

## Supplement Information

### Highly selective oxidation of organic sulfides by a conjugated polymer as the photosensitizer for singlet oxygen generation

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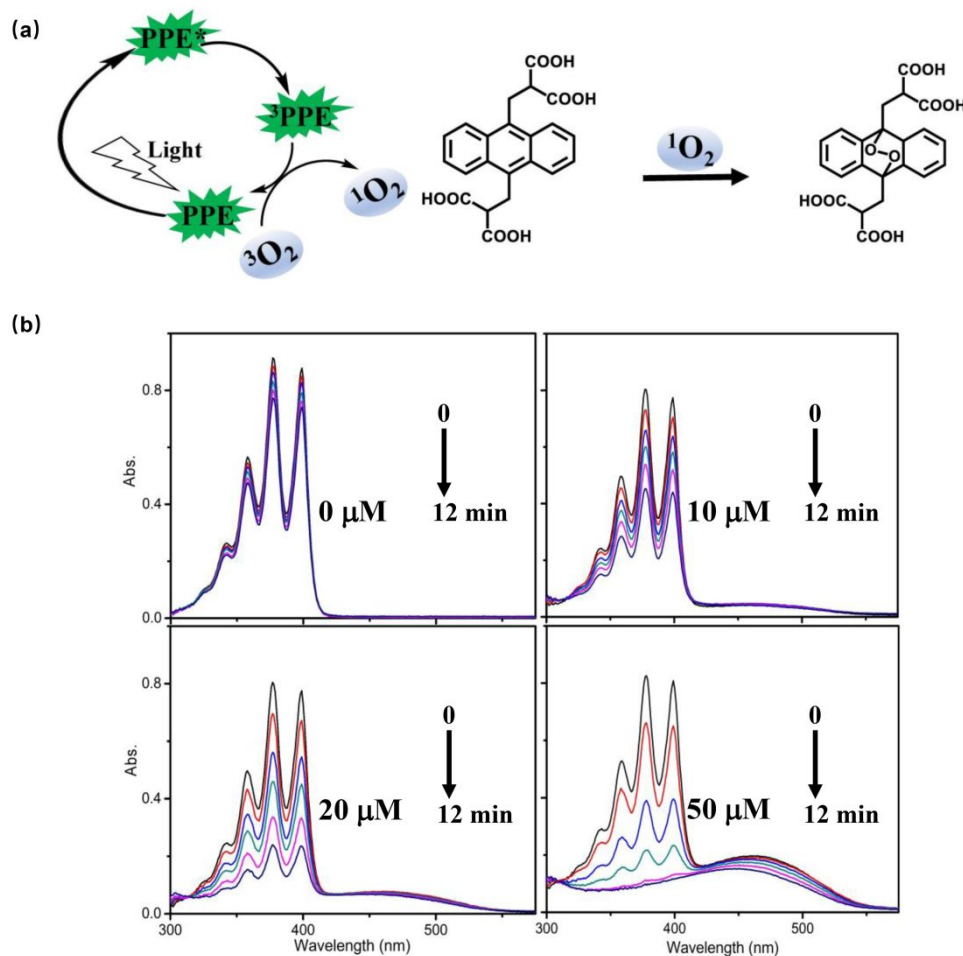
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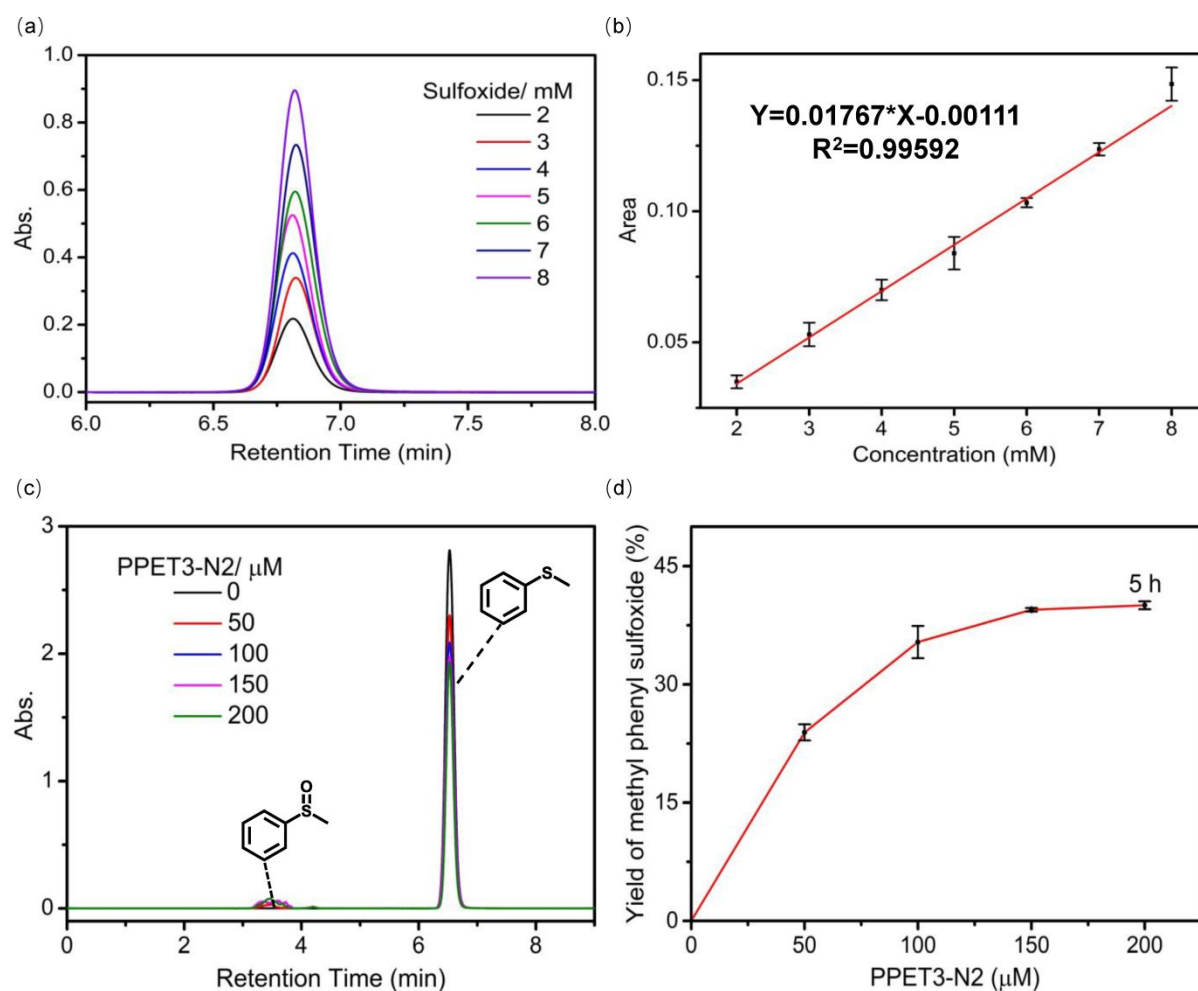
## Results

### Determination of singlet oxygen generation.

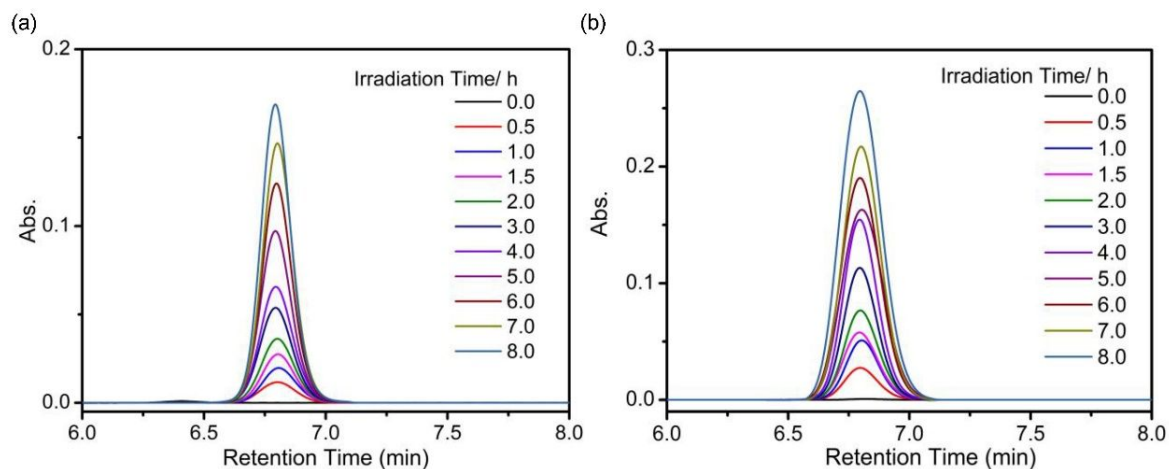


**Figure S1.** (a) Schematic diagram of  $^1\text{O}_2$  generation and chemical reaction of ABDA with  $^1\text{O}_2$ . (b) Absorption spectral changes of ABDA in the presence of 0, 10, 20, and 50  $\mu\text{M}$  PPET3-N<sub>2</sub> over different periods of exposure time. A white light LED lamp (400–800 nm, power: 120 W, 3.8 mW/cm<sup>2</sup>) was employed as the light source.

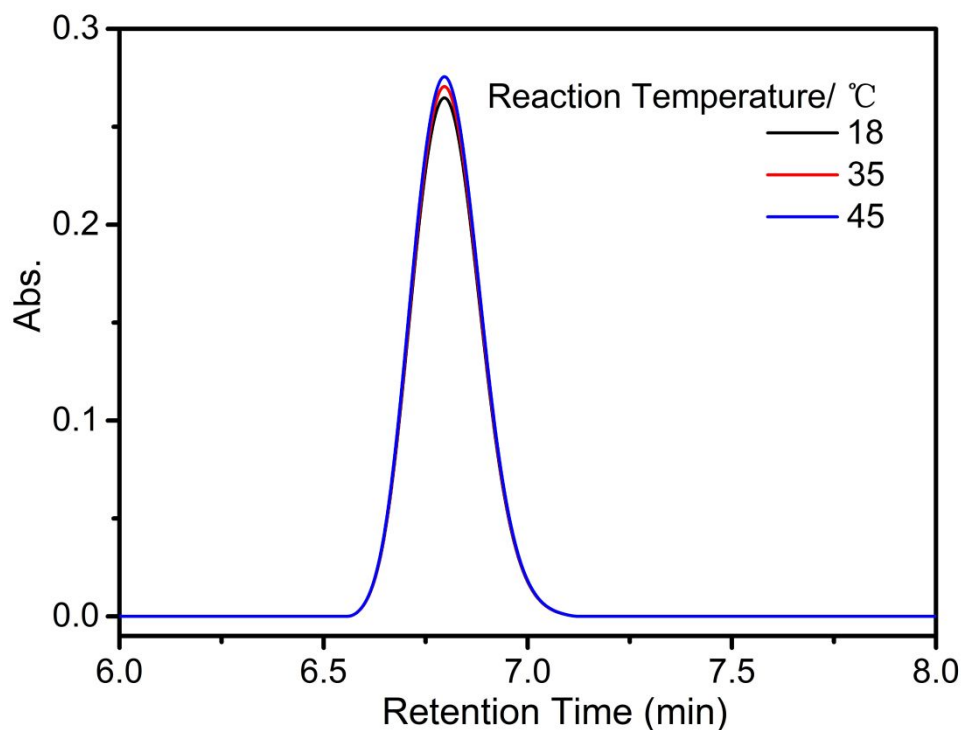
## Batch experiment of thioanisole



**Figure S2.** (a) HPLC chromatogram (Detection: 253.314 nm; Eluent: 4:1 (v/v)  $\text{H}_2\text{O}/\text{CH}_3\text{CN}$ ; Flow rate: 0.5 mL/min; Retention Time: 6.0-8.0 min) of 2.0-8.0 mM methyl phenyl sulfoxide; (b) The average area (integral area of 6.5-7.1 min in (a)) values at various thioanisole concentration. Error bars are  $\pm$  SD,  $n=3$ ; (c) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v)  $\text{H}_2\text{O}/\text{CH}_3\text{CN}$  solution was used as the eluent; (d) photosensitized conversion of thioanisole into methyl phenyl sulfoxide in a batch reaction. Reaction conditions: 10 mM thioanisole with different concentrations of PPET3-N2 in 4 mL methanol under 3.8  $\text{mW}/\text{cm}^2$  white LED light irradiation, 5 h.



**Figure S3.** Photosensitized production of methyl phenyl sulfoxide at different reaction time periods under 1.6 mW/cm<sup>2</sup> (a) and 3.8 mW/cm<sup>2</sup> (b) white LED light. The HPLC chromatograms were acquired after dilution of 400  $\mu$ L reaction solution to 400  $\mu$ L methanol in a sample bottle, and the photodiode array detector was set at 253.314 nm. The reaction conditions are the same as Figure 1.



**Figure S4.** Photosensitized production of methyl phenyl sulfoxide at different reaction temperature under 3.8 mW/cm<sup>2</sup> white LED light.; Reaction conditions: 10 mM thioanisole with 150  $\mu$ M PPET3-N2 in 4 mL methanol, 8 h.

## $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR spectra

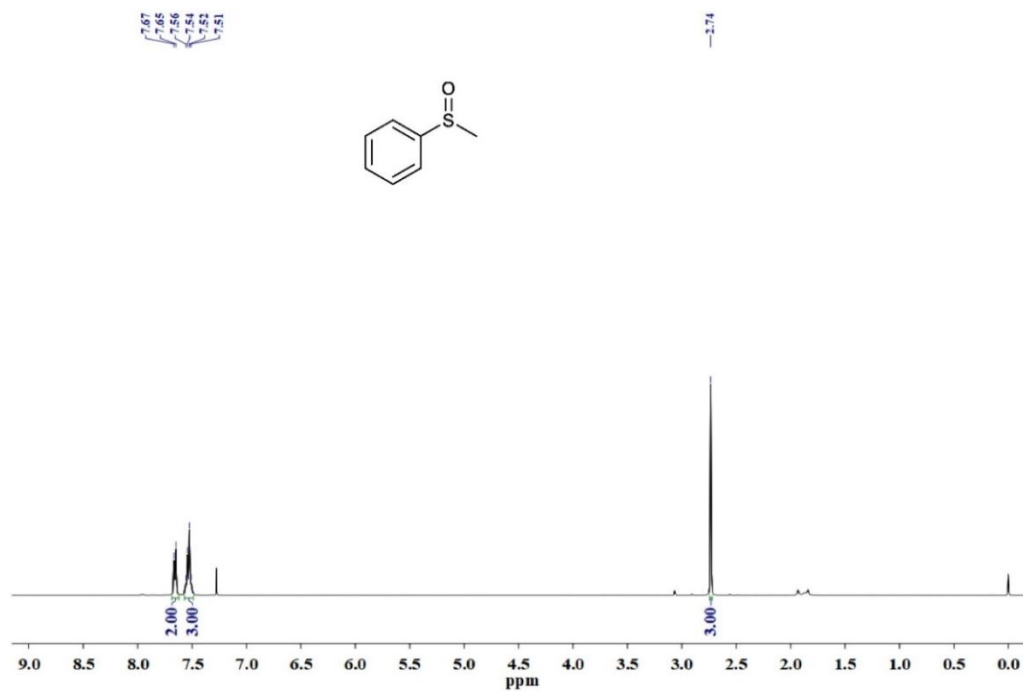


Figure S5.  $^1\text{H}$ -NMR spectrum of methyl phenyl sulfoxide.

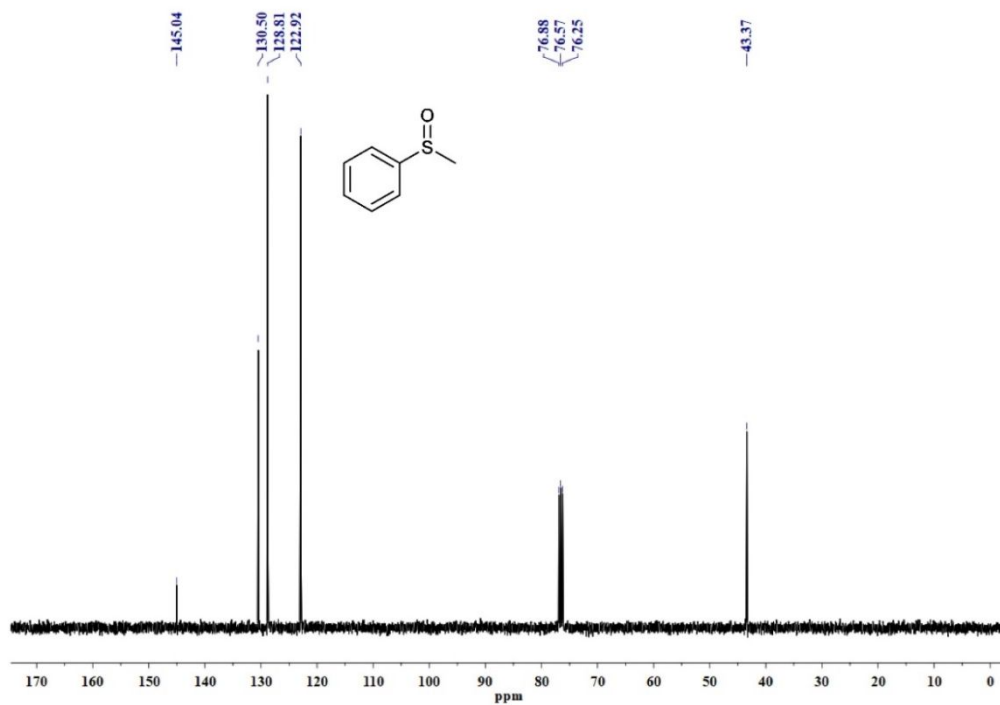
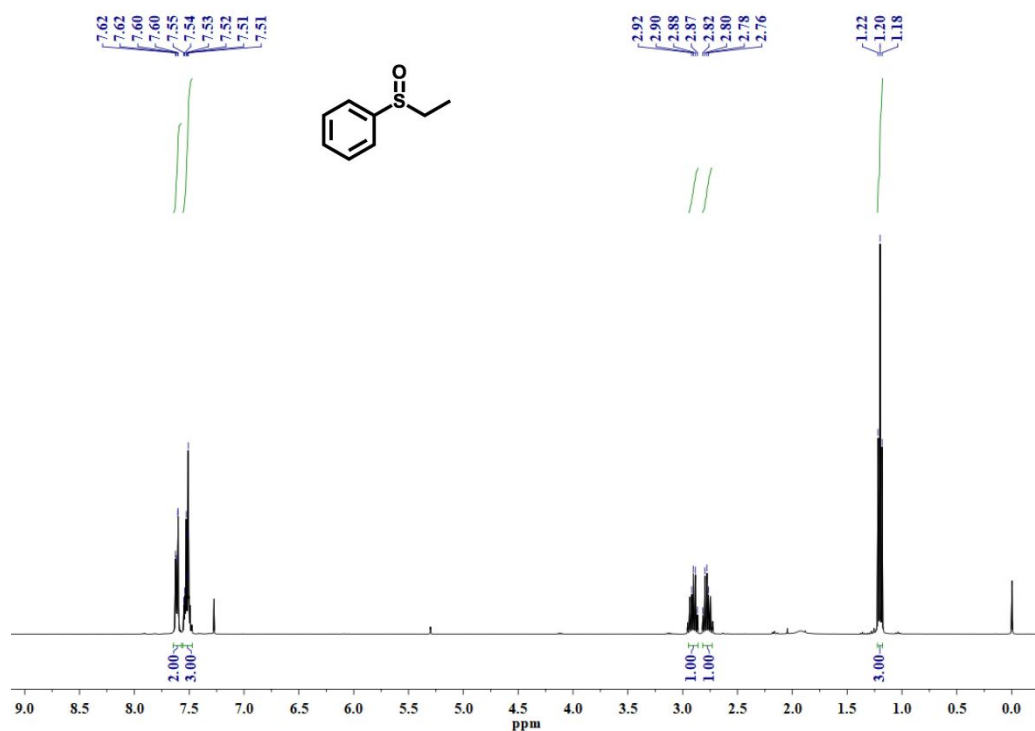
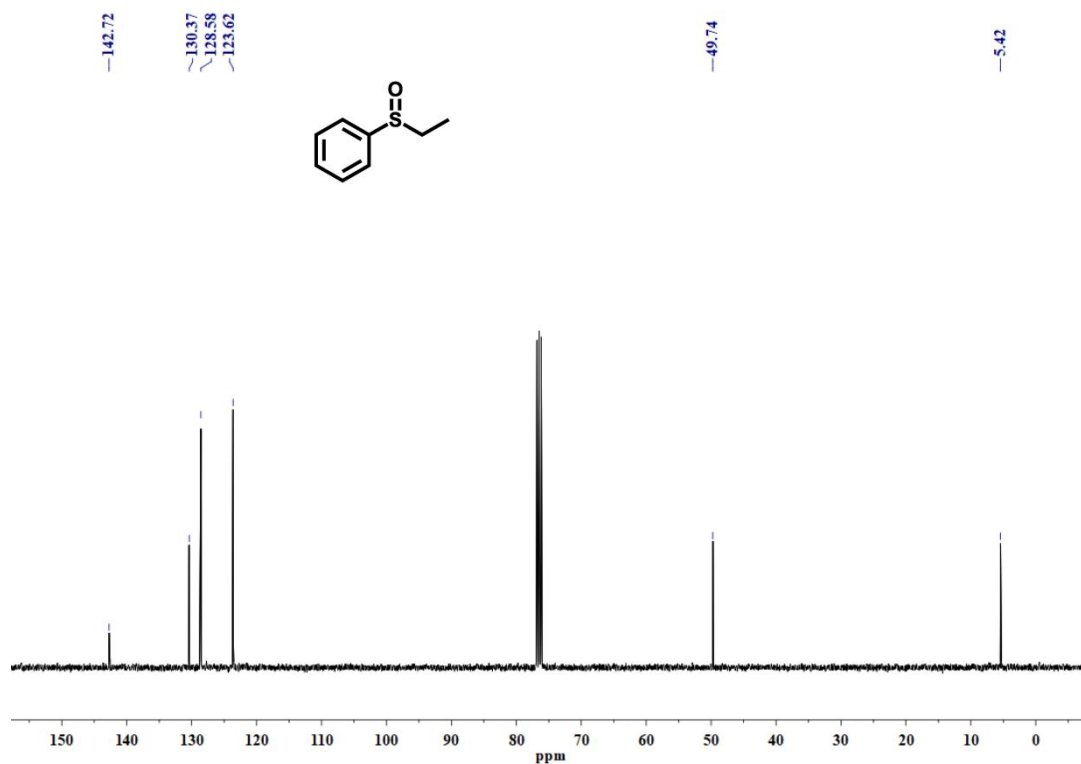


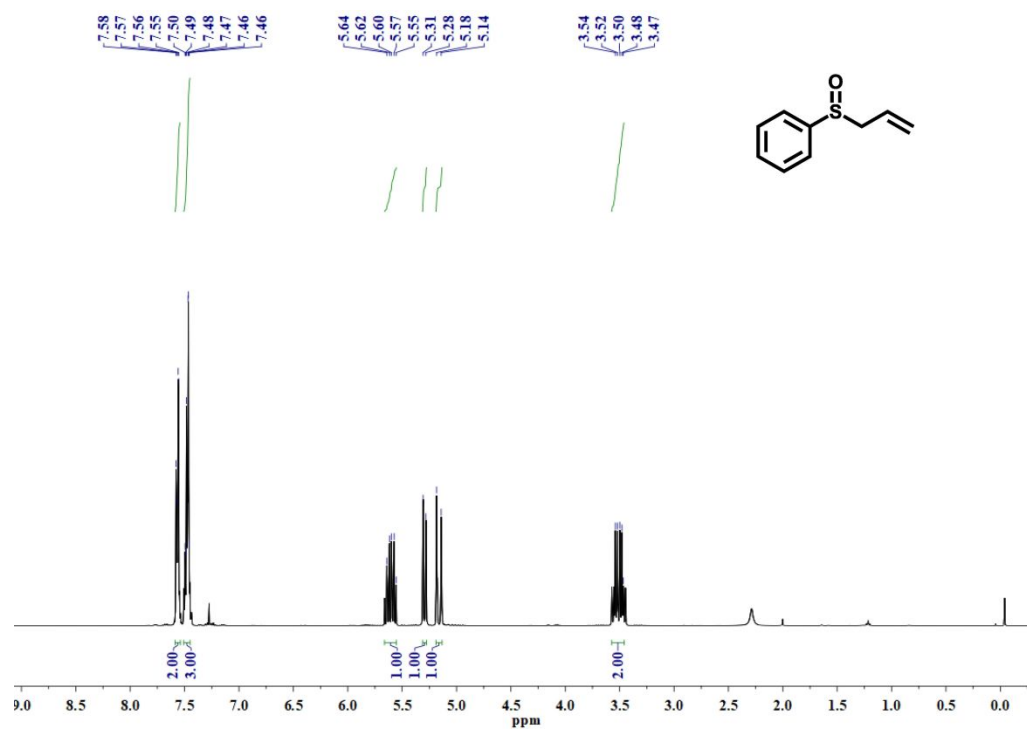
Figure S6.  $^{13}\text{C}$ -NMR spectrum of methyl phenyl sulfoxide.



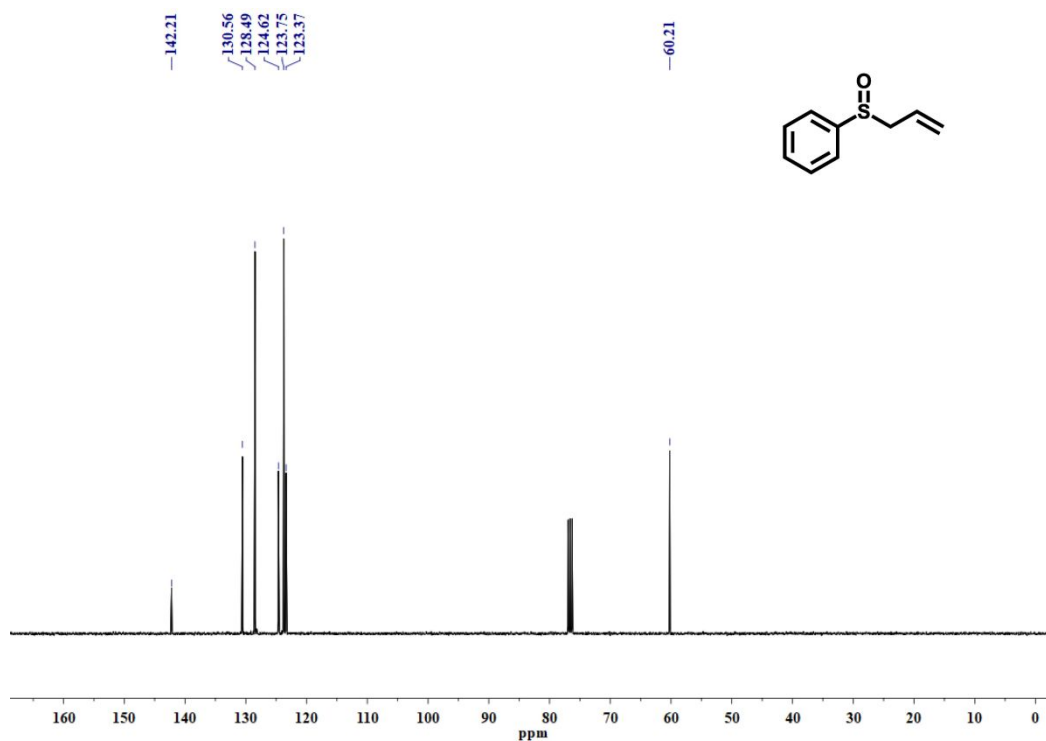
**Figure S7.**  $^1\text{H}$ -NMR spectrum of ethyl phenyl sulfoxide.



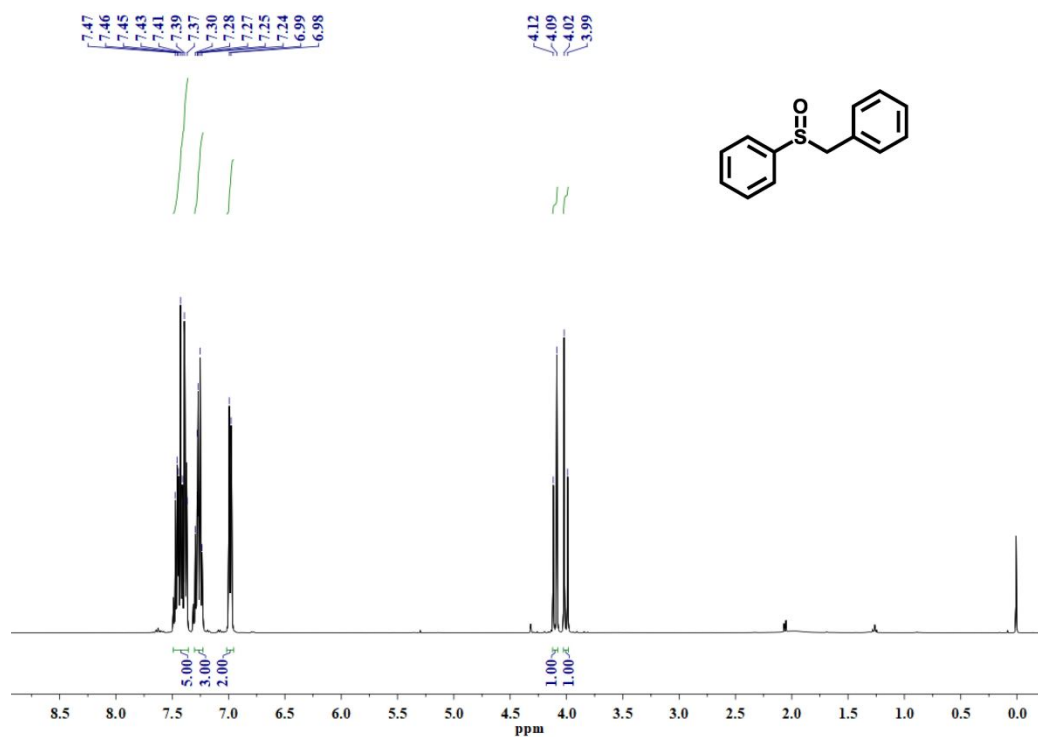
**Figure S8.**  $^{13}\text{C}$ -NMR spectrum of ethyl phenyl sulfoxide.



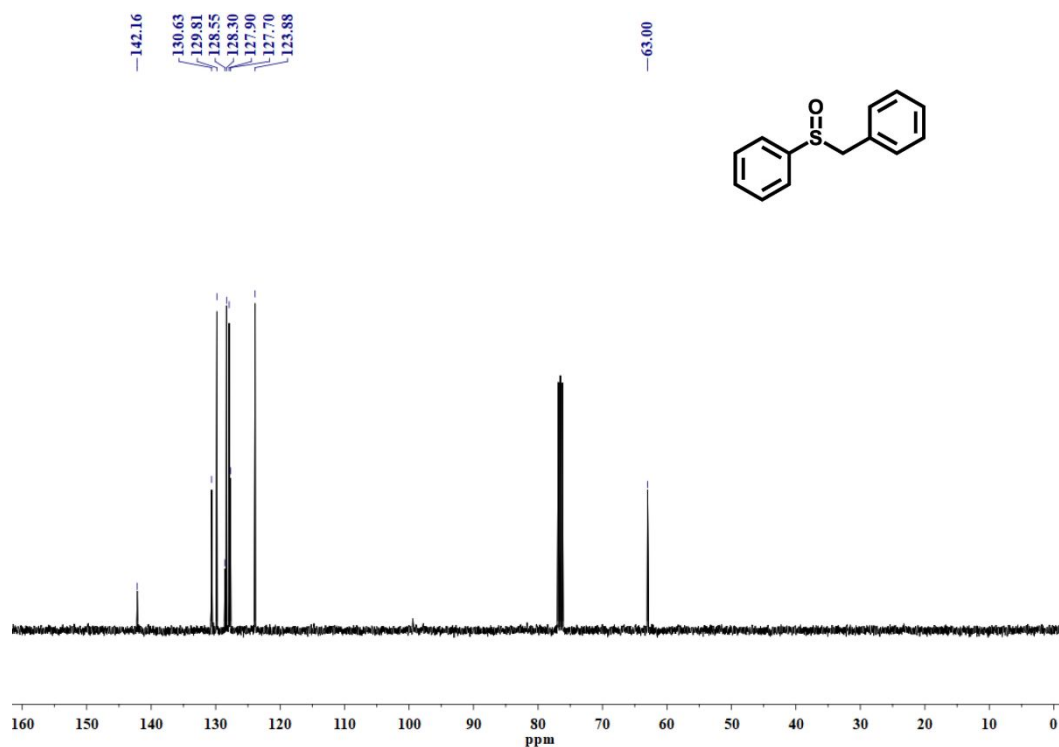
**Figure S9.** <sup>1</sup>H-NMR spectrum of phenyl allyl sulfoxide.



**Figure S10.** <sup>13</sup>C-NMR spectrum of phenyl allyl sulfoxide.

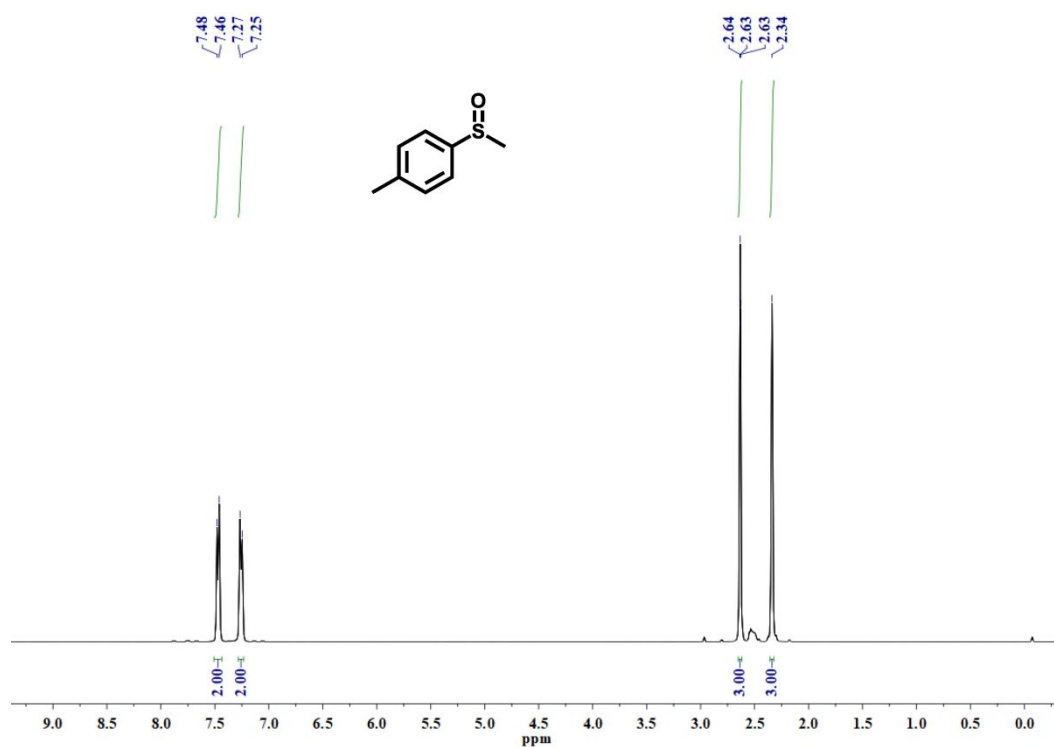


**Figure S11.** <sup>1</sup>H-NMR spectrum of phenyl benzyl sulfoxide.

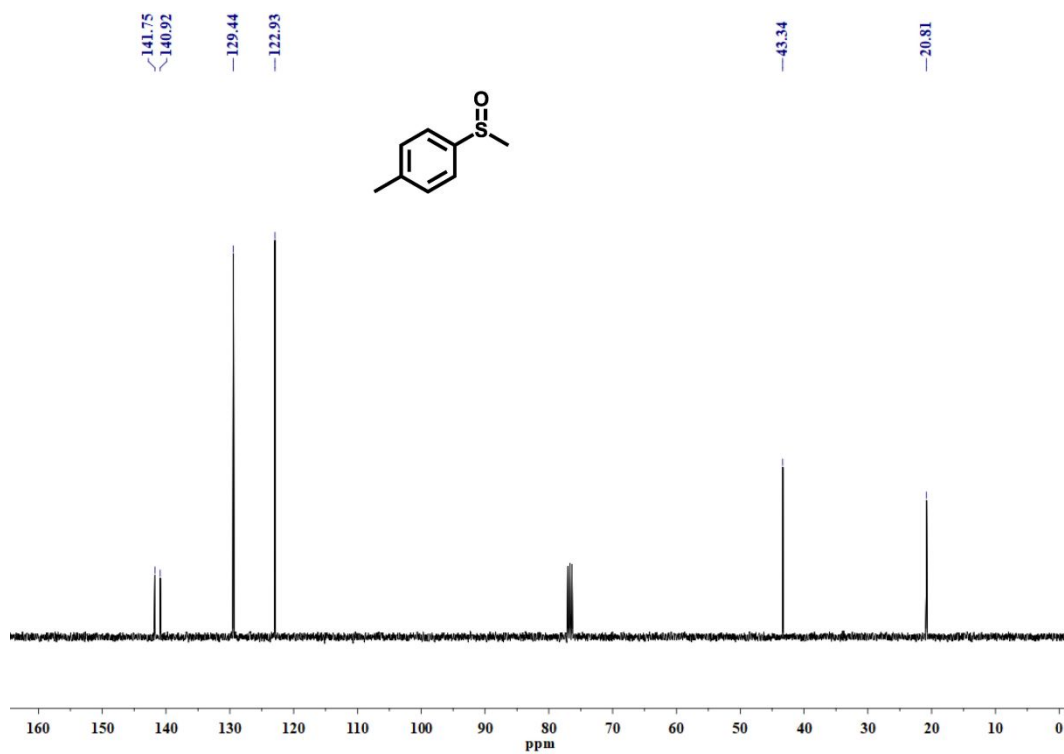


**Figure S12.** <sup>13</sup>C-NMR spectrum of phenyl benzyl sulfoxide.

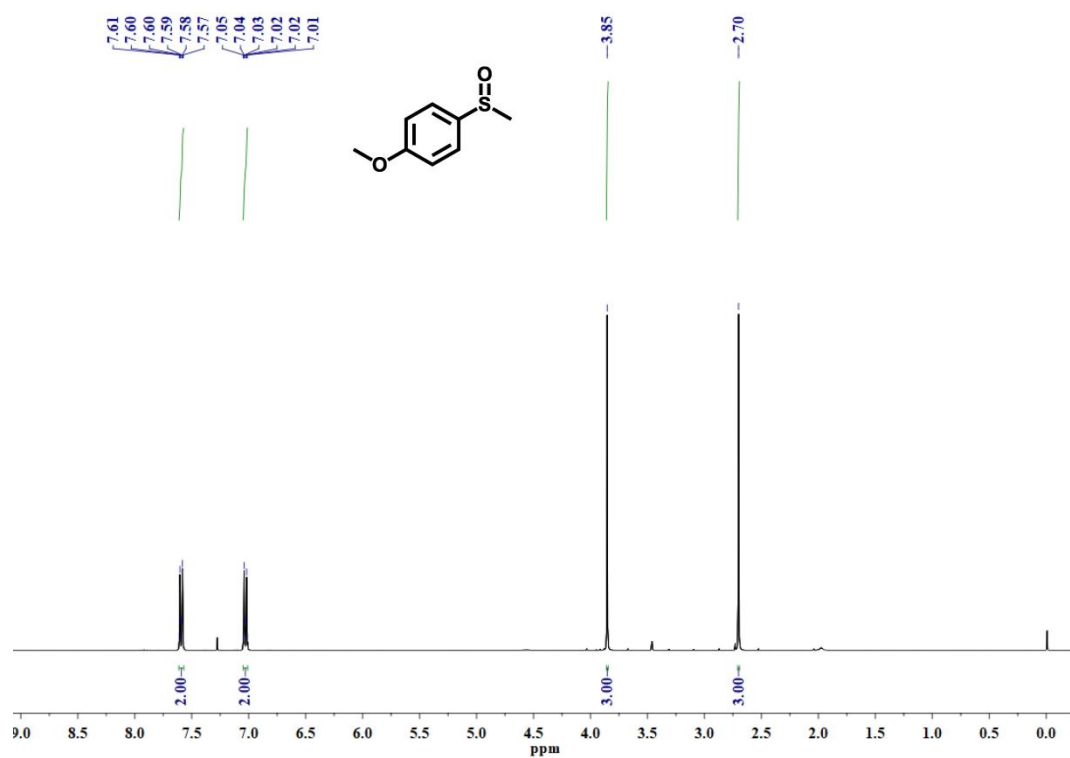




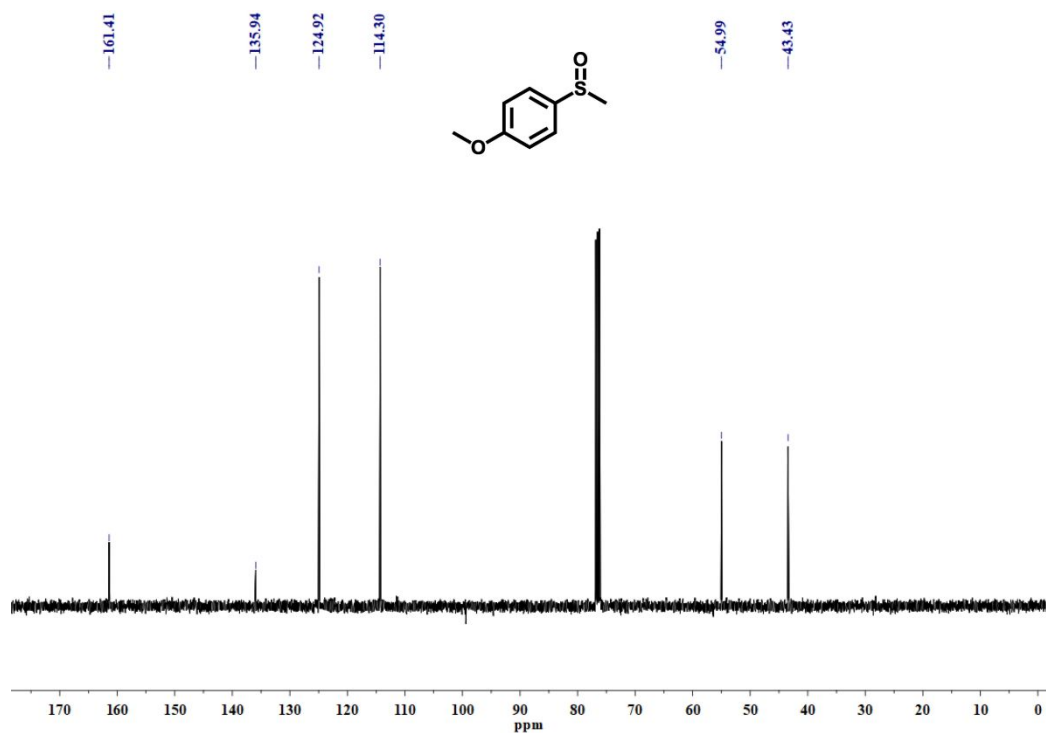
**Figure S13.** <sup>1</sup>H-NMR spectrum of methyl 4-methylphenyl sulfoxide.



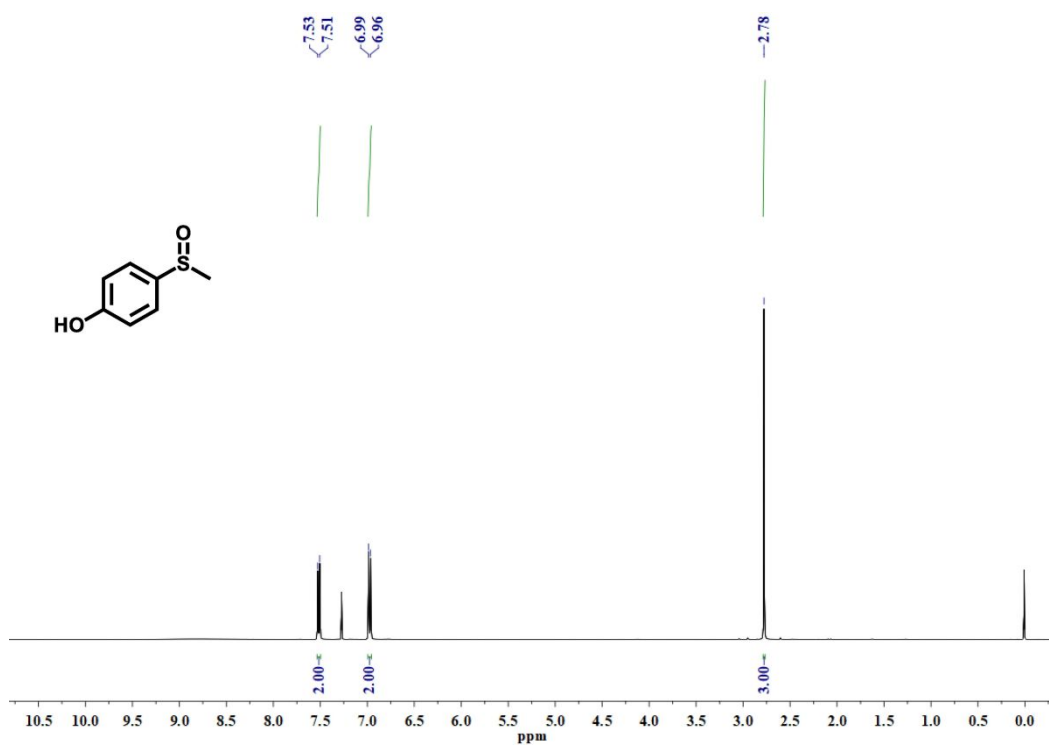
**Figure S14.**  $^{13}\text{C}$ -NMR spectrum of methyl 4-methylphenyl sulfoxide.



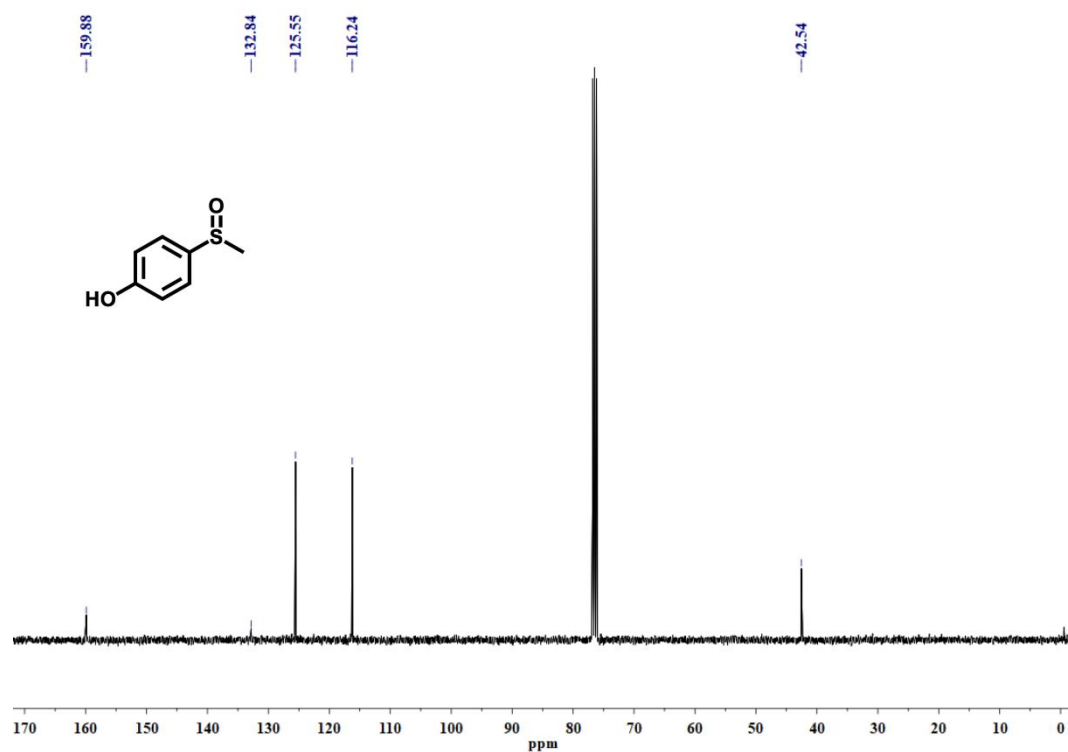
**Figure S15.**  $^1\text{H}$ -NMR spectrum of methyl 4-methoxyphenyl sulfoxide.



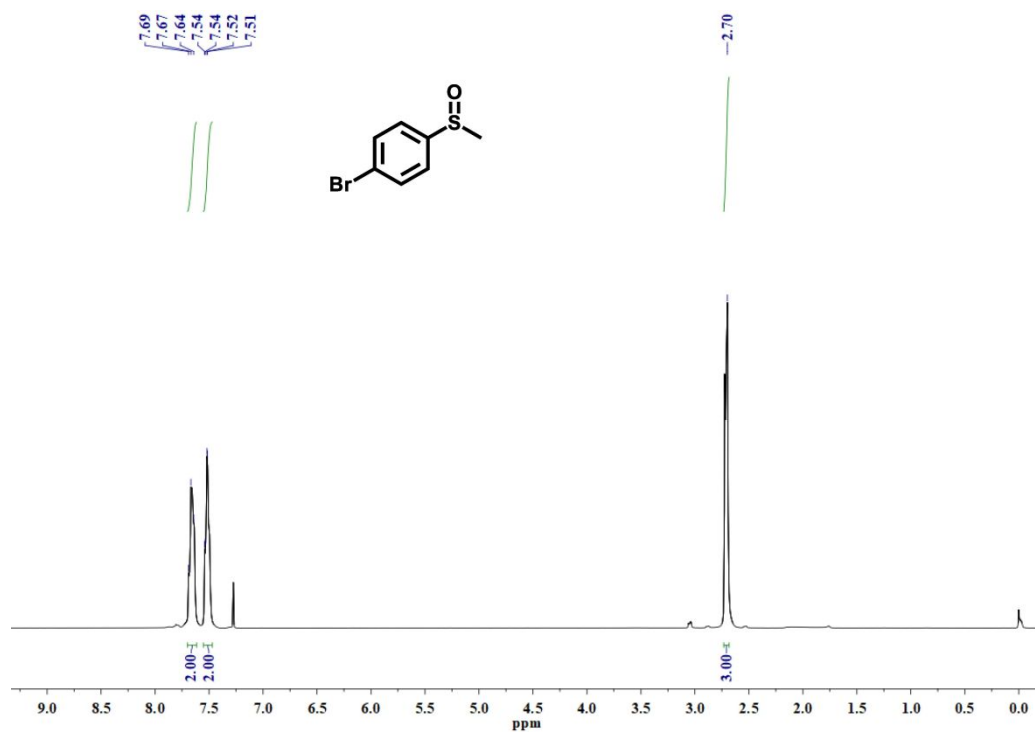
**Figure S16.** <sup>13</sup>C-NMR spectrum of methyl 4-methoxyphenyl sulfoxide.



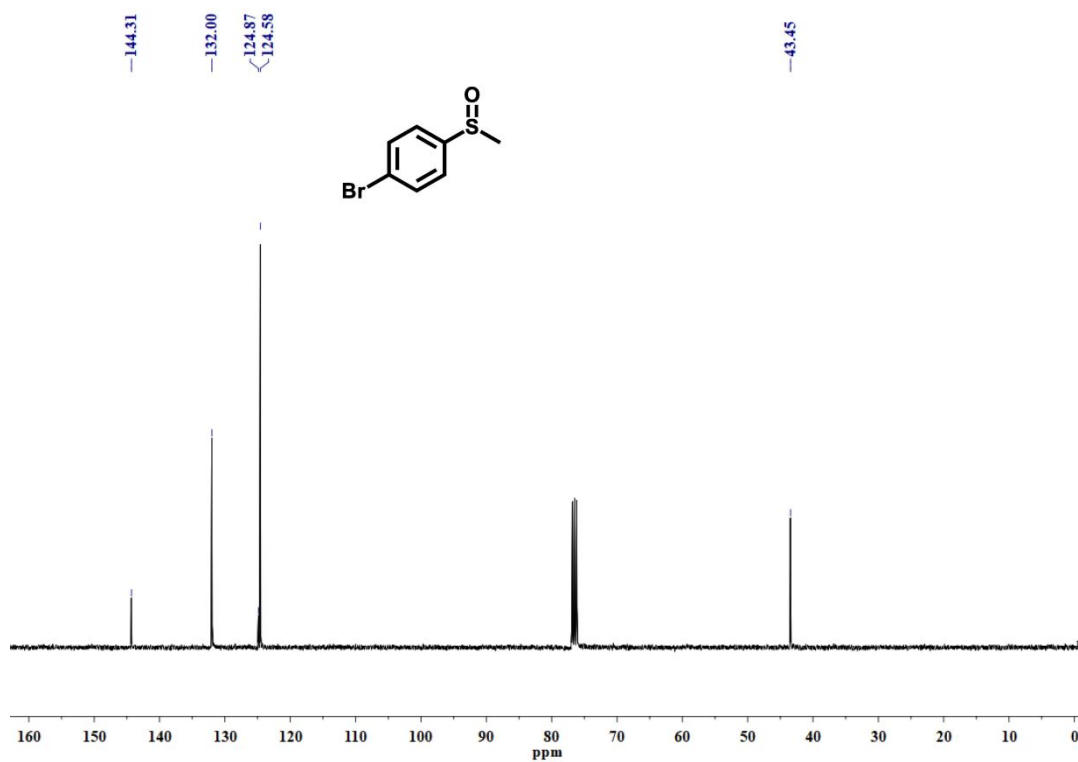
**Figure S17.** <sup>1</sup>H-NMR spectrum of 4-(methylsulfinyl)phenol.



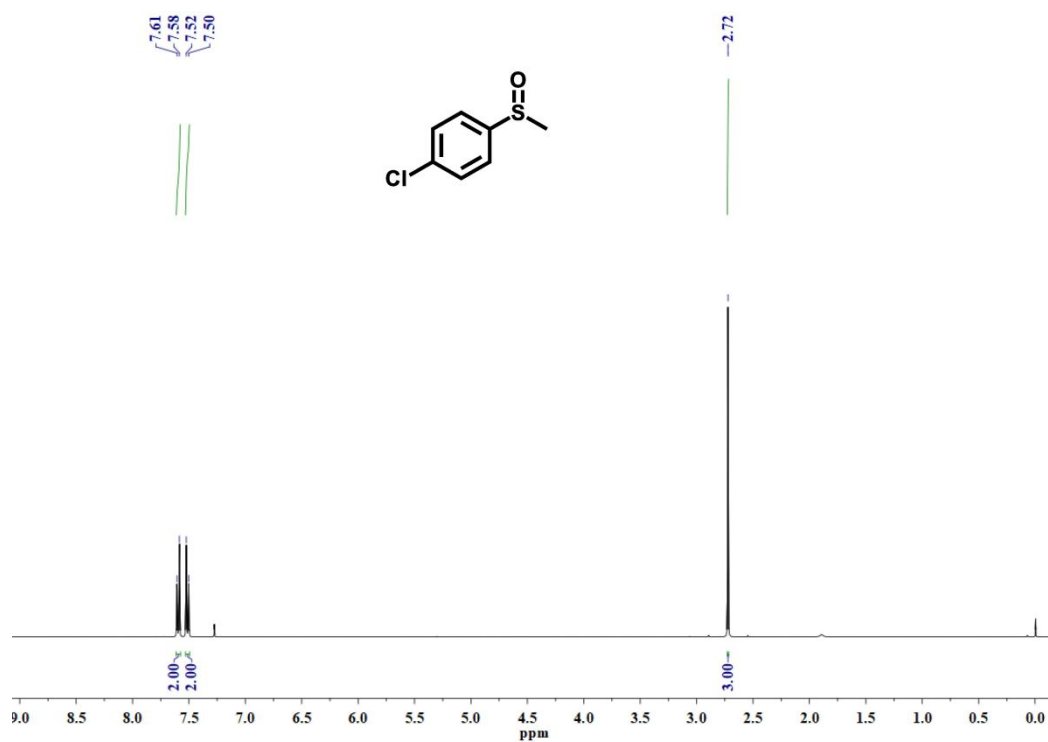
**Figure S18.** <sup>13</sup>C-NMR spectrum of methyl 4-(methylsulfinyl)phenol.



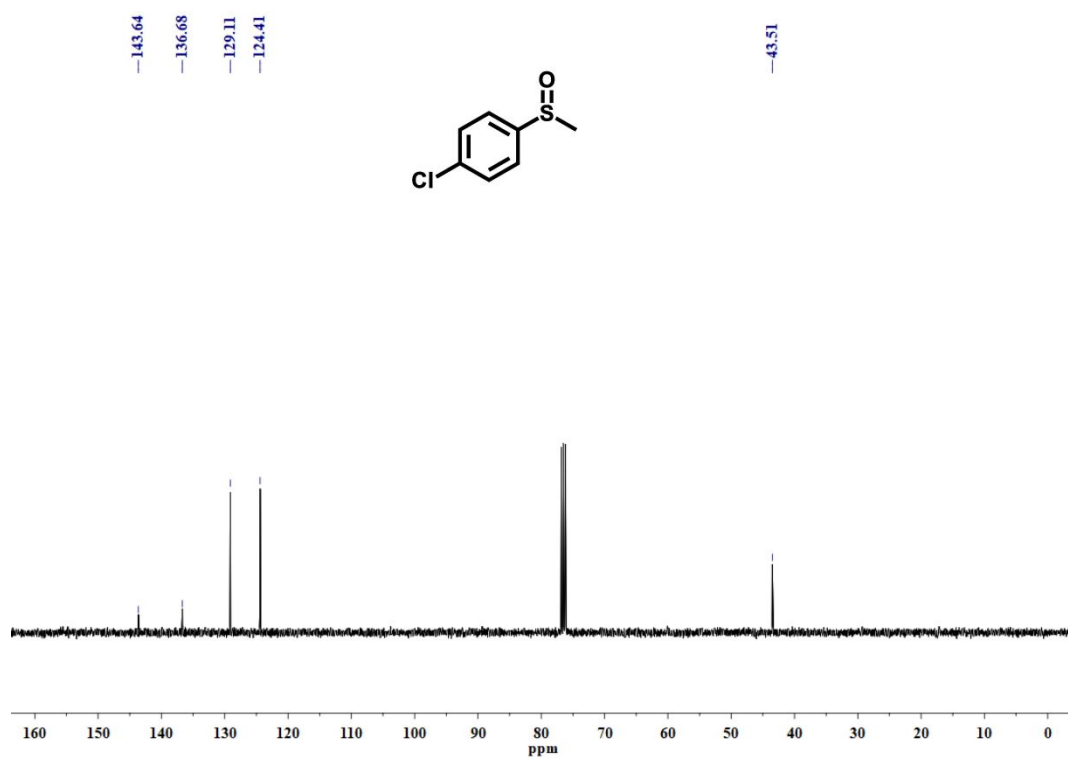
**Figure S19.** <sup>1</sup>H-NMR spectrum of 4-bromophenylmethylsulfoxide.



**Figure S20.** <sup>13</sup>C-NMR spectrum of 4-bromophenylmethanesulfoxide.

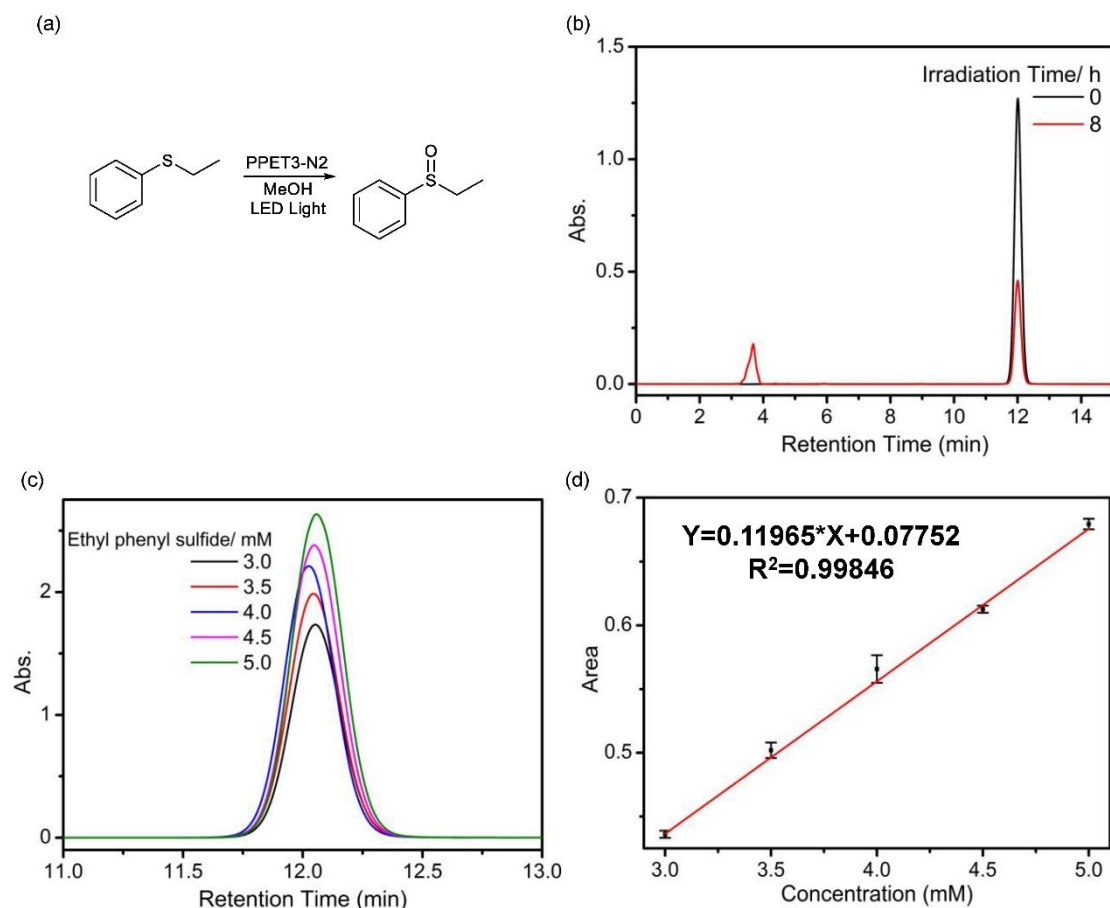


**Figure S21.** <sup>1</sup>H-NMR spectrum of 4-chlorophenylmethanesulfoxide.

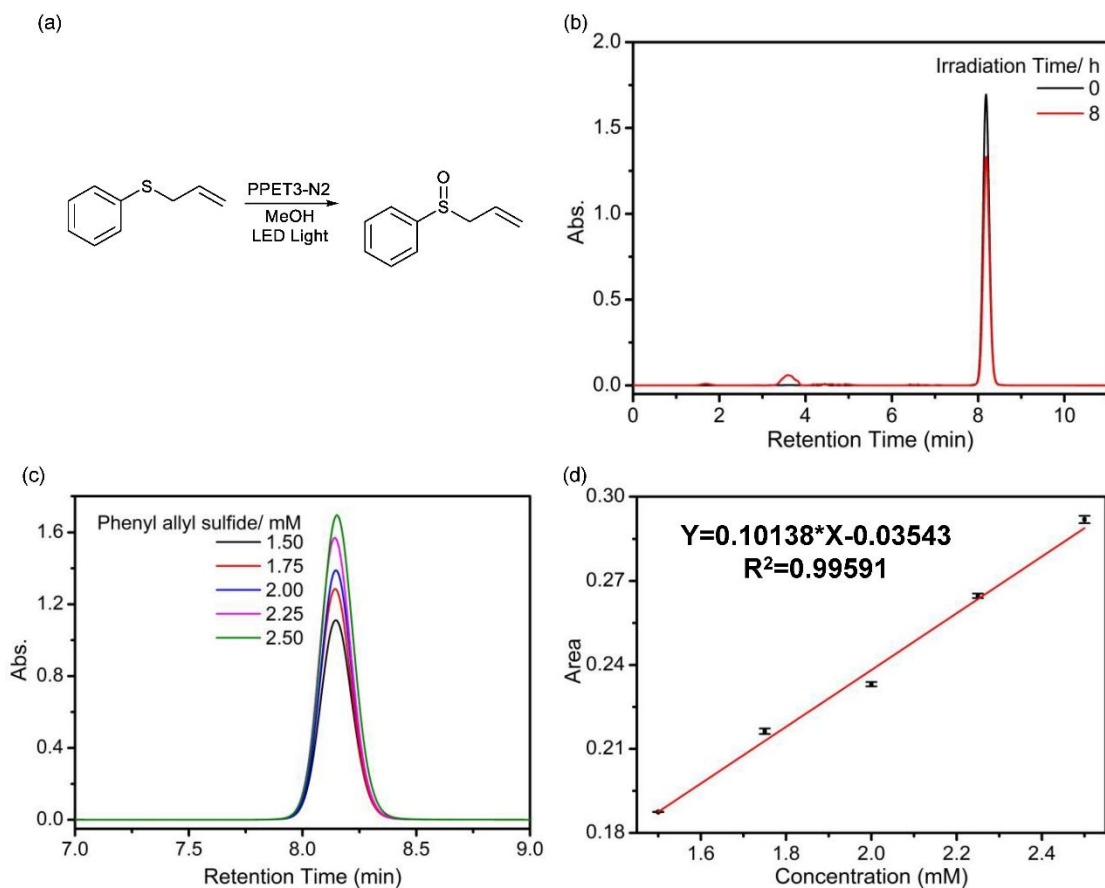


**Figure S22.**  $^{13}\text{C}$ -NMR spectrum of 4-chlorophenylmethanesulfoxide.

## Batch experiment of thioether derivative

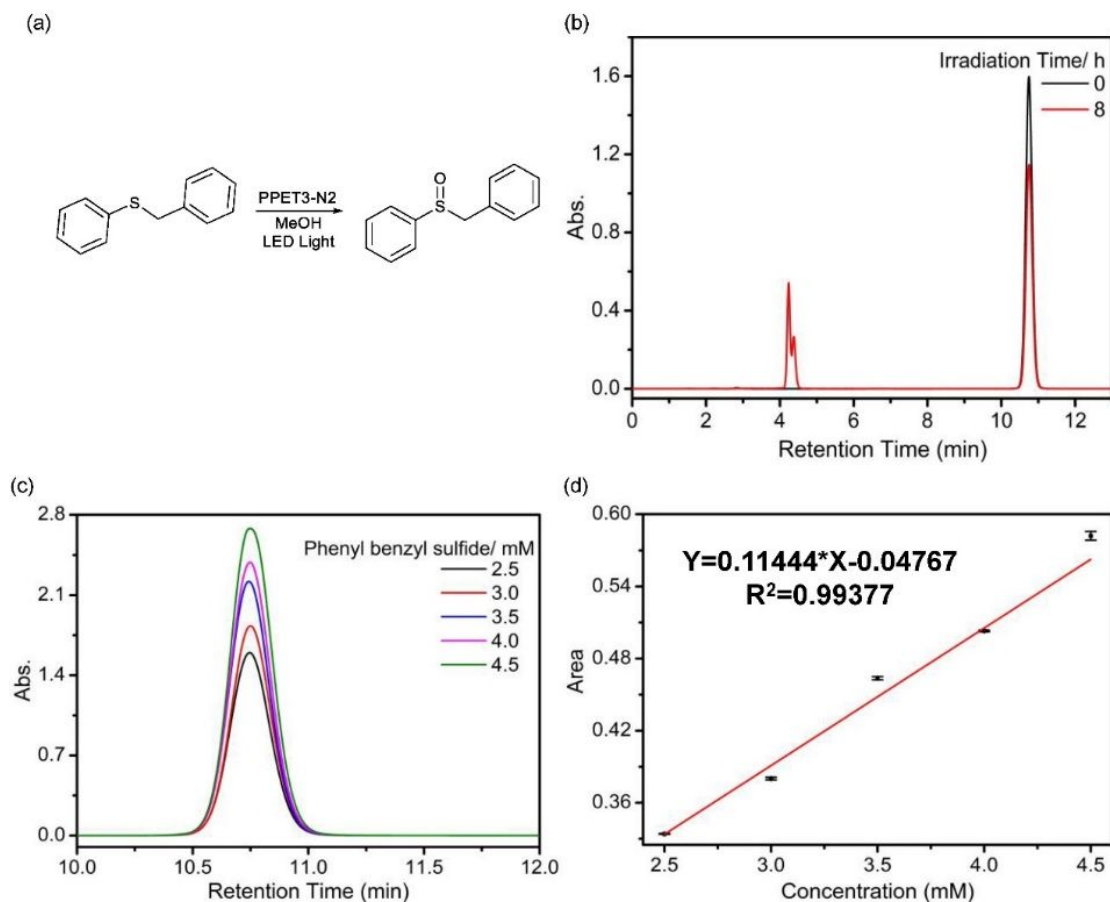


**Figure S23.** (a) Oxidation of ethyl phenyl sulfide by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 2:3 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 254.493 nm; (c) HPLC chromatogram (Retention Time: 11.0-13.0 min) of 3.0-5.0 mM ethyl phenyl sulfide; (d) The average area (integral area of 11.8-12.6 min in (c)) values at various ethyl phenyl sulfide concentration. Error bars are  $\pm$  SD,  $n=3$ . Reaction conditions: 10 mM ethyl phenyl sulfide with 150  $\mu$ M PPET3-N<sub>2</sub> in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.

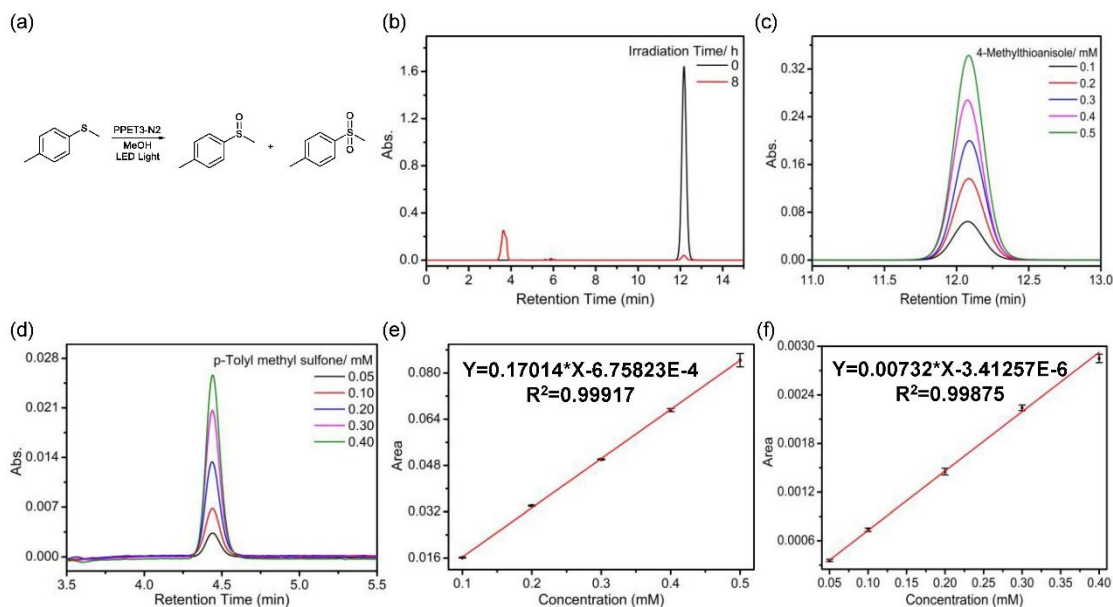


**Figure S24.** (a) Oxidation of phenyl allyl sulfide by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 253.314 nm; (c) HPLC chromatogram (Retention Time: 7.0-9.0 min) of 1.5-2.5 mM phenyl allyl sulfide; (d) The average area (integral area of 7.85-8.45 min in (c)) values at various phenyl allyl sulfide concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM phenyl allyl sulfide with 150  $\mu$ M PPET3-N2 in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.

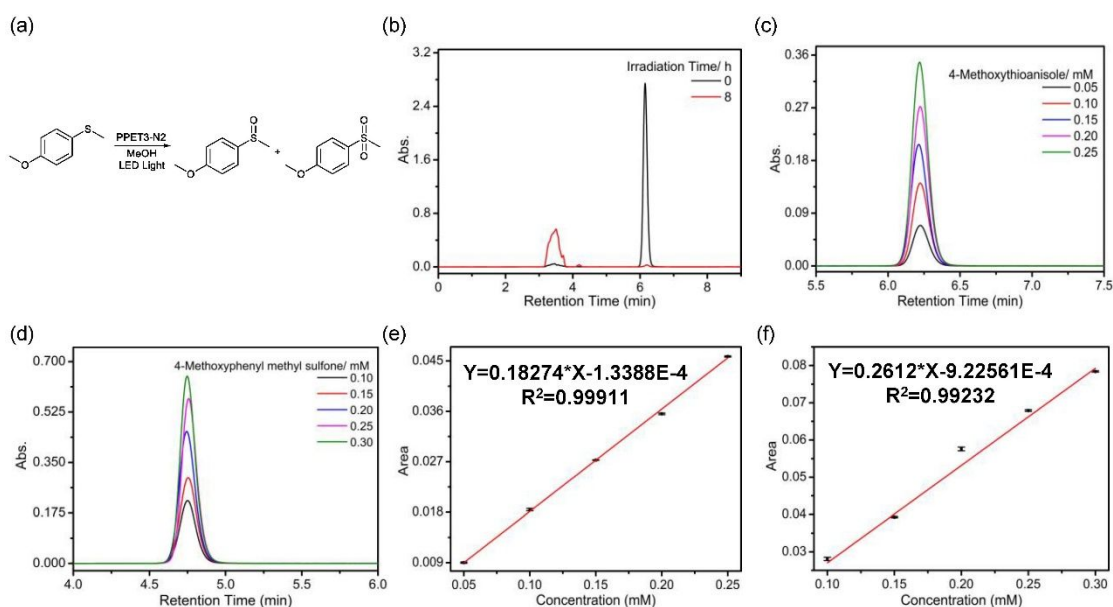




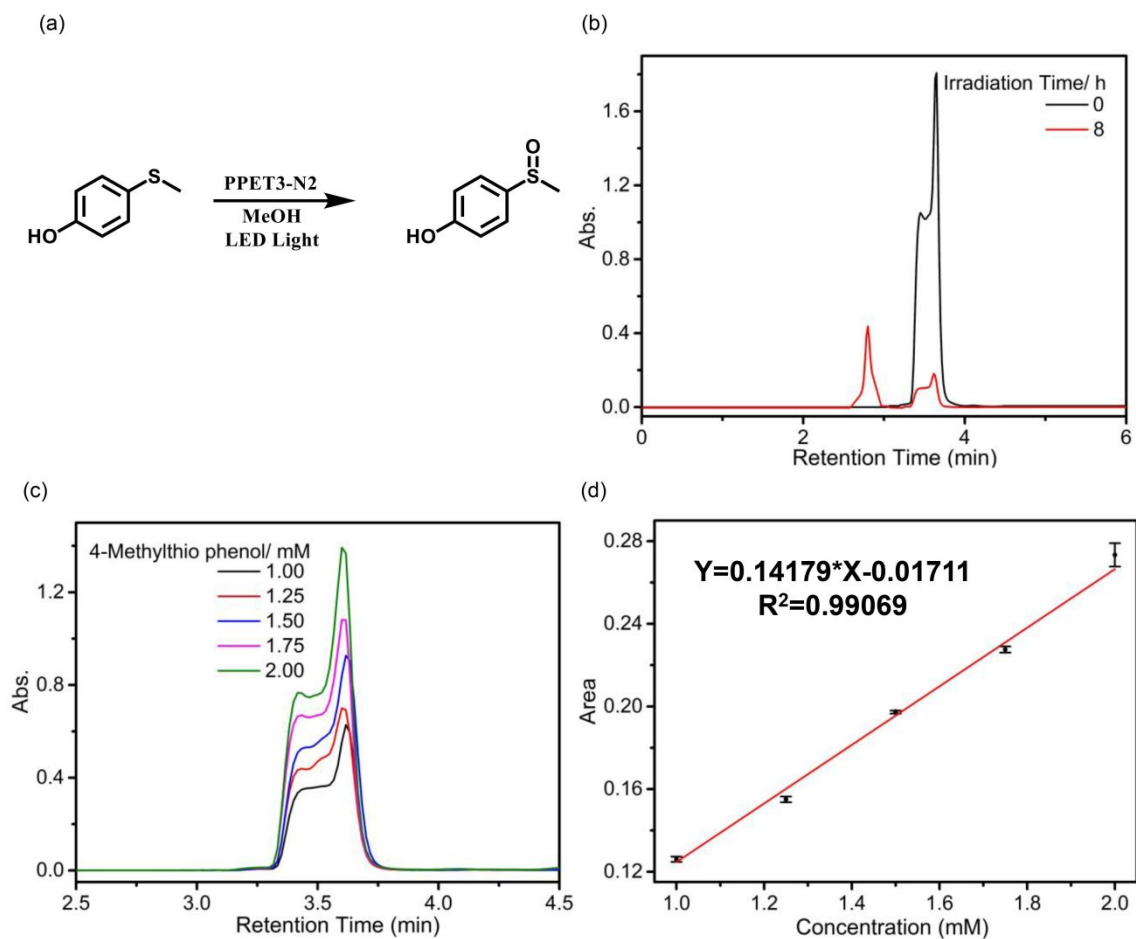
**Figure S25.** (a) Oxidation of phenyl benzyl sulfide by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v)  $\text{H}_2\text{O}/\text{CH}_3\text{CN}$  solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 253.314 nm; (c) HPLC chromatogram (Retention Time: 10.0-12.0 min) of 2.5-4.5 mM phenyl benzyl sulfide; (d) The average area (integral area of 10.4-11.2 min in (c)) values at various phenyl benzyl sulfide concentration. Error bars are  $\pm$  SD,  $n=3$ . Reaction conditions: 10 mM phenyl benzyl sulfide with 150  $\mu\text{M}$  PPET3-N2 in 4 mL methanol under 3.8  $\text{mW}/\text{cm}^2$  white LED light irradiation.



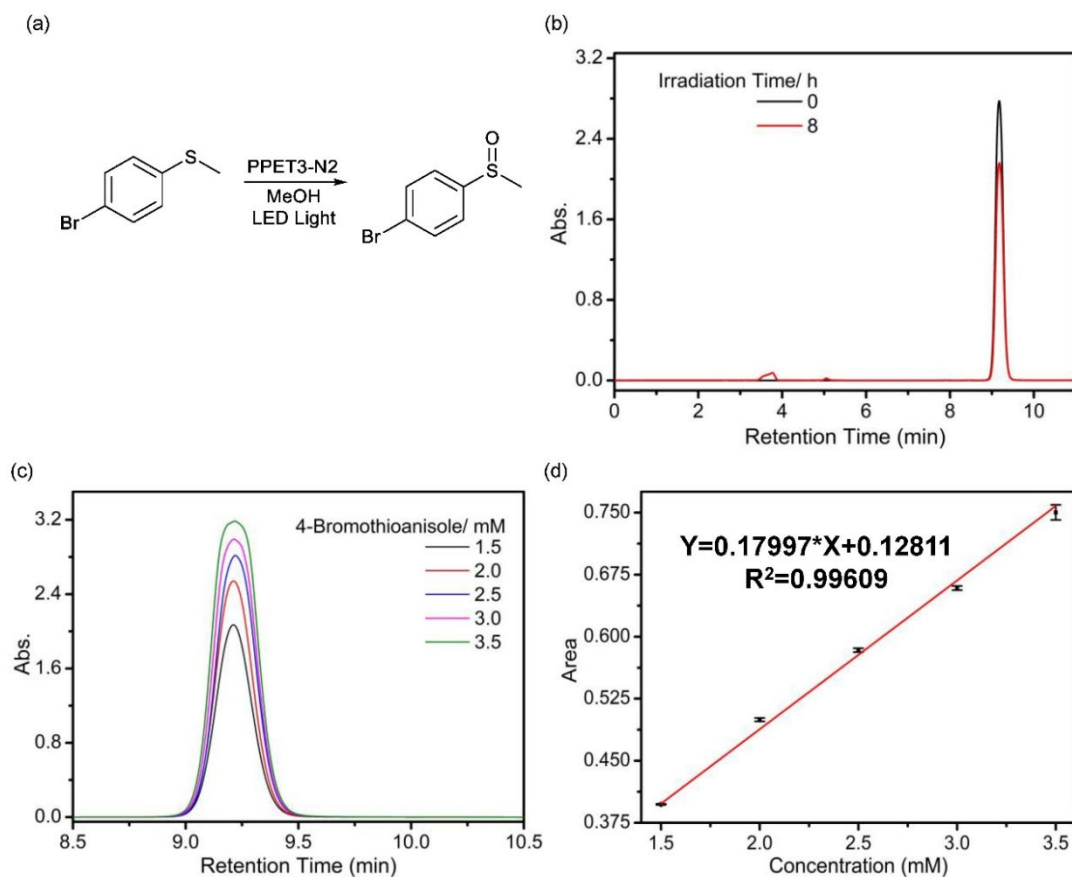
**Figure S26.** (a) Oxidation of 4-Methylthioanisole by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 2:3 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 254.493 nm; (c) HPLC chromatogram (Retention Time: 11.0-13.0 min) of 0.1-0.5 mM 4-Methylthioanisole; (d) HPLC chromatogram (Retention Time: 3.5-5.5 min) of 0.1-0.5 mM p-Tolyl methyl sulfone; (e) The average area (integral area of 11.8-12.6 min in (c)) values at various 4-Methylthioanisole concentration. Error bars are  $\pm$  SD, n=3; (f) The average area (integral area of 4.3-4.6 min in (d)) values at various p-Tolyl methyl sulfone concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM 4-Methylthioanisole with 150  $\mu$ M PPET3-N<sub>2</sub> in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.



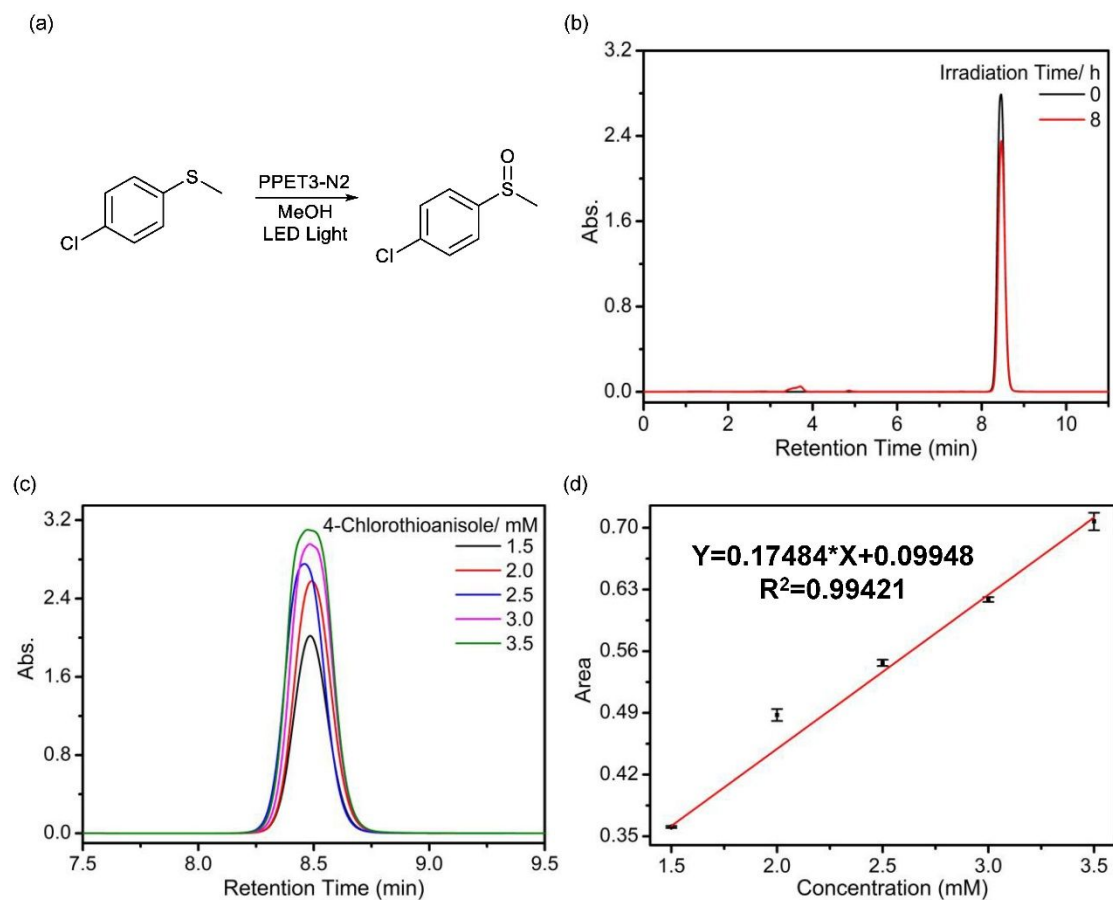
**Figure S27.** (a) Oxidation of 4-Methoxythioanisole by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 255.672 nm; (c) HPLC chromatogram (Retention Time: 5.5-7.5 min) of 0.05-0.25 mM 4-Methoxythioanisole; (d) HPLC chromatogram (Detection: 239.182 nm; Eluent: 1:1 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN; Retention Time: 4.0-6.0 min) of 0.1-0.5 mM 4-Methoxyphenyl methyl sulfone; (e) The average area (integral area of 6.0-6.4 min in (c)) values at various 4-Methoxythioanisole concentration. Error bars are  $\pm$  SD, n=3; (f) The average area (integral area of 4.55-4.95 min in (d)) values at various 4-Methoxyphenyl methyl sulfone concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM 4-Methoxythioanisole with 150  $\mu$ M PPET3-N2 in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.



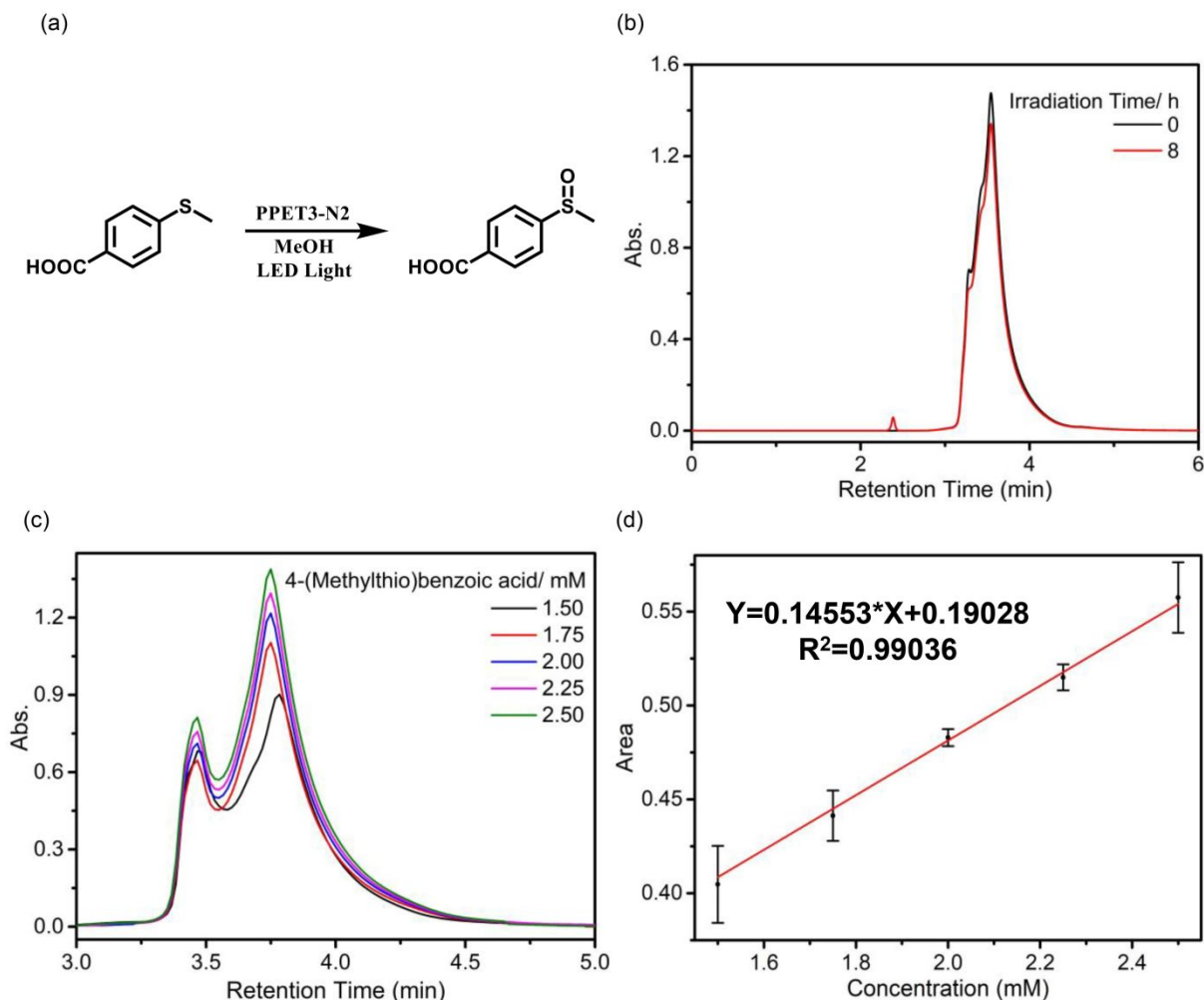
**Figure S28.** (a) Oxidation of 4-Methylthio phenol by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 255.672 nm; (c) HPLC chromatogram (Retention Time: 2.5-4.5 min) of 1.0-2.0 mM 4-Methylthio phenol; (d) The average area (integral area of 3.25-3.85 min in (c)) values at various 4-Methylthio phenol concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM 4-Methylthio phenol with 150  $\mu$ M PPET3-N2 in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.



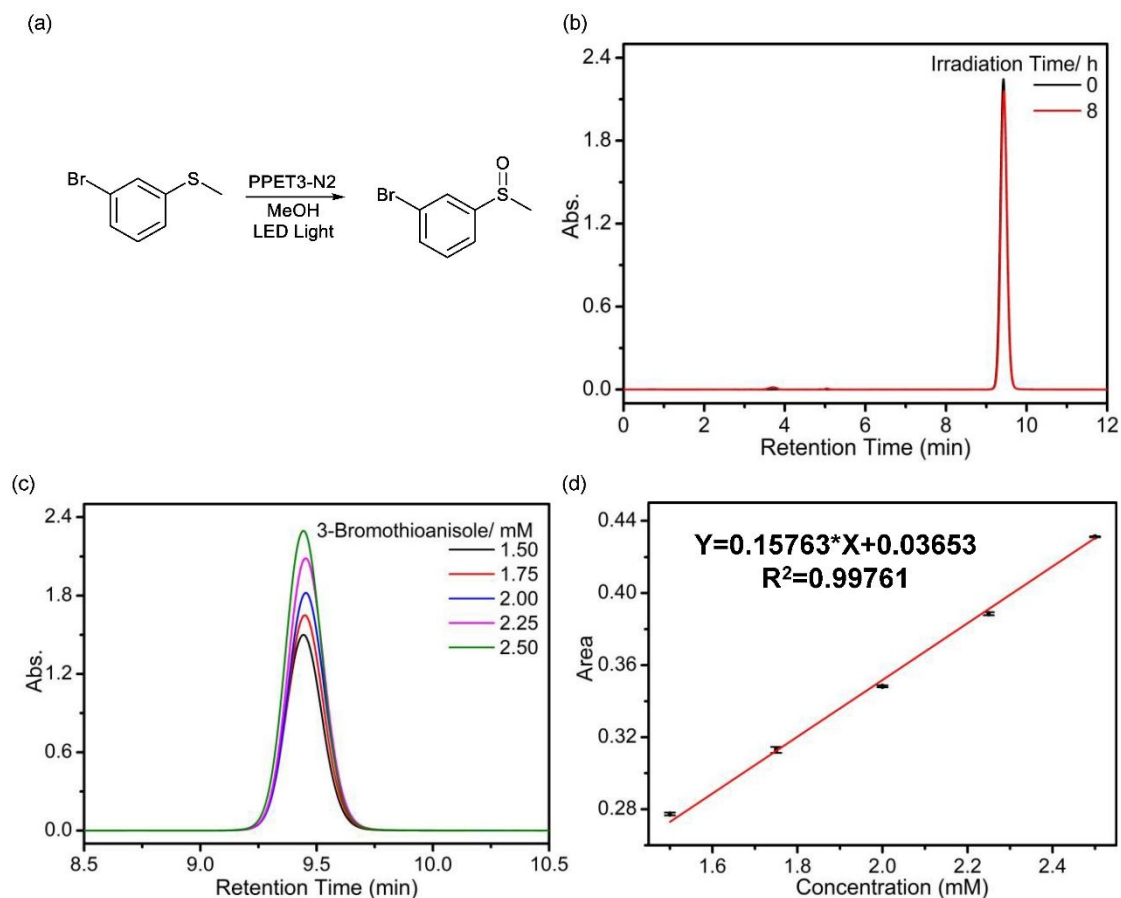
**Figure S29.** (a) Oxidation of 4-bromothioanisole by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 260.390 nm; (c) HPLC chromatogram (Retention Time: 8.5-10.5 min) of 1.5-3.5 mM 4-bromothioanisole; (d) The average area (integral area of 8.9-9.7 min in (c)) values at various 4-bromothioanisole concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM 4-bromothioanisole with 150  $\mu$ M PPET3-N<sub>2</sub> in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.



**Figure S30.** (a) Oxidation of 4-chlorothioanisole by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 259.211 nm; (c) HPLC chromatogram (Retention Time: 7.5-9.5 min) of 1.5-3.5 mM 4-chlorothioanisole; (d) The average area (integral area of 8.2-9.0 min in (c)) values at various 4-chlorothioanisole concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM 4-chlorothioanisole with 150  $\mu$ M PPET3-N2 in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.

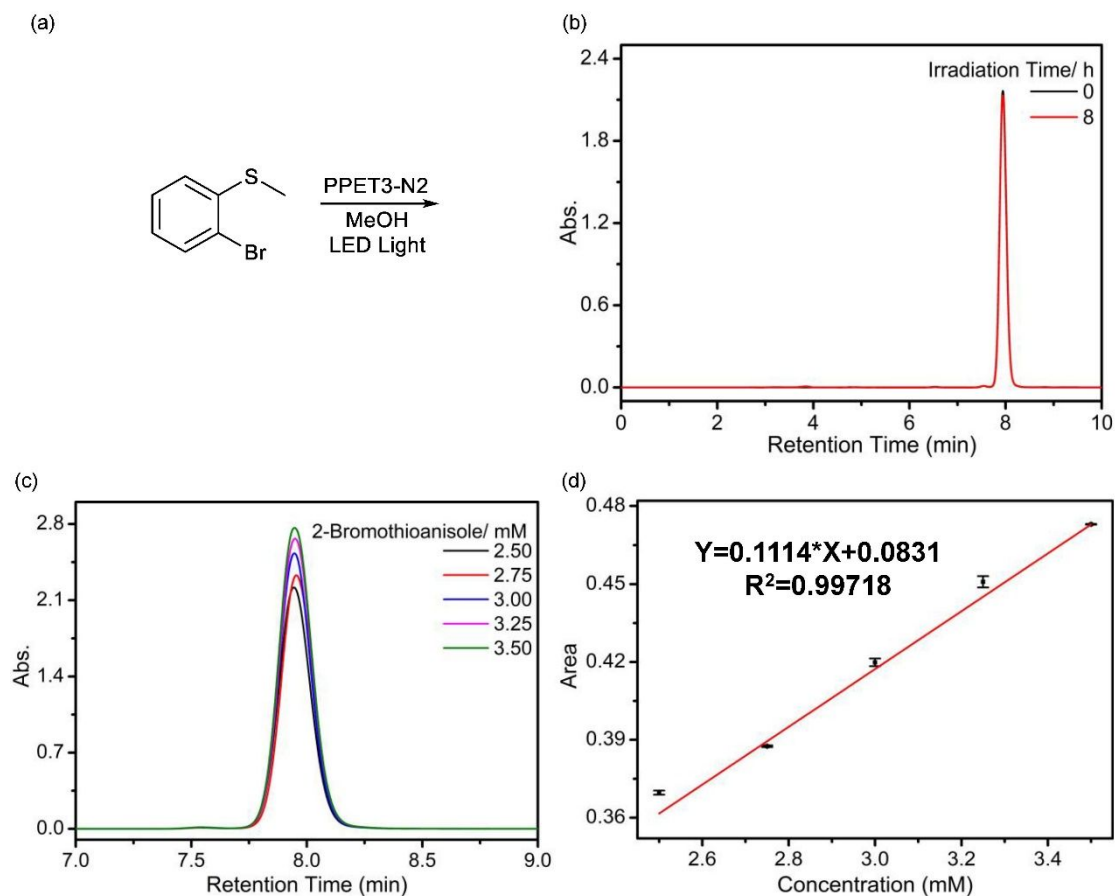


**Figure S31.** (a) Oxidation of 4-Methylthiobenzoic acid by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 1:4 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 281.662 nm; (c) HPLC chromatogram (Retention Time: 3.0-5.0 min) of 1.5-2.5 mM 4-Methylthiobenzoic acid; (d) The average area (integral area of 3.2-5.0 min in (c)) values at various 4-Methylthiobenzoic acid concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM 4-Methylthiobenzoic acid with 150  $\mu$ M PPET3-N2 in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.



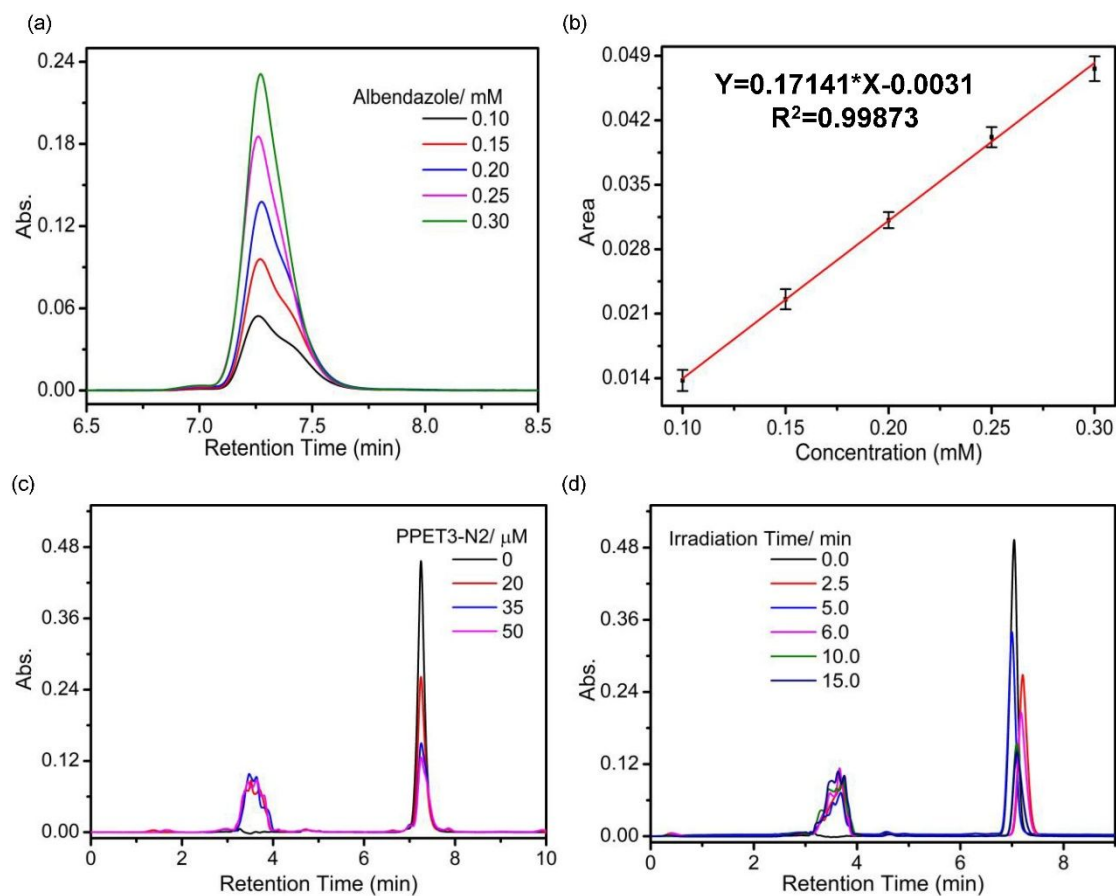
**Figure S32.** (a) Oxidation of 3-bromothioanisole by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 258.031 nm; (c) HPLC chromatogram (Retention Time: 8.5-10.5 min) of 1.5-2.5 mM 3-bromothioanisole; (d) The average area (integral area of 9.1-9.9 min in (c)) values at various 3-bromothioanisole concentration. Error bars are  $\pm$  SD, n=3. Reaction conditions: 10 mM 3-bromothioanisole with 150  $\mu$ M PPET3-N<sub>2</sub> in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.





**Figure S33.** (a) Oxidation of 2-bromothioanisole by singlet oxygen via the heteroatom oxidation reaction; (b) HPLC chromatogram of the reaction solution. Procedures. a 3:7 (v/v)  $H_2O/CH_3CN$  solution was used as the eluent with a flow rate of 0.5 mL/min, and the photodiode array detector was set at 252.135 nm; (c) HPLC chromatogram (Retention Time: 7.0-9.0 min) of 2.5-3.5 mM 2-bromothioanisole; (d) The average area (integral area of 7.5-8.3 min in (c)) values at various 2-bromothioanisole concentration. Error bars are  $\pm$  SD,  $n=3$ . Reaction conditions: 10 mM 2-bromothioanisole with 150  $\mu$ M PPET3-N2 in 4 mL methanol under 3.8 mW/cm<sup>2</sup> white LED light irradiation.





**Figure S34.** (a) HPLC chromatogram (Detection: 254.493 nm; Eluent: 1:1 (v/v) H<sub>2</sub>O/CH<sub>3</sub>CN; Flow rate: 0.5 mL/min; Retention Time: 6.5-8.5 min) of 0.1-0.3 mM albendazole; (b) The average area (integral area of 7.0-7.6 min in (a)) values at various albendazole concentration. Error bars are  $\pm$  SD, n=3; (c) HPLC chromatogram of the reaction solution in batch; (d) HPLC chromatogram of the reaction solution in microfluidic reactor.