Supplementary Information

Visible-light-induced selective synthesis of sulfoxides from alkenes and thiols using air as the oxidant

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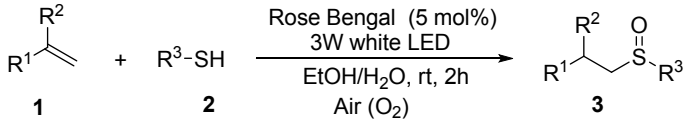
1. General information

All commercially available reagent grade chemicals were purchased from Aldrich, Acros, Alfa Aesar and Beijing Ouhe Chemical Company and used as received without further purification unless otherwise stated. All solvents were dried according to standard procedures. ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ on a Bruker Avance III 400 spectrometer with TMS as internal standard (500 MHz ^{1}H, 125 MHz ^{13}C) at room temperature, the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). Mass analyses and HRMS were obtained on a Finnigan-LCQDECA mass spectrometer and a Bruker Daltonics Bio-TOF-Q mass spectrometer by the ESI method, respectively. Column chromatography was performed on silica gel (200-300 mesh). There is 3.0 cm distance between the reactor and LEDs.

2. General procedure for visible-light-induced selective synthesis of sulfoxides from alkenes and thiols under air.

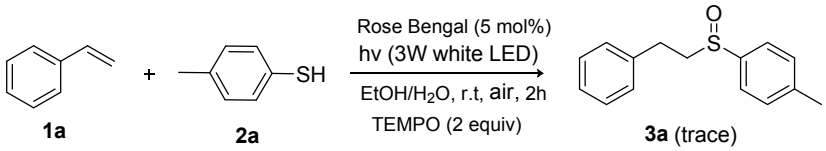


1 2 3

To a solution of thiol **2** (0.3 mmol) and Rose Bengal (0.01mmol, 5 mol %) in EtOH/H_2O (v_1/v_2=1/1) 2 mL was added alkene **1** (0.2 mmol). The reaction mixture was open to the air and stirred under the irradiation of 3w white LEDs at room temperature for 2h. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **3**.

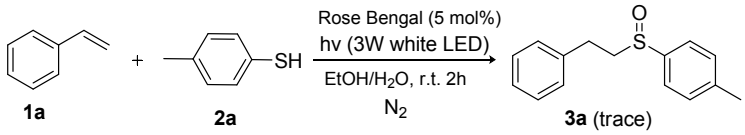
3. Preliminary mechanistic studies

3.1 The addition of TEMPO in the model reaction system.



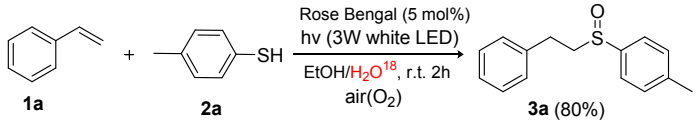
To a solution of 4-methylbenzenethiol **2a** (0.3 mmol), TEMPO (0.4 mmol), and Rose Bengal (0.01 mmol, 5 mol %) in EtOH/H_2O (v_1/v_2=1/1) 2 mL was added styrene **1a** (0.2 mmol). The reaction mixture was open to the air and stirred under the irradiation of 3w white LEDs at room temperature for 2h. After completion of the reaction, the solution was concentrated in vacuum, only a trace amount of desired product was detected.

3.2 The model reaction was carried out under N_2.



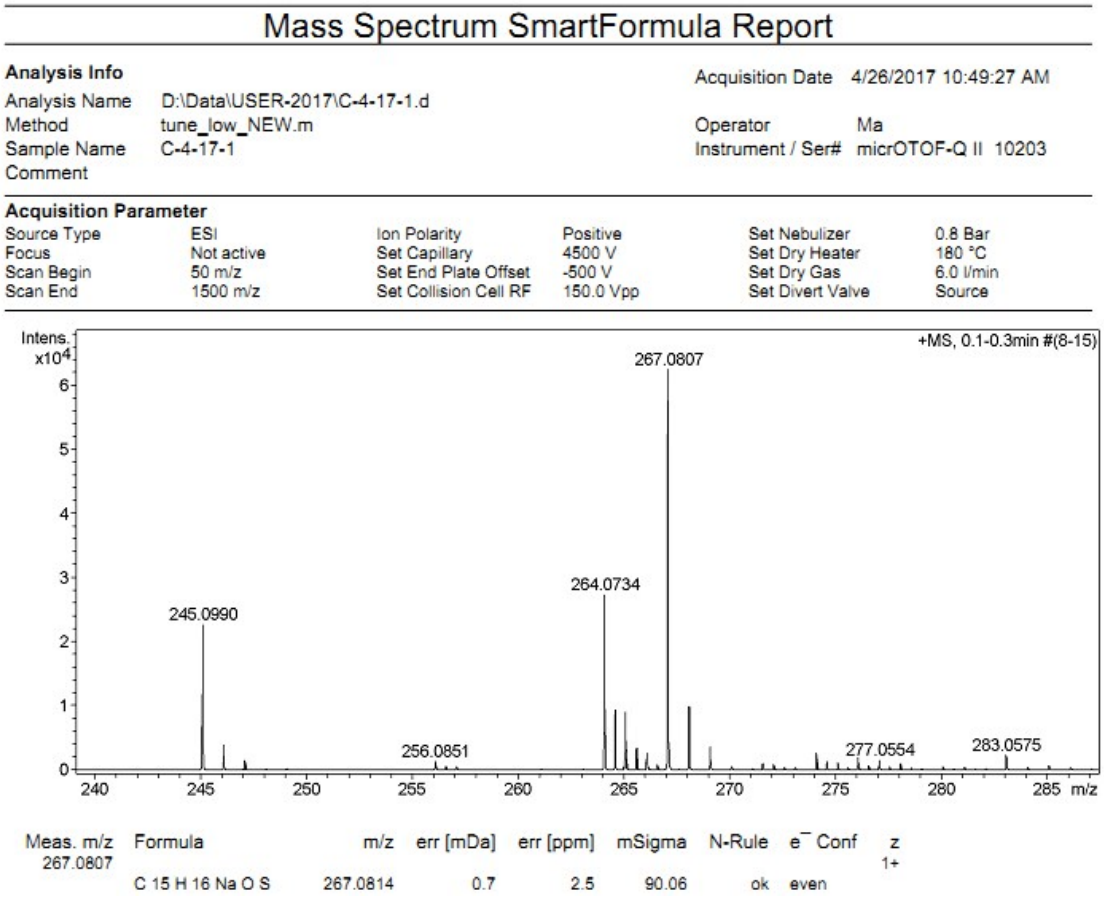
To a solution of 4-methylbenzenethiol **2a** (0.3 mmol), and Rose Bengal (0.01mmol, 5 mol %) in EtOH/H_2O (v_1/v_2=1/1) 2 mL was added styrene **1a** (0.2 mmol) under N_2. The reaction mixture was stirred under the irradiation of 3w white LEDs at room temperature for 2h. After completion of the reaction, the solution was concentrated in vacuum, only a trace amount of desired product was detected.

3.3 The model reaction was carried out under H_2O^{18} (^{18}O-labeling experiment).



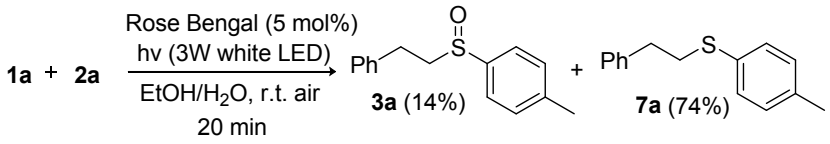
To a solution of 4-methylbenzenethiol **2a** (0.15 mmol), and Rose Bengal (0.005 mmol, 5 mol %) in EtOH/H_2O (v_1/v_2=1/1) 1 mL was added styrene **1a** (0.1 mmol). The reaction mixture was open to the air and stirred under the irradiation of 3w white LEDs at room temperature for 2h. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **3a** in 80% yield.

The HRMS spectrum of **3a** is demonstrated as bellow



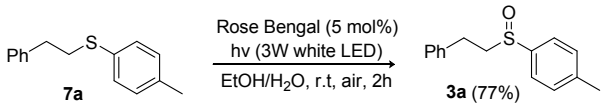
HRMS spectra of 3a

3.4 The model reaction was carried out for 20 min.



To a solution of 4-methylbenzenethiol **2a** (0.3 mmol) and Rose Bengal (0.01 mmol, 5 mol %) in EtOH/H_2O (v_1/v_2=1/1) 2 mL was added styrene **1a** (0.2 mmol). The reaction mixture was open to the air and stirred under the irradiation of 3w white LEDs at room temperature for 20min. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the product **3a** and **7a** in 14% and 74% yields, respectively.

3.5 The transformation of 7a under the standard conditions.



To a solution of Rose Bengal (0.005 mmol, 5 mol %) in EtOH/H_2O (v_1/v_2=1/1) 2 mL was added sulfide **7a** (0.1 mmol). The reaction mixture was open to the air and stirred under the irradiation of 3w white LEDs at room temperature for 2h. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the product **3a** in 77% yield.

3.6 The UV-visible spectroscopy and Fluorescence quenching studies (Stern–Volmer Studies)

UV-visible spectroscopy of reaction solution was recorded on a SHIMADZU UV-3600 UV-visible spectrophotometer. The sample was prepared by mixing Bengal Rose, styrene and thiophenol with solvent (V[ethanol] : V[H_2O] = 1:1) (M[Bengal Rose] = 1.0×10^{-5}mol/L, M[styrene] = 2.0×10^{-4}mol/L, M[thiophenol] = 3.0×10^{-4}mol/L in a light path quartz UV cuvette. The UV-visible spectroscopy indicated that the maximum absorption wavelength of reaction solution was found to be 558 nm. The absorption was collected and the result was listed in Figure S1.

The fluorescence emission intensity of reaction solution was recorded on a Fluoromax-4600 spectrofluorimeter. The excitation wavelength was fixed at 521nm, and the emission wavelength was masured at 576 nm. The sample was prepared by mixing Bengal Rose, styrene, thiophenol with solvent (V[ethanol] : V[H_2O] = 1:1) (M[Bengal Rose] = 1.0×10^{-5}mol/L, M[styrene] = 2.0×10^{-4}mol/L, M[thiophenol] = 3.0×10^{-4}mol) in a light path quartz fluoresence cuvette. The emission intensity was collected and the result was listed in Figure S2.

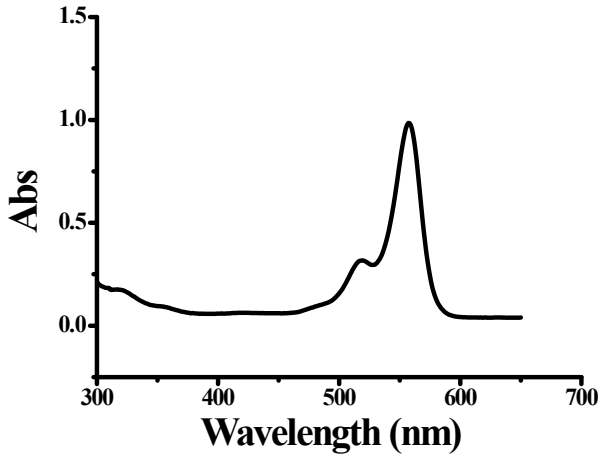


Figure S1. UV–vis spectra of the reaction mixture.

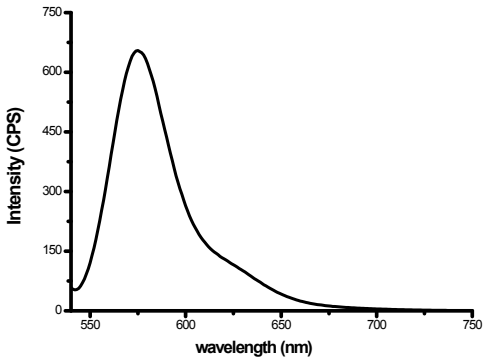


Figure S2. Fluorescence spectra of the photooxysulfonylation reaction mixture

Fluorescence quenching experiments

The fluorescence emission intensities were recorded on a Fluormax-4600 spespectrofluorimeter. The excitation wavelength was fixed at 521nm, and the emission wavelength was measured at 576 nm (emission maximum). The samples were prepared by mixing by Rose Bengal (1.0×10^{-5}mol/L) and different amount of Thiophenol in ethanol (total volume = 0.1 mL) in a light path quartz fluorescence cuvette. The concentration of Thiophenol stock solution is 3.0×10^{-6}mol/L in ethanol. For each quenching experiment, 0.1mL of Thiophenol stock solution was titrated to a mixed solution of Bengal Rose (0.1mL, in a total volume = 1.0 mL). Then the emission intensity was collected and the results were presented in Figure S3.

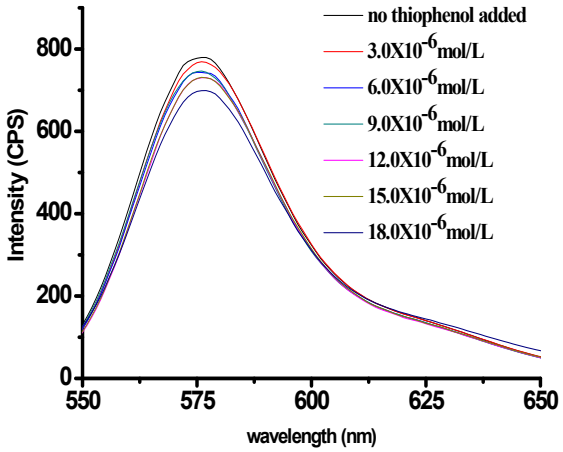


Figure S3. Quenching of Rose Bengal fluorescence emission in the presence of Thiophenol

An indeed fluorescence quenching phenomenon of Rose Bengal under various concentrations of Thiophenol was demonstrated in a curve of $[I_0/I]$ vs $C_{[Thiophenol]}$, as shown in Figure S4 (Stern-Volmer plots). For example, when $C_{[Thiophenol]}$ is 9×10^{-6}mol/L, the non-liner Stern-Volmer plots indicated energy transfer event operating between Bengal Rose's excited state and Thiophenol.

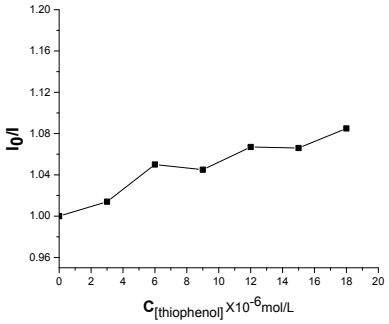


Figure S4. Stern-volmer plots

The fluorescence emission intensities were recorded on a Fluormax-4600 spespectrofluorimeter. The excitation wavelength was fixed at 521nm, and the emission wavelength was measured at 576 nm (emission maximum). The samples were prepared by mixing by Rose Bengal (1.0×10^{-5}mol/L) and different amount of styrene in ethanol (total volume = 0.1 mL) in a light path quartz fluorescence cuvette. The concentration of styrene stock solution is 2.0×10^{-6}mol/L in ethanol. For each quenching experiment,

0.1mL of Thiophenol stock solution was titrated to a mixed solution of Rose Bengal (0.1mL, in a total volume = 1.0 mL). Then the emission intensity was collected and the results were presented in Figure S5. An fluorescence quenching phenomenon of Bengal Rose under various concentrations of styrene was shown in Figure 6 (Stern-Volmer plots).

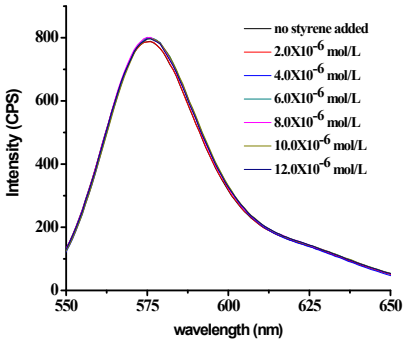


Figure S5. Quenching of Rose Bengal fluorescence emission in the presence of styrene

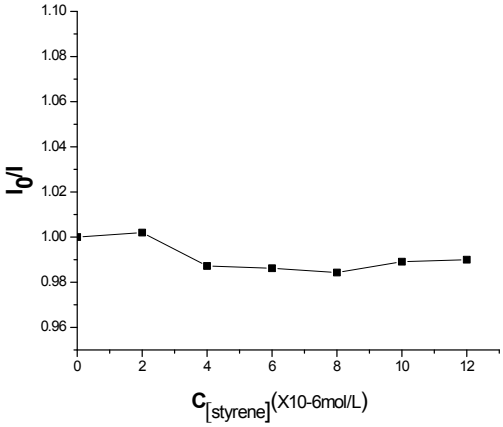
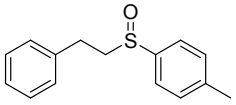
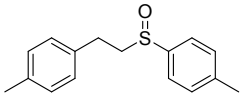


Figure S6. Stern-volmer plots

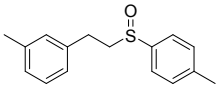
4. Characterization data of products 3a-3v



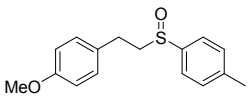
1-methyl-4-(phenethylsulfinyl)benzene, Compound **3a** was obtained in 89% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.55 (d, J = 8.2 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.31 (t, J = 7.2 Hz, 2H), 7.24 (t, J = 7.3 Hz, 1H), 7.20 (d, J = 7.1 Hz, 2H), 3.11-3.04 (m, 3H), 2.94-2.90 (m, 1H), 3.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.5, 140.4, 138.9, 130.0, 128.7, 128.5, 126.7, 124.1, 58.4, 28.2, 21.4; HRMS calc. for $C_{15}H_{16}OSNa$ $(M+Na)^+$, 267.0820, found, 267.0813.



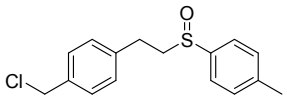
1-methyl-4-(4-methylphenethylsulfinyl)benzene, Compound **3b** was obtained in 72% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 8.1 Hz, 2H), 7.06 (d, J = 8.1 Hz, 2H), 3.05-2.99 (m, 3H), 2.88-2.82 (m, 1H), 2.41 (s, 3H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.5, 140.5, 136.2, 135.8, 130.0, 129.4, 128.4, 124.1, 58.5, 27.8, 21.4, 21.0; HRMS calc. for $C_{16}H_{18}OSNa$ $(M+Na)^+$, 281.0976, found, 281.0979.



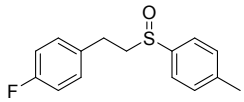
1-methyl-3-(2-(p-tolylsulfinyl)ethyl)benzene, Compound **3c** was obtained in 72% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.44 (d, J = 8.2 Hz, 2H), 7.25 (d, J = 8.1 Hz, 2H), 7.09 (t, J = 7.5 Hz, 1H), 6.95-6.88 (m, 3H), 2.98-2.92 (m, 3H), 2.81-2.76 (m, 1H), 2.34 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 140.4, 139.4, 137.8, 137.3, 128.9, 128.3, 127.6, 126.3, 124.5, 123.0, 57.3, 27.1, 20.4, 20.3; HRMS calc. for $C_{16}H_{18}OSNa$ $(M+Na)^+$, 281.0976; found, 281.0981.



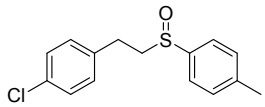
1-methoxy-4-(2-(p-tolylsulfinyl)ethyl)benzene, Compound **3d** was obtained in 71% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 8.6 Hz, 2H), 6.82 (d, J = 8.6 Hz, 2H), 3.77 (s, 3H), 3.04-2.98 (m, 3H), 2.85-2.82 (m, 1H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 158.4, 141.5, 140.5, 130.8, 130.0, 129.5, 124.1, 114.1, 58.7, 55.3, 27.4, 21.4; HRMS calc. for $C_{16}H_{18}O_2SNa$ $(M+Na)^+$, 297.0925; found, 297.0921.



1-(chloromethyl)-4-(2-(p-tolylsulfinyl)ethyl)benzene, Compound **3f** was obtained in 55% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.2 Hz, 2H), 7.34-7.30 (m, 4H), 7.17 (d, J = 8.1 Hz, 2H), 4.55 (s, 2H), 3.11-2.99 (m, 3H), 2.91-2.85 (m, 1H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.6, 140.3, 139.2, 135.9, 130.0, 129.0, 129.0, 124.1, 58.1, 46.0, 27.8, 21.4; HRMS calc. for $C_{16}H_{17}ClOSNa$ $(M+Na)^+$, 315.0586; found, 315.0589.

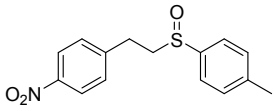


1-fluoro-4-(2-(p-tolylsulfinyl)ethyl)benzene, Compound **3g** was obtained in 53% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.15-7.12 (m, 2H), 6.97 (t, J = 8.7 Hz, 2H), 3.08-2.98 (m, 3H), 2.89-2.84 (m, 1H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 161.7 (d, 243.4), 141.6, 140.3, 134.5 (d, J = 3.2 Hz), 130.1 (d, J = 7.9 Hz), 130.0, 124.0, 115.5 (d, J = 21.2 Hz), 58.4, 27.4, 21.4; HRMS calc. for $C_{15}H_{15}FOSNa$ $(M+Na)^+$, 285.0725; found, 285.0723.

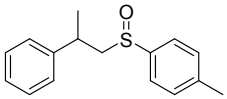


1-chloro-4-(2-(p-tolylsulfinyl)ethyl)benzene, Compound **3e** was obtained in 61% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.1 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.4 Hz, 2H), 7.10 (d, J = 8.4 Hz, 2H), 3.09-

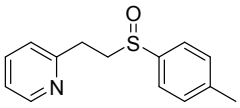
2.97 (m, 3H), 2.88-2.82 (m, 1H), 2.42 (s, 3H); [1]; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.6, 140.2, 137.3, 132.5, 130.0, 130.0, 128.9, 124.0, 58.0, 27.5, 21.4; HRMS calc. for $C_{15}H_{15}ClOSNa$ $(M+Na)^+$, 301.0430; found, 301.0431.



1-methyl-4-(4-nitrophenethylsulfinyl)benzene, Compound **3h** was obtained in 40% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.15 (d, J = 8.7 Hz, 2H), 7.51 (d, J = 8.1 Hz, 2H), 7.34 (d, J = 8.4 Hz, 4H), 3.25-3.19 (m, 1H), 3.11-2.95 (m, 3H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 146.9, 146.6, 141.9, 139.8, 130.1, 129.5, 124.0, 124.0, 57.1, 27.8, 21.4; HRMS calc. for $C_{15}H_{15}NO_3SNa$ $(M+Na)^+$, 312.0670; found, 312.0675.

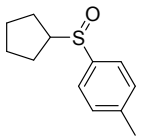


1-methyl-4-(2-phenylpropylsulfinyl)benzene, Compound **3i** was obtained in 60% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.1 Hz, 1H), 7.47 (d, J = 8.2 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.31-7.27 (m, 4H), 7.26-7.18 (m, 2H), 3.41-3.30 (m, 1H), 3.12 (dd, J_1 = 4.6 Hz, J_2 = 12.9 Hz, 0.51H), 3.06 (dd, J_1 = 5.5 Hz, J_2 = 12.9 Hz, 0.52H), 2.89 (dd, J_1 = 9.7 Hz, J_2 = 12.9 Hz, 0.52H), 2.79 (dd, J_1 = 10.3 Hz, J_2 = 12.9 Hz, 0.51H), 2.40 (s, 3H), 1.51 (d, J = 6.9 Hz, 1.51H), 1.40 (d, J = 7.0 Hz, 1.55H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 144.6, 143.9, 141.6, 141.5, 141.4, 141.0, 130.0, 130.0, 128.8, 128.7, 127.2, 127.0, 126.9, 126.8, 124.1, 123.9, 67.3, 66.7, 35.4, 34.6, 22.3, 21.4, 20.7; HRMS calc. for $C_{16}H_{18}OSNa$ $(M+Na)^+$, 281.0976; found, 281.0977.

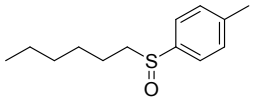


3-(2-(p-tolylsulfinyl)ethyl)pyridine, Compound **3j** was obtained in 90% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.50 (d, J = 4.7 Hz, 1H), 7.60-7.57 (m, 1H), 7.53 (d, J = 7.9 Hz, 2H), 7.31 (d, J = 7.4 Hz, 2H), 7.18 (d, J = 7.7 Hz,

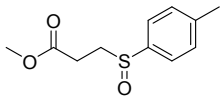
1H), 7.14-7.11 (m, 1H), 3.36-3.24 (m, 2H), 3.19-3.14 (m, 1H), 3.08-3.03 (m, 1H), 2.40 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 158.6, 149.4, 141.4, 140.4, 136.6, 129.9, 124.1, 123.4, 121.7, 56.0, 30.2, 21.4; HRMS calc. for $C_{14}H_{15}NOSNa$ $(M+Na)^+$, 268.0772; found, 268.0779.



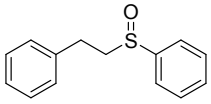
1-(cyclopentylsulfinyl)-4-methylbenzene，Compound **3k** was obtained in 16% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.52 (d, J = 8.1 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 3.13-3.07 (m, 1H), 2.41 (s, 3H), 2.12-2.08 (m, 1H), 1.79-1.67 (m, 5H), 1.63-1.59 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.3, 140.4, 129.7, 124.7, 64.4, 27.6, 26.1, 25.7, 25.2, 21.4; HRMS calc. for $C_{12}H_{16}OSNa$ $(M+Na)^+$, 231.0820; found, 231.0825.



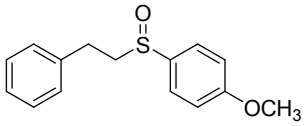
1-(hexylsulfinyl)-4-methylbenzene, Compound **3l** was obtained in 18% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 2.82-2.72 (m, 2H), 2.42 (s, 3H), 1.76-1.56 (m, 3H), 1.47-1.37 (m, 2H), 1.29-1.27 (m, 3H), 0.87 (t, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.4, 140.9, 129.9, 124.1, 57.5, 31.4, 28.4, 22.4, 22.2, 21.4, 14.0; HRMS calc. for $C_{13}H_{20}OSNa$ $(M+Na)^+$, 247.1133; found, 247.1135.



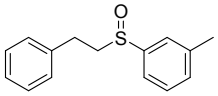
Methyl3-(p-tolylsulfinyl)propanoate, Compound **3m** was obtained in 43% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.51 (d, J = 8.1 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 3.66 (s, 3H), 3.23-3.18 (m, 1H), 2.98-2.93 (m, 1H), 2.85-2.79 (m, 1H), 2.58-2.51 (m, 1H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 171.7, 141.7, 139.6, 130.0, 124.1, 52.1, 51.2, 26.0, 21.4; HRMS calc. for $C_{11}H_{14}O_3SNa$ $(M+Na)^+$, 249.0561; found, 249.0563.



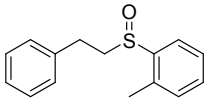
Phenethylsulfinylbenzene, Compound **3n** was obtained in 60% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.64-7.63 (m, 2H), 7.54-7.49 (m, 3H), 7.30-7.27 (m, 2H), 7.23-7.17 (m, 3H), 3.13-2.99 (m, 3H), 2.92-2.86 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 143.7, 138.8, 131.0, 129.3, 128.8, 128.6, 126.7, 124.0, 58.3, 28.2; HRMS calc. for $C_{14}H_{14}OSNa$ $(M+Na)^+$, 253.0663; found, 253.0661.



1-methoxy-4-(phenethylsulfinyl)benzene, Compound **3o** was obtained in 68% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.58 (d, J = 8.8 Hz, 2H), 7.29 (t, J = 7.3 Hz, 2H), 7.22 (t, J = 7.4 Hz, 1H), 7.18 (d, J = 7.2 Hz, 2H), 7.03 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H), 3.06-3.01 (m, 3H), 2.91-2.88 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 162.0, 138.9, 134.5, 128.7, 128.5, 126.7, 126.0, 114.8, 58.5, 55.5, 28.3; HRMS calc. for $C_{15}H_{16}O_2SNa$ $(M+Na)^+$, 283.0769; found, 283.0773.

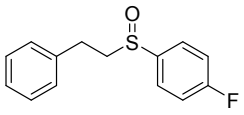


1-methyl-3-(phenethylsulfinyl)benzene, Compound **3p** was obtained in 65% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.47 (s, 1H), 7.40-7.39 (m, 2H), 7.30-7.27 (m, 3H), 7.23-7.17 (m, 3H), 3.13-3.01 (m, 3H), 2.93-2.88 (m, 1H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 143.6, 139.5, 138.9, 131.8, 129.1, 128.7, 128.6, 126.7, 124.3, 121.1, 58.3, 28.3, 21.4; HRMS calc. for $C_{13}H_{16}OSNa$ $(M+Na)^+$, 267.0820; found, 267.0825.

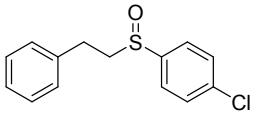


1-methyl-2-(phenethylsulfinyl)benzene, Compound **3q** was obtained in 63% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.94 (dd, J_1 =

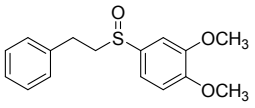
1.3 Hz, J_2 = 1.2 Hz, 1H), 7.43 (t, J = 7.3 Hz, 1H), 7.39-7.36 (m, 1H), 7.29 (t, J = 7.2 Hz, 2H), 7.23-7.18 (m, 4H), 3.16-3.03 (m, 2H), 2.99-2.92 (m, 2H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.9, 138.9, 134.3, 130.7, 128.7, 128.5, 127.2, 126.7, 124.0, 56.4, 29.7, 28.5, 18.1; HRMS calc. for $C_{15}H_{16}OSNa$ $(M+Na)^+$, 267.0820; found, 267.0823.



1-fluoro-4-(phenethylsulfinyl)benzene, Compound **3r** was obtained in 56% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.65-7.62 (m, 2H), 7.29 (t, J = 7.2 Hz, 2H), 7.25-7.21 (m, 3H), 7.18 (d, J = 7.1 Hz, 2H), 3.12-3.01 (m, 3H), 2.92-2.87 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 164.4 (d, J = 250.0 Hz), 139.1 (d, J = 3.1 Hz), 138.6, 128.8, 128.5, 126.8, 126.3 (d, J = 8.8 Hz), 116.6 (d, J = 22.4 Hz), 58.6, 28.2; HRMS calc. for $C_{14}H_{13}FOSNa$ $(M+Na)^+$, 271.0569; found, 271.0571.

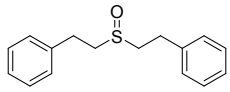


1-chloro-4-(phenethylsulfinyl)benzene, Compound **3s** was obtained in 71% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.57 (d, J = 8.5 Hz, 2H), 7.51 (d, J = 8.5 Hz, 2H), 7.29 (t, J = 7.3 Hz, 2H), 7.22 (t, J = 7.3 Hz, 1H), 7.17 (d, J = 7.3 Hz, 2H), 3.13-2.98 (m, 3H), 2.91-2.85 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 142.2, 138.5, 137.3, 129.6, 128.8, 128.5, 126.8, 125.5, 58.4, 28.1; HRMS calc. for $C_{14}H_{13}ClOSNa$ $(M+Na)^+$, 287.0273; found, 287.0276.

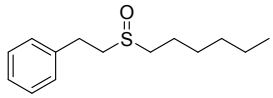


1,2-dimethoxy-4-(phenethylsulfinyl)benzene, Compound **3t** was obtained in 61% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.29 (t, J = 7.2 Hz, 2H), 7.24-7.21 (m, 2H), 7.18 (d, J = 7.1 Hz, 2H), 7.13 (dd, J_1 = 2.0 Hz, J_2 = 8.3 Hz, 1H), 6.96 (d, J = 8.4 Hz, 1H), 3.95 (s, 3H), 3.93 (s, 3H), 3.07-3.01 (m, 3H), 2.95-2.90 (m,

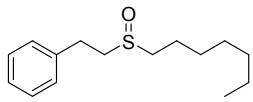
1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 151.4, 150.1, 138.8, 134.9, 128.7, 128.5, 126.7, 117.4, 111.2, 106.4, 58.6, 56.2, 56.1, 28.4; HRMS calc. for $C_{16}H_{18}O_3SNa$ $(M+Na)^+$, 313.0874; found, 313.0877.



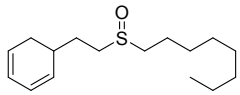
2,2'-sulfinylbis(ethane-2,1-diyl)dibenzene, Compound **3u** was obtained in 90% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.24 (t, J = 7.2 Hz, 4H), 7.18-7.14 (m, 6H), 3.08-2.96 (m, 4H), 2.94-2.89 (m, 2H), 2.85-2.79 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 137.8, 127.8, 127.5, 125.8, 52.9, 27.9; HRMS calc. for $C_{16}H_{18}OSNa$ $(M+Na)^+$, 281.0976; found, 281.0973.



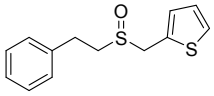
(2-(hexylsulfinyl)ethyl)benzene, Compound **3v** was obtained in 84% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.32 (t, J = 7.6 Hz, 2H), 7.26-7.23 (m, 3H), 3.15-3.04 (m, 2H), 2.98-2.86 (m, 2H), 2.76-2.70 (m, 1H), 2.65-2.59 (m, 1H), 1.78-1.72 (m, 2H), 1.47-1.41 (m, 2H), 1.32-1.29 (m, 4H), 0.89 (t, J = 6.9 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 139.0, 128.8, 128.6, 126.7, 53.8, 52.6, 31.3, 28.9, 28.5, 22.6, 22.4, 14.0; HRMS calc. for $C_{14}H_{22}OSNa$ $(M+Na)^+$, 261.1289; found, 261.1287.



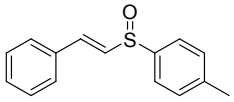
(2-(heptylsulfinyl)ethyl)benzene, Compound **3w** was obtained in 75% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.32 (t, J = 7.6 Hz, 2H), 7.26-7.23 (m, 3H), 3.17-3.05 (m, 2H), 2.98-2.87 (m, 2H), 2.76-2.71 (m, 1H), 2.66-2.60 (m, 1H), 1.80-1.72 (m, 2H), 1.46-1.35 (m, 2H), 1.33-1.27 (m, 6H), 0.88 (t, J = 6.7 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 139.0, 128.8, 128.6, 126.8, 53.8, 52.6, 31.5, 28.9, 28.9, 28.8, 22.6, 22.5, 14.0; HRMS calc. for $C_{15}H_{24}OSNa$ $(M+Na)^+$, 275.1446; found, 275.1447.



(2-(octylsulfinyl)ethyl)benzene, Compound **3x** was obtained in 82% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.32 (t, J = 7.7 Hz, 2H), 7.26-7.23 (m, 3H), 3.17-3.04 (m, 2H), 2.98-2.86 (m, 2H), 2.76-2.70 (m, 1H), 2.65-2.59 (m, 1H), 1.78-1.73 (m, 2H), 1.46-1.40 (m, 2H), 1.33-1.26 (m, 8H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 139.0, 128.8, 128.6, 126.8, 53.8, 52.6, 31.7, 30.9, 29.2, 29.0, 28.9, 22.6, 22.6, 14.1; HRMS calc. for $C_{16}H_{26}OSNa$ $(M+Na)^+$, 289.1602; found, 289.1605.

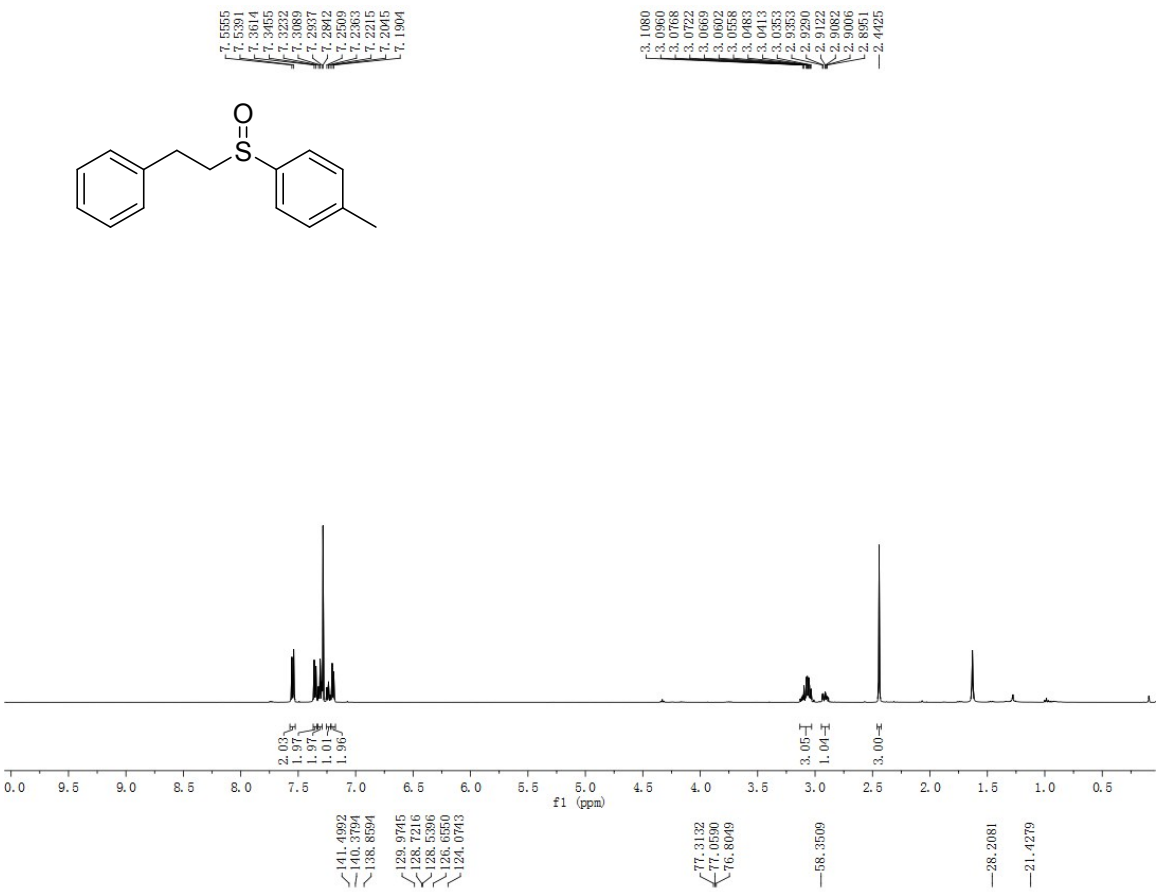


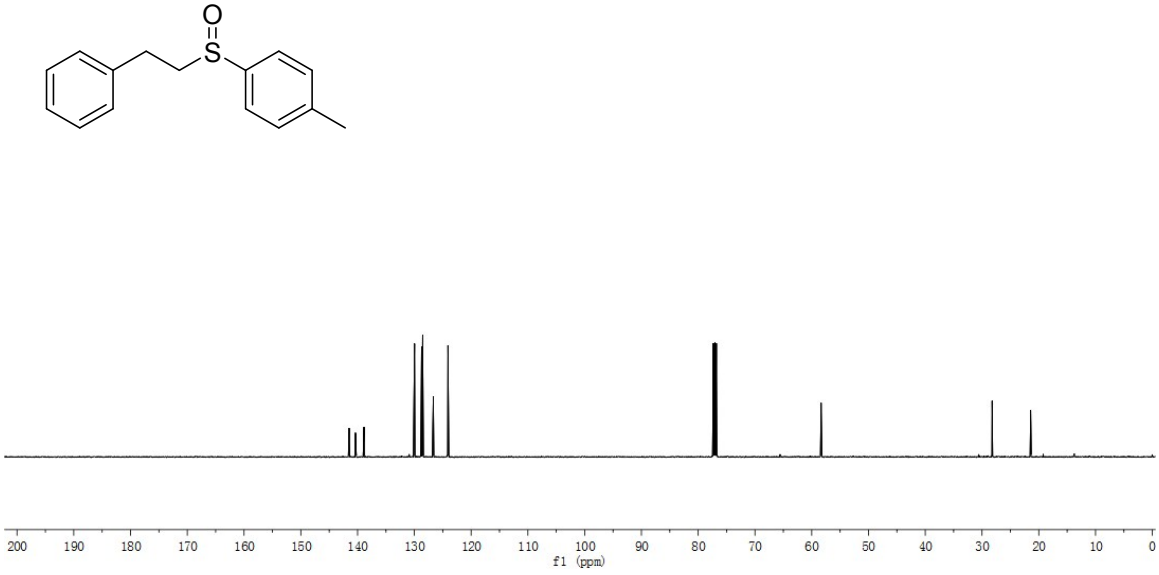
2-(2-(phenethylsulfinyl)ethyl)thiophene, Compound **3y** was obtained in 60% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.32-7.29 (m, 3H), 7.25-7.19 (m, 3H), 7.04-7.02 (m, 2H), 4.19 (s, 2H), 3.13-3.00 (m, 2H), 2.88-2.84 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 138.8, 130.2, 128.8, 128.8, 128.6, 127.6, 126.8, 126.8, 52.1, 52.1, 28.5; HRMS calc. for $C_{13}H_{14}OS_2Na$ $(M+Na)^+$, 273.0384; found, 273.0381.

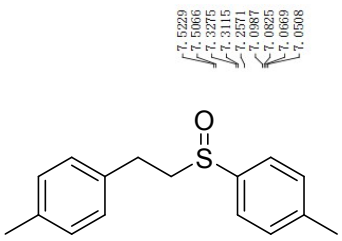


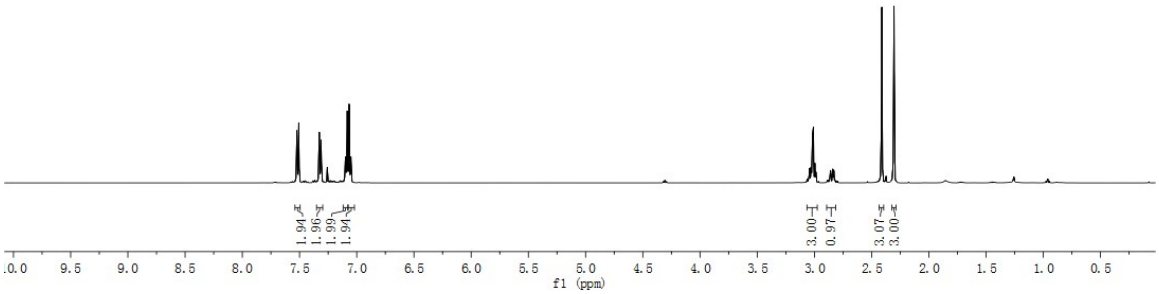
(*E*)-1-methyl-4-(styrylsulfinyl)benzene, Compound **3z** was obtained in 29% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.57 (d, J = 8.2 Hz, 2H), 7.46-7.44 (m, 2H), 7.38-7.31 (m, 6H), 6.81 (d, J = 15.5 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 141.8, 140.7, 136.1, 133.8, 133.1, 130.2, 130.0, 128.9, 127.8, 125.0, 21.5; HRMS calc. for $C_{15}H_{14}OSNa$ $(M+Na)^+$, 265.0663; found, 265.0661.

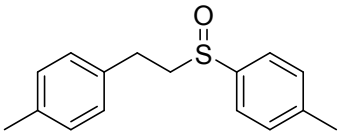
5. Copies of NMR Spectra for 3a−3z

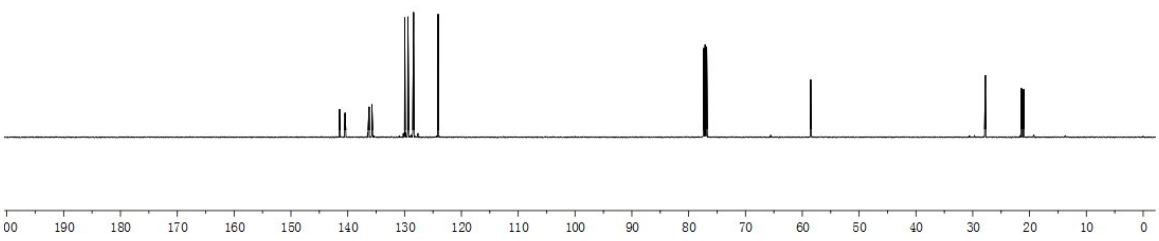


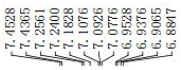








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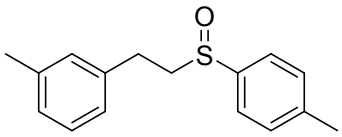
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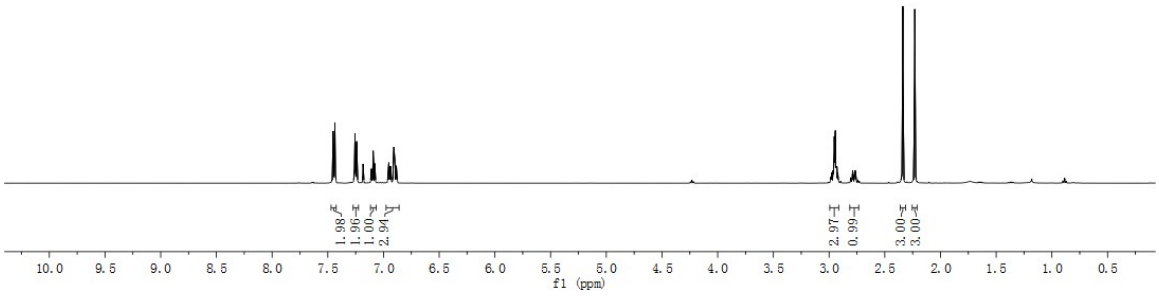
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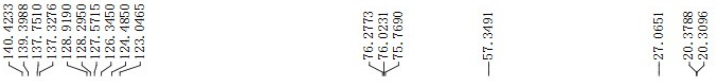
f1 (ppm)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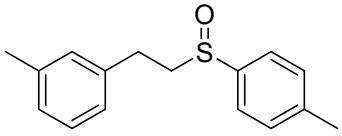
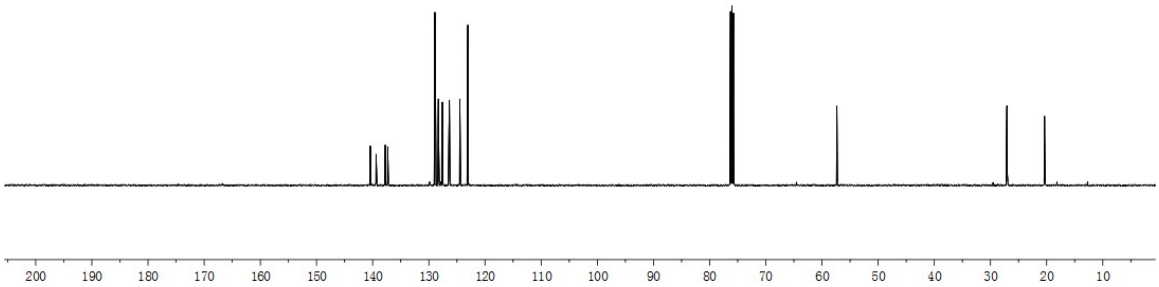
137.7510
137.3276
128.9190
128.2950
127.5715
126.3450
124.4850
123.0465
76.2773
76.0231
75.7690
57.3491
27.0651
20.3788
20.3096


O
S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90
80
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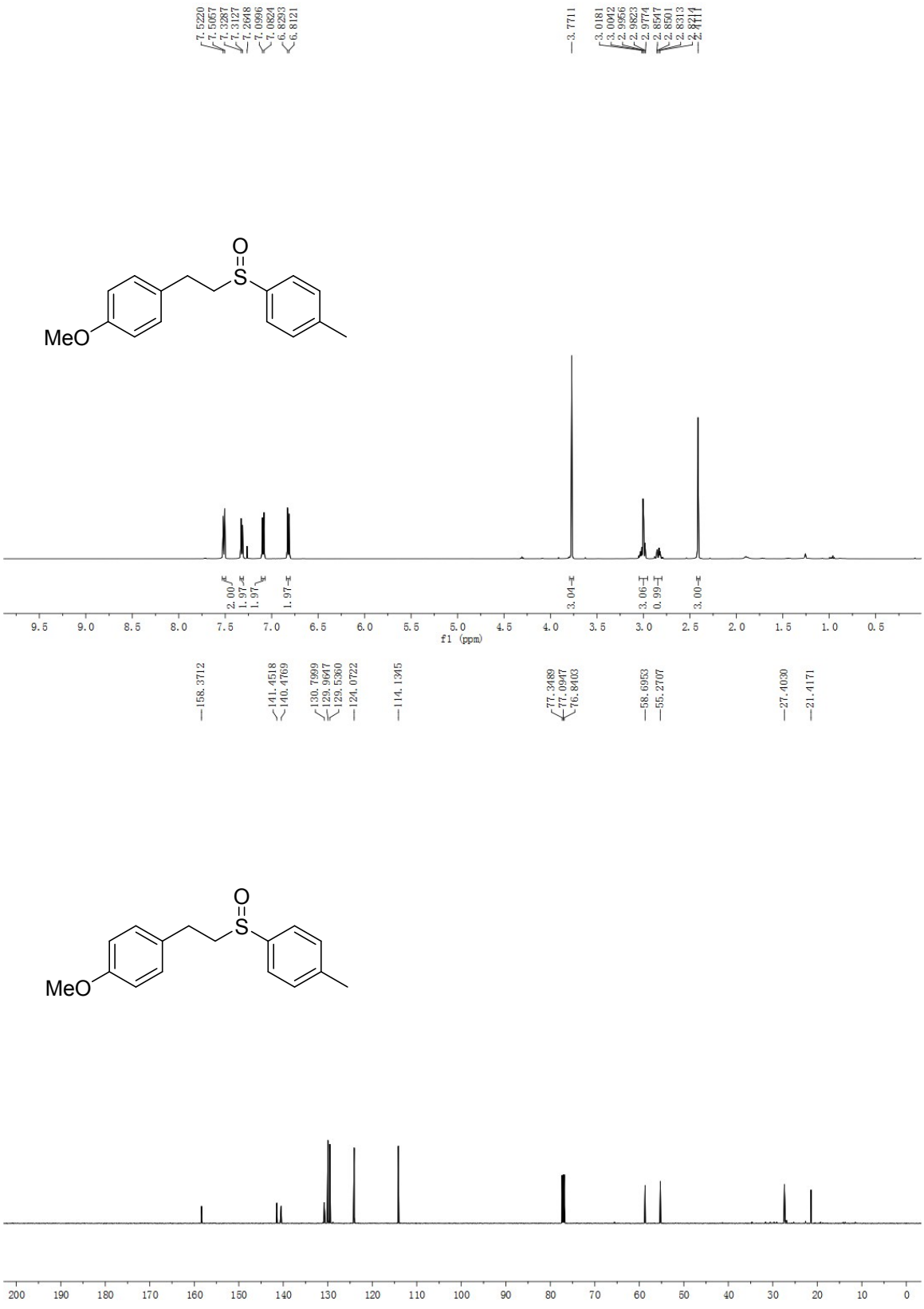
60
50
40
30
20
10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7.3287
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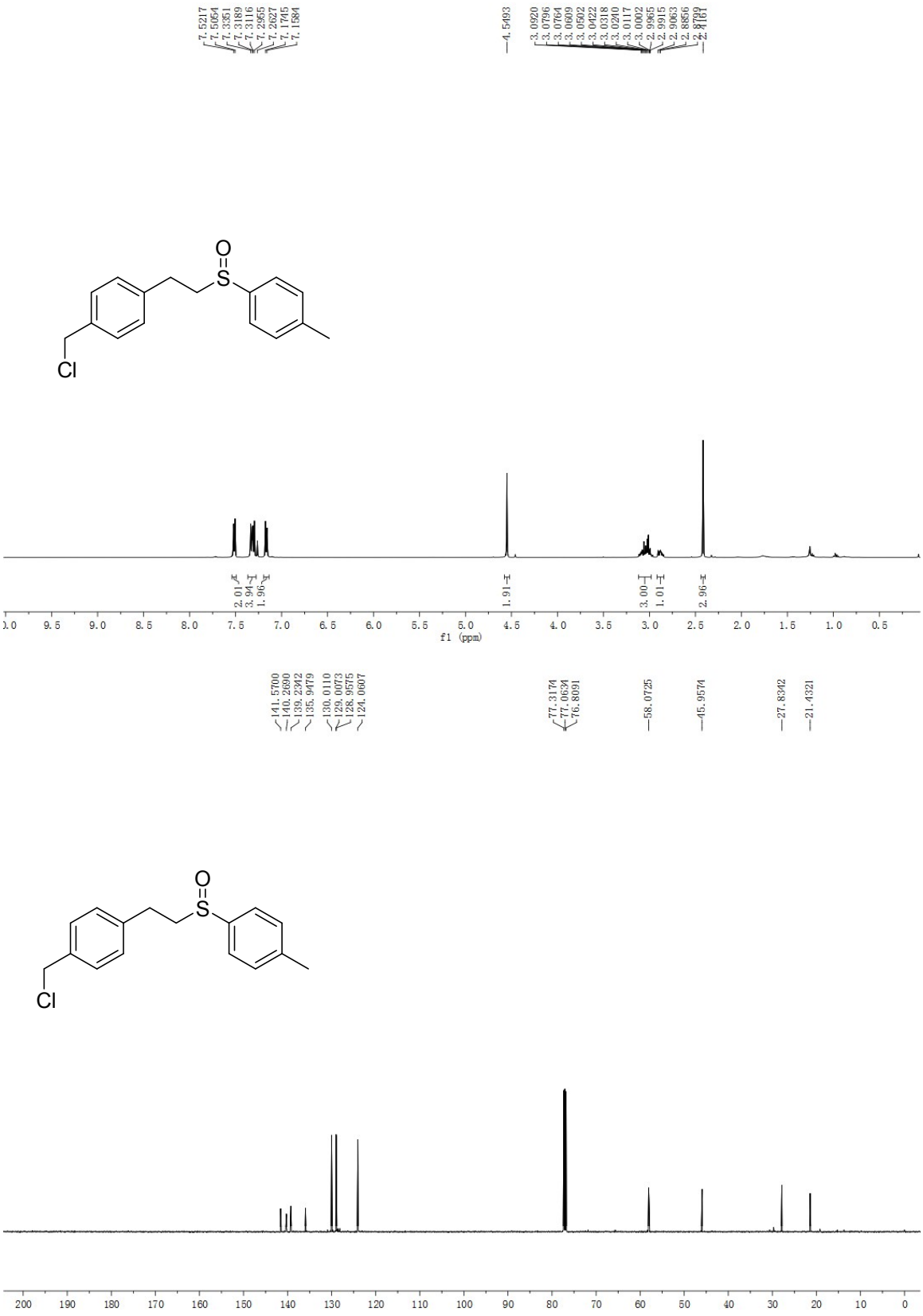
7.2648
7.0996
7.0824
6.8293
6.8121
3.7711
3.0181
3.0042
2.9956
2.9823
2.9774
2.8547
2.8501
2.8313
2.8214
O
S
MeO
2.00
1.97
1.97
1.97
3.04
3.06
0.99
3.00
f1 (ppm)
158.3712
141.4518
140.4769
130.7999
129.9647
129.5360
124.0722
114.1345
77.3489
77.0947
76.8403
58.6953
55.2707
27.4030
21.4171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7.1745
7.1584
4.5493
3.0920
3.0796
3.0764
3.0609
3.0502
3.0422
3.0318
3.0240
3.0117
3.0002
2.9965
2.9915
2.9063
2.8856
O
S
Cl
2.01
3.94
1.96
1.91
3.00
1.01
2.96
f1 (ppm)
141.5700
140.2690
139.2342
135.9479
130.0110
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124.0607
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77.0634
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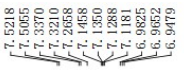
27.8342
21.4321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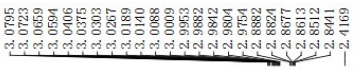
7.1350
7.1288
7.1181
6.9825
6.9652
6.9479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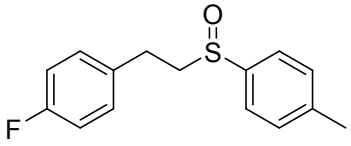
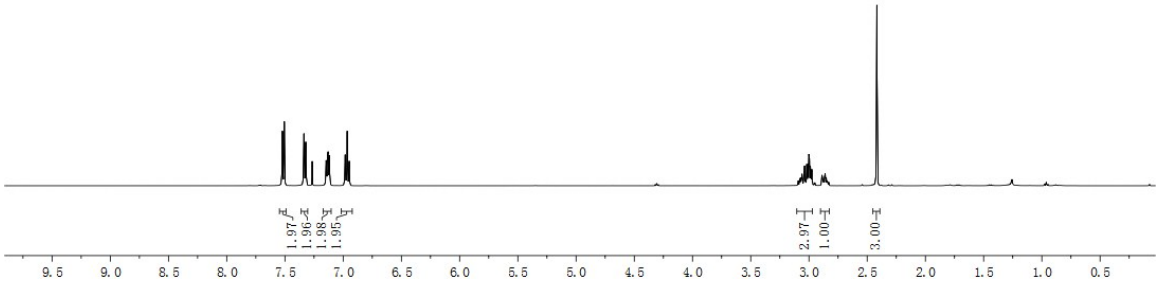
3.0723
3.0659
3.0594
3.0406
3.0375
3.0303
3.0267
3.0189
3.0140
3.0088
3.0009
2.9953
2.9882
2.9842
2.9804
2.9754
2.8824
2.8677
2.8613
2.8512
2.8441
2.4169


O
S
F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1.96
1.98
1.95
2.97
1.00
3.00
9.5
9.0
8.5
8.0
7.5
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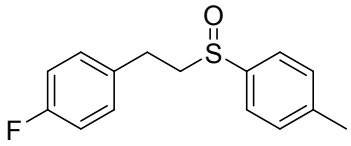
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5


162.6571
160.7098
141.5629
140.3252
134.5217
130.0500
130.0046
129.9871
124.0381
115.6284
115.4588
77.3071
77.0530
76.7988
58.3628
27.4132
21.4131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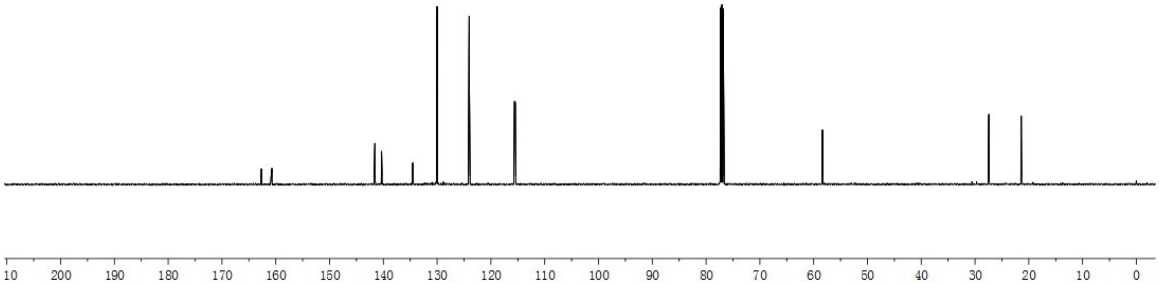
S
F


210
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190
180
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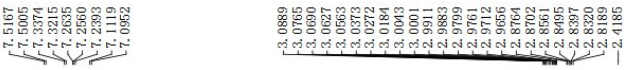
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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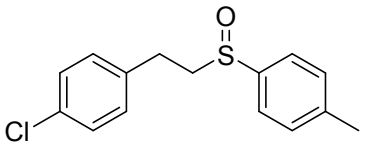
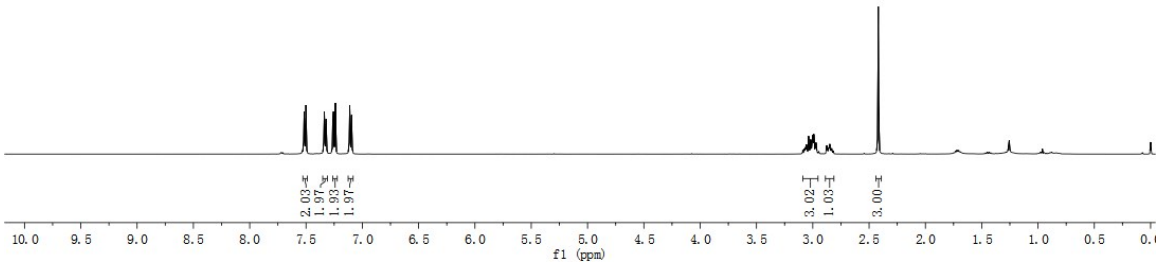
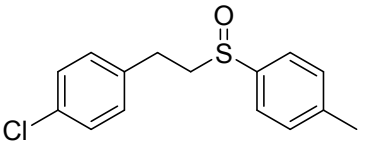
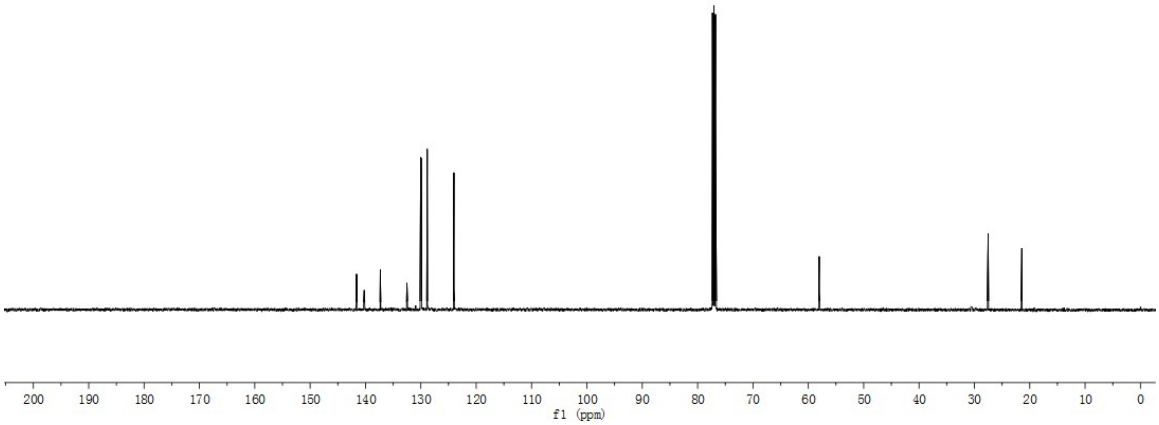
7.3374
7.3215
7.2635
7.2560
7.2393
7.1119
7.0952
3.0889
3.0765
3.0690
3.0627
3.0563
3.0373
3.0272
3.0184
3.0043
3.0001
2.9911
2.9883
2.9799
2.9761
2.9712
2.9656
2.8764
2.8702
2.8561
2.8495
2.8397
2.8320
2.8189
2.4185

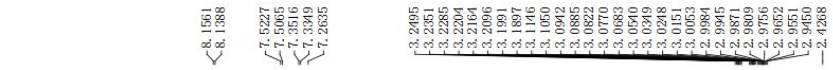

O
S
Cl


2.03
1.97
1.93
1.97
3.02
1.03
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


141.6159
140.2153
137.3200
132.5120
130.0288
129.9184
126.8510
124.0403
77.2965
77.0424
76.7884
58.0470
27.5126
21.4238


O
S
Cl


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5227
7.5065
7.3516
7.3349
7.2635
3.2495
3.2351
3.2285
3.2204
3.2164
3.2096
3.1991
3.1897
3.1146
3.1050
3.0942
3.0885
3.0822
3.0770
3.0683
3.0540
3.0349
3.0218
3.0151
3.0053
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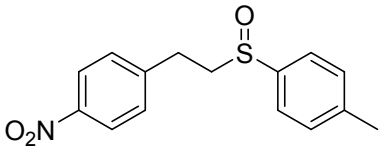
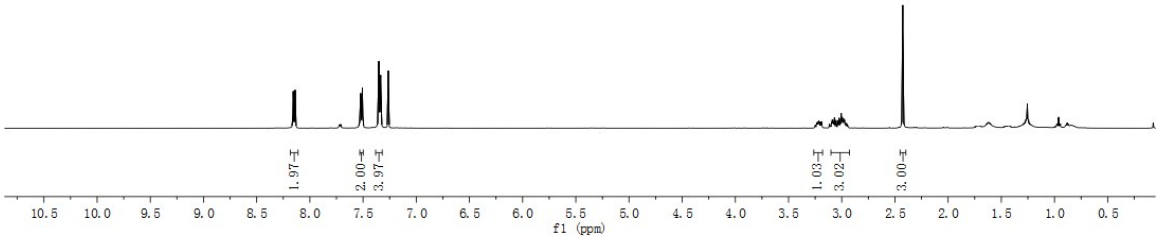
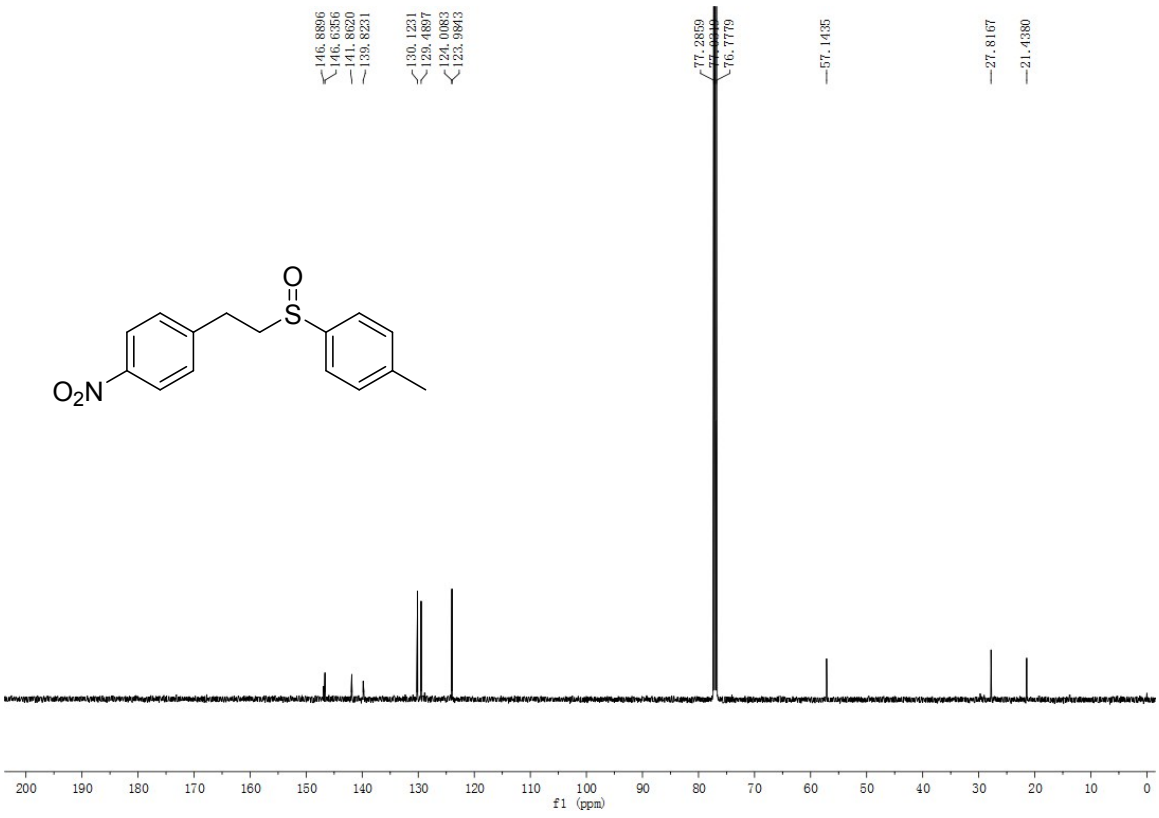
2.9945
2.9871
2.9809
2.9756
2.9652
2.9551
2.9450
2.4268


O
S
O2N


1.97
2.00
3.97
1.03
3.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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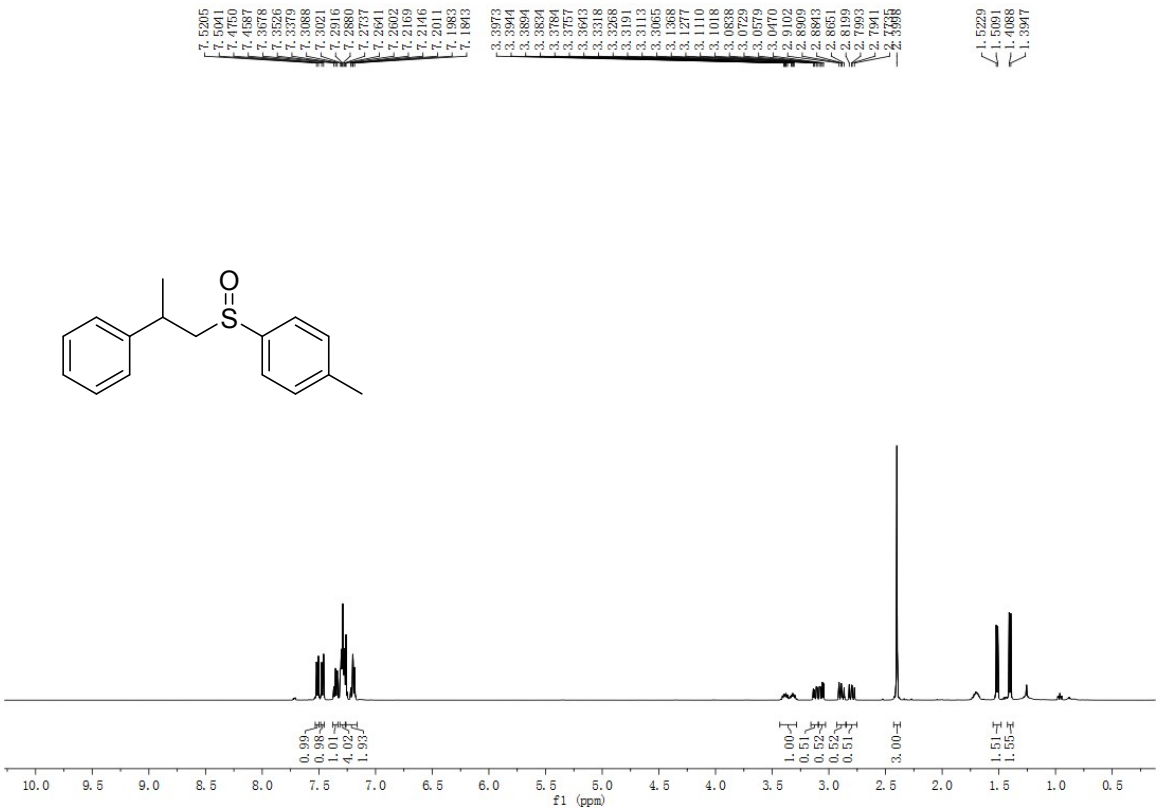
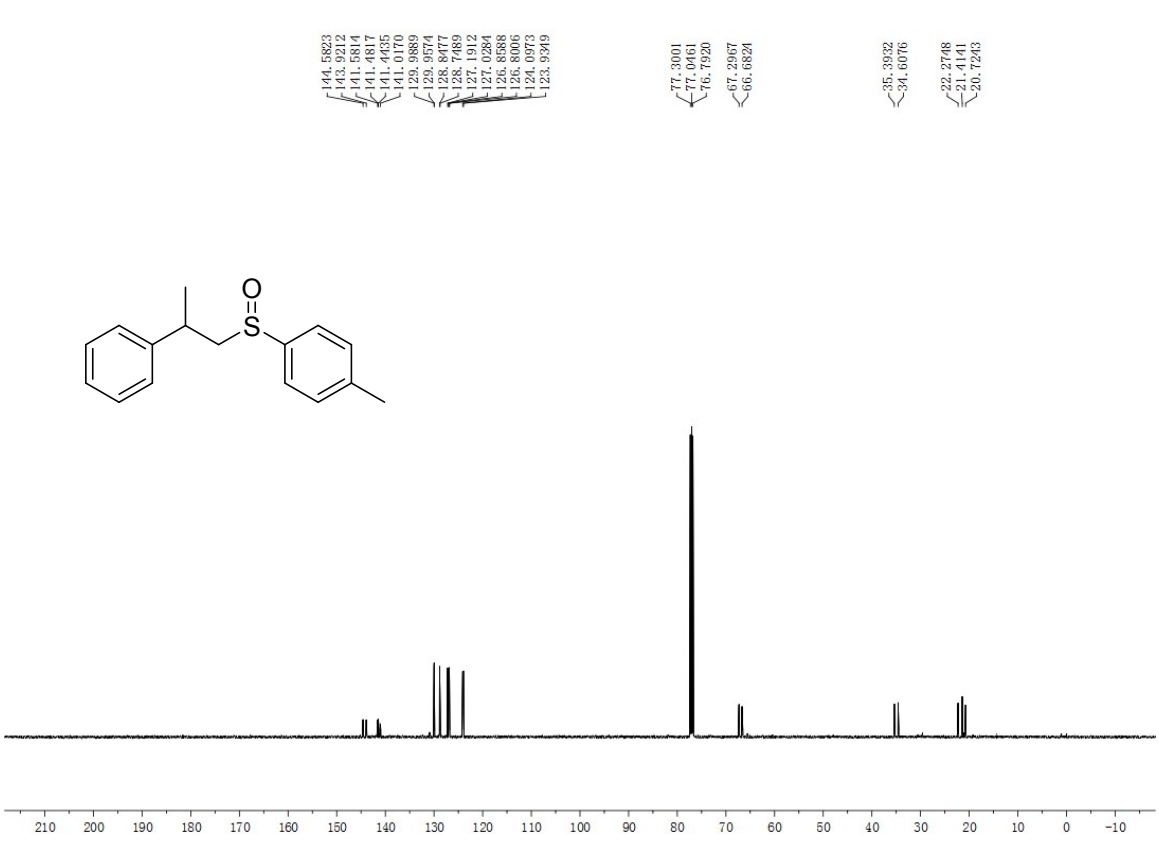
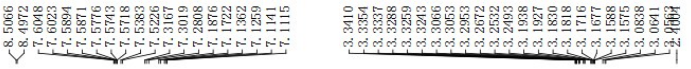
146.6356
141.8620
139.8231
130.1231
129.4897
124.0083
123.9843
77.2859
76.7779
57.1435
27.8167
21.4380
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

O
S
O2N



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7.5718
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7.3167
7.3019
7.2808
7.1876
7.1722
7.1362
7.1259
7.1141
7.1115
3.3410
3.3354
3.3337
3.3288
3.3259
3.3243
3.3066
3.3053
3.2953
3.2672
3.2532
3.2493
3.1938
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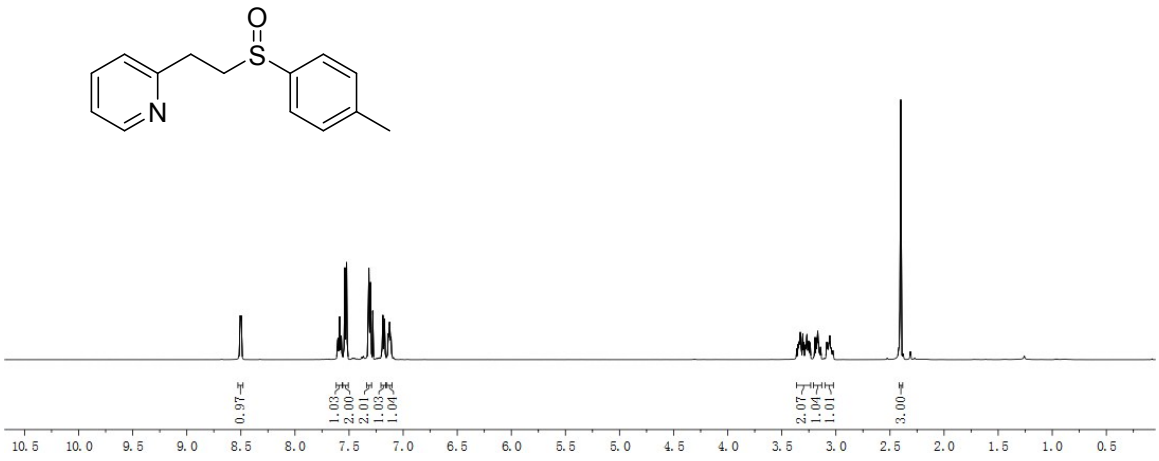
3.1830
3.1818
3.1716
3.1677
3.1588
3.1575
3.0838
3.0641


O
S
N
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1.03
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2.01
1.03
1.04
2.07
1.04
1.01
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5


158.5572
149.4456
141.3601
140.3949
136.5927
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123.3664
121.6891
77.3467
77.0925
76.8380
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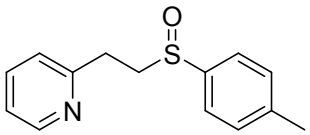
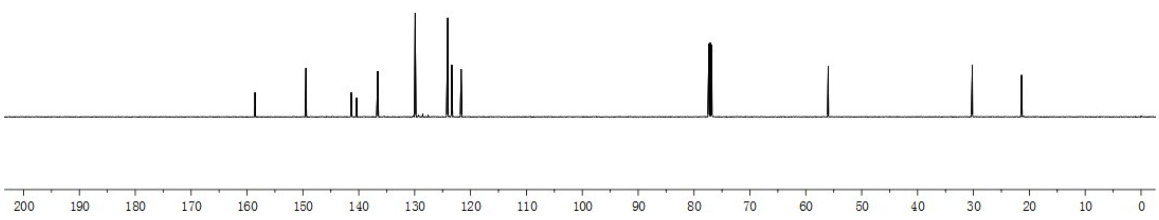
21.3836


O
S
N


200
190
180
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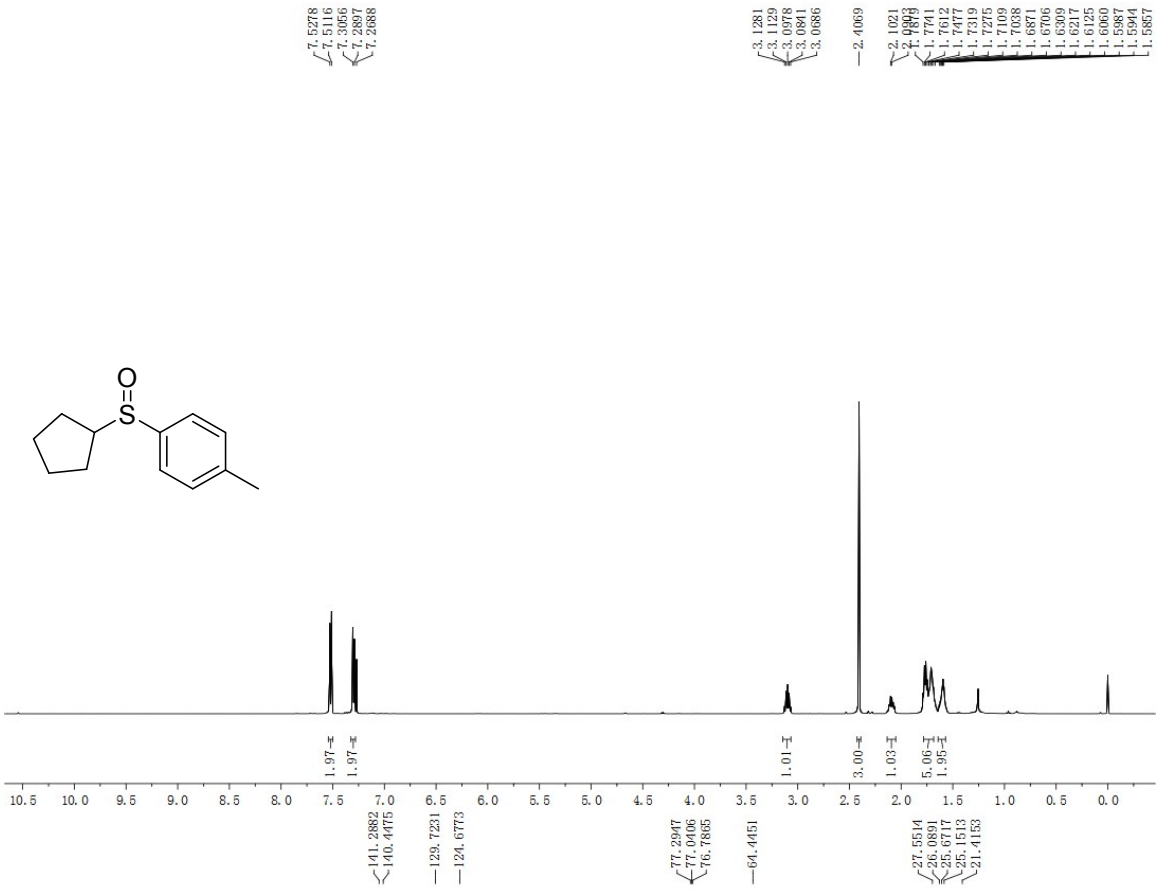
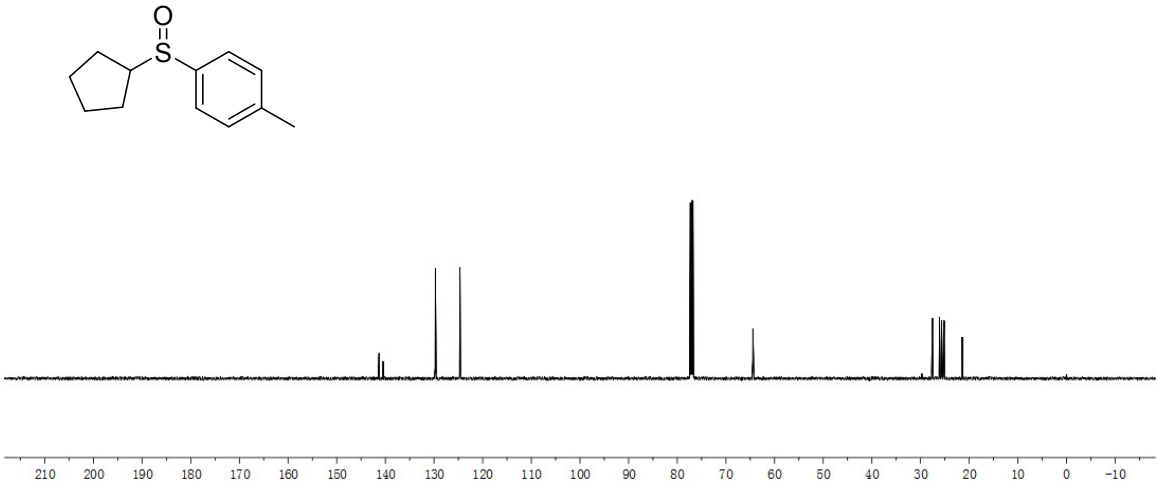
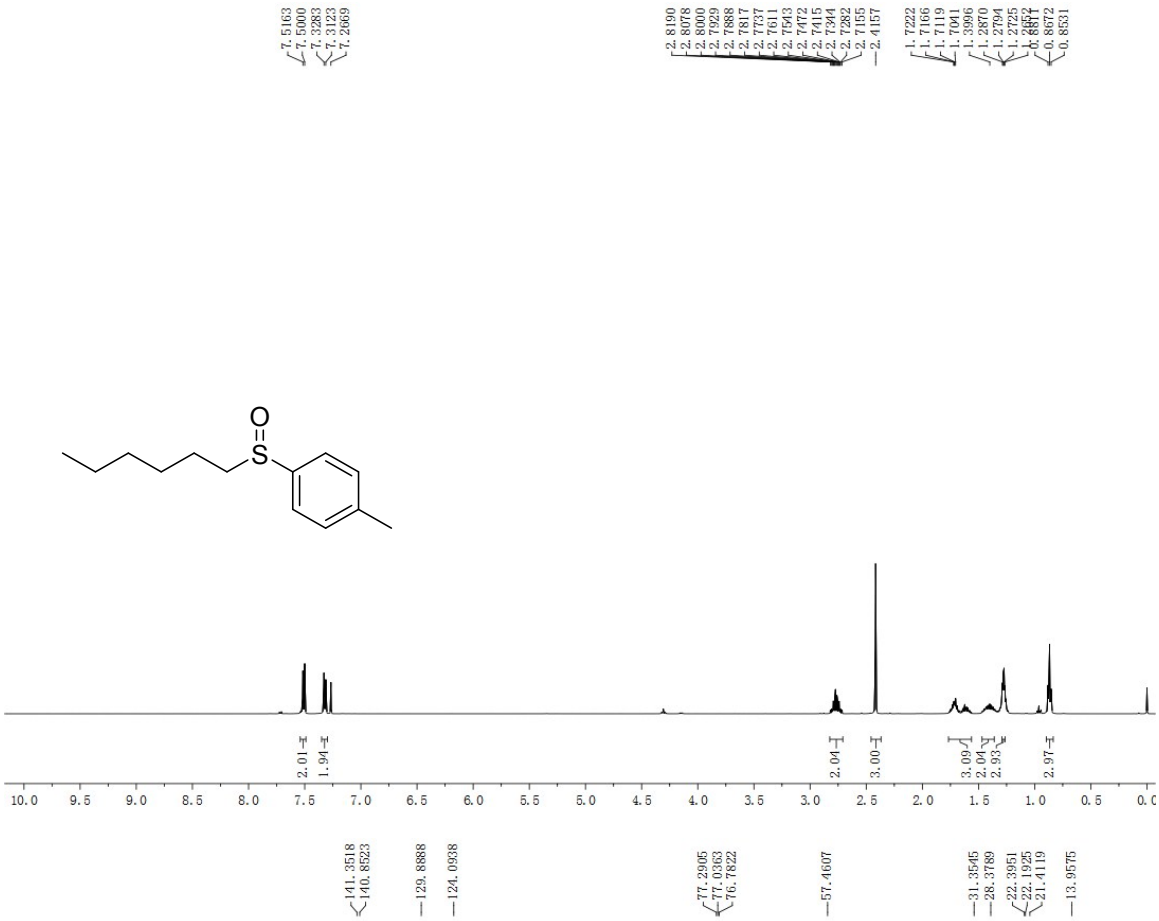
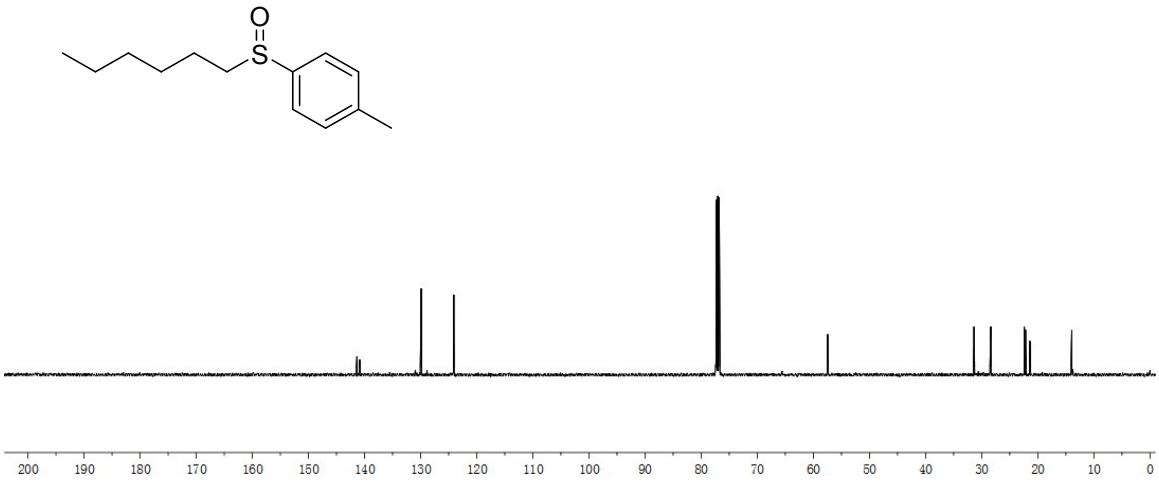
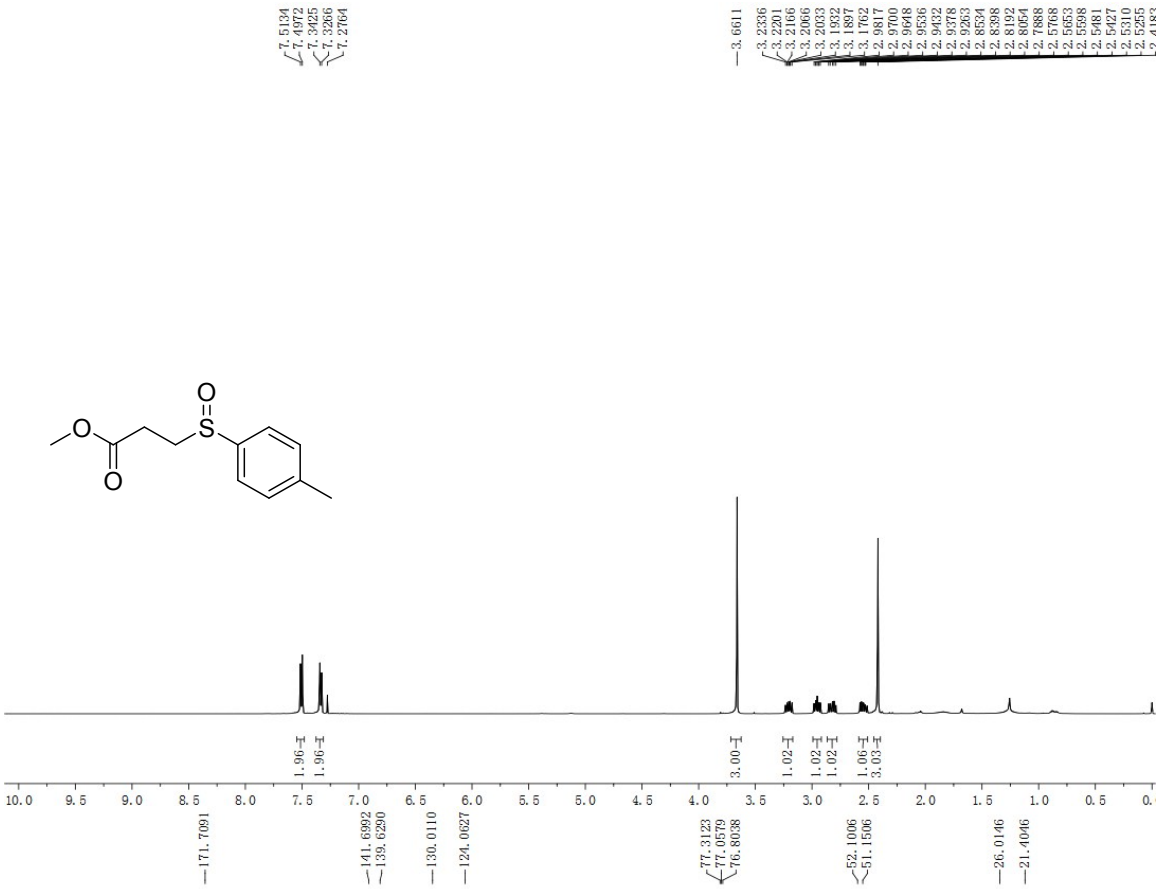
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

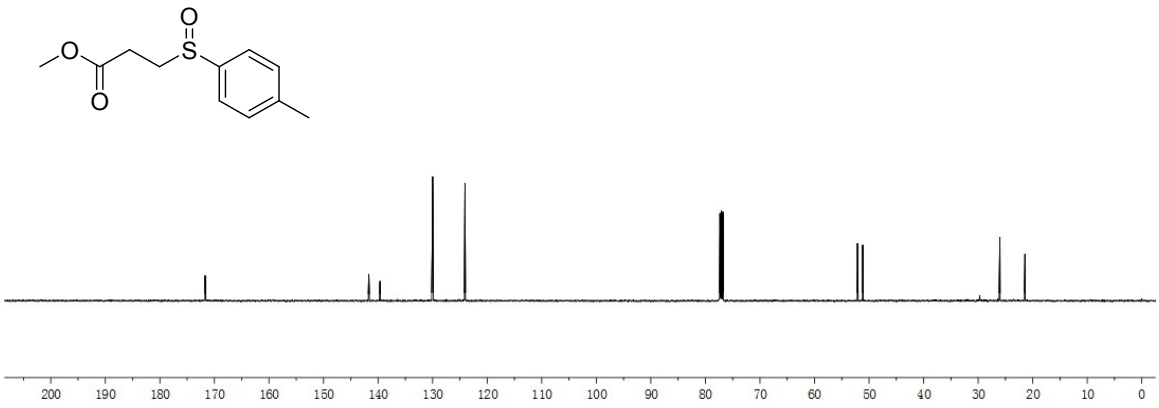













7.6443
7.6410
7.6369
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7.2231
7.2107
7.2065
7.1960
7.1830
7.1804
7.1664


3.1296
3.1178
3.1088
3.1045
3.0949
3.0842
3.0800
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3.0704
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3.0584
3.0520
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3.0399
3.0272
3.0242
3.0191
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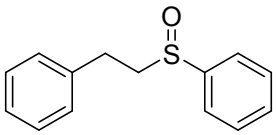
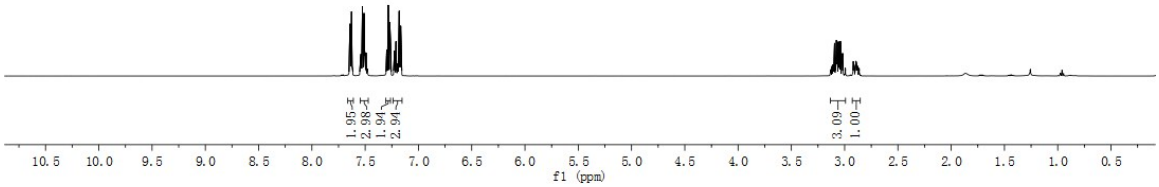
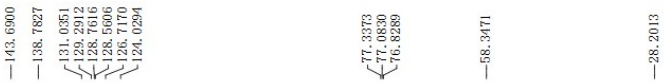
2.8639


O
S


1.95
2.98
1.94
2.94
3.09
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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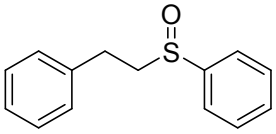
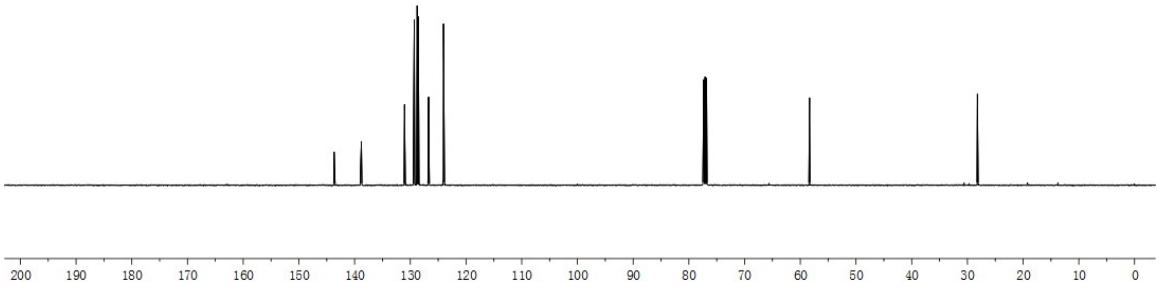
77.0830
76.8289
58.3471
28.2013


O
S


200
190
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80
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50
40
30
20
10
0


7.5853
7.5678
7.3008
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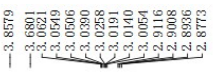
7.0235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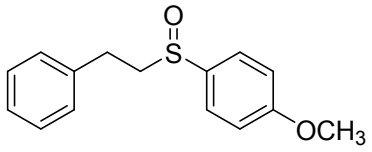
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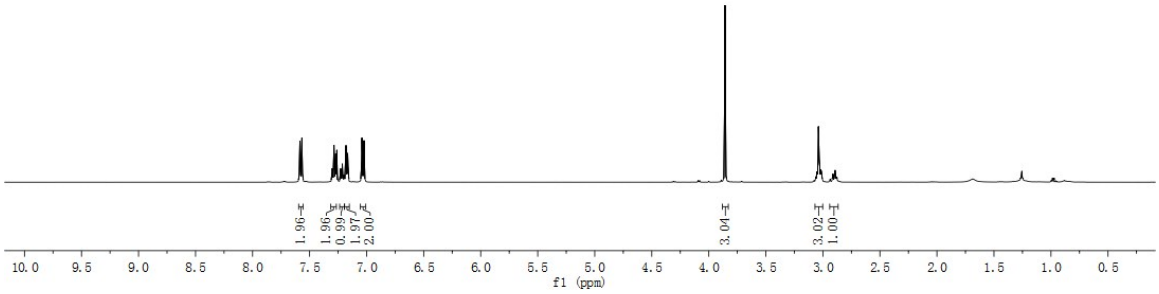
S
OCH3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3.02
1.00
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f1 (ppm)


162.0018
138.8779
134.5276
128.7349
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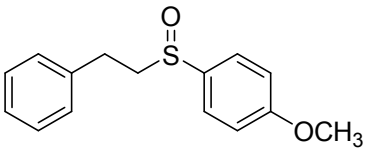
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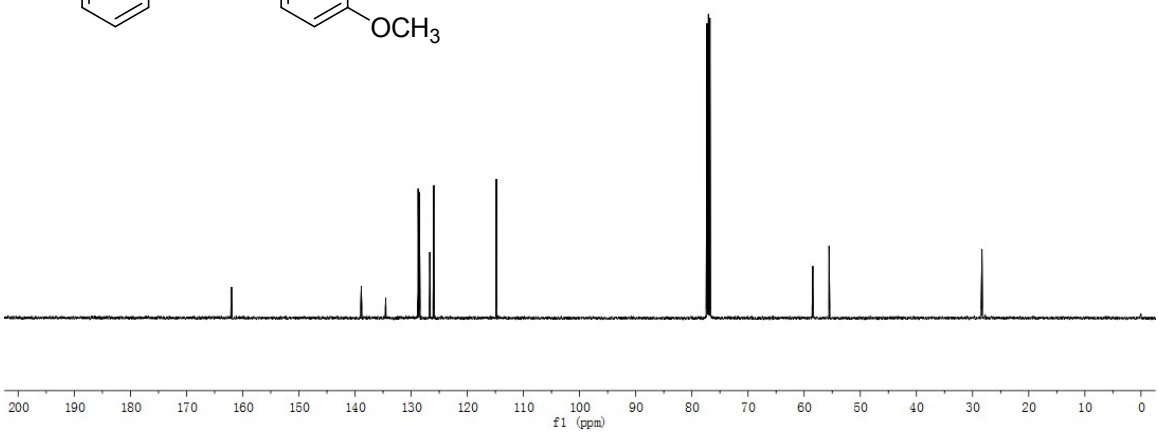
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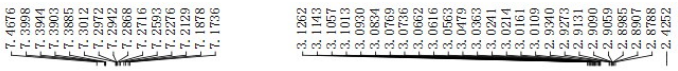
f1 (ppm)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7.2129
7.1878
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3.0834
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3.0736
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3.0616
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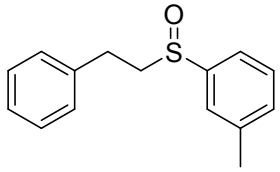

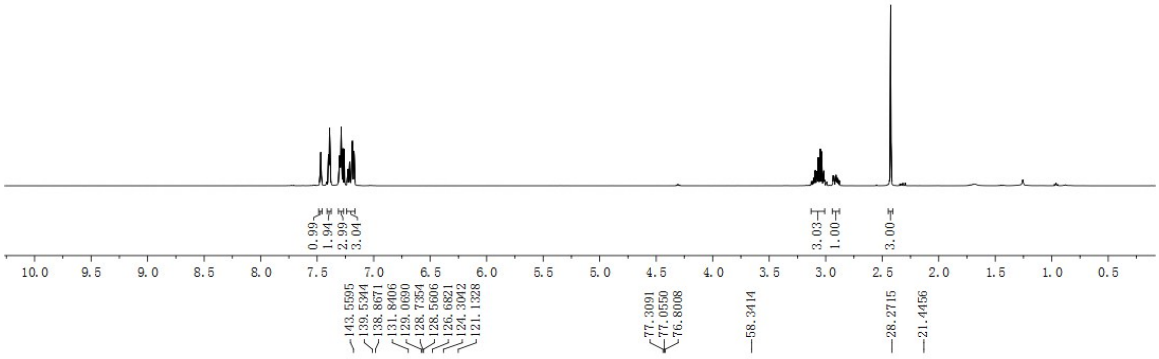
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10.0
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9.0
8.5
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
143.5595
139.5304
138.8671
131.8406
129.0690
128.7354
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124.3042
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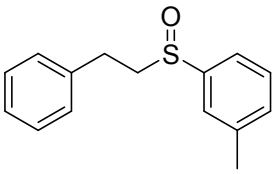
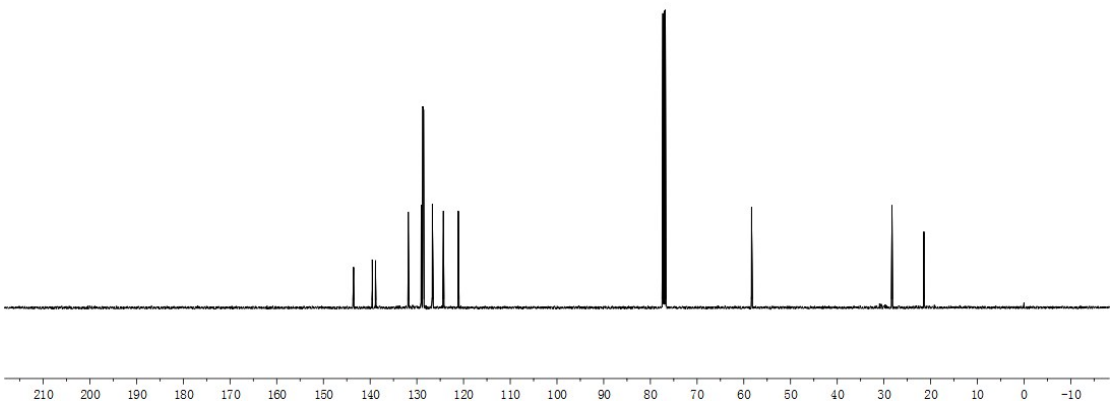
21.4456

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100
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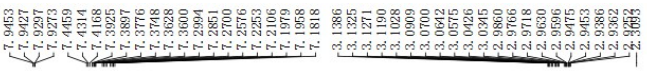
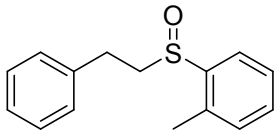
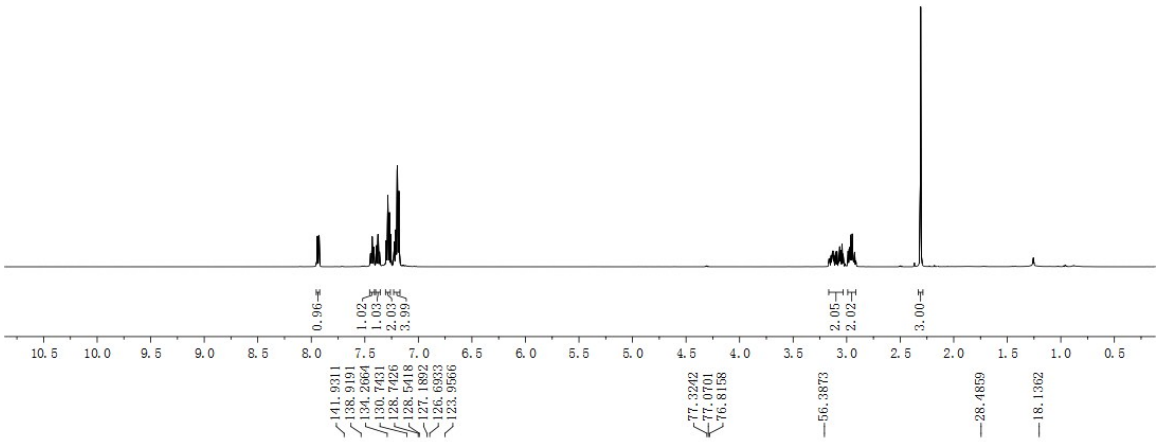
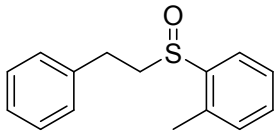
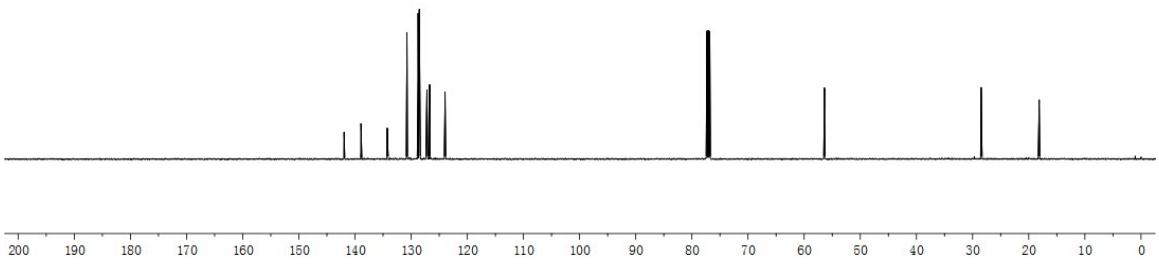
10
0
-10









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7.2939
7.2787
7.2613
7.2498
7.2442
7.2400
7.2382
7.2271
7.2235
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7.2098
7.1823
7.1681
3.1197
3.1077
3.0996
3.0949
3.0869
3.0779
3.0706
3.0607
3.0509
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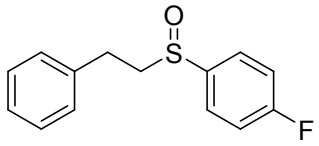
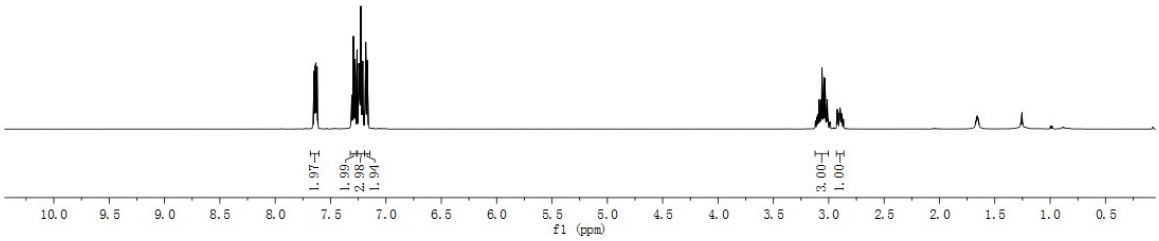
2.8801
2.8682


O
S
F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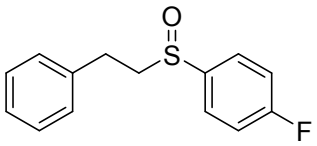
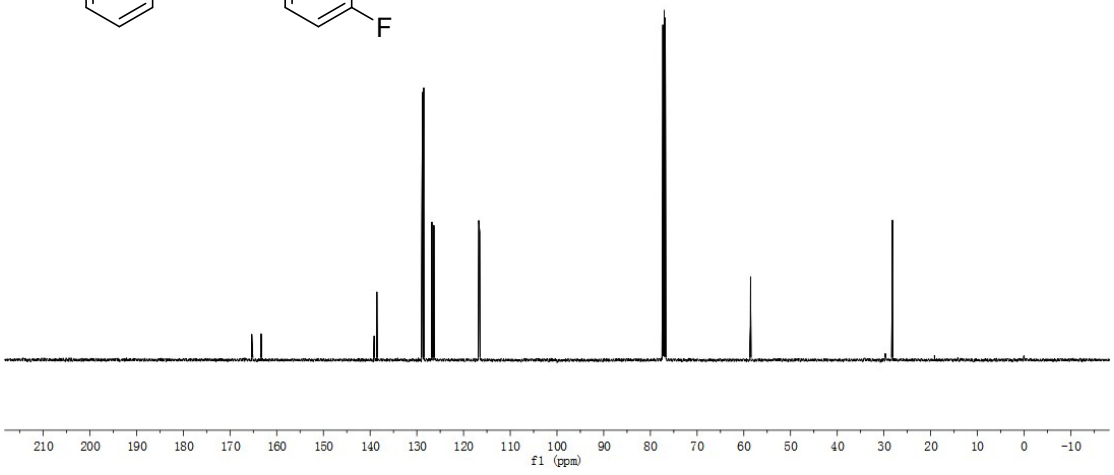
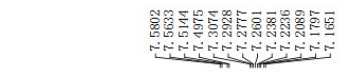
1.99
2.98
1.94
3.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


165.3523
163.3526
139.1427
139.1182
138.5691
128.8003
128.5368
126.7910
116.5577
77.3118
77.0576
76.8035
58.5590
28.1792


O
S
F


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)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7.2777
7.2601
7.2381
7.2236
7.2089
7.1797
7.1651


3.1309
3.1189
3.1105
3.1053
3.0982
3.0949
3.0896
3.0806
3.0716
3.0611
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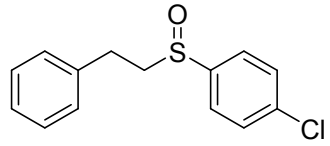
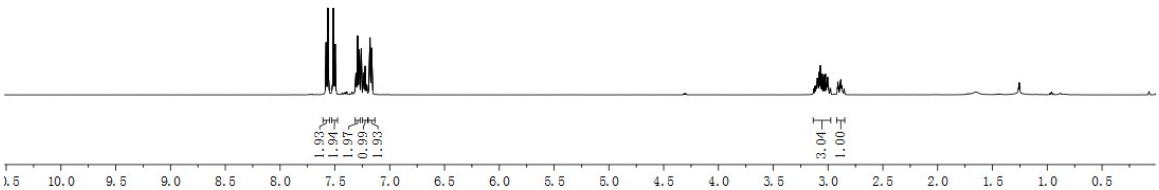
2.8747
2.8662
2.8535


O
S
Cl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1.94
1.97
0.99
1.93
3.04
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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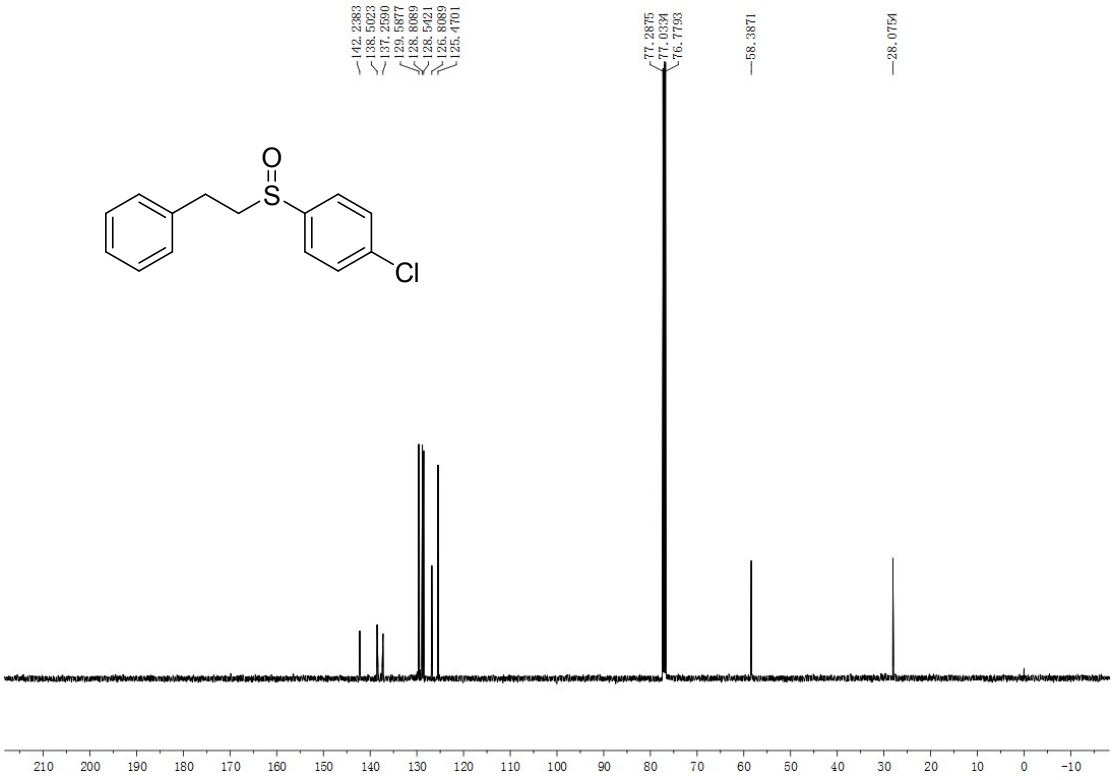
0.5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76.7793
58.3871
28.0754
O
S
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


7.3080
7.2936
7.2784
7.2642
7.2387
7.2350
7.2202
7.2054
7.1904
7.1762
7.1404
7.1365
7.1238
7.1199
6.9731
6.9564
3.9484
3.9291
3.0675
3.0515
3.0438
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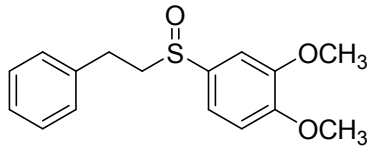
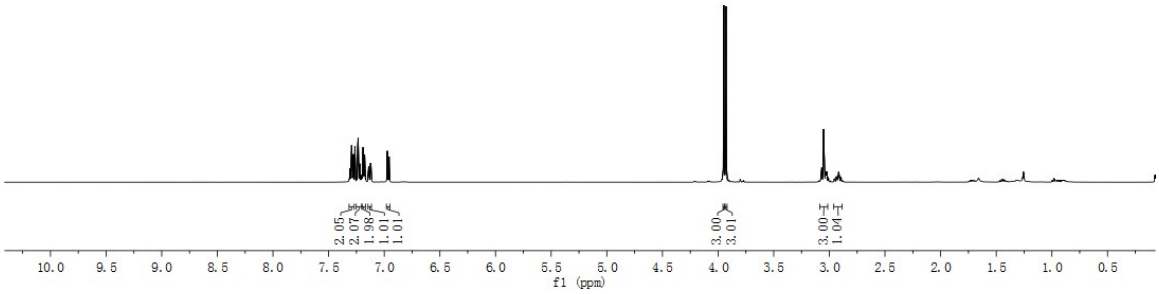
2.8953


O
S
OCH3
OCH3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1.01
3.00
3.01
3.00
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


151.4479
150.1221
138.8294
134.9448
128.7442
128.5376
126.6952
117.4244
111.1795
106.3665
77.2981
77.0440
76.7899
58.6418
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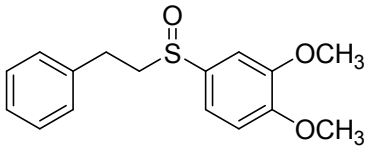
56.1722
28.4424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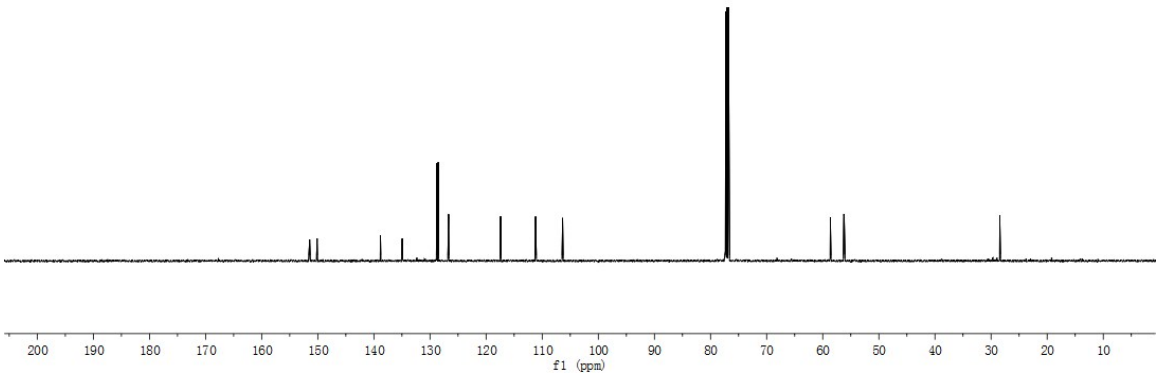
OCH3
OCH3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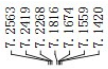
f1 (ppm)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7.1559
7.1420


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3.0674
3.0596
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3.0401
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3.0102
3.0056
2.9918
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2.9643
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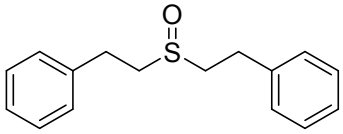
2.7891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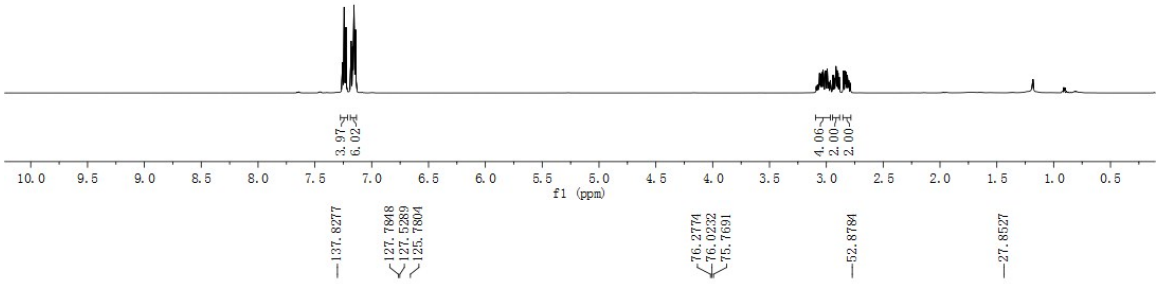
S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9.0
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6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
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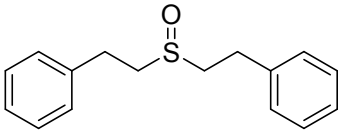
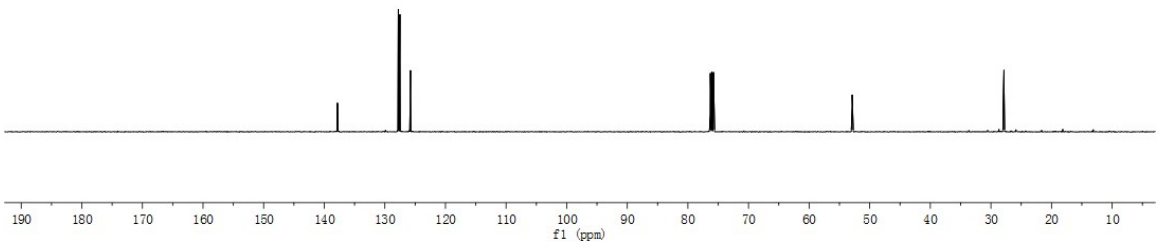
127.7848
127.5289
125.7804
76.2774
76.0232
75.7691
52.8784
27.8527


O
S


190
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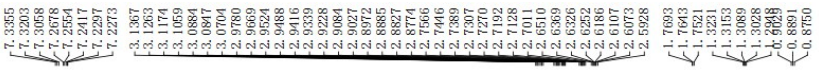
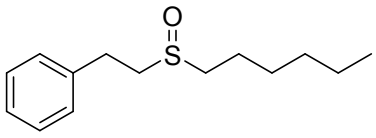
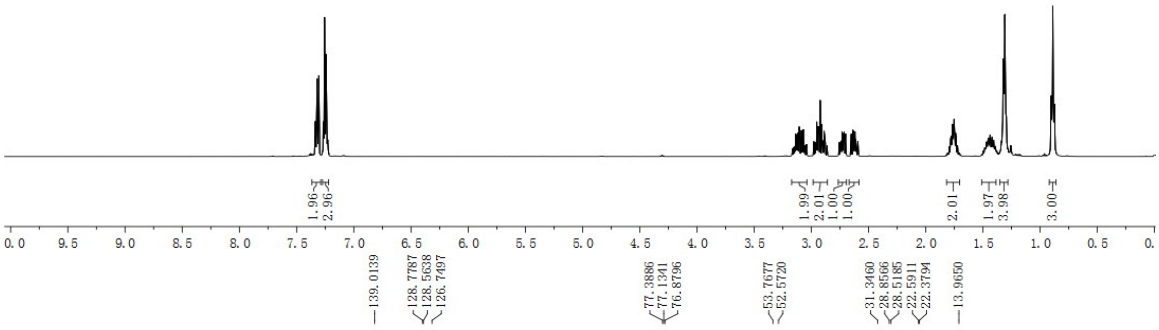
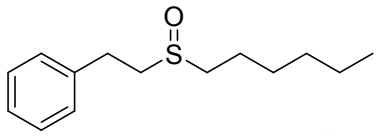
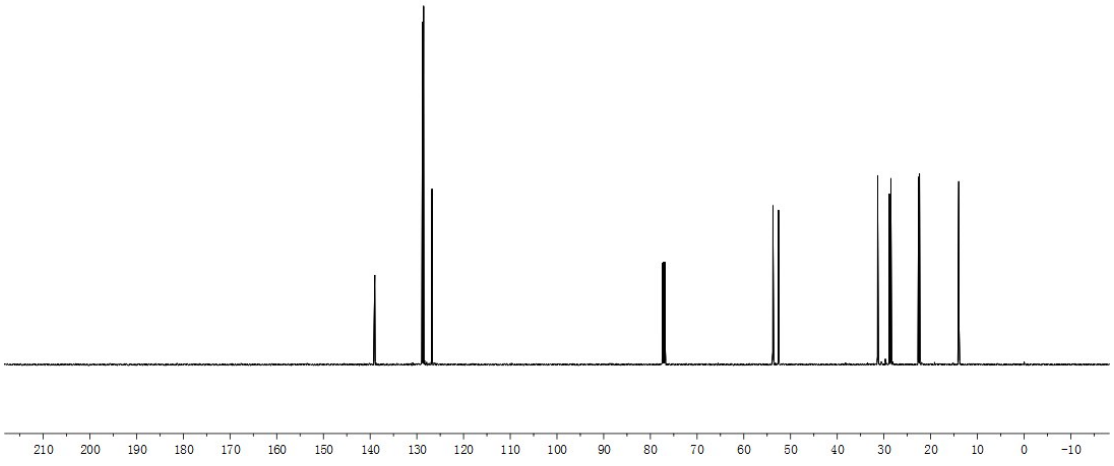
40
30
20
10
f1 (ppm)

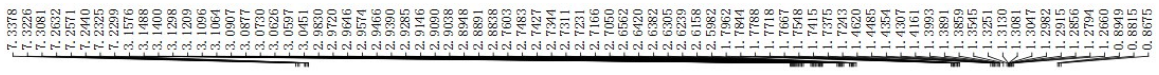


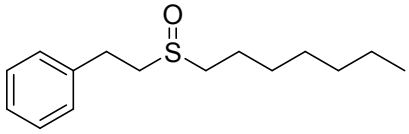


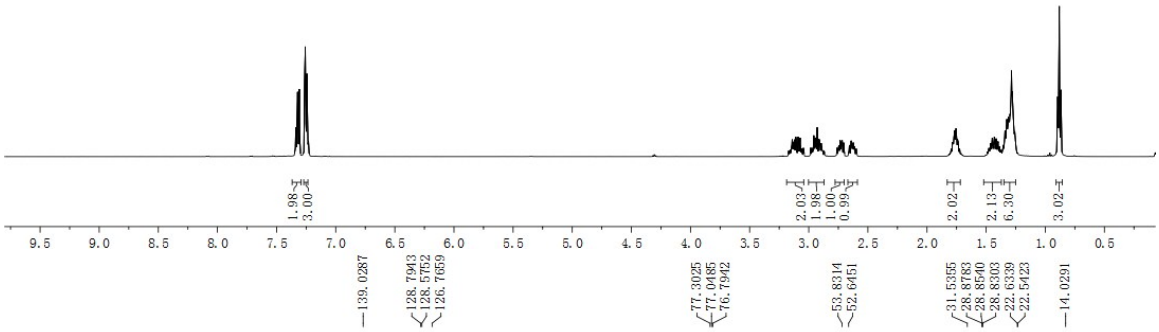


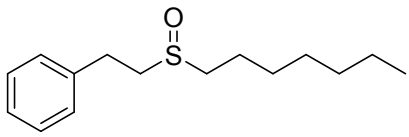


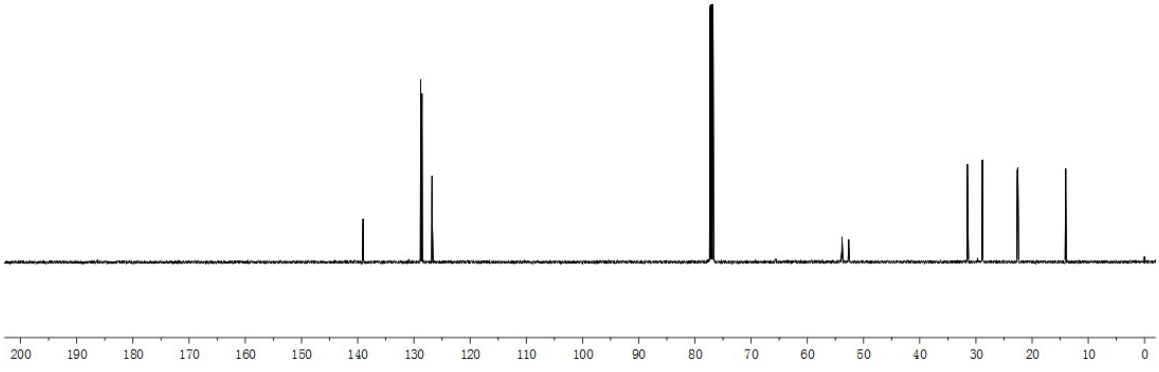


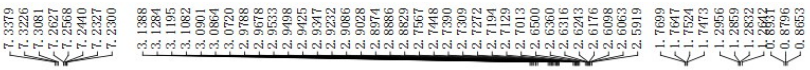


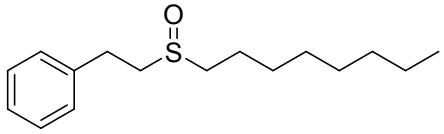


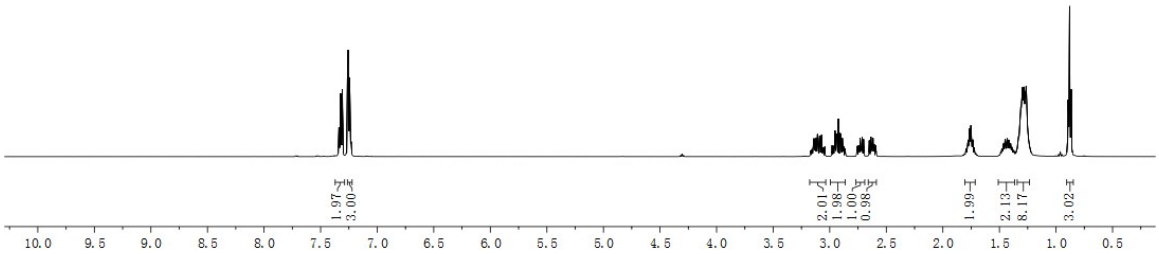


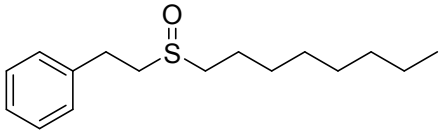


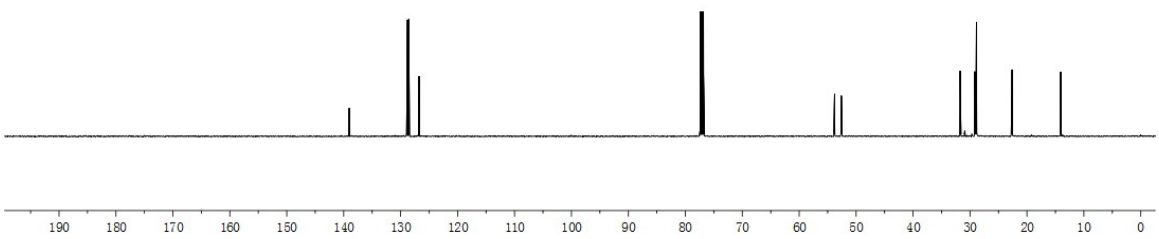


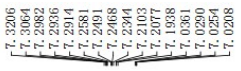








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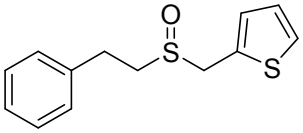
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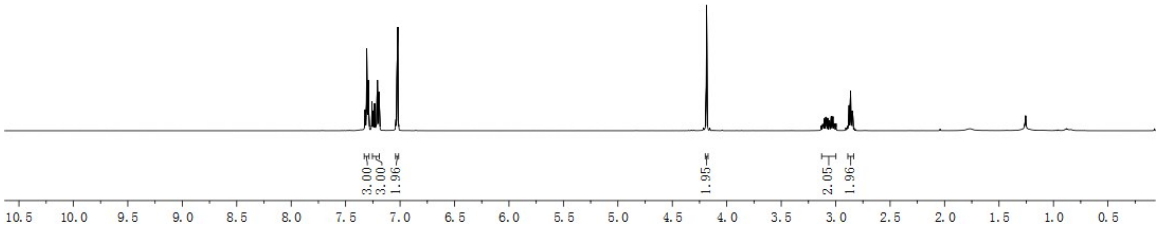
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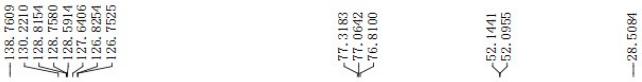
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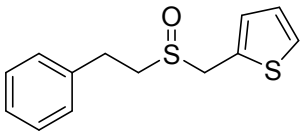
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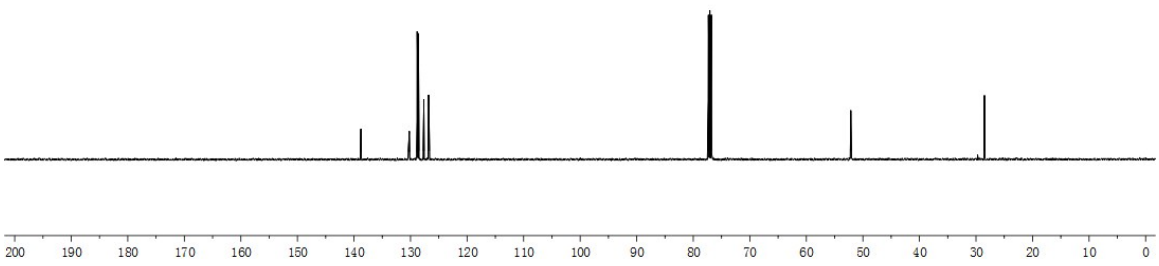
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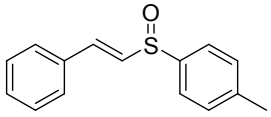
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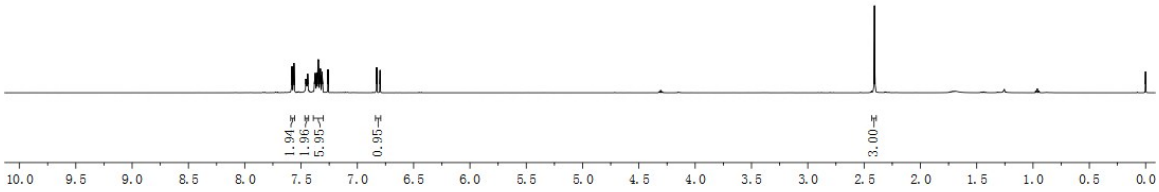
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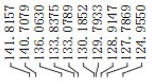
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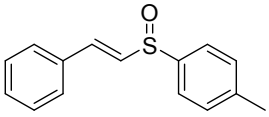
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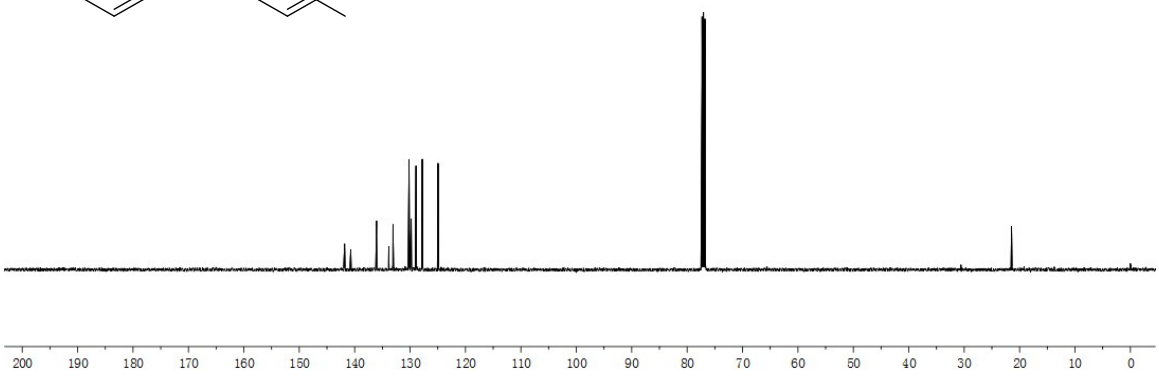
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