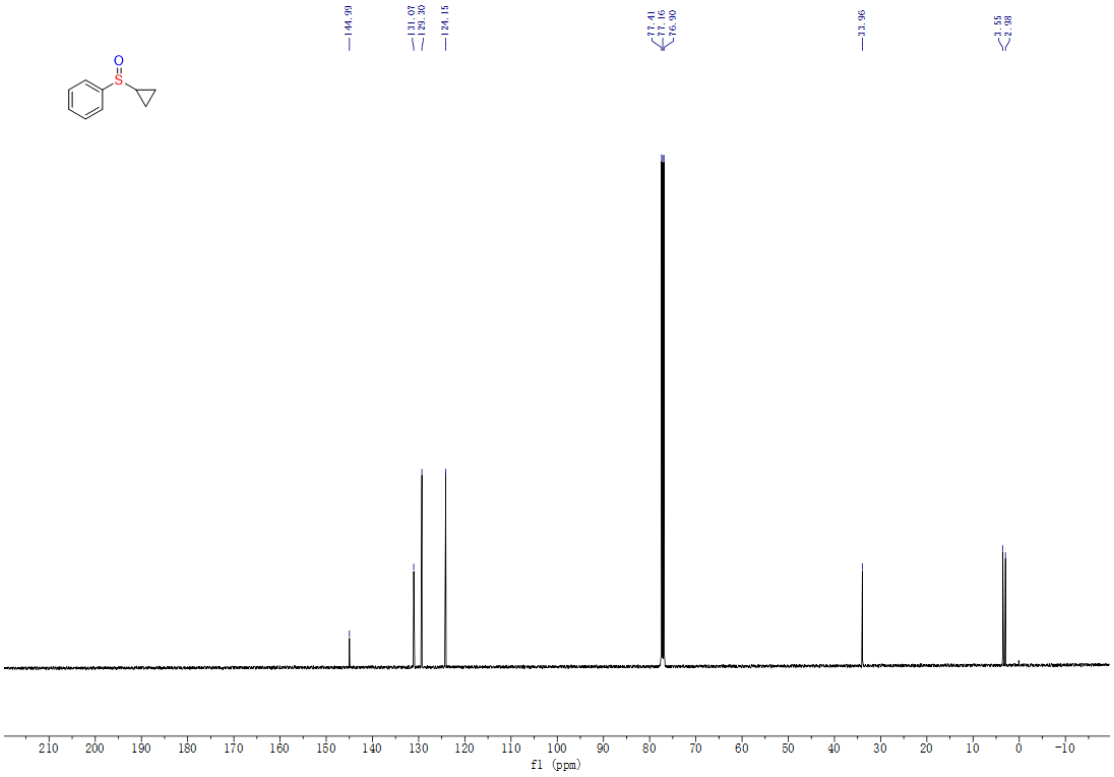

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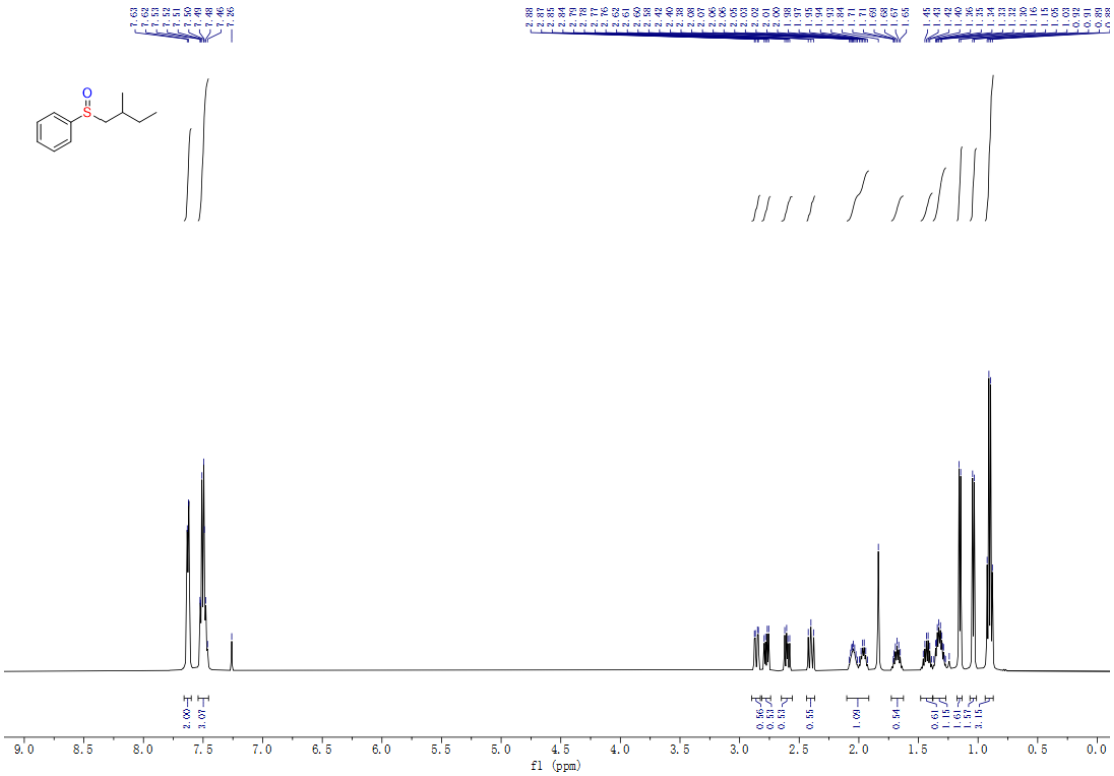

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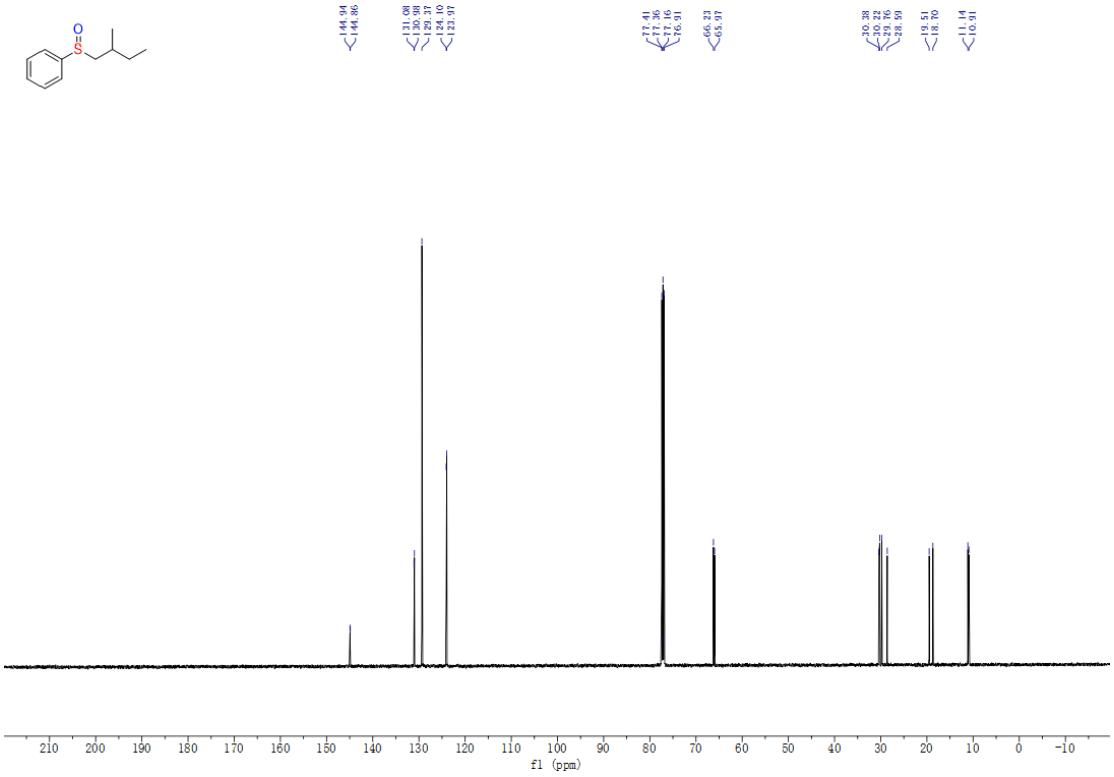

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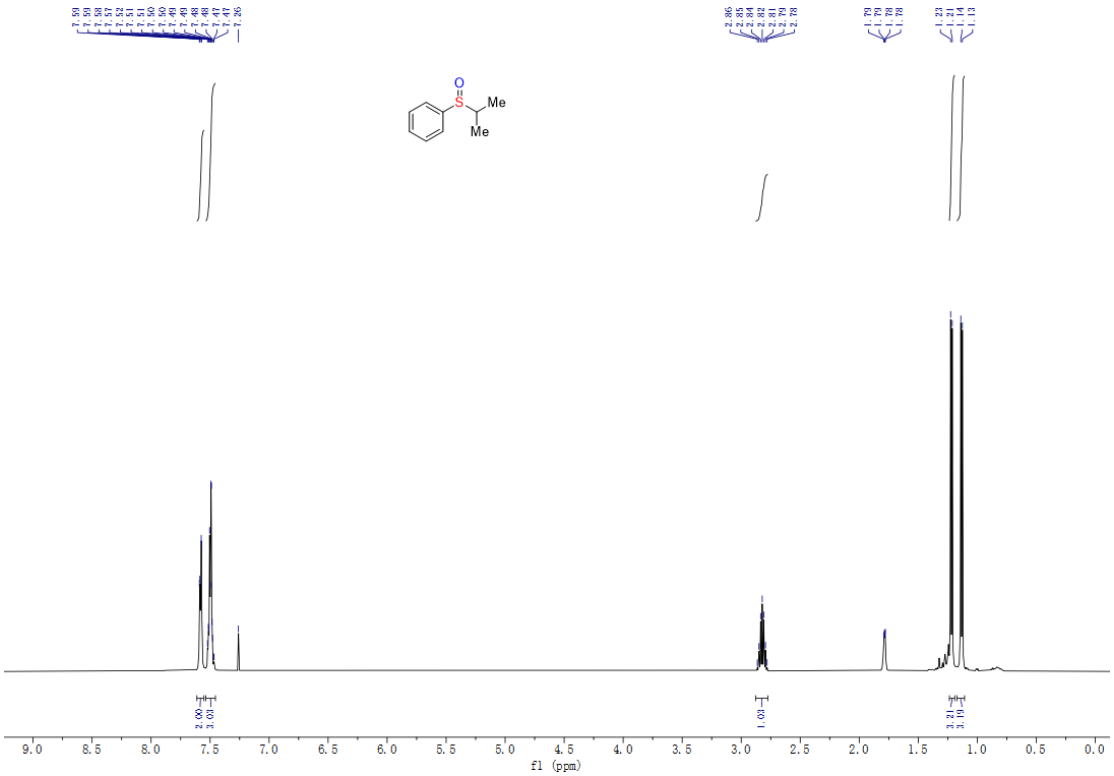

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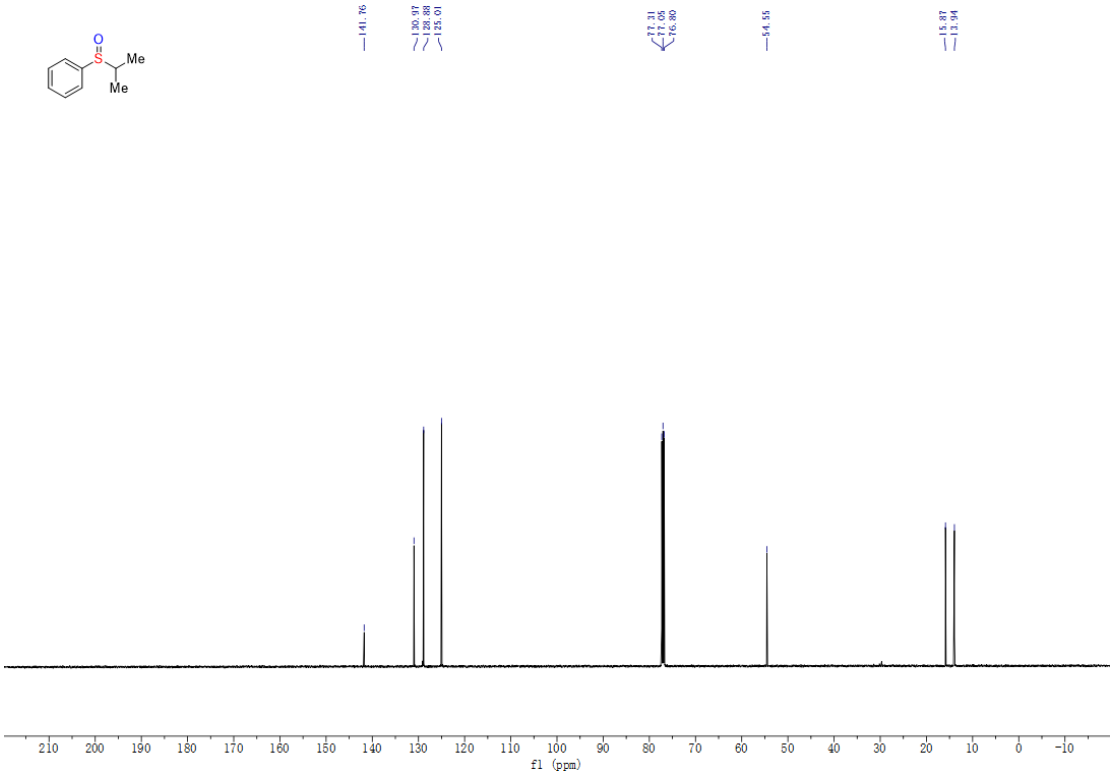

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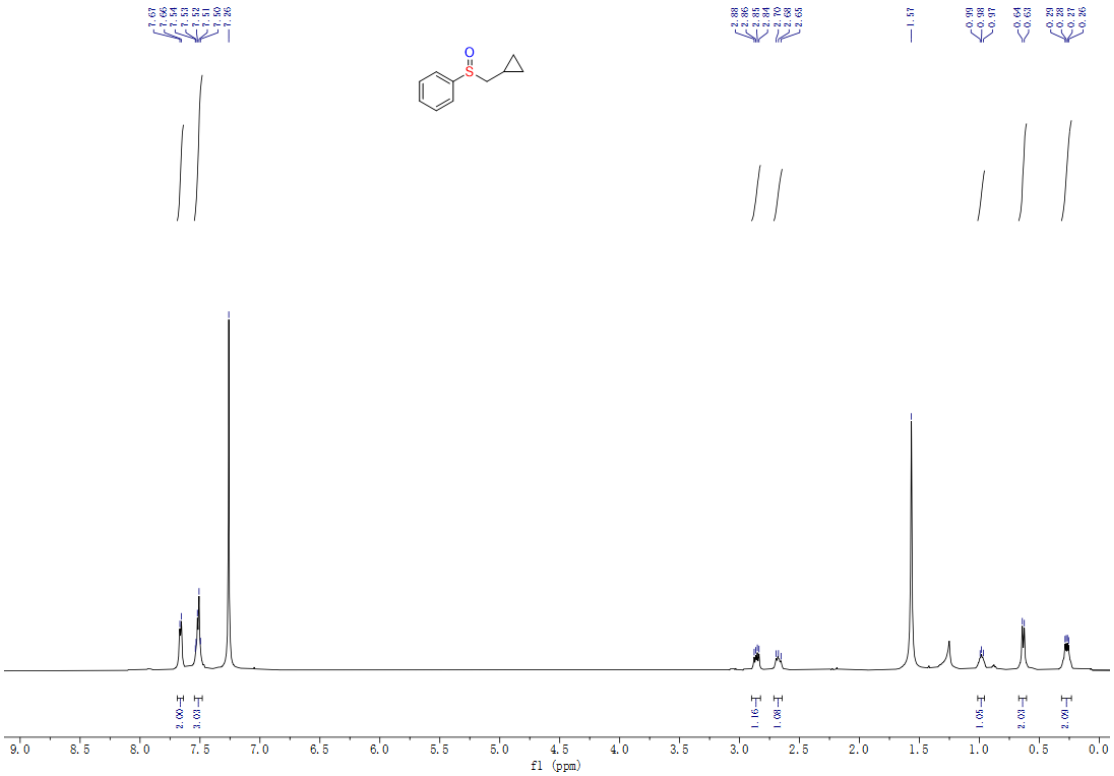
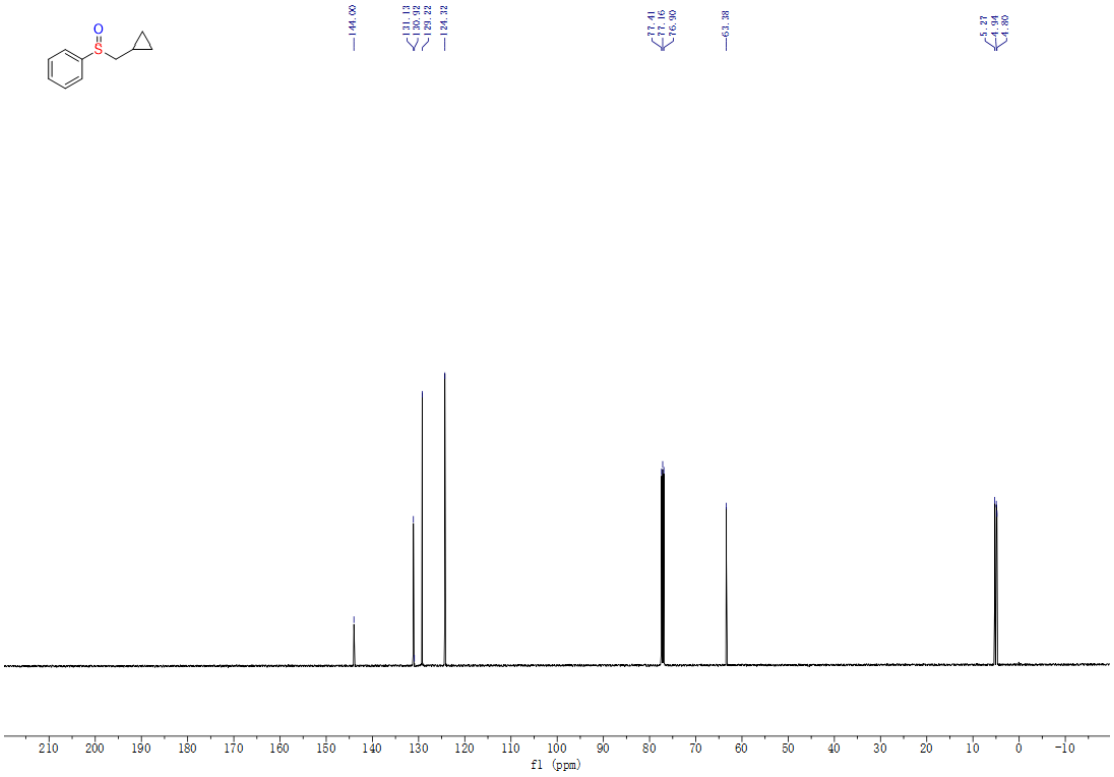
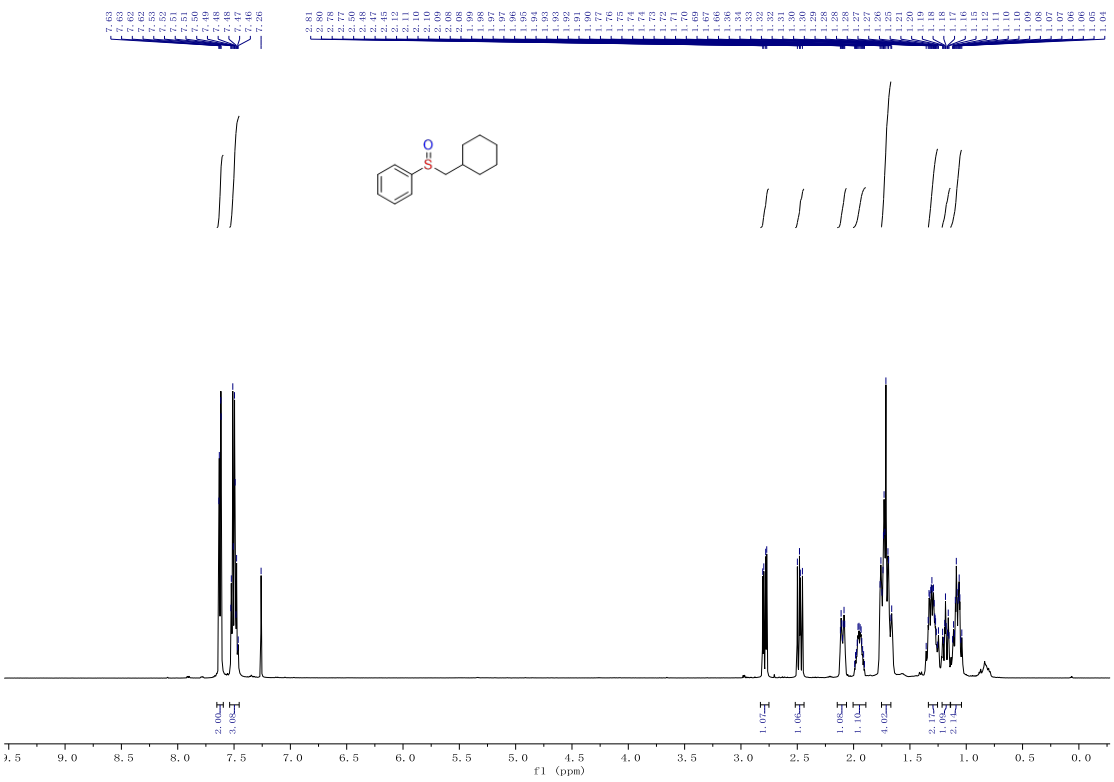


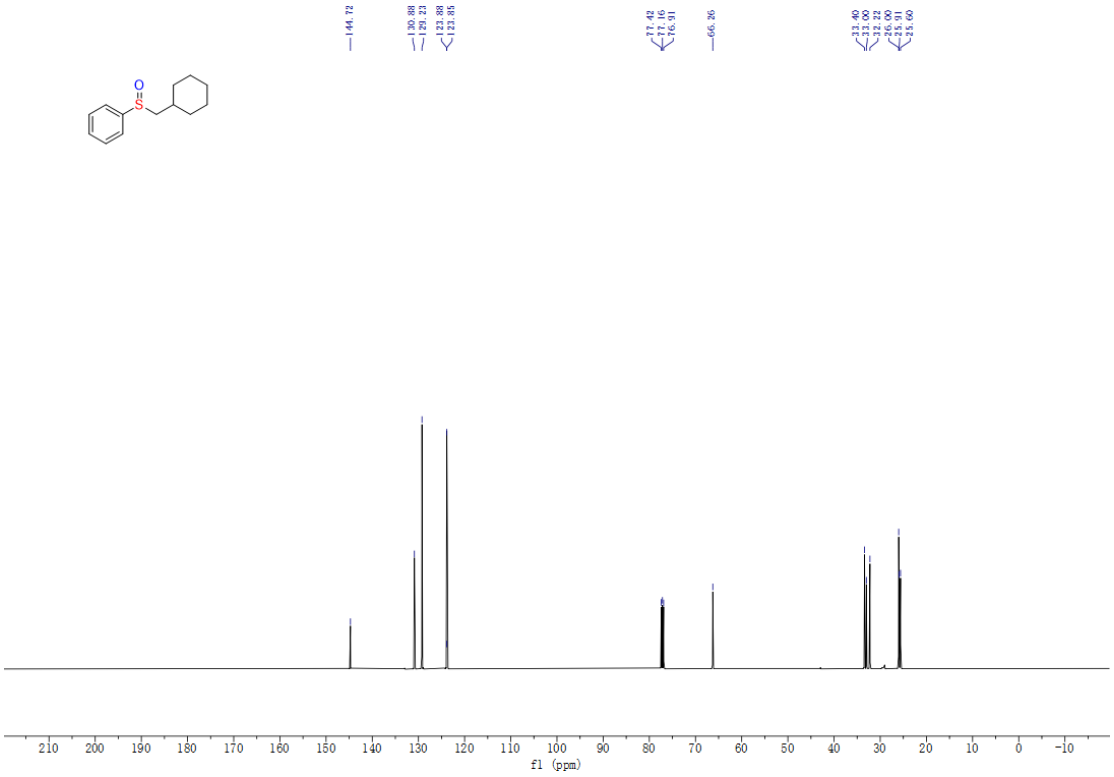
^{1}H NMR of compound **2u**



^{13}C NMR of compound **2u**



^{1}H NMR of compound **2v**



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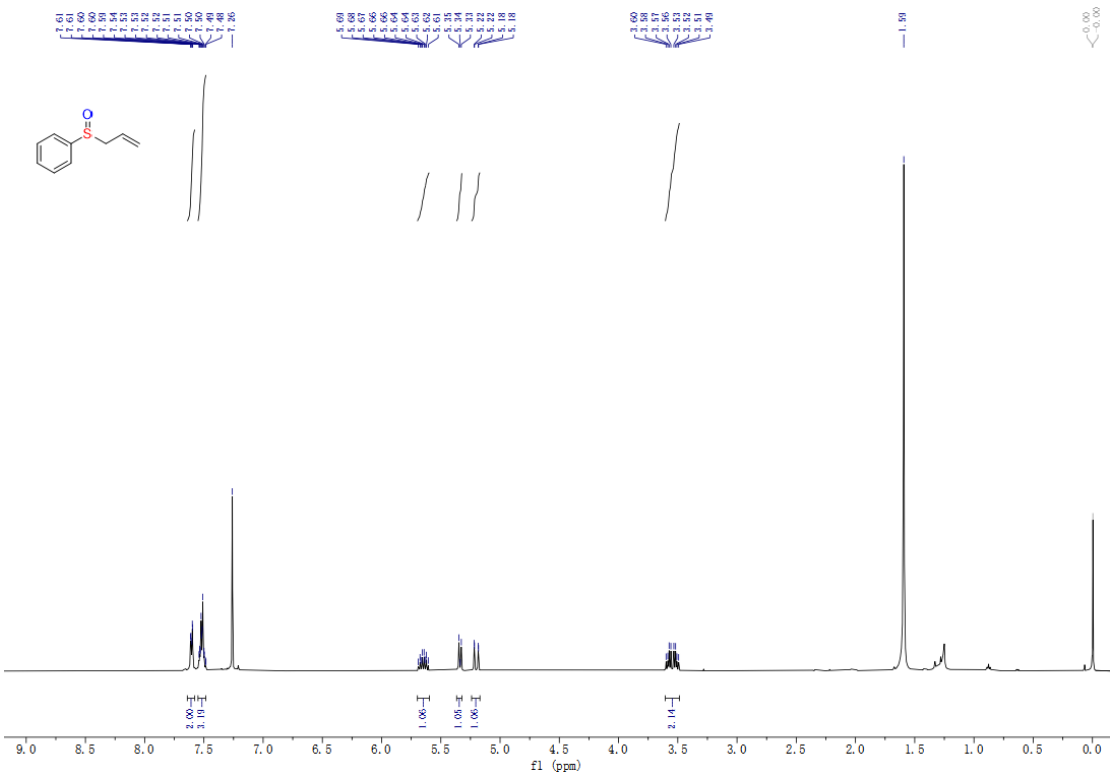
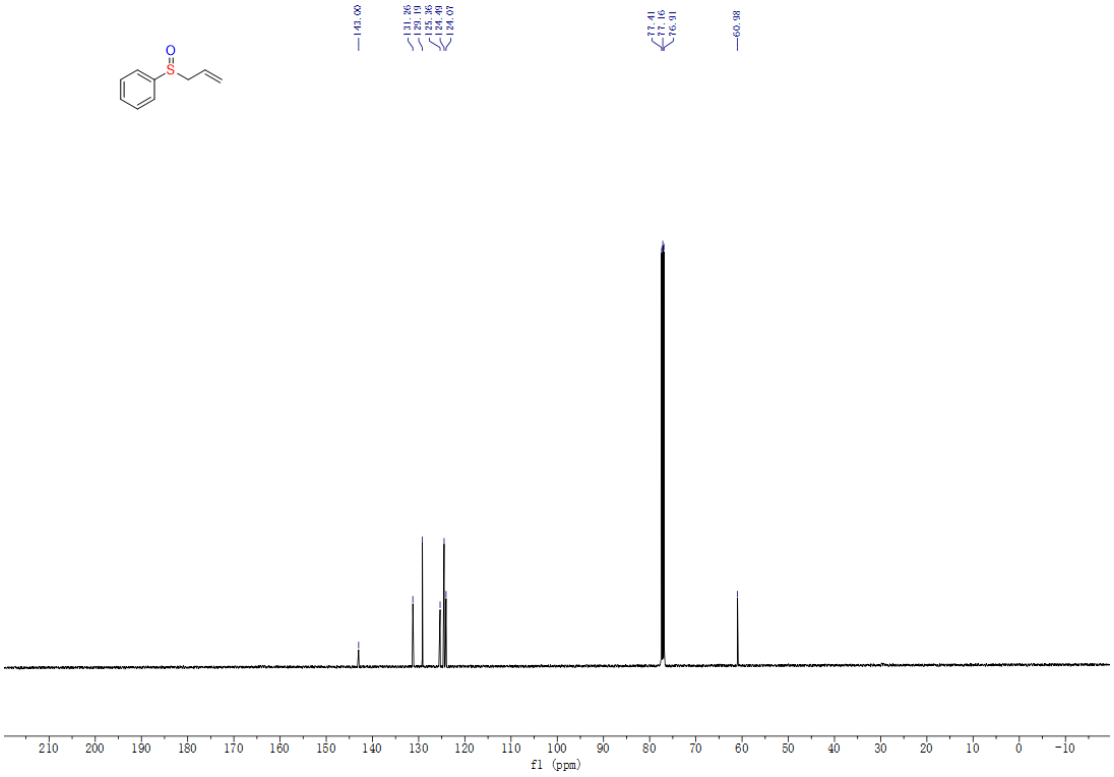
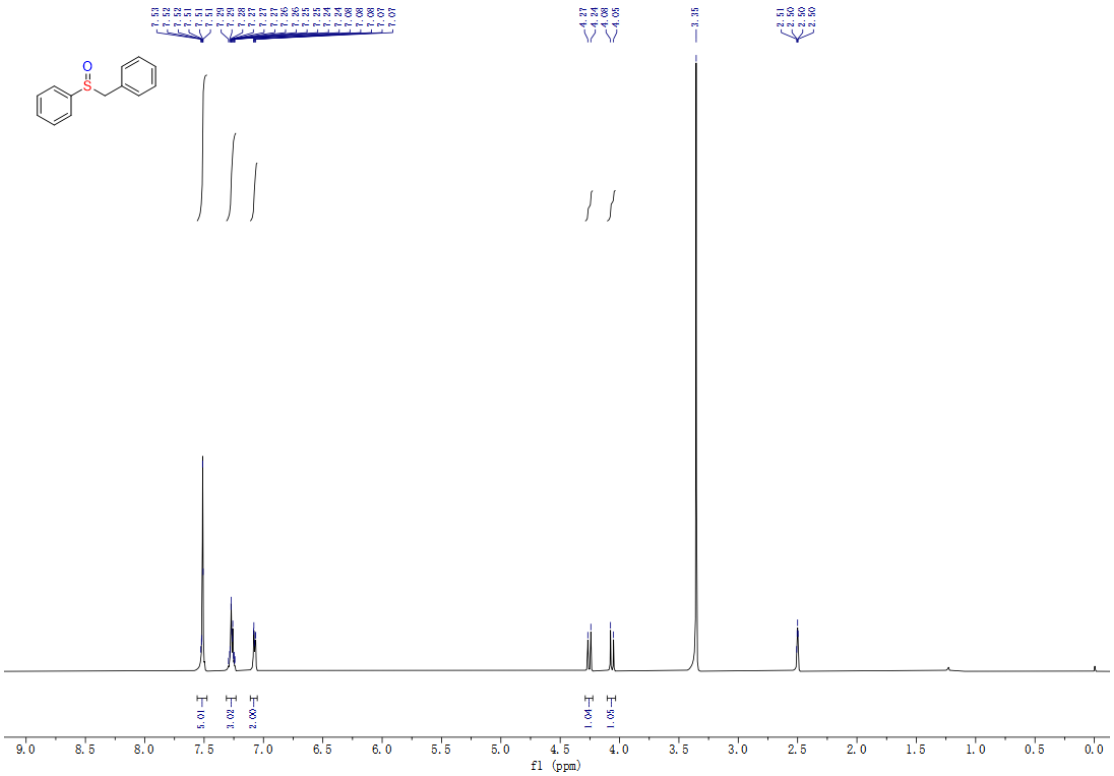


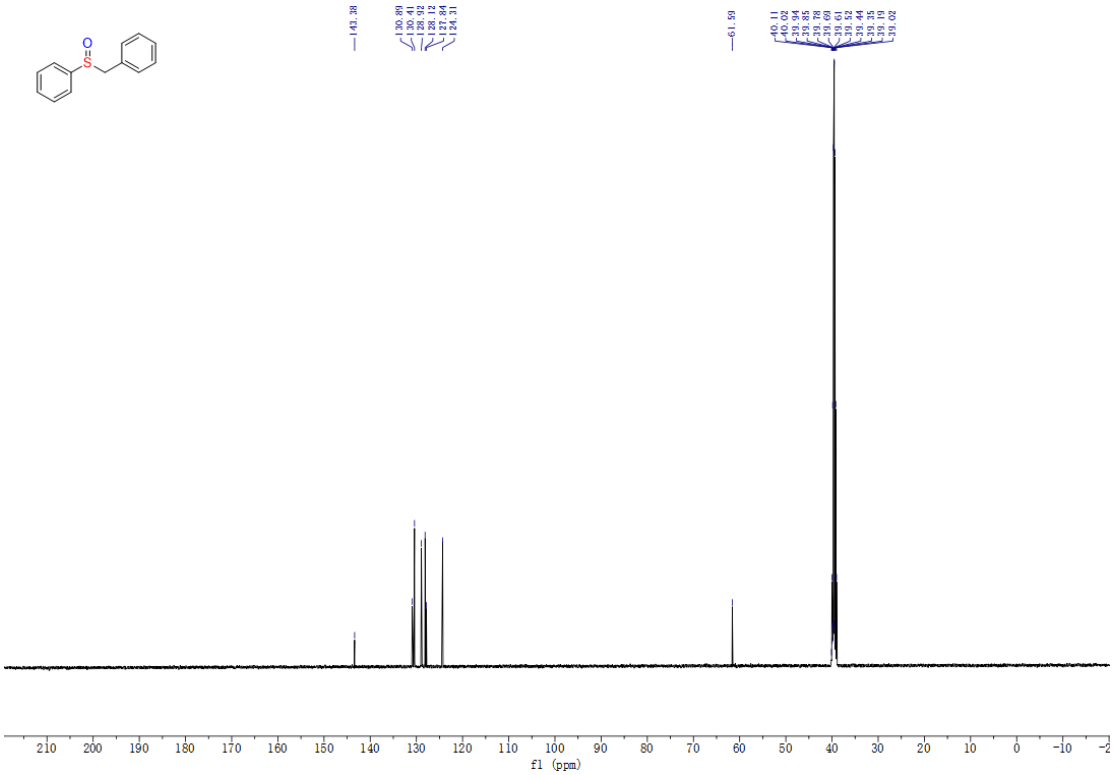
^{1}H NMR of compound **2w**



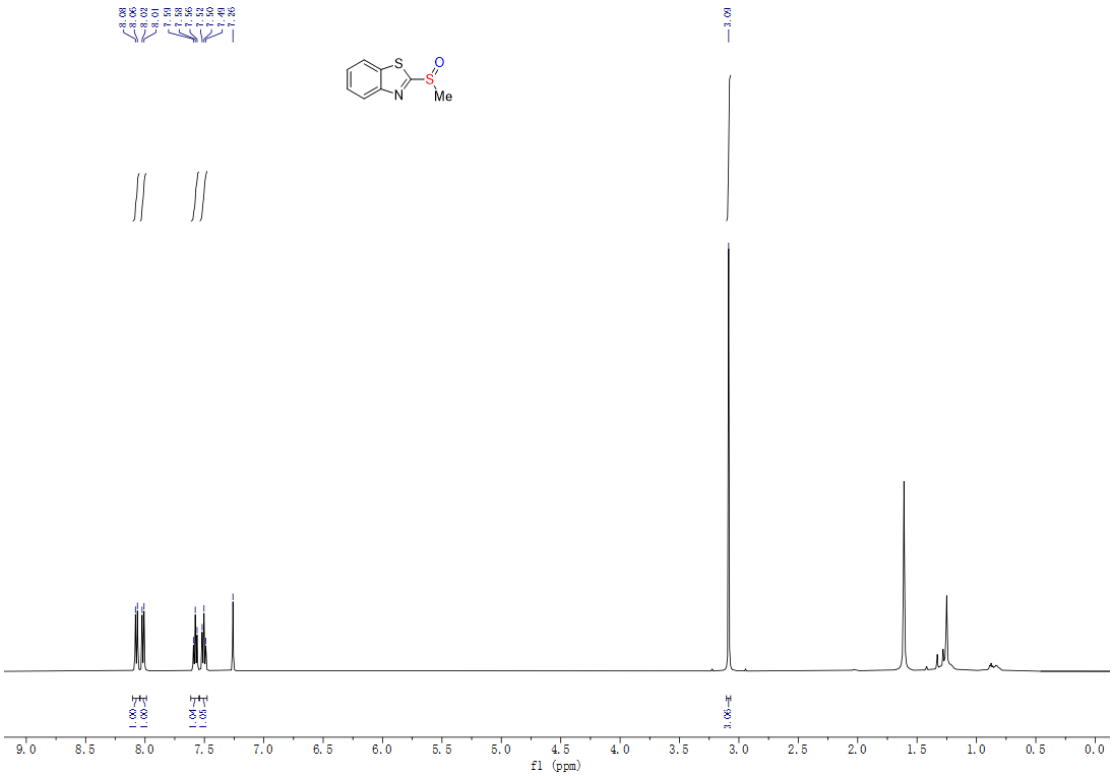
^{13}C NMR of compound **2w**



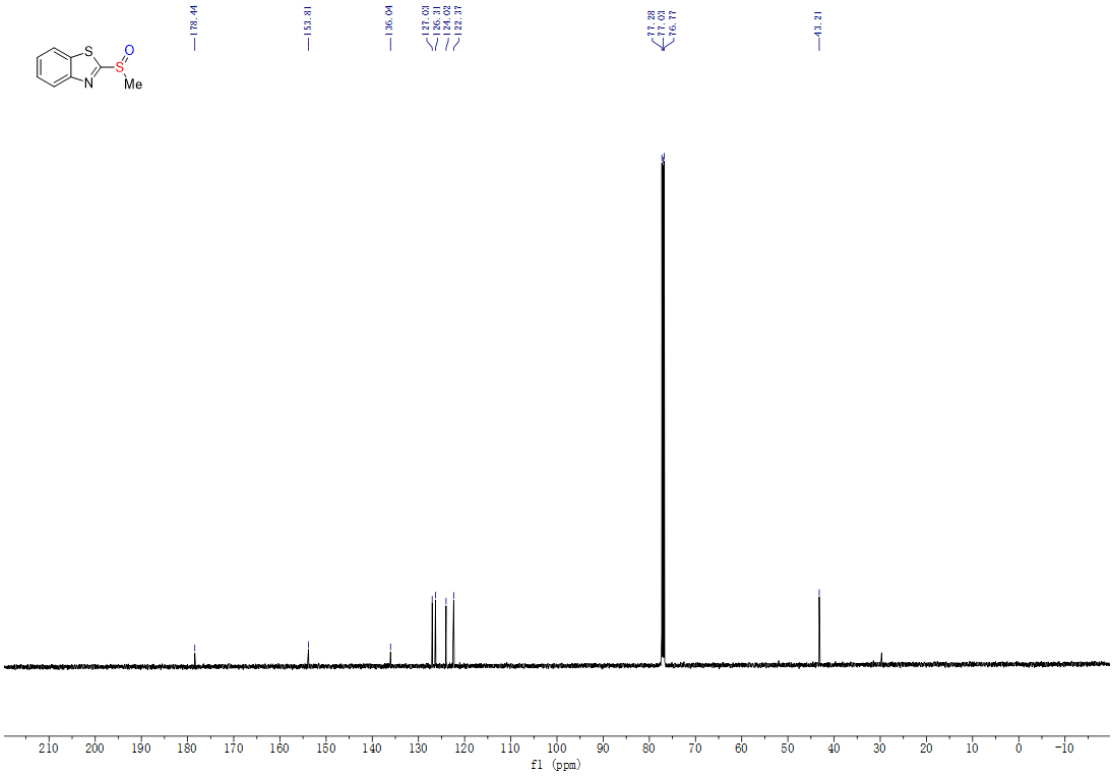
^{1}H NMR of compound **2x**



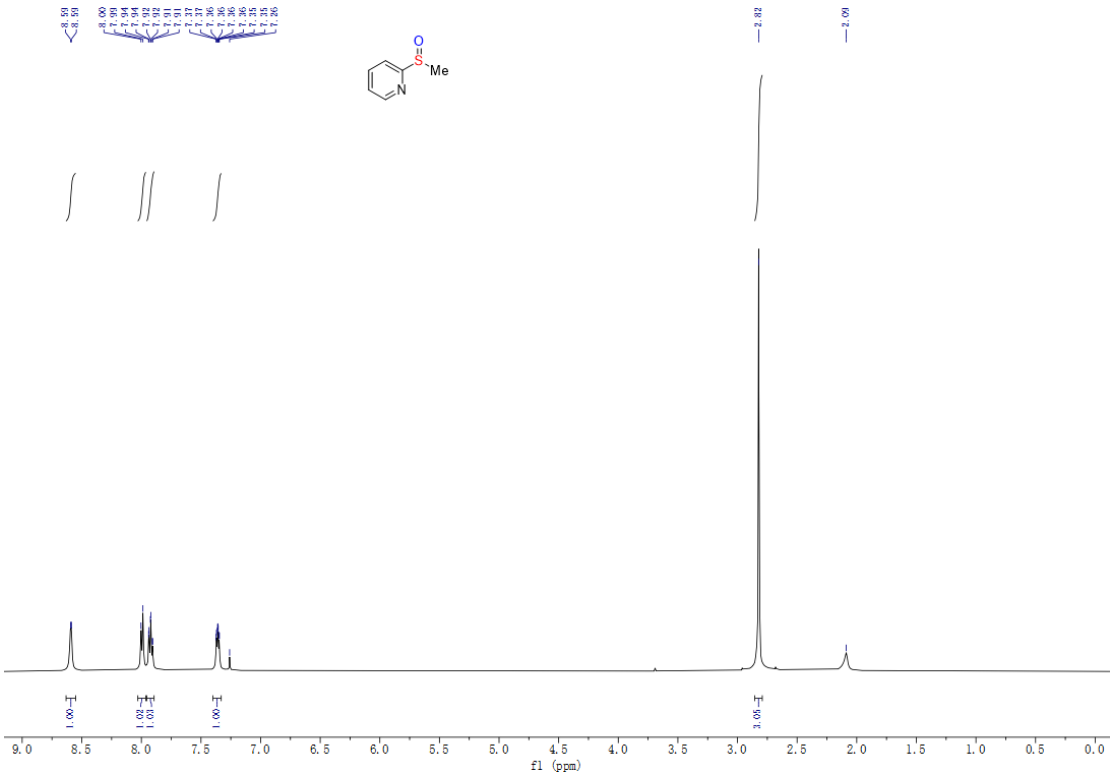
^{13}C NMR of compound **2x**



^{1}H NMR of compound **2y**



^{13}C NMR of compound **2y**



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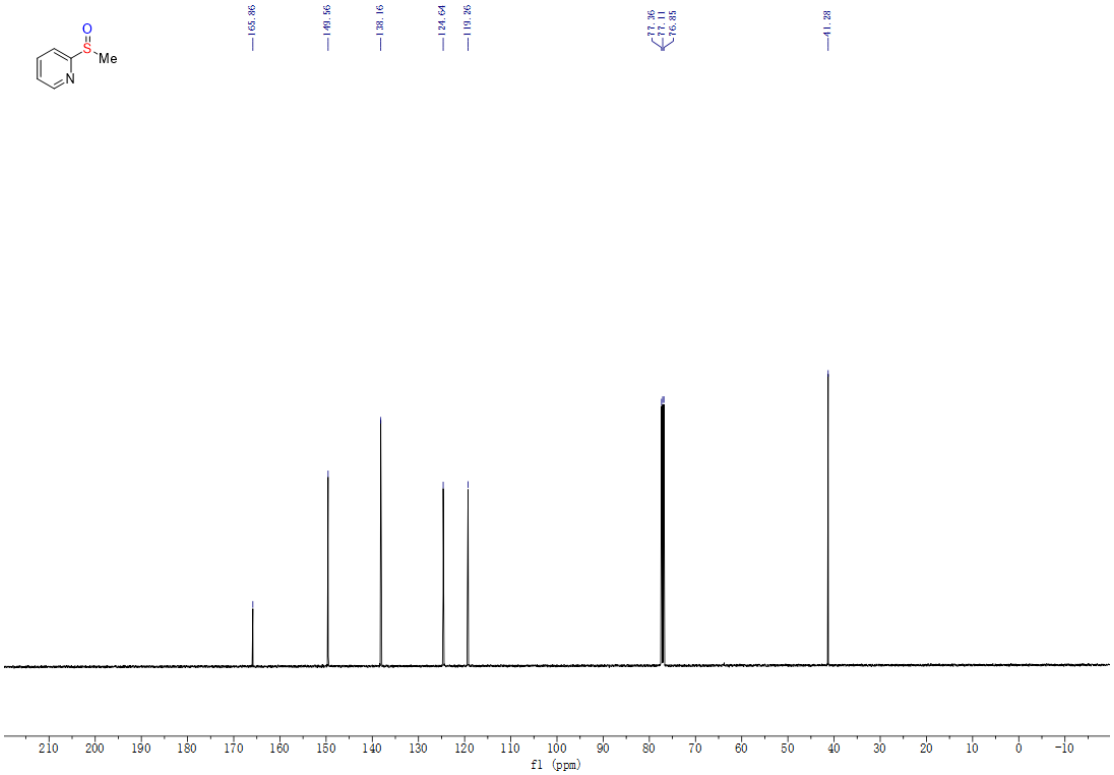
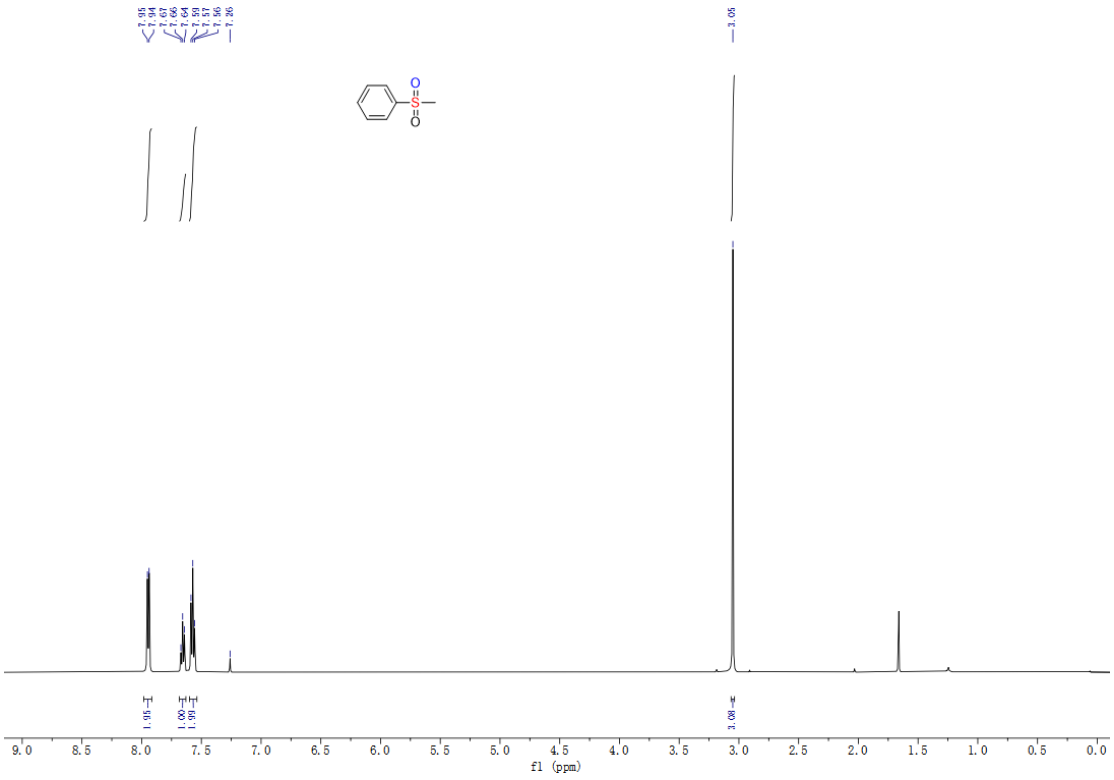
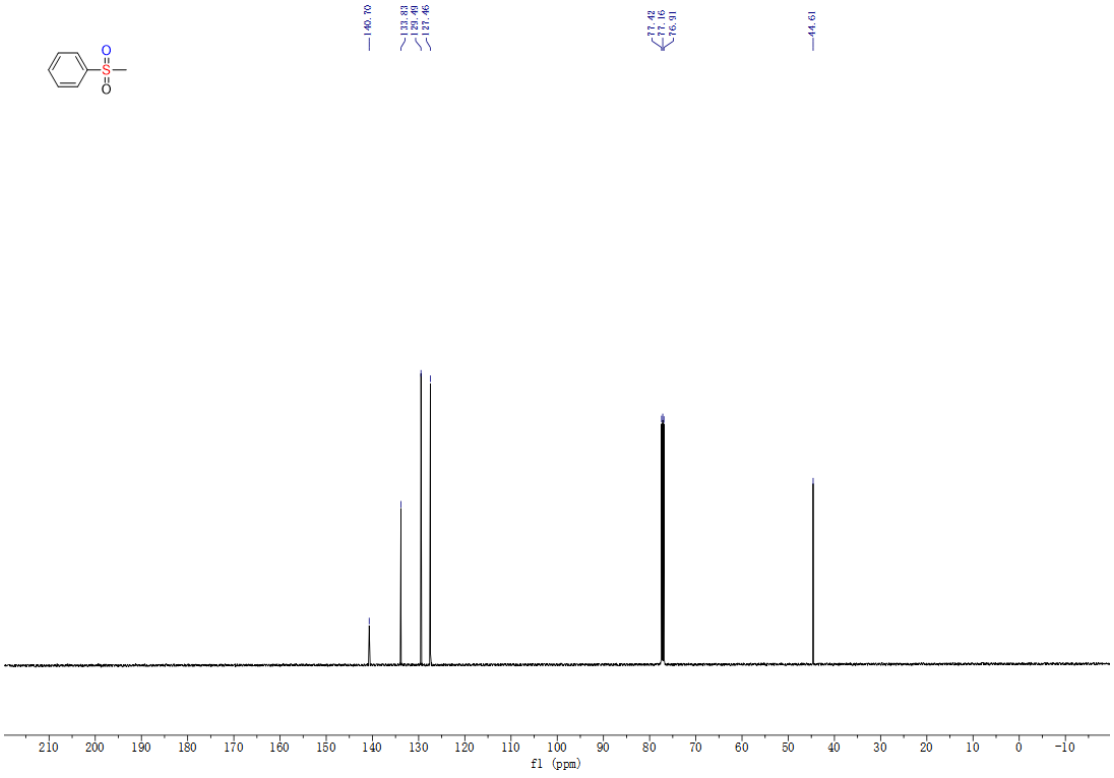


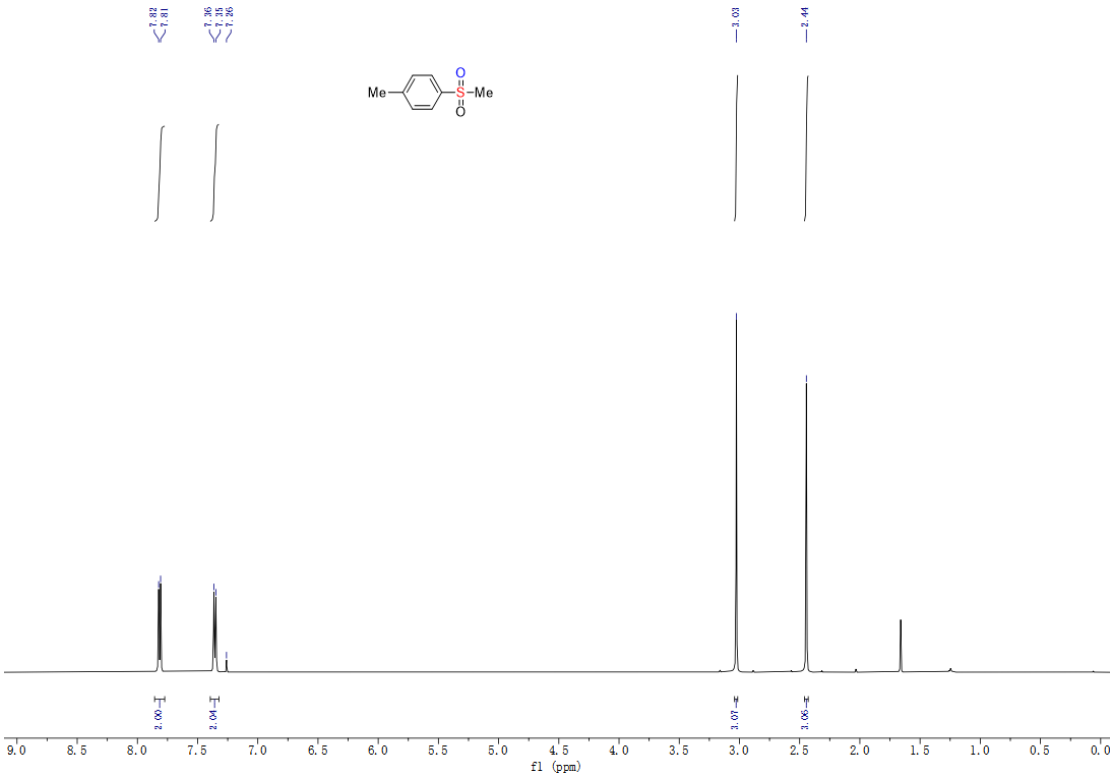
^{13}C NMR of compound **2z**



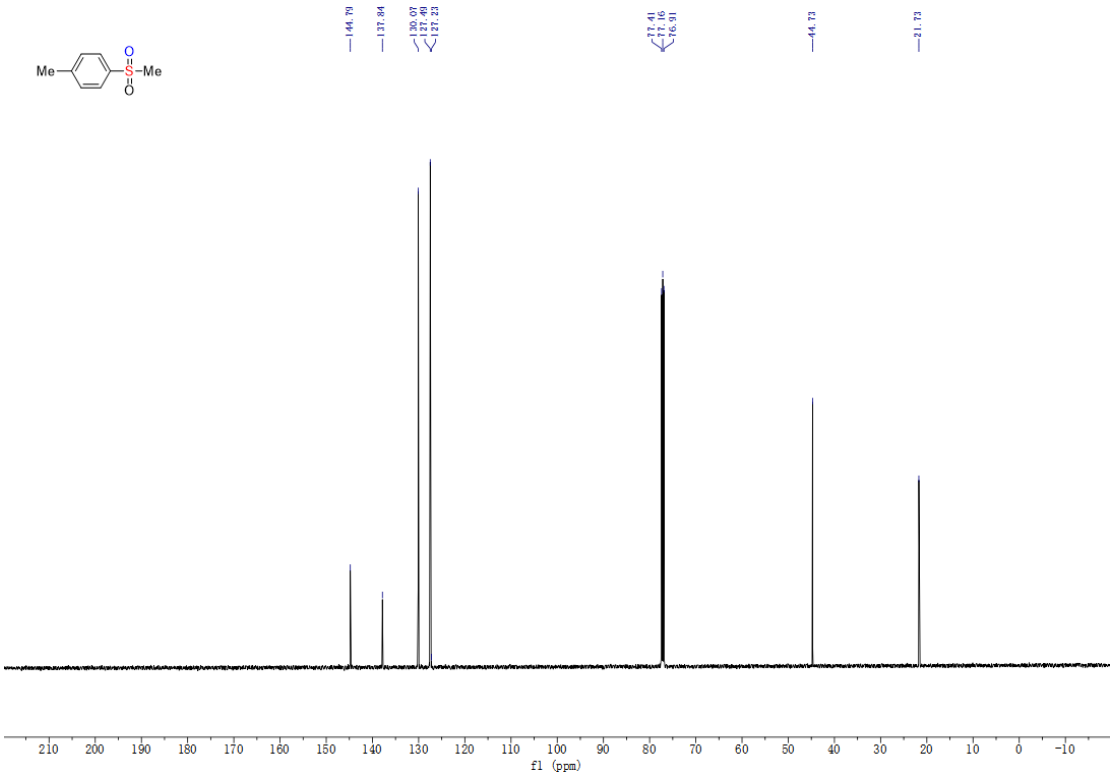
^{1}H NMR of compound **3a**



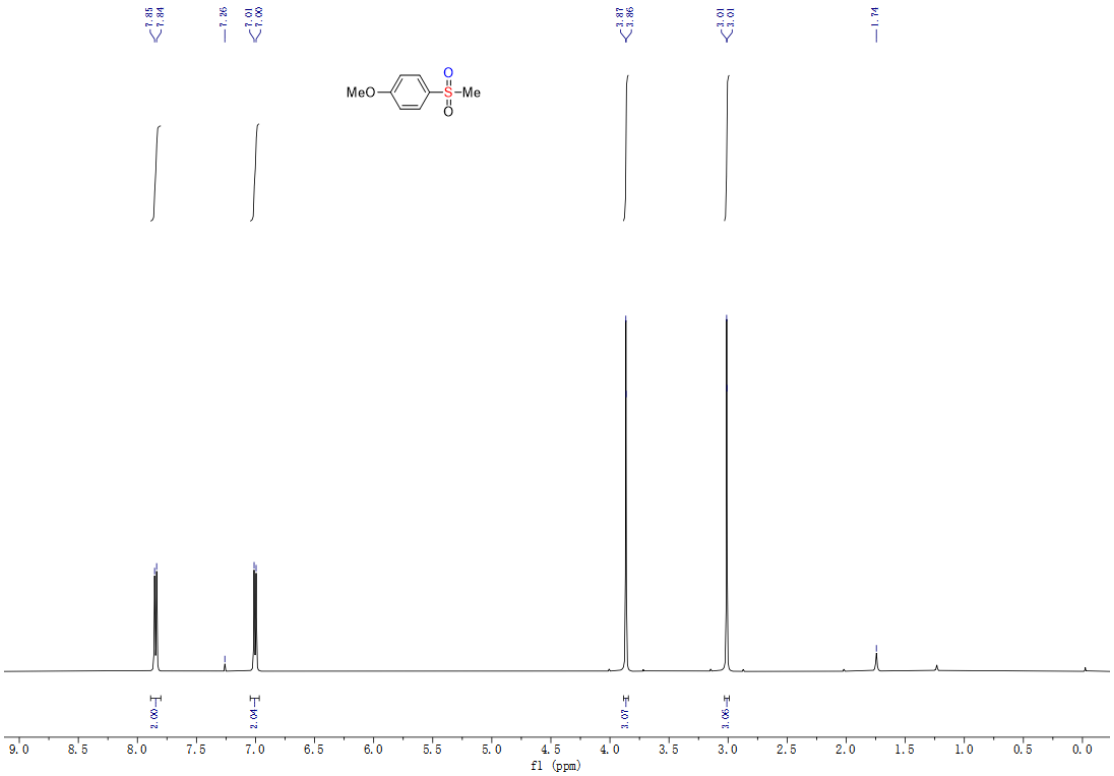
^{13}C NMR of compound **3a**



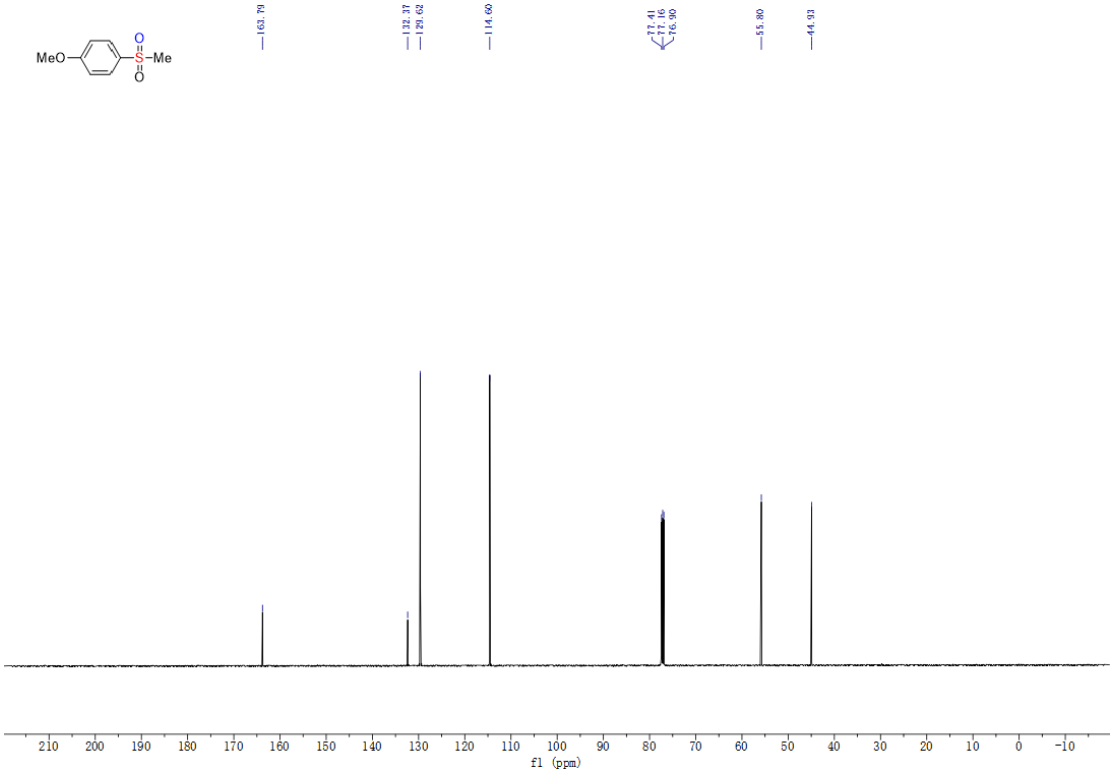
^{1}H NMR of compound **3b**



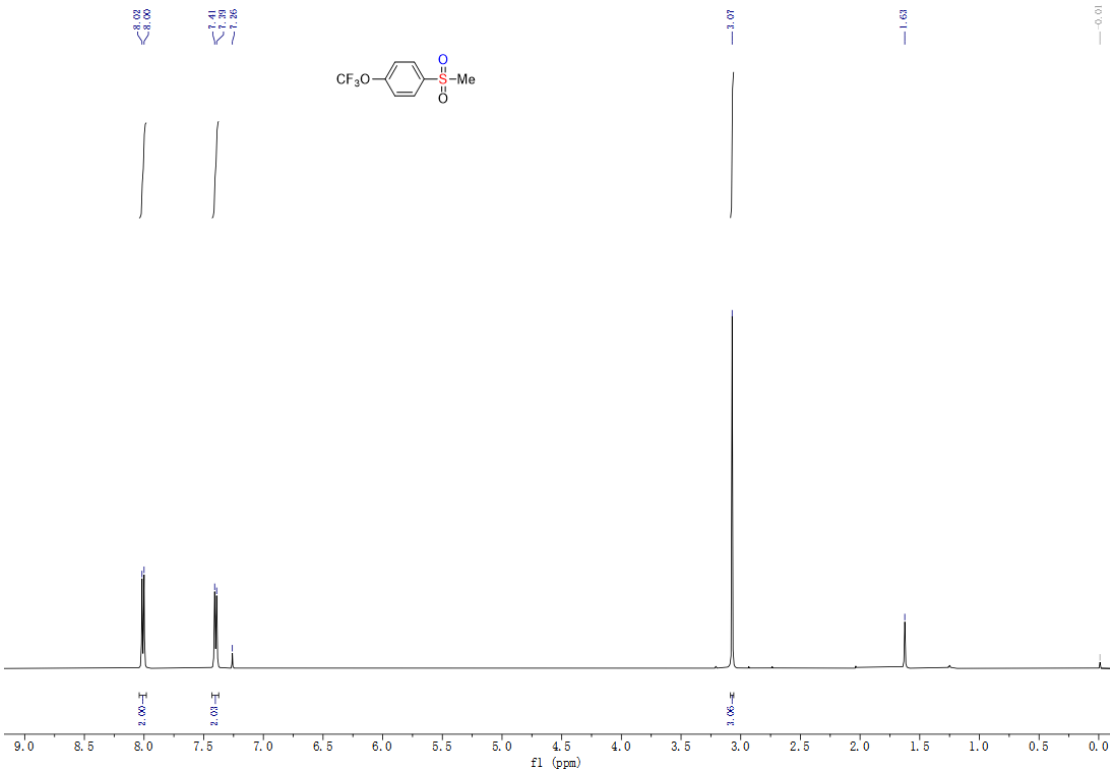
^{13}C NMR of compound **3b**



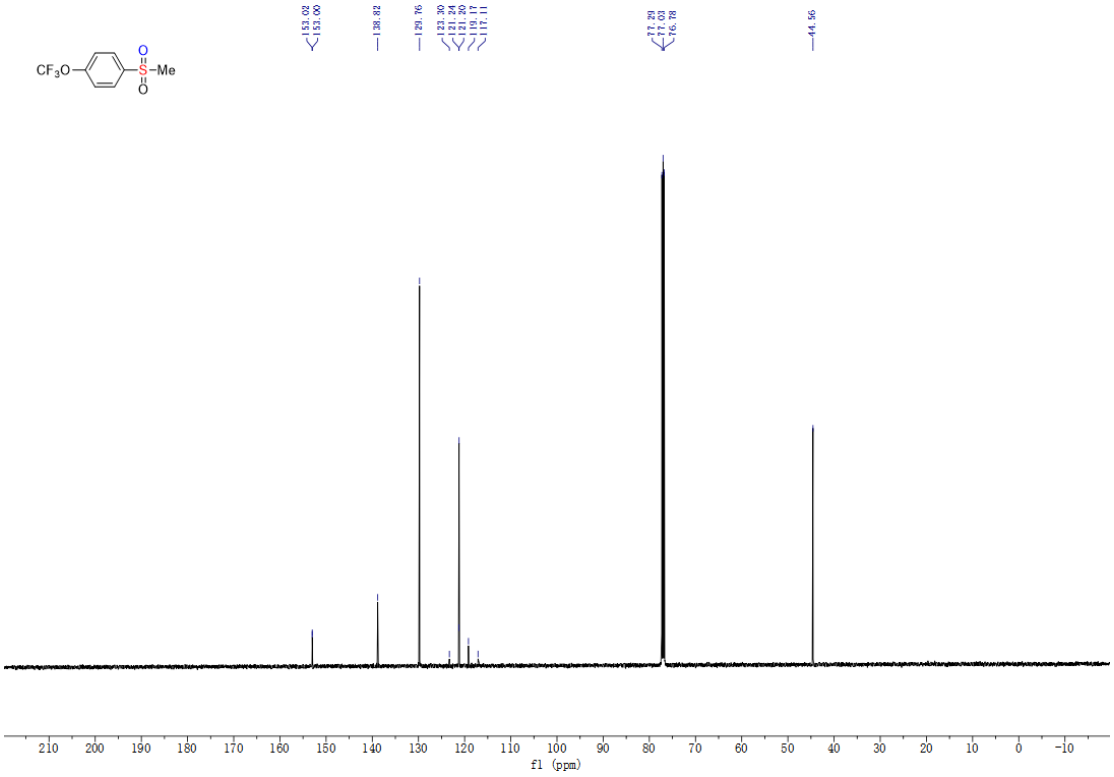
^{1}H NMR of compound **3c**



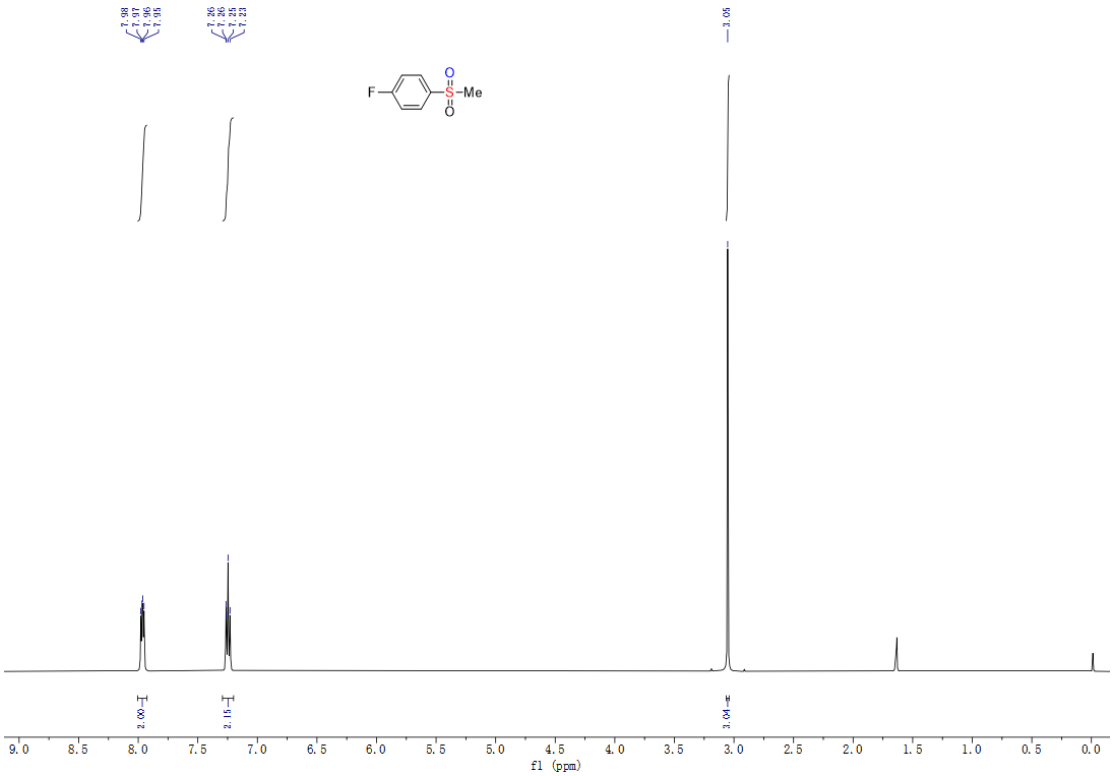
^{13}C NMR of compound **3c**



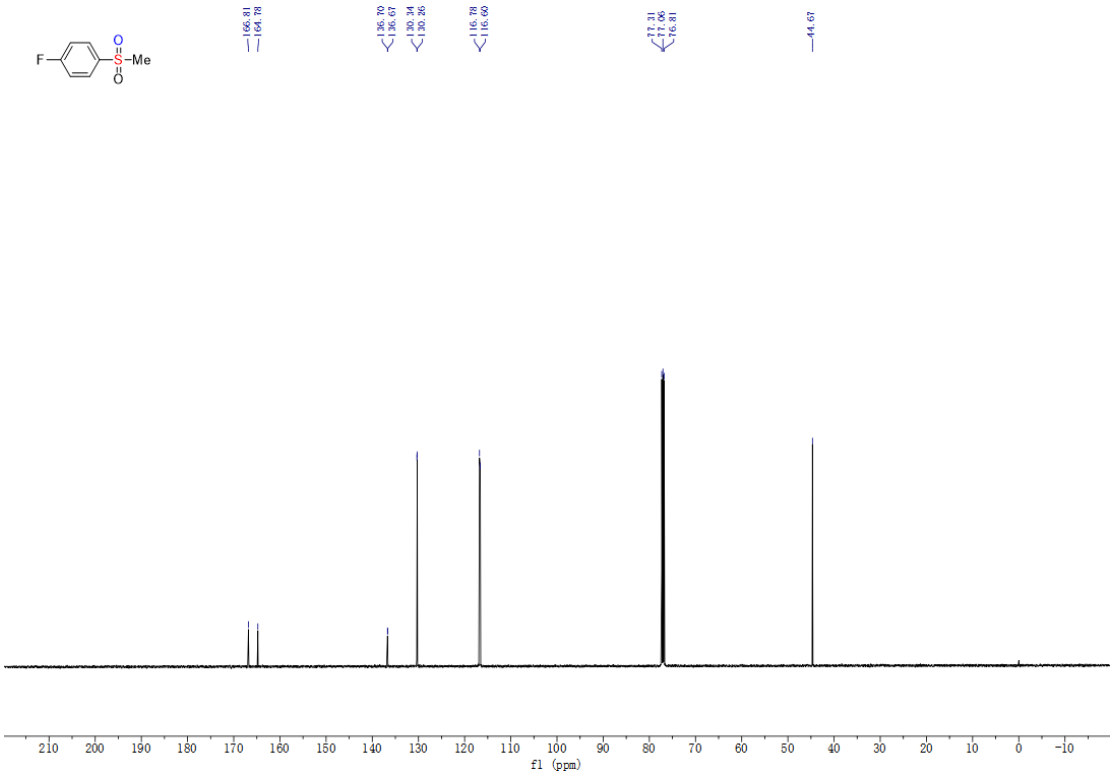
^{1}H NMR of compound **3d**



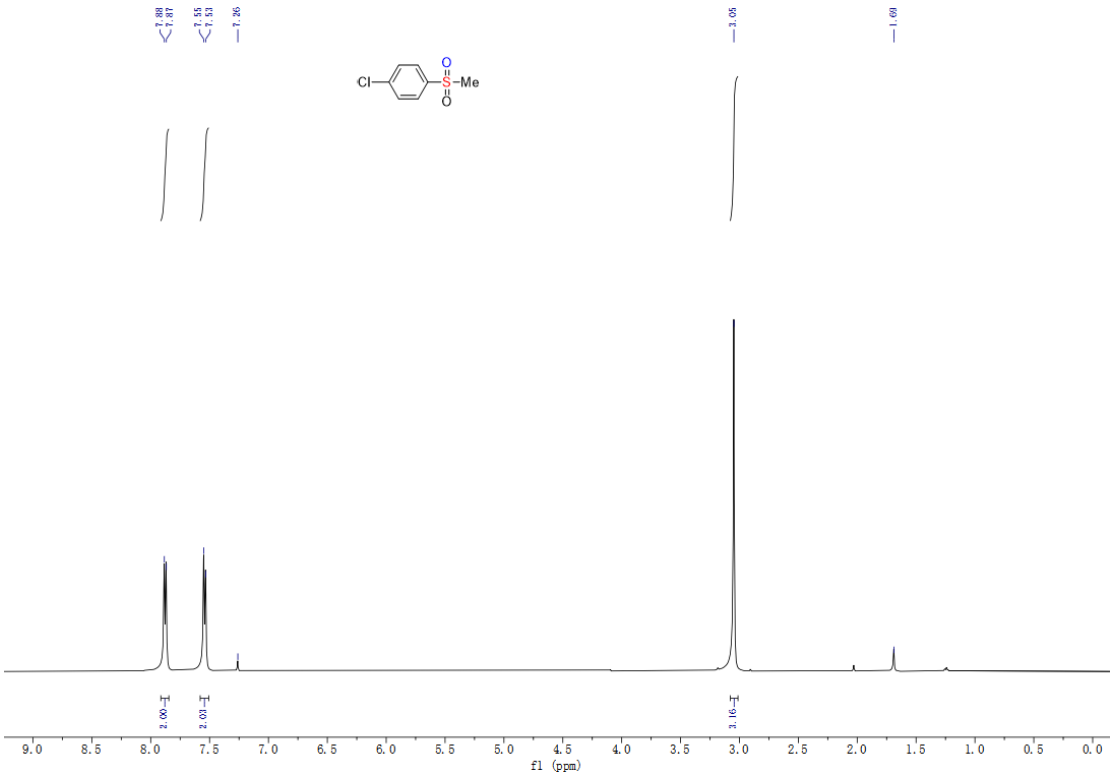
^{13}C NMR of compound **3d**



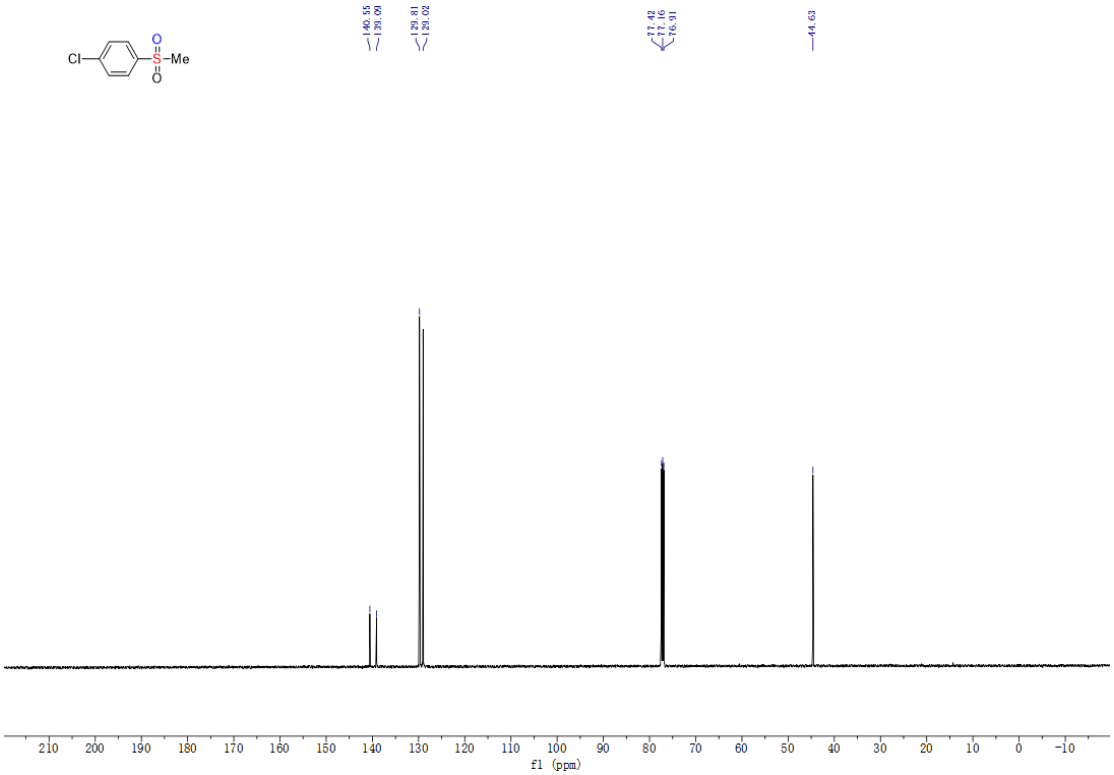
^{1}H NMR of compound **3e**



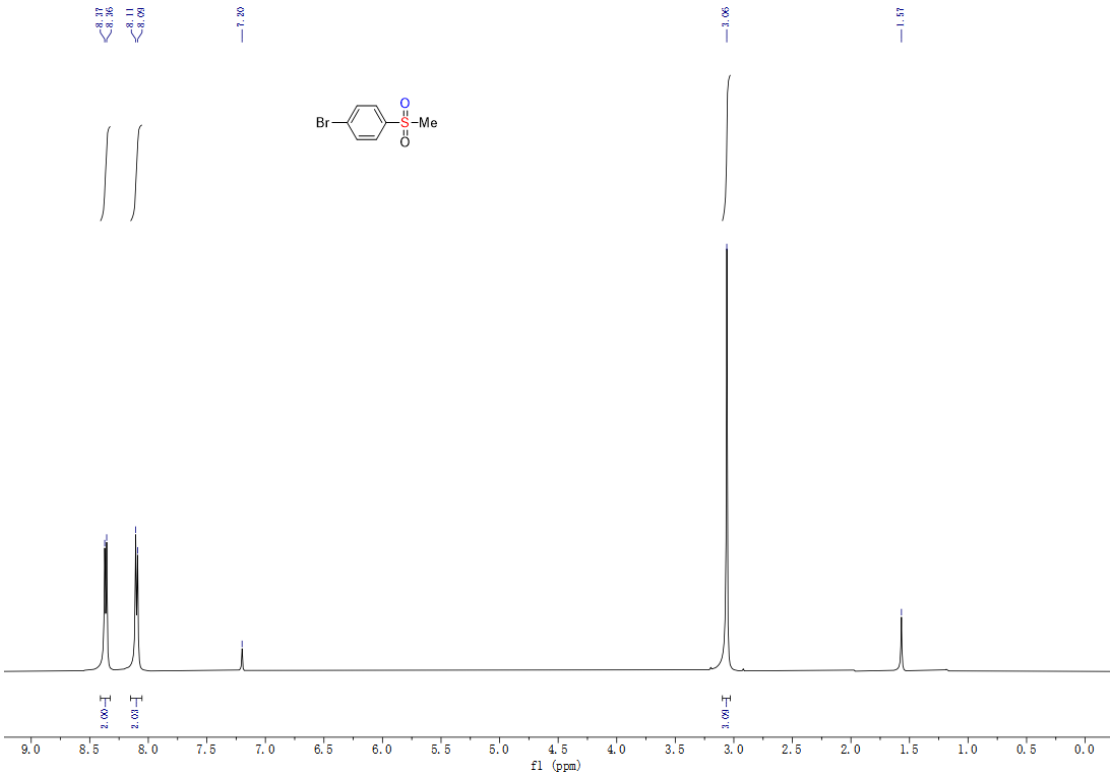
^{13}C NMR of compound **3e**



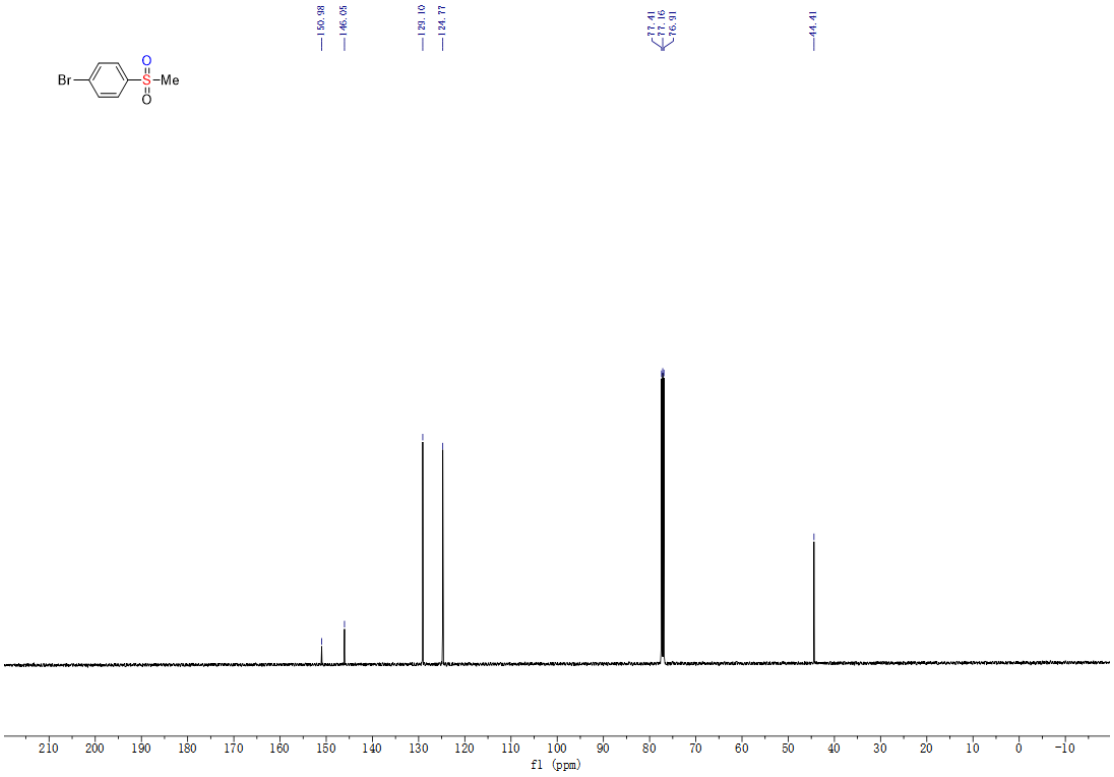
^{1}H NMR of compound **3f**



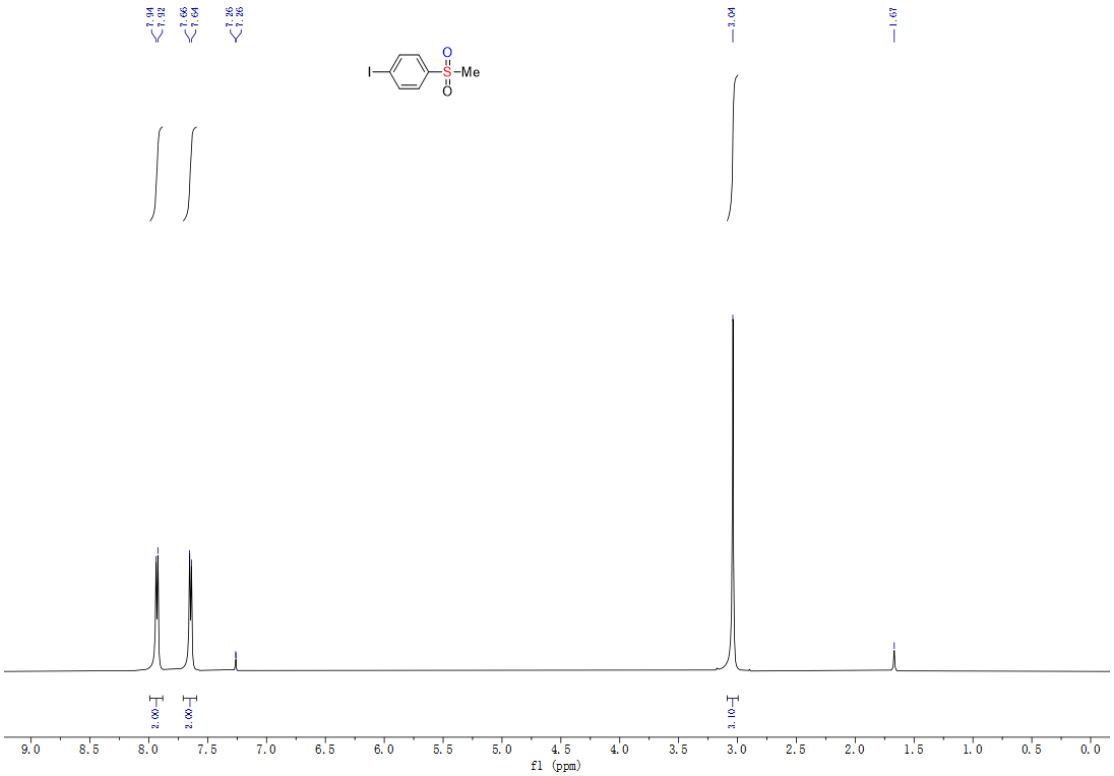
^{13}C NMR of compound **3f**



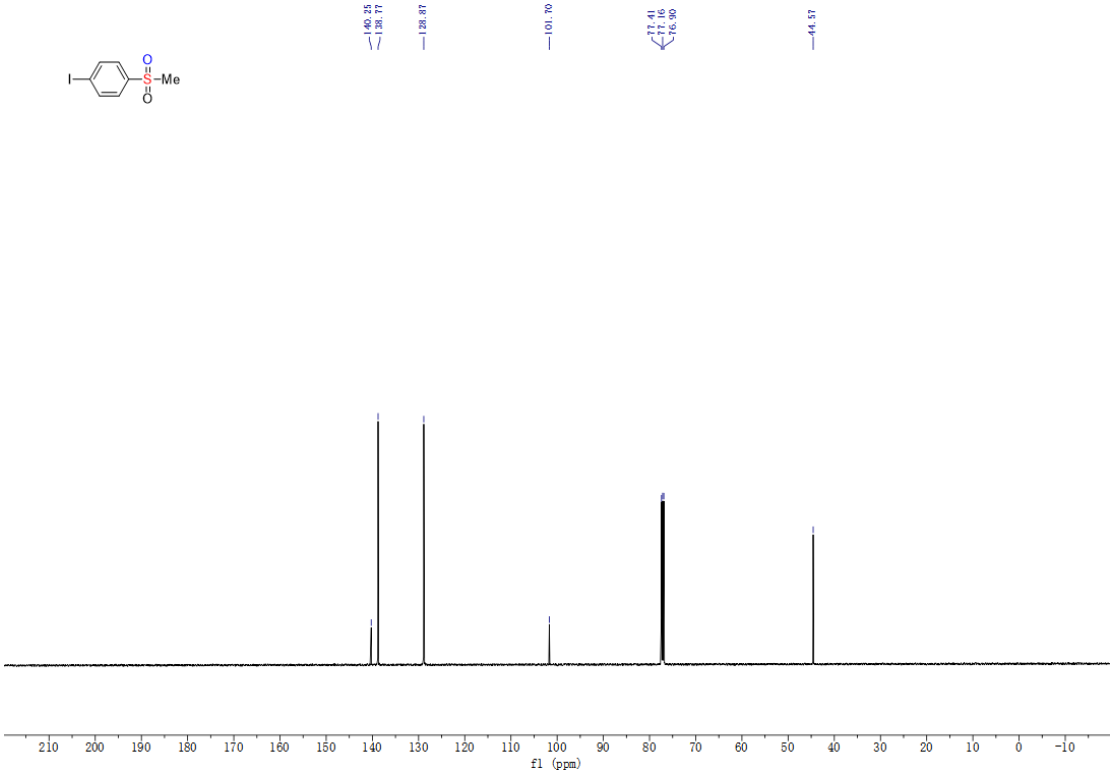
^{1}H NMR of compound **3g**



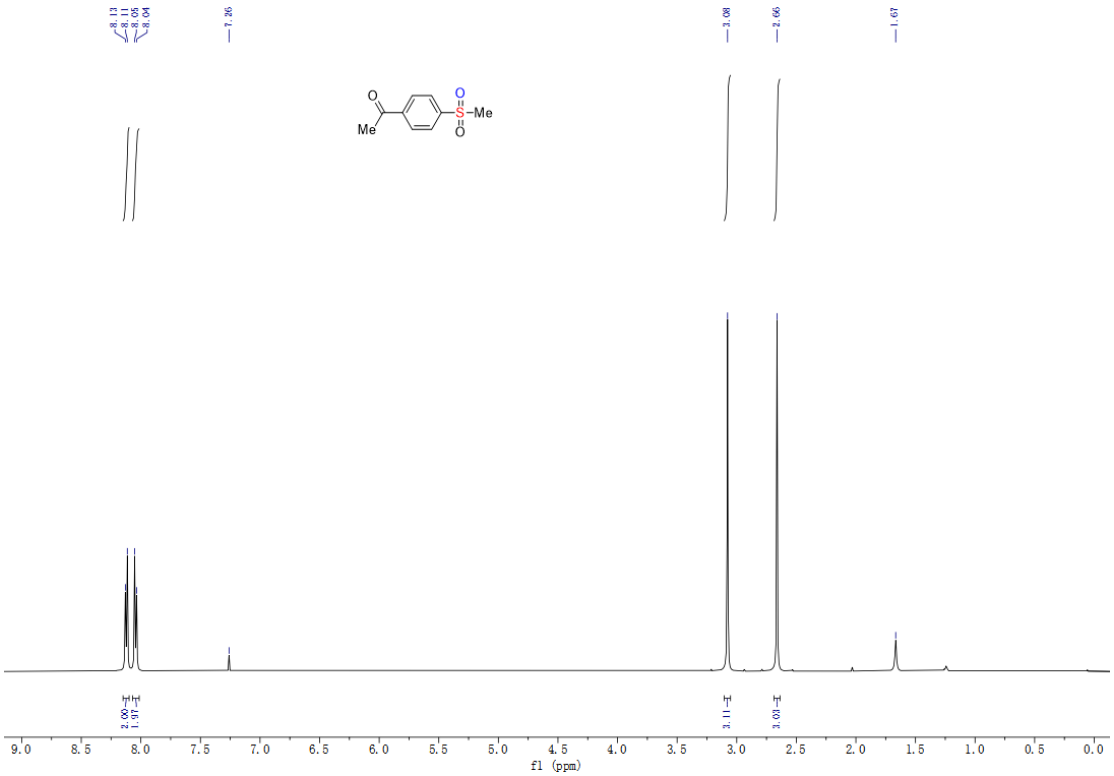
^{13}C NMR of compound **3g**



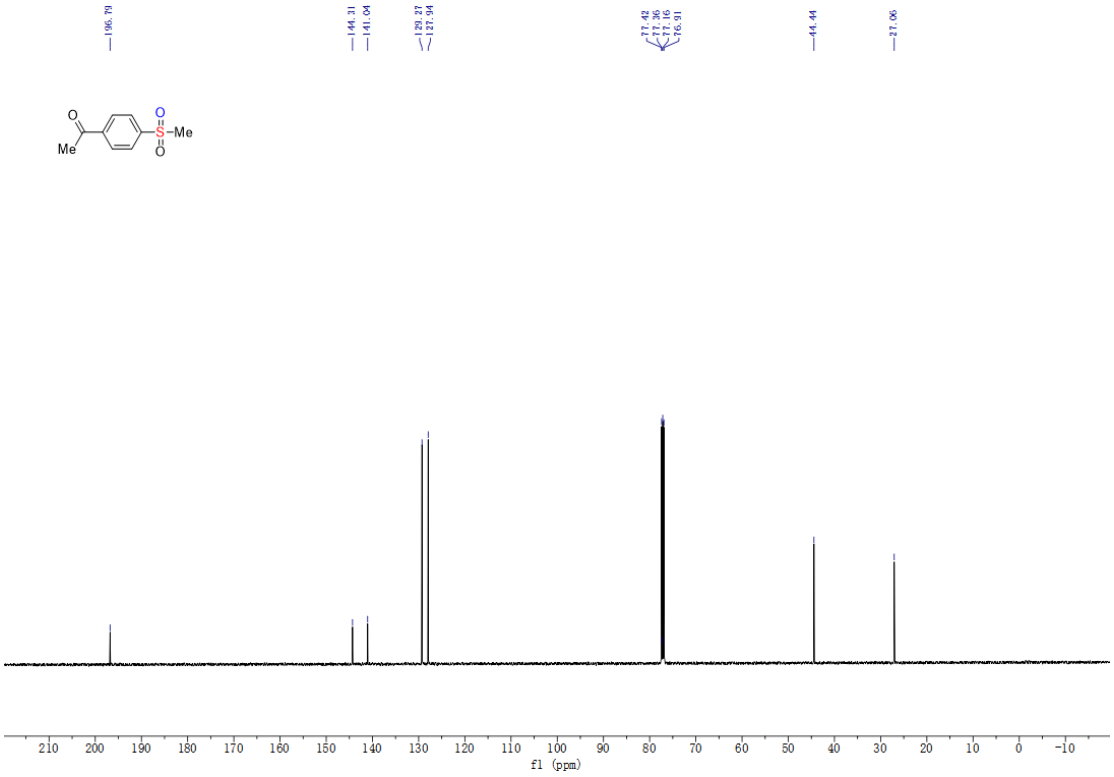
^{1}H NMR of compound **3h**



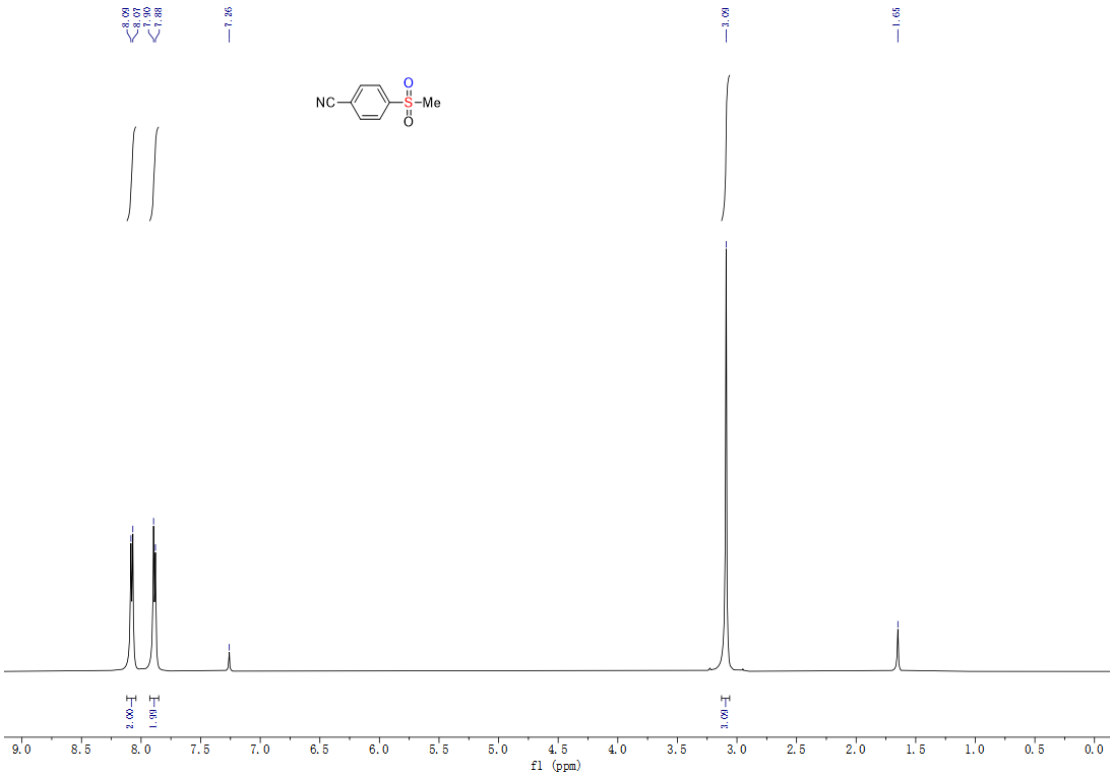
^{13}C NMR of compound **3h**



^{1}H NMR of compound **3j**



^{13}C NMR of compound **3j**



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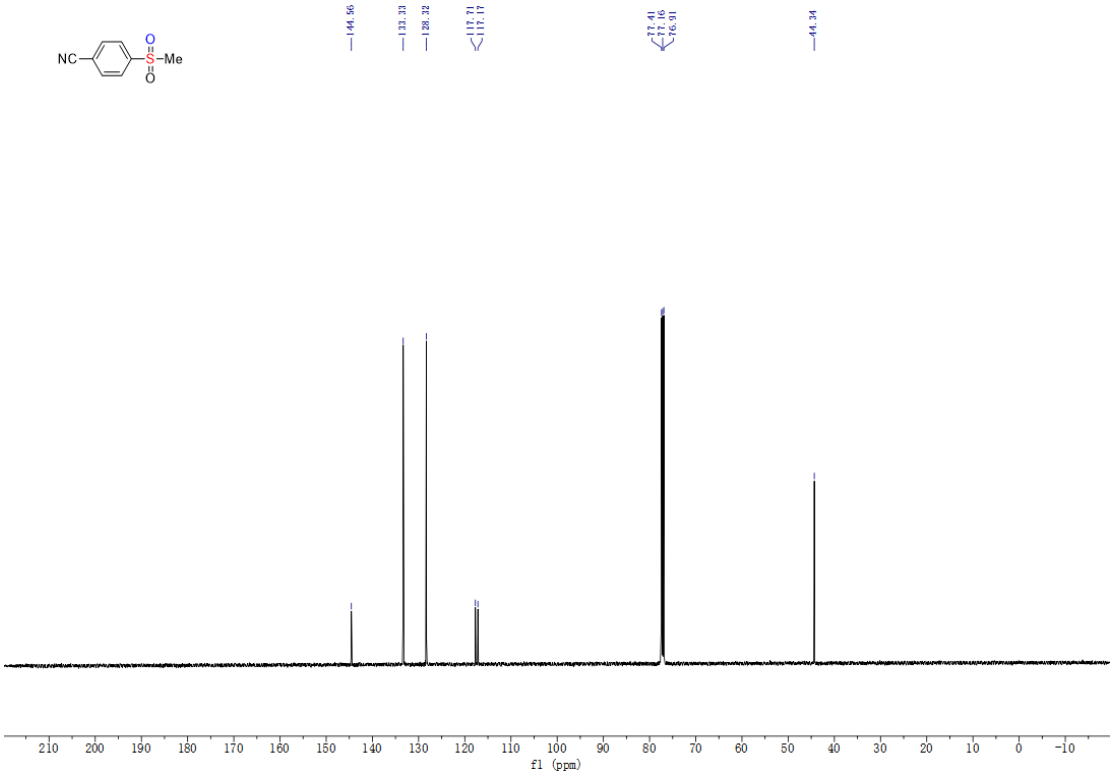
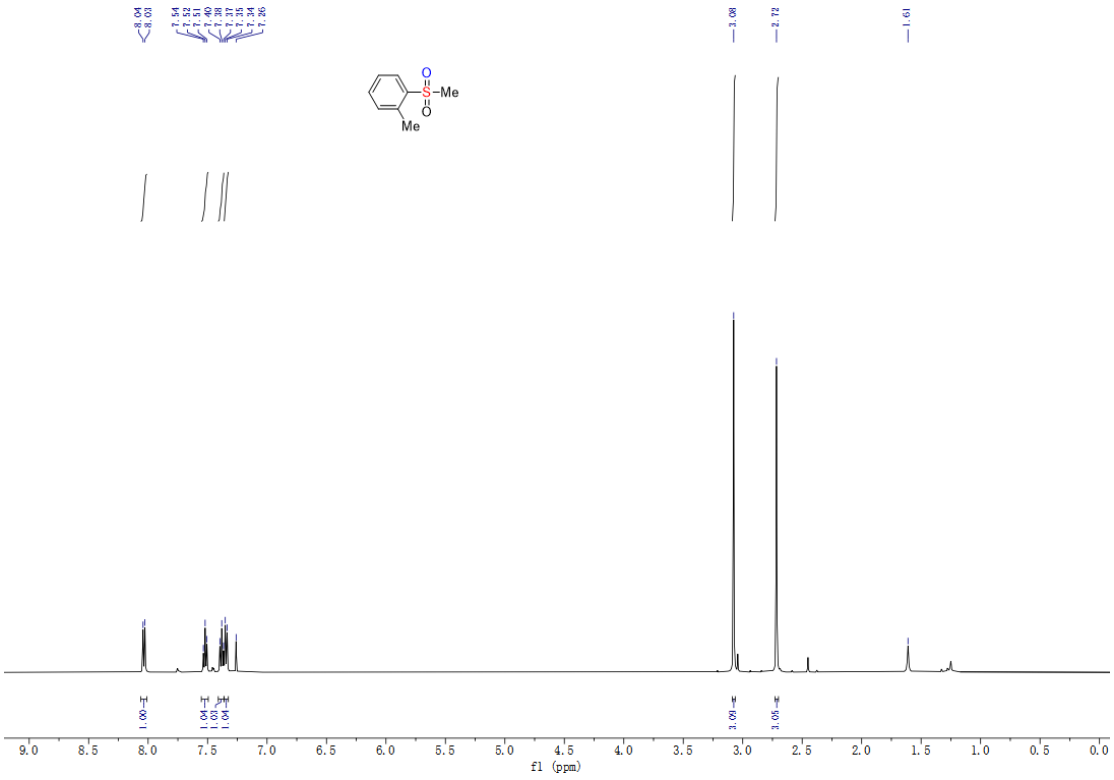
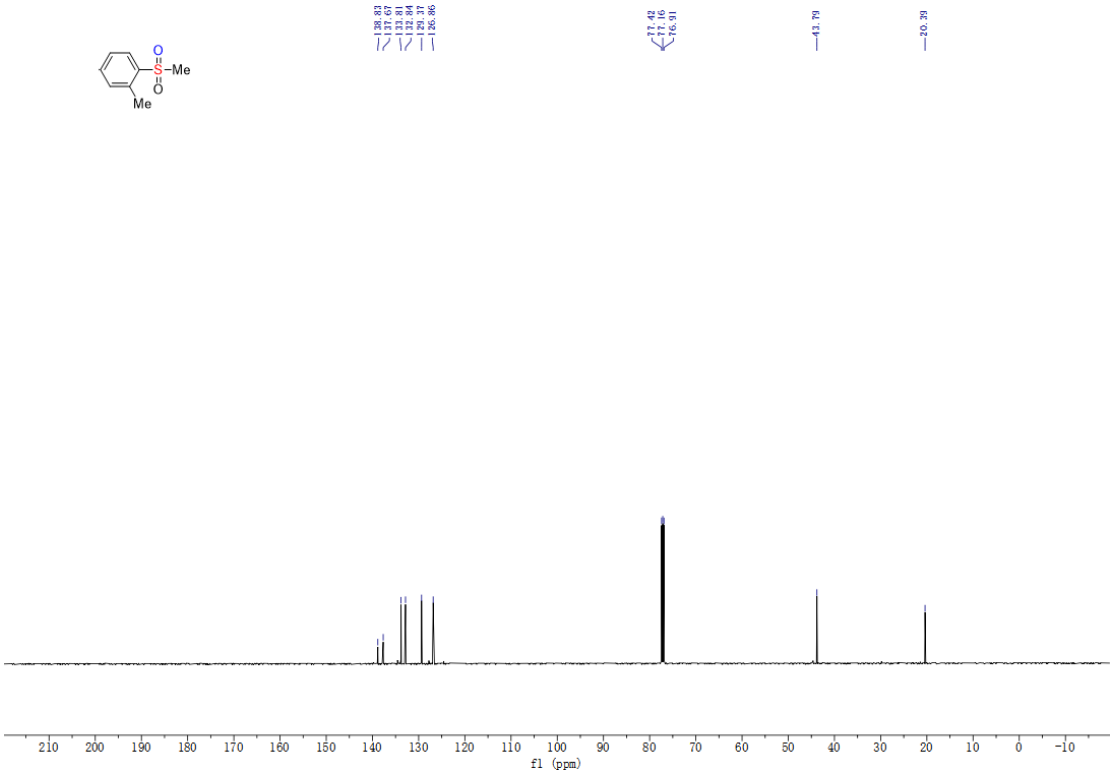


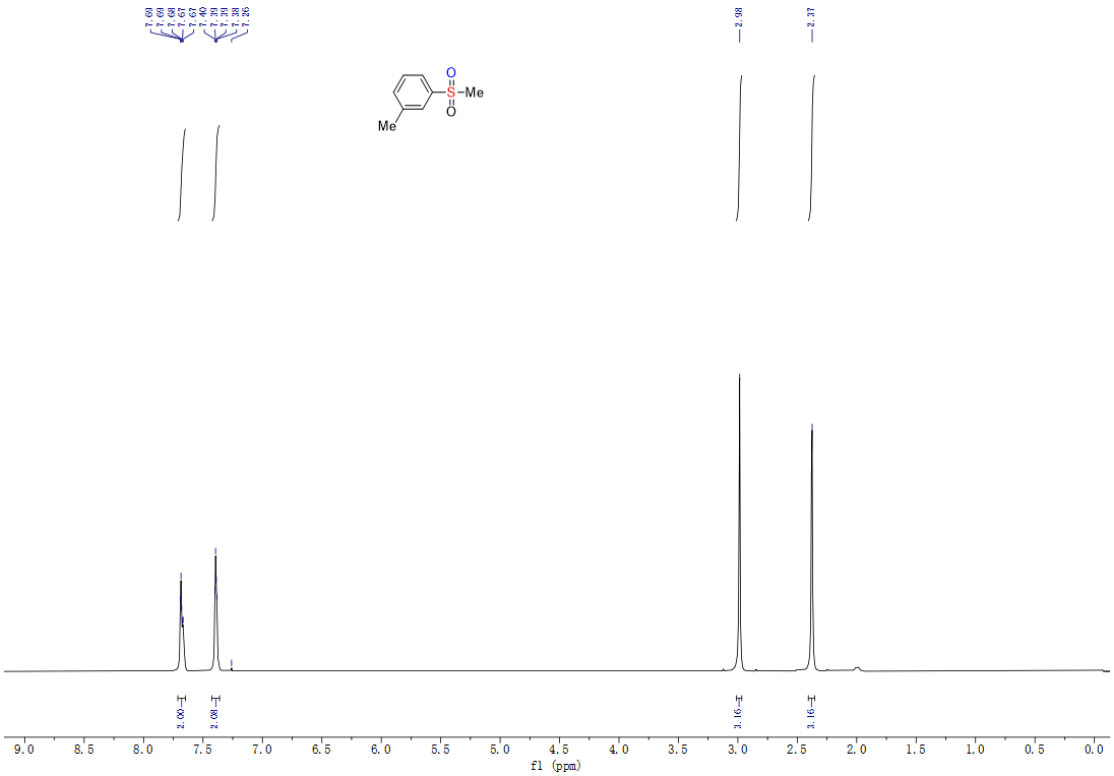
^{13}C NMR of compound **3k**



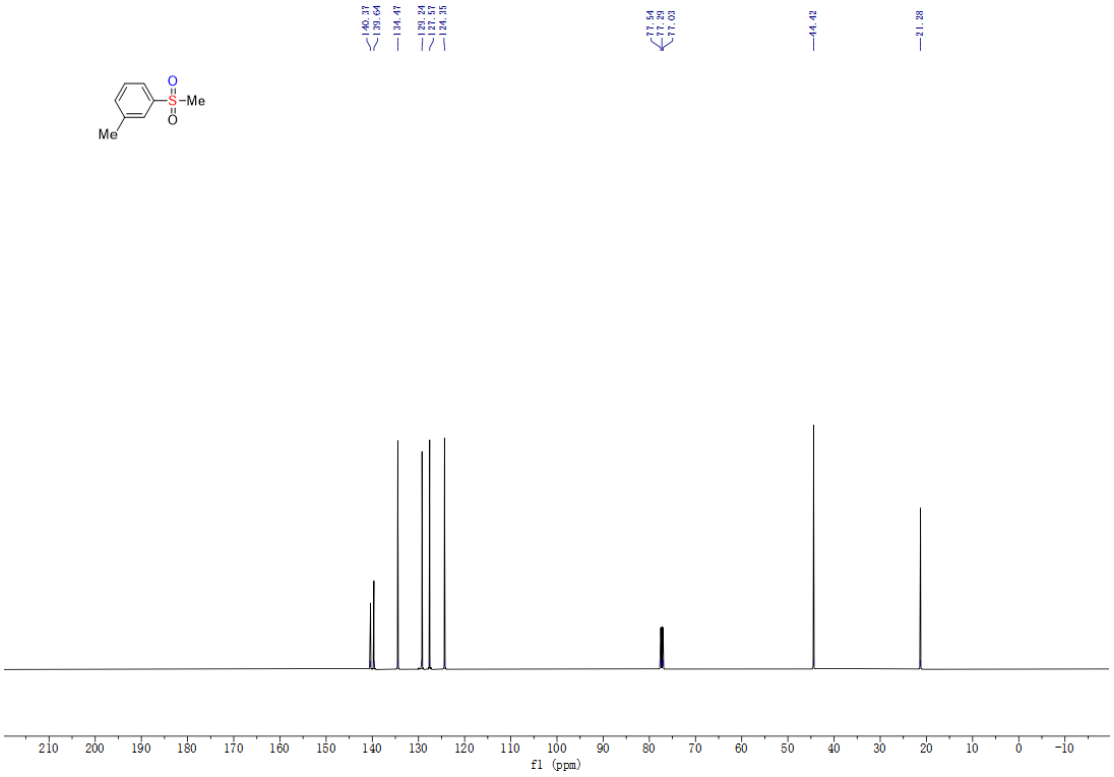
^{1}H NMR of compound **3m**



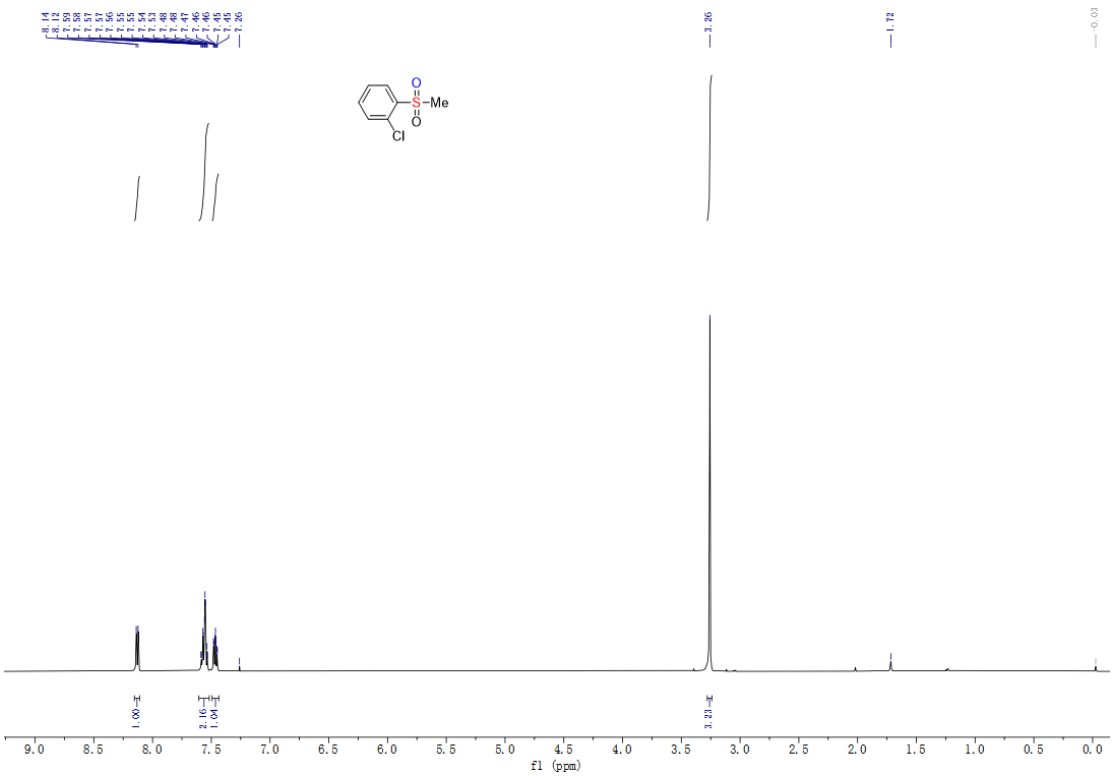
^{13}C NMR of compound **3m**



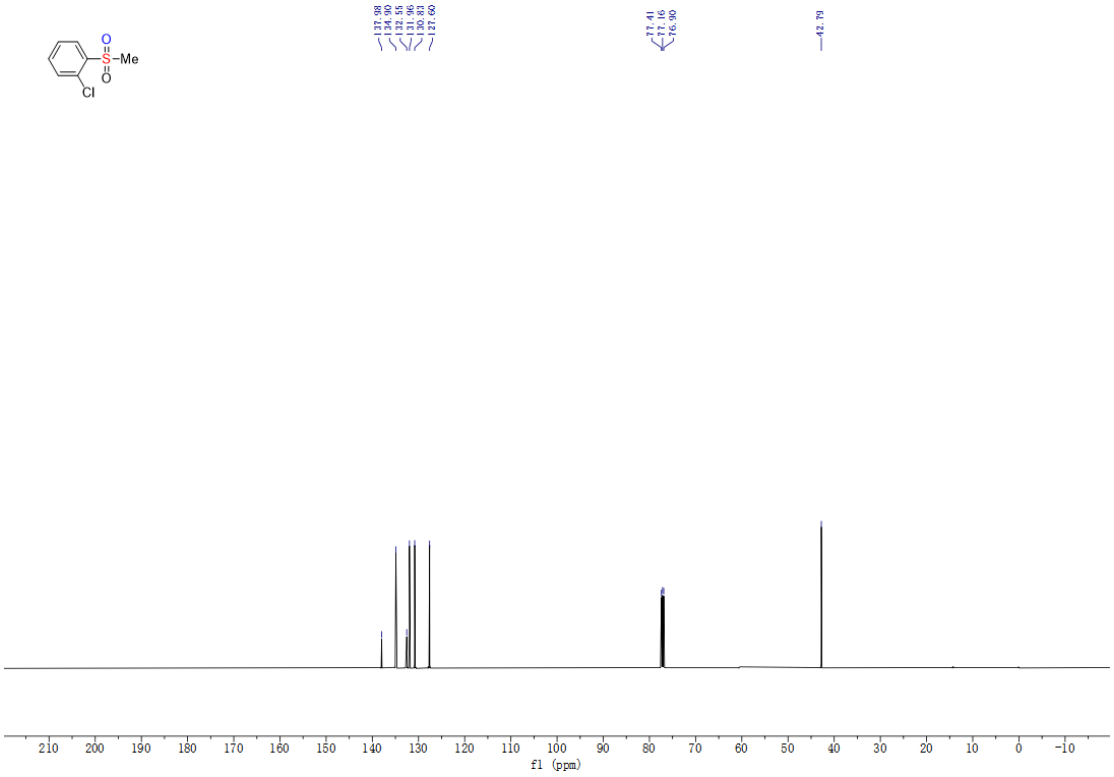
^{1}H NMR of compound **3n**



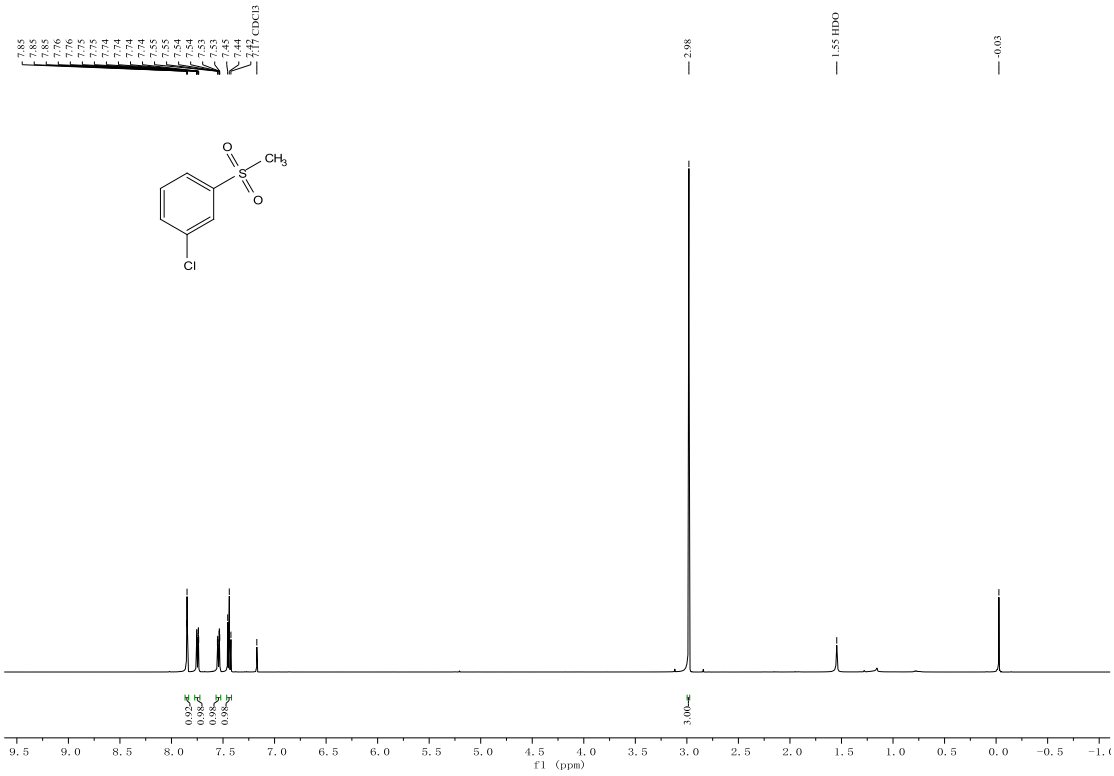
^{13}C NMR of compound **3n**



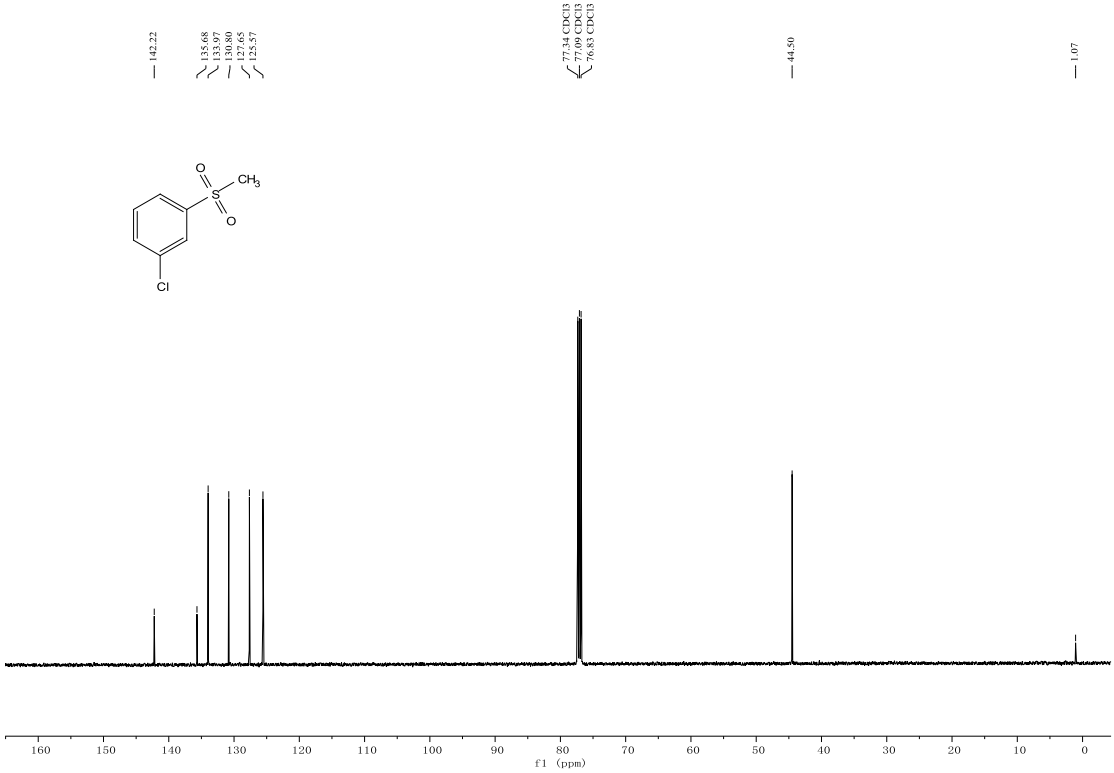
^{1}H NMR of compound **3o**



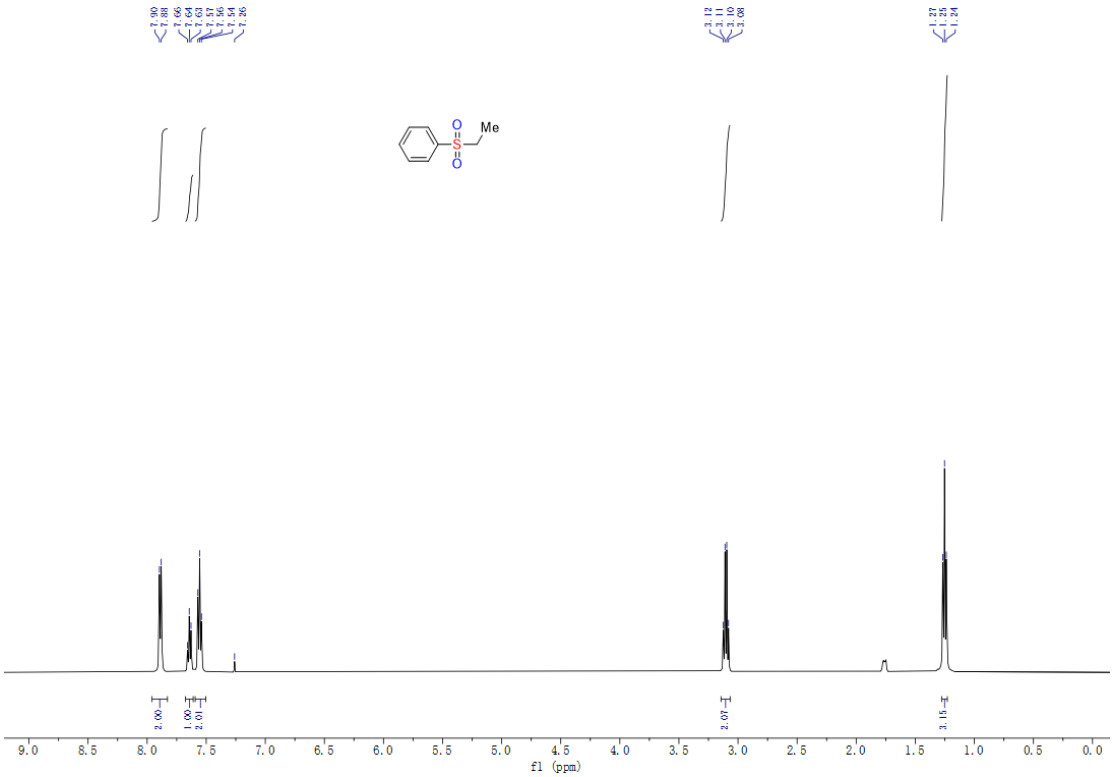
^{13}C NMR of compound **3o**



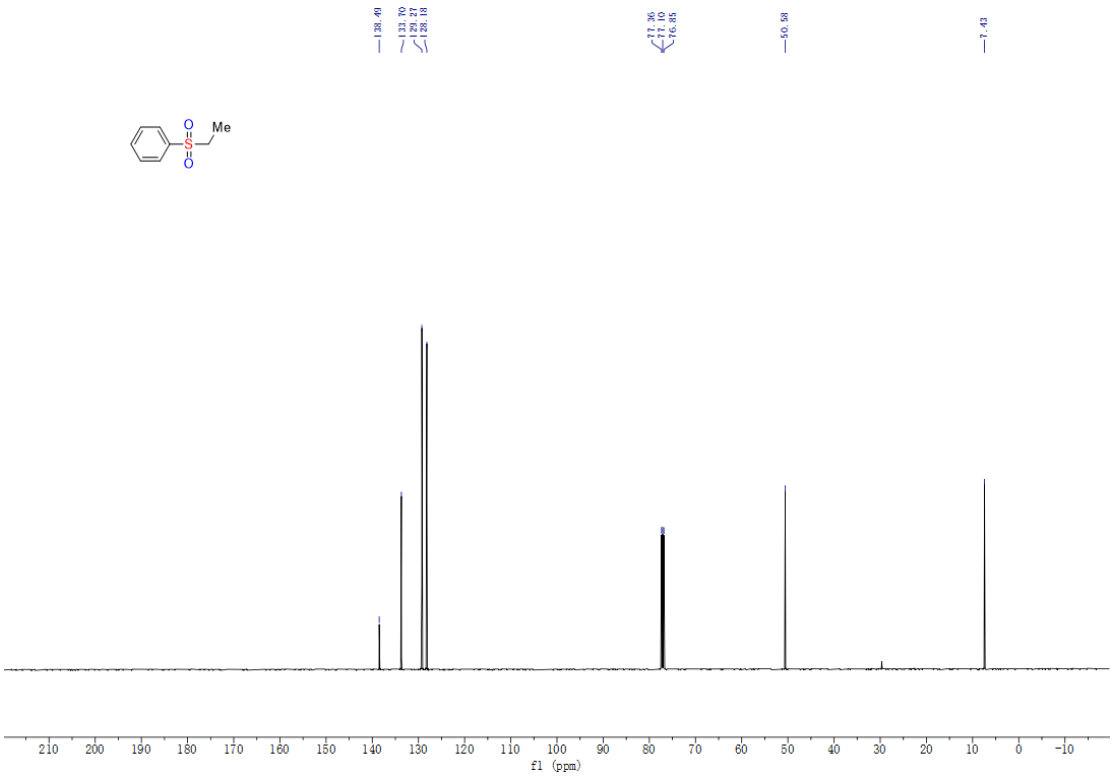
^{1}H NMR of compound **3p**



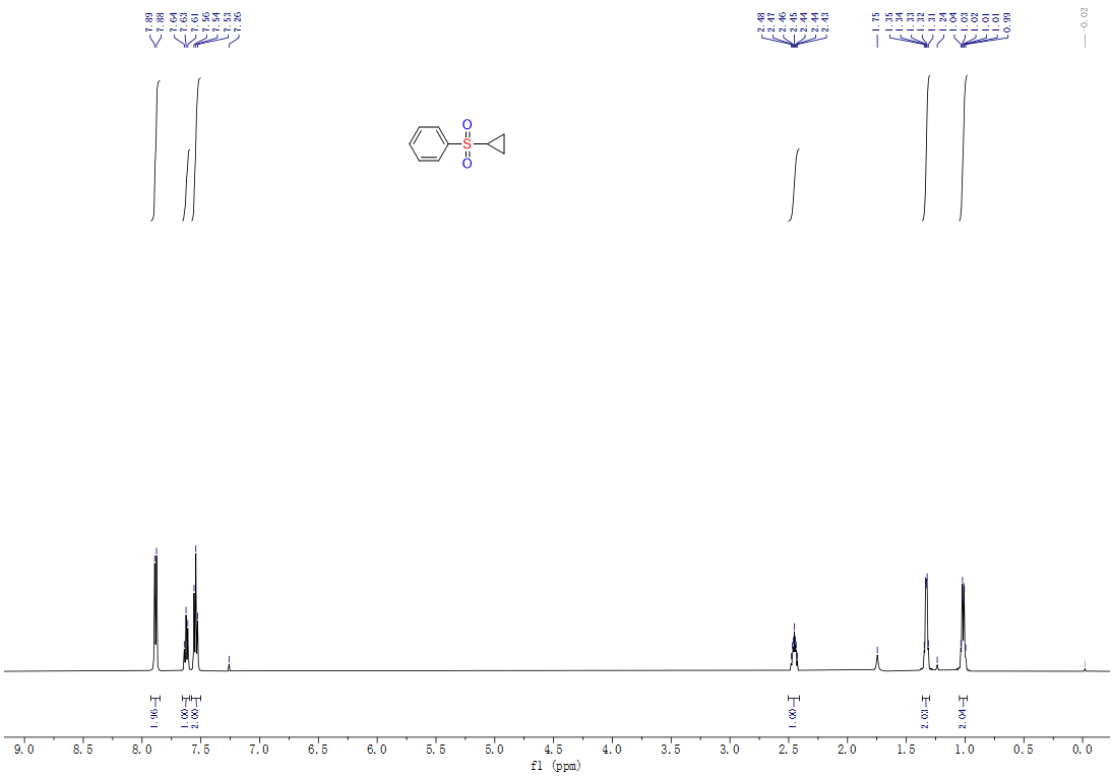
^{13}C NMR of compound **3p**



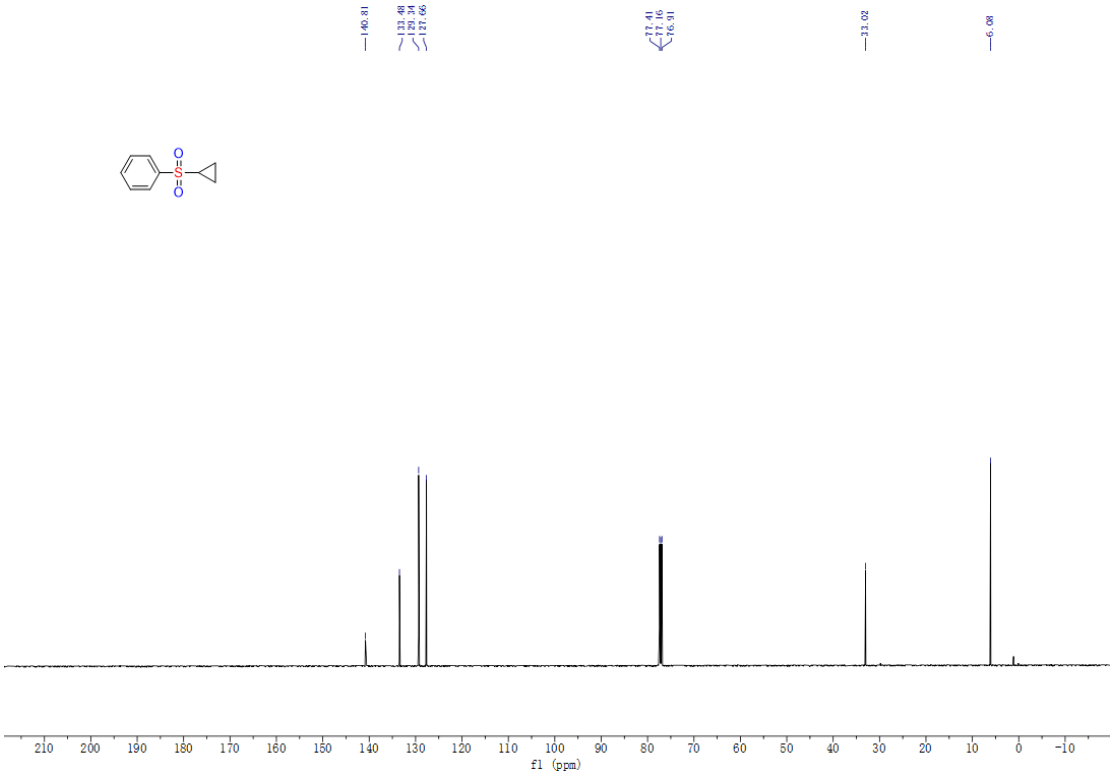
^{1}H NMR of compound **3q**



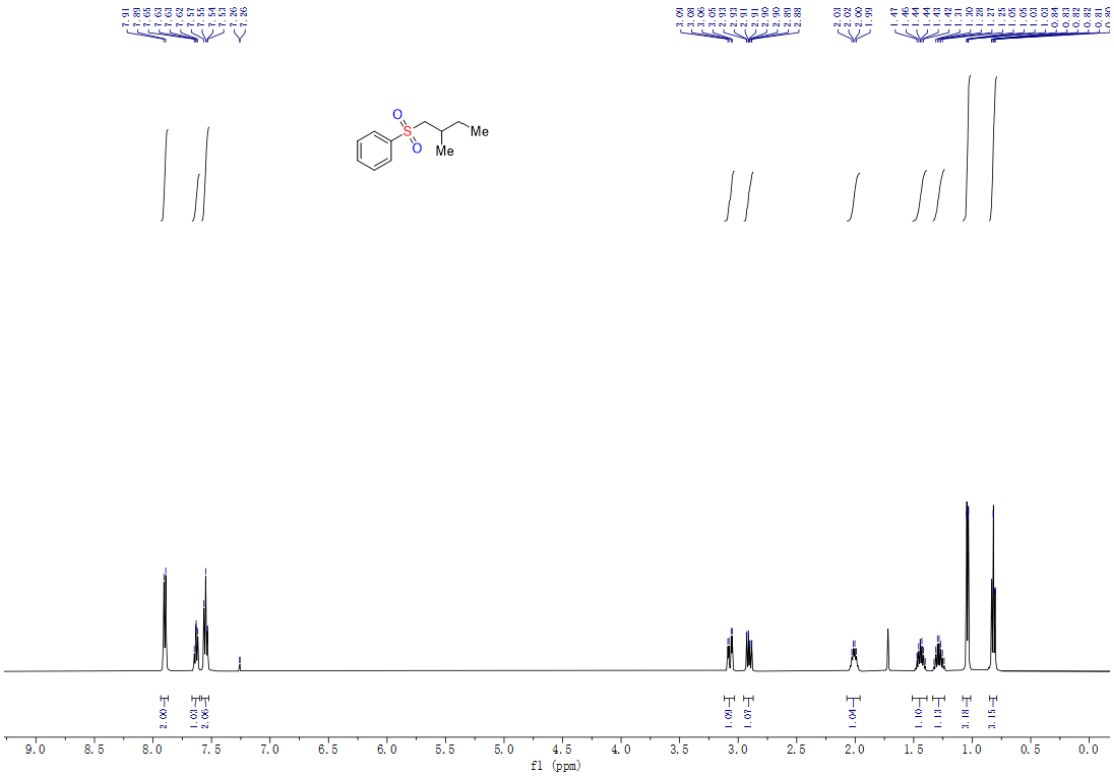
^{13}C NMR of compound **3q**



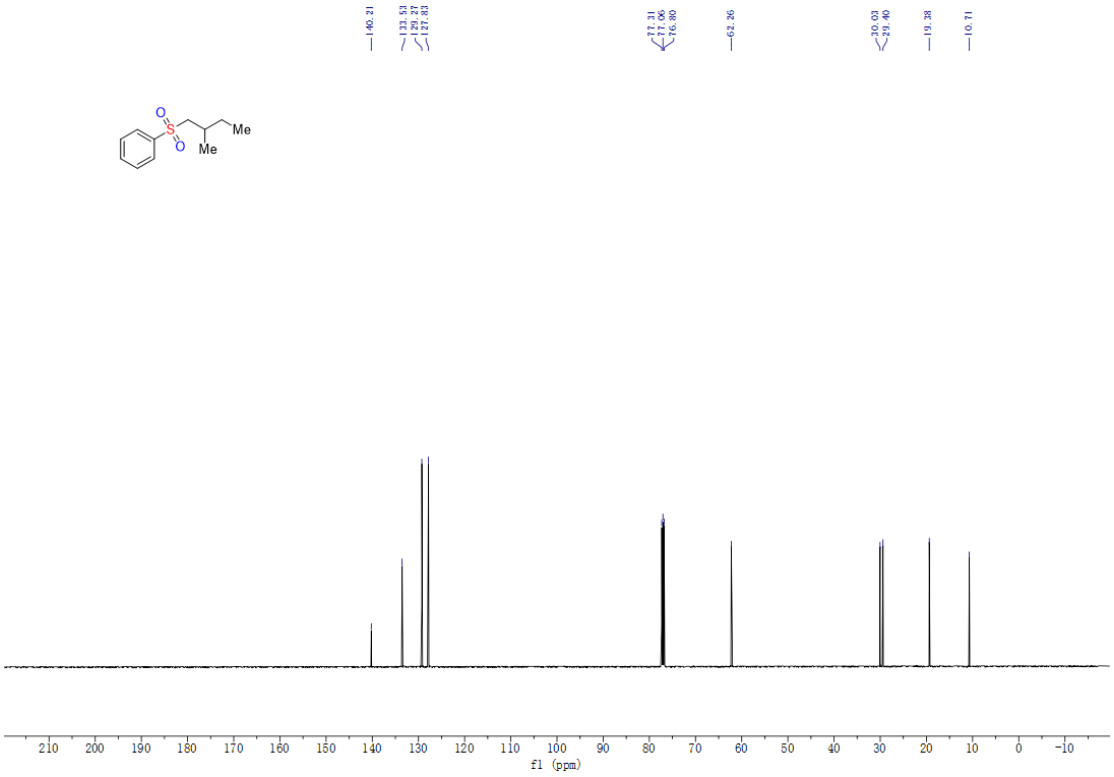
^{1}H NMR of compound **3r**



^{13}C NMR of compound **3r**



^{1}H NMR of compound **3s**



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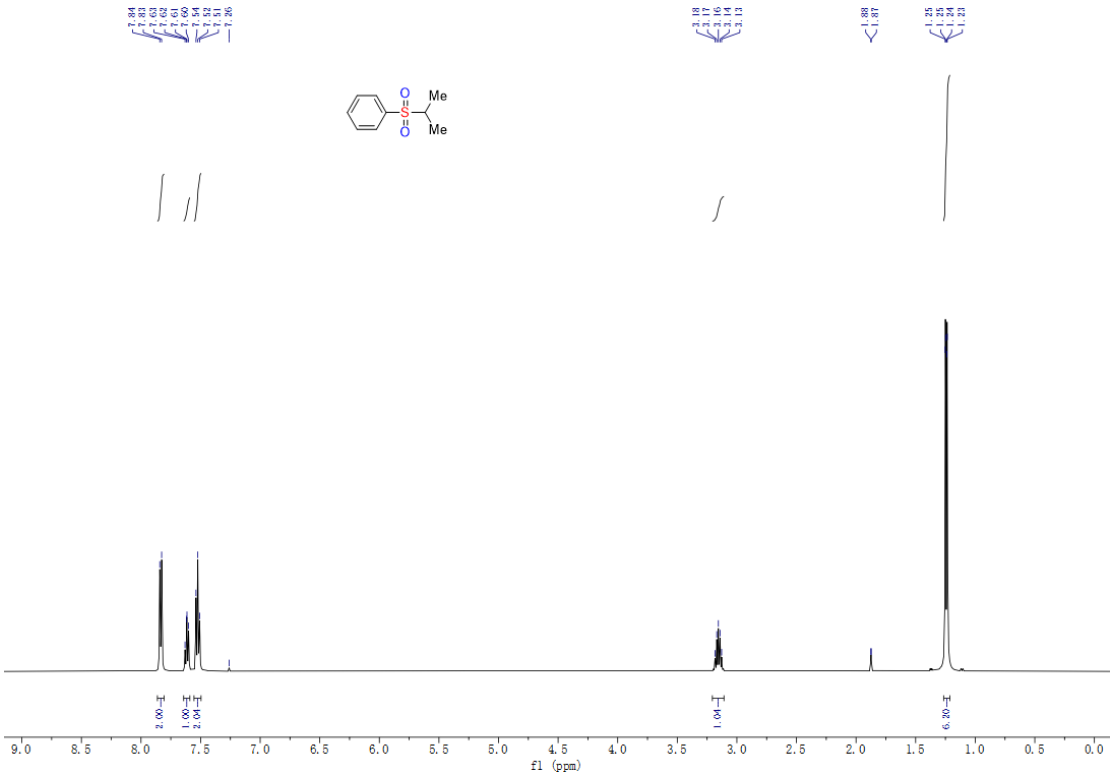

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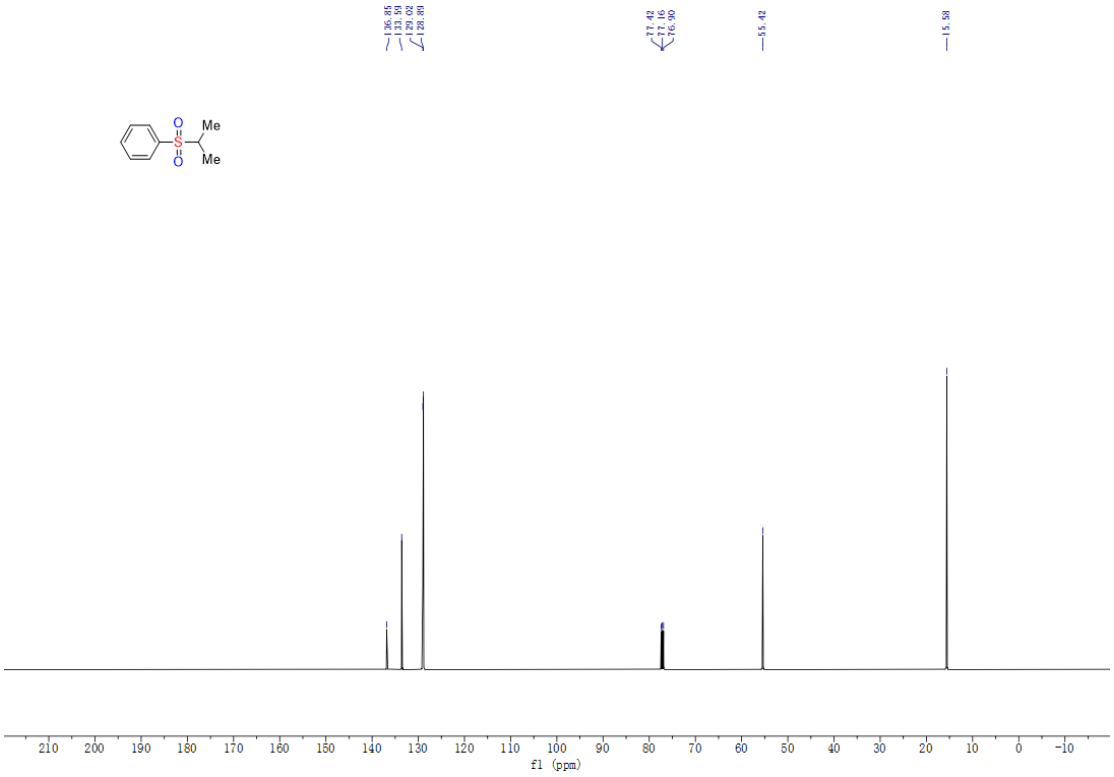
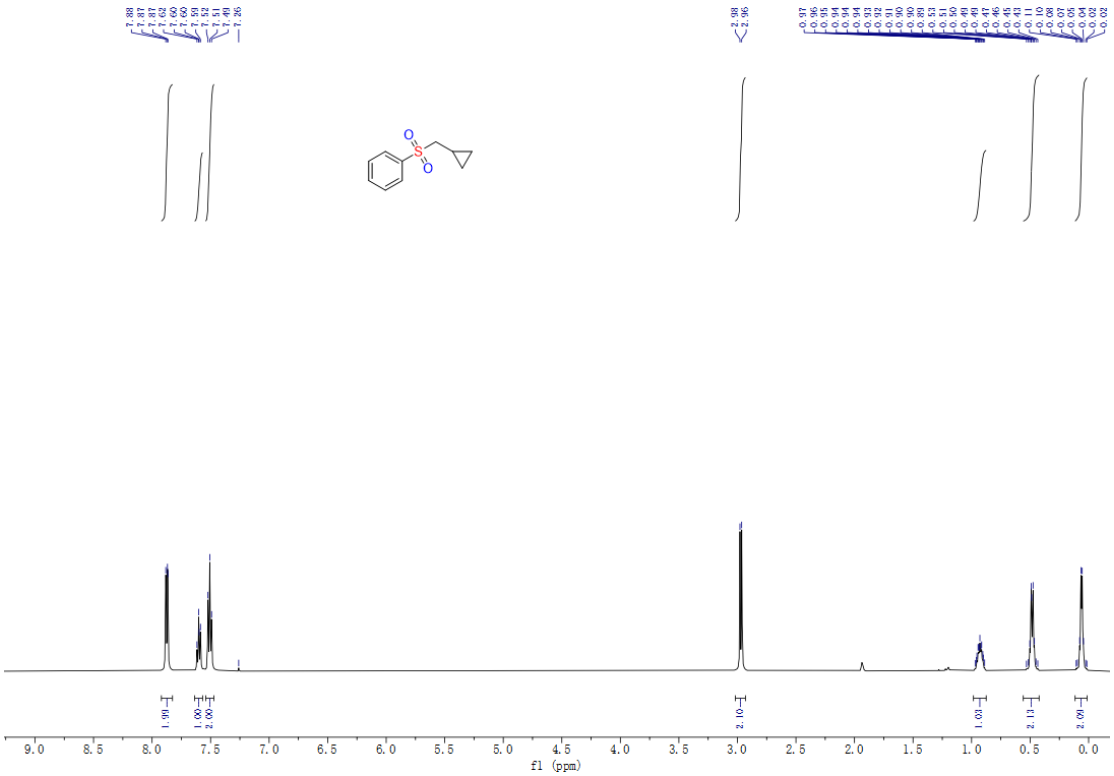
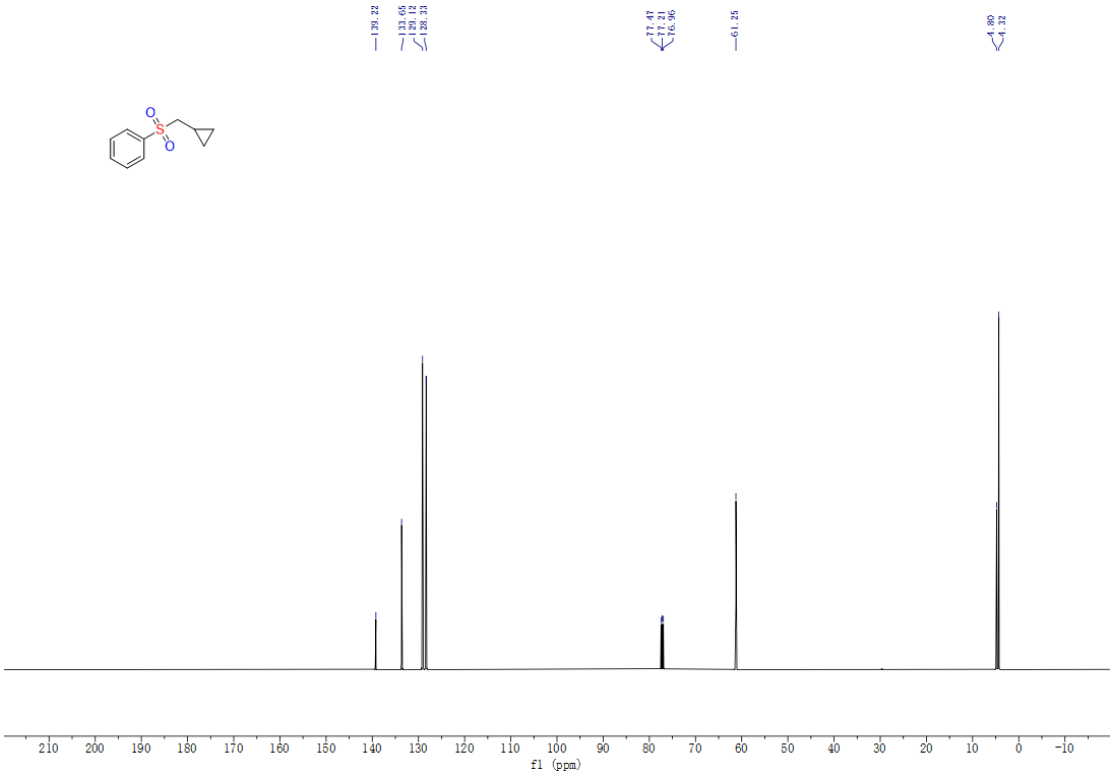


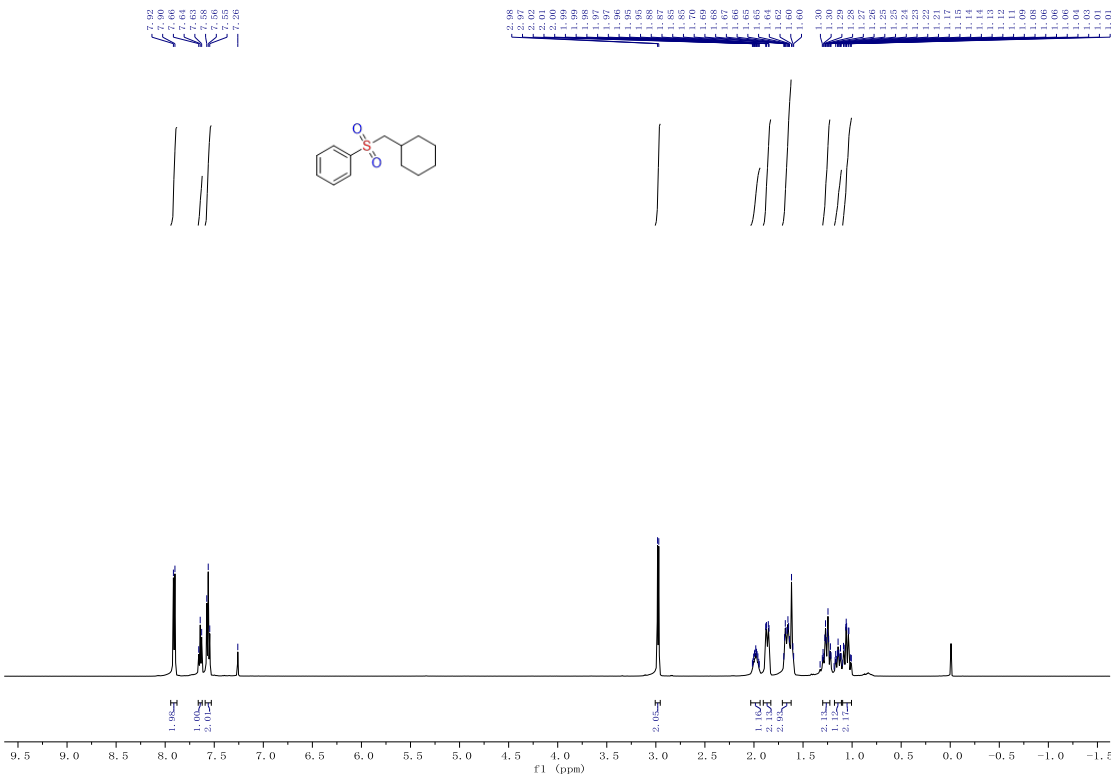
^{13}C NMR of compound **3t**



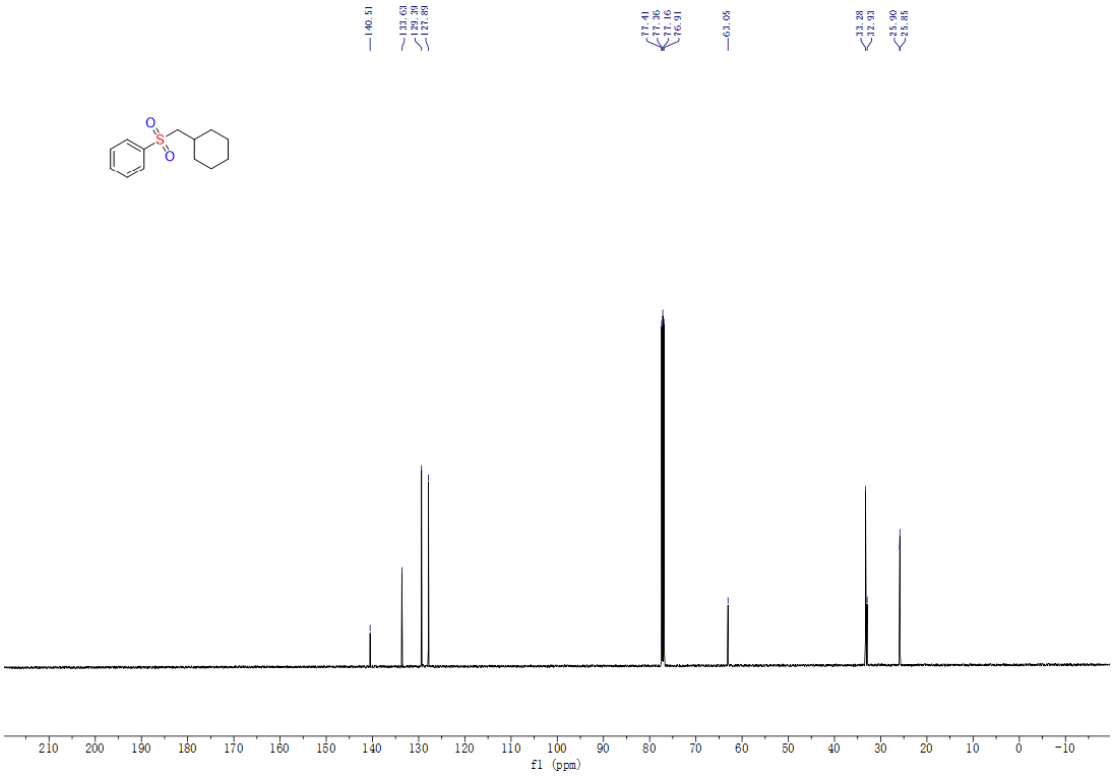
^{1}H NMR of compound **3u**



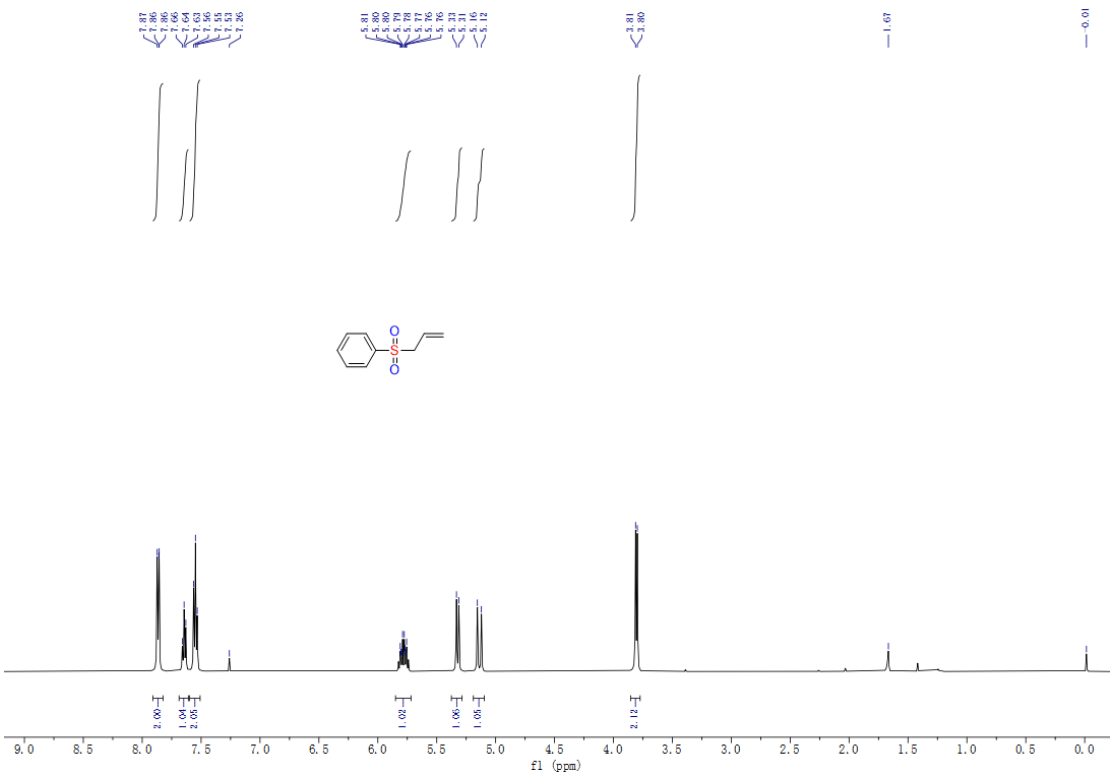
^{13}C NMR of compound **3u**



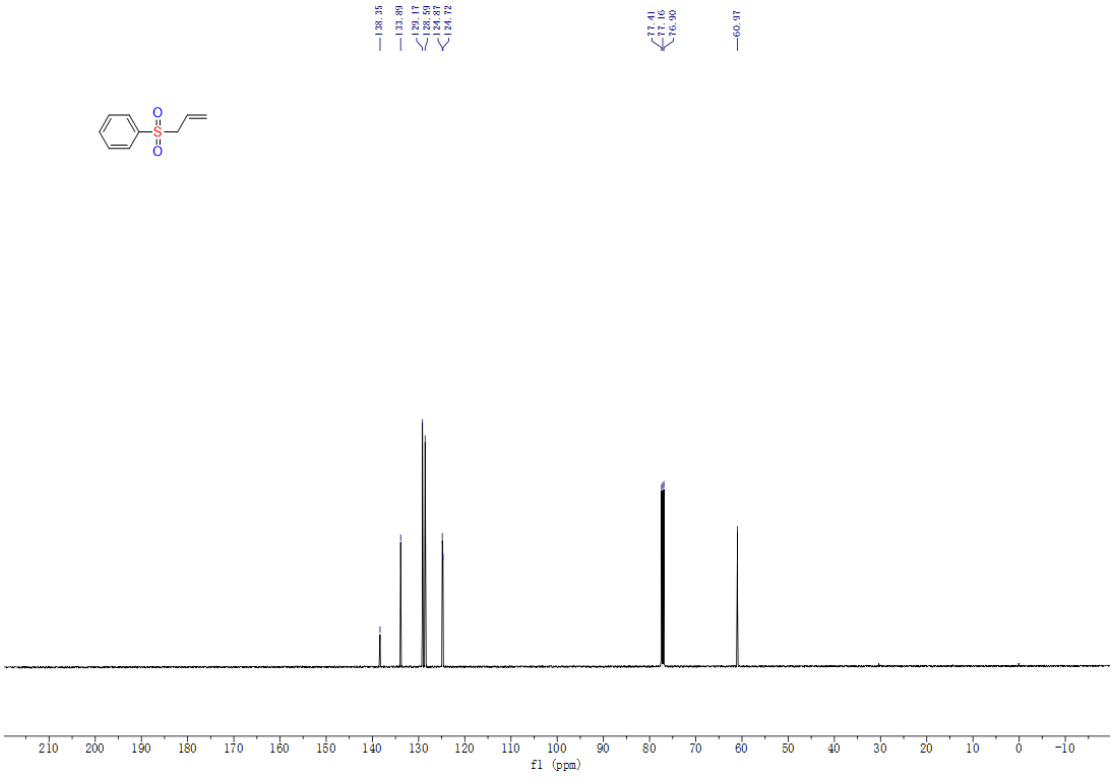
^{1}H NMR of compound **3v**



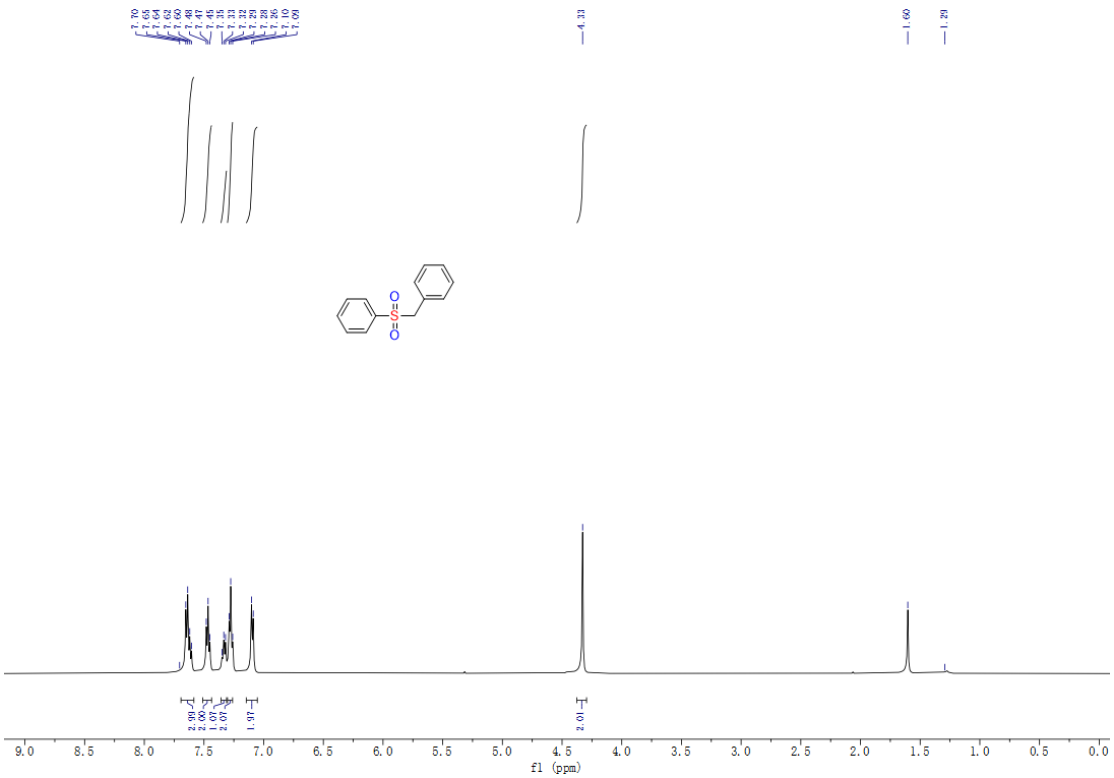
^{13}C NMR of compound **3v**



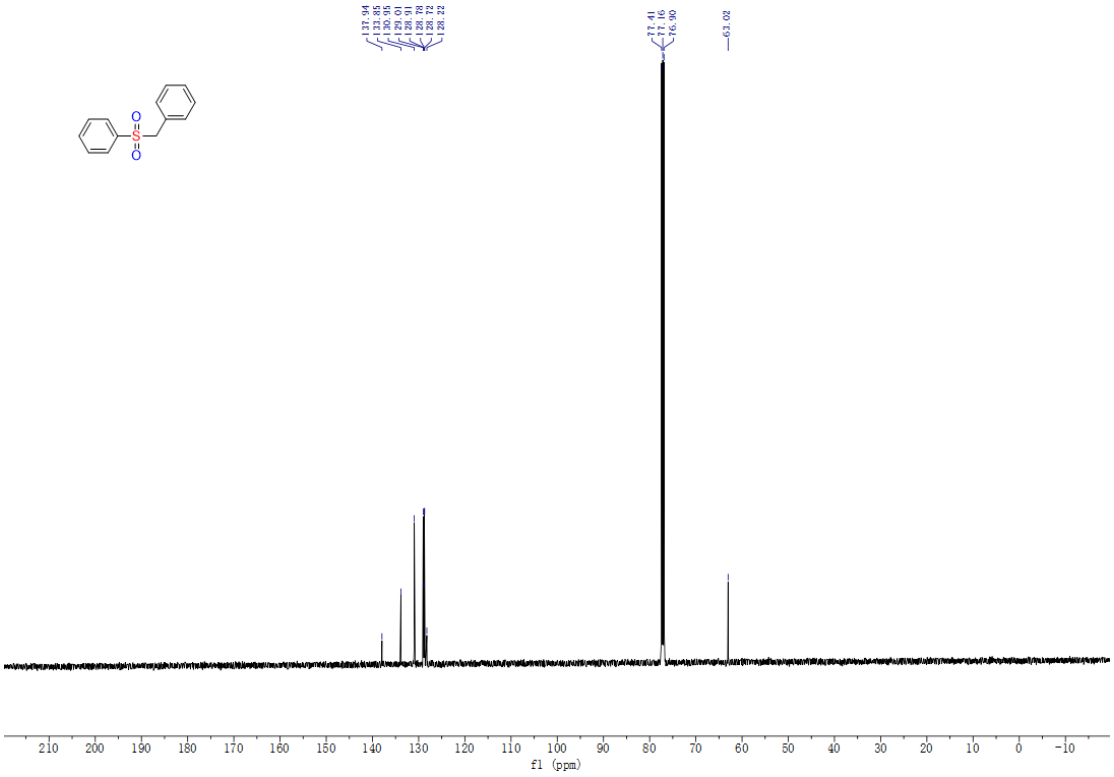
^{1}H NMR of compound **3w**



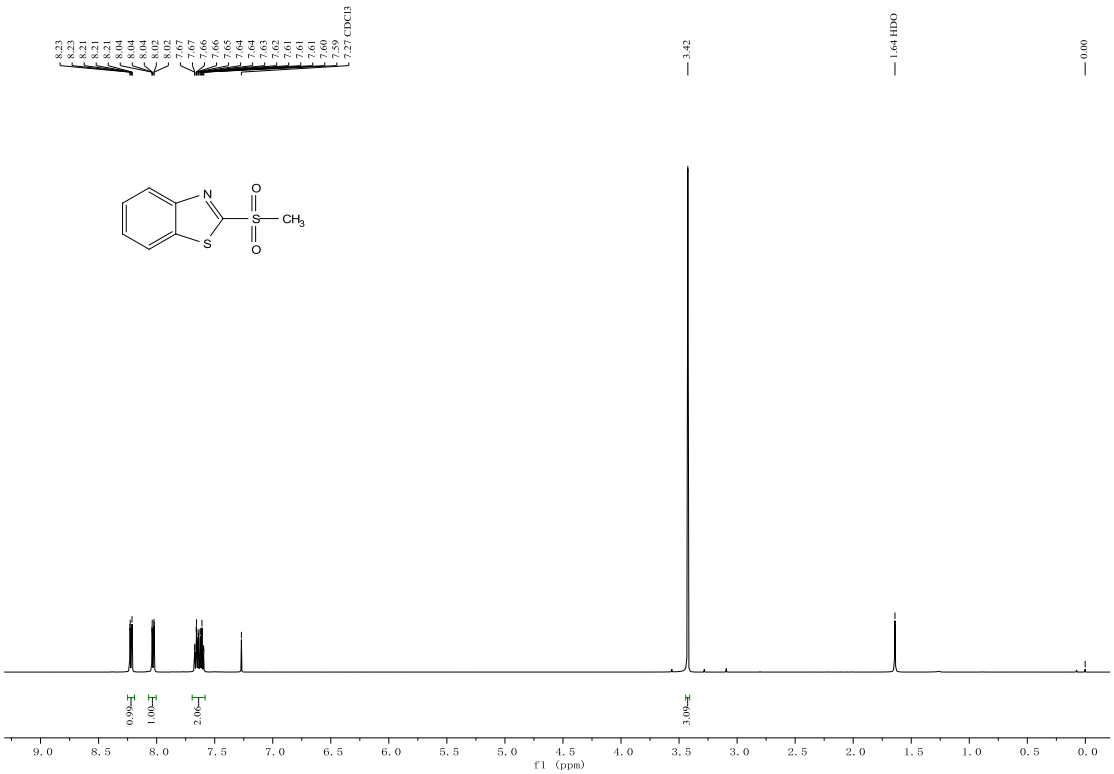
^{13}C NMR of compound **3w**



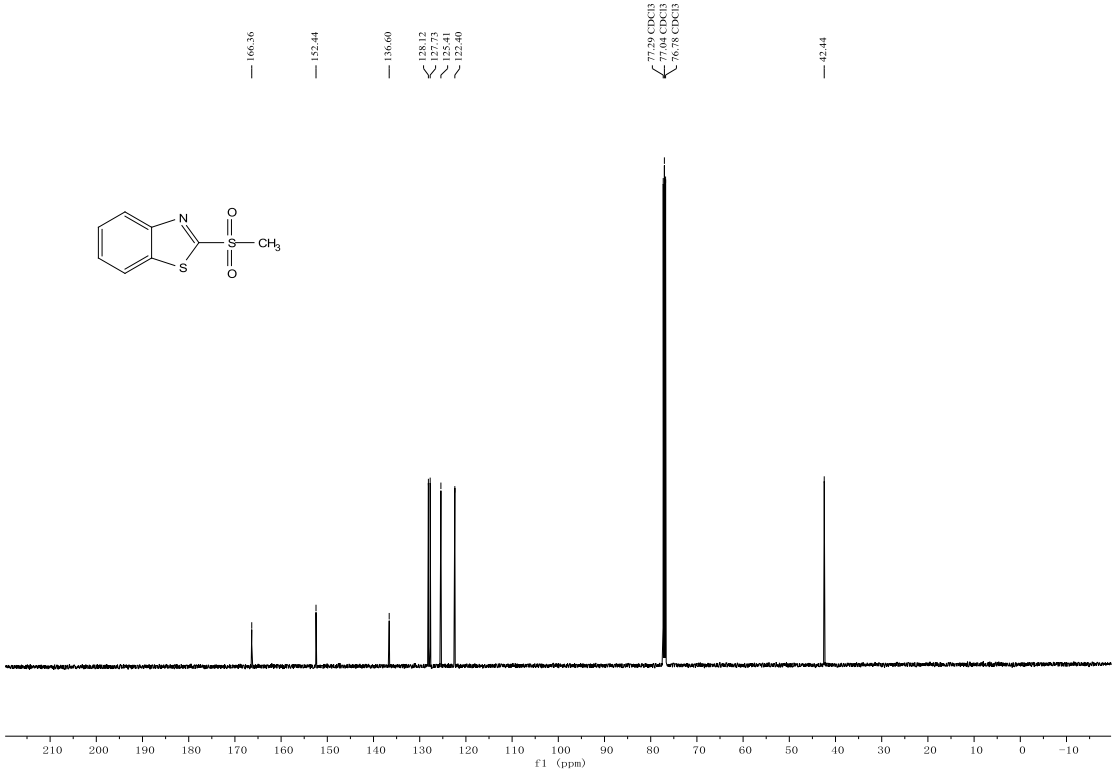
^{1}H NMR of compound **3x**



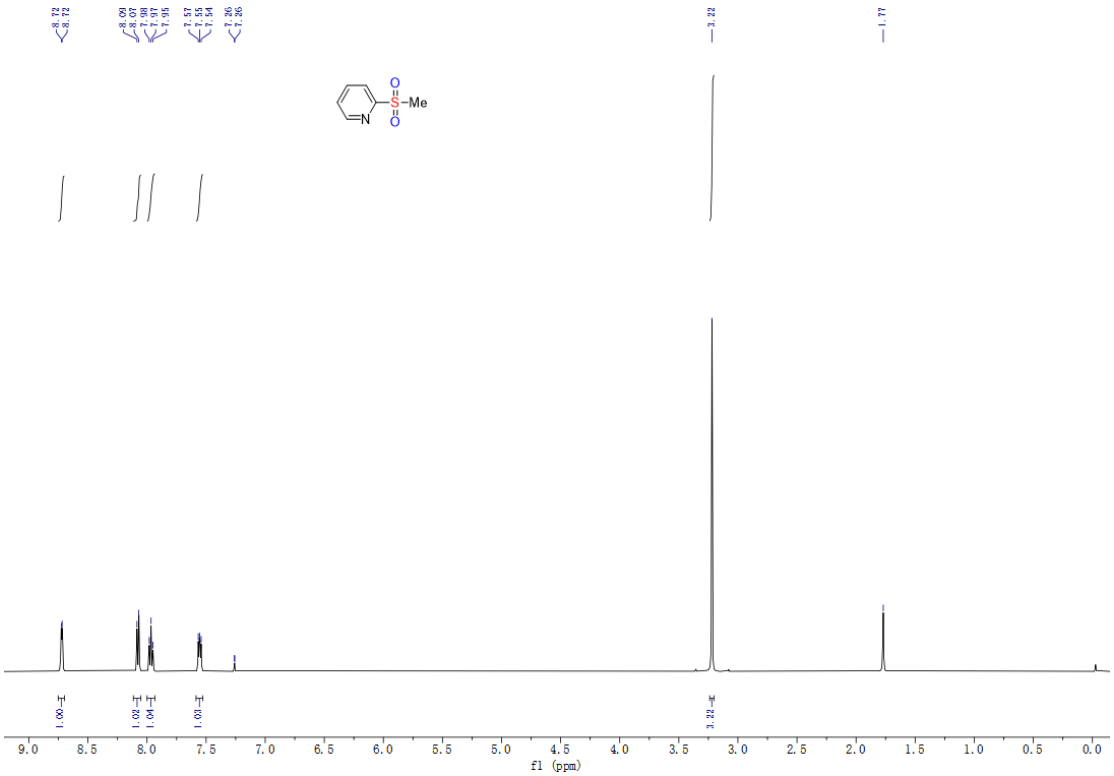
^{13}C NMR of compound **3x**



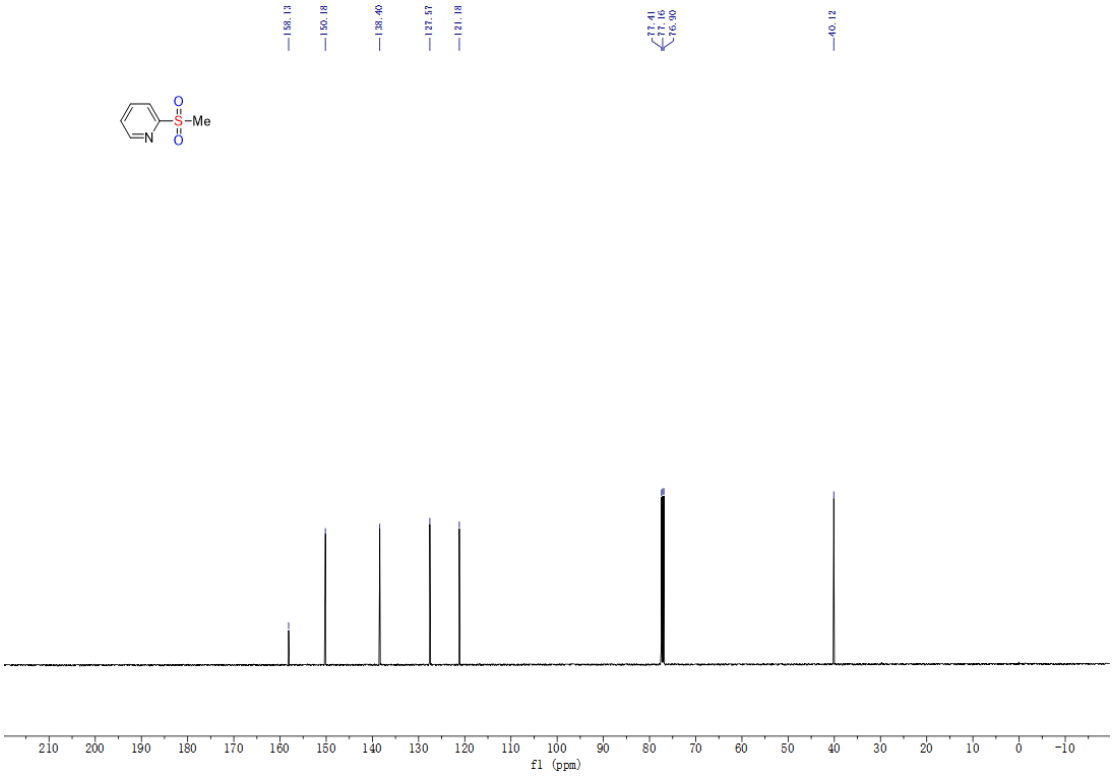
^{1}H NMR of compound **3y**



^{13}C NMR of compound **3y**



^{1}H NMR of compound **3z**



^{13}C NMR of compound **3z**