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Supporting Information

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Supporting information

Metal-free chemoselective oxidation of sulfides to sulfoxides by hydrogen peroxide catalyzed by the *in situ* generated dodecyl hydrogen sulfate in the absence of any organic co-solvents

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**General procedure for sulfoxidation of sulfides (Table 2, entries 1, 4, 7-11):**

A 10 mL flask was charged with 1 mL (8.0 mmol) of aqueous solution of H<sub>2</sub>O<sub>2</sub> (35%), 0.029 g (0.10 mmol) of SDS, and 2 mmol sulfide. To the resulting mixture, 20 μL (0.2 mmol) of aqueous HCl solution was added and stirred at room temperature. The progress of the reaction was followed by TLC. After complete disappearance of the reactant, the excess amount of H<sub>2</sub>O<sub>2</sub> was destroyed by the addition of saturated aqueous solution of Na<sub>2</sub>SO<sub>3</sub> to the reaction mixture. The product was extracted with EtOAc which was separated and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. Evaporation of the solvent under diminished pressure resulted the almost pure product.

**Methyl Phenyl Sulfoxide [MeS(O)Ph]:<sup>[1]</sup>**

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 250 MHz): δ= 2.73 (s, 3 H), 7.51–7.55 (m, 3 H), 7.64–7.69 (m, 2 H).

<sup>13</sup>C NMR (CHCl<sub>3</sub>, 63 MHz): δ= 43.83, 123.36, 129.24, 130.92, 145.51.

**Ethyl Phenyl Sulfoxide [PhS(O)Et]:<sup>[1]</sup>**

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 250 MHz): δ= 1.20 (t, 3 H, *J* = 7.5 Hz), 2.69–3.15 (m, 2 H), 7.40–7.61 (m, 5 H), 7.52–7.58 (m, 3 H).

<sup>13</sup>C NMR (CHCl<sub>3</sub>, 63 MHz): δ= 5.8, 50.3, 124.1, 129.1, 130.1, 143.1.

**Dibutyl Sulfoxide [CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>S(O)CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>]:<sup>[1]</sup>**

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 0.92 (t, 6 H,  $J$  = 7.5 Hz), 1.37–1.50 (m, 4 H), 1.70 (m, 4 H), 2.57–2.66 (m, 4 H).

$^{13}\text{C}$  NMR ( $\text{CHCl}_3$ , 63 MHz):  $\delta$  = 13.3, 21.7, 24.2, 51.8.

**Diallyl Sulfoxide [ $\text{CH}_2=\text{CHCH}_2\text{S(O)CH}_2\text{CH}=\text{CH}_2$ ]:<sup>[3]</sup>**

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 3.43–3.59 (m, 4 H), 5.36–5.52 (m, 4 H), 5.83–5.92 (m, 2 H).

$^{13}\text{C}$  NMR ( $\text{CHCl}_3$ , 63 MHz):  $\delta$  = 54.2, 123.9, 126.0.

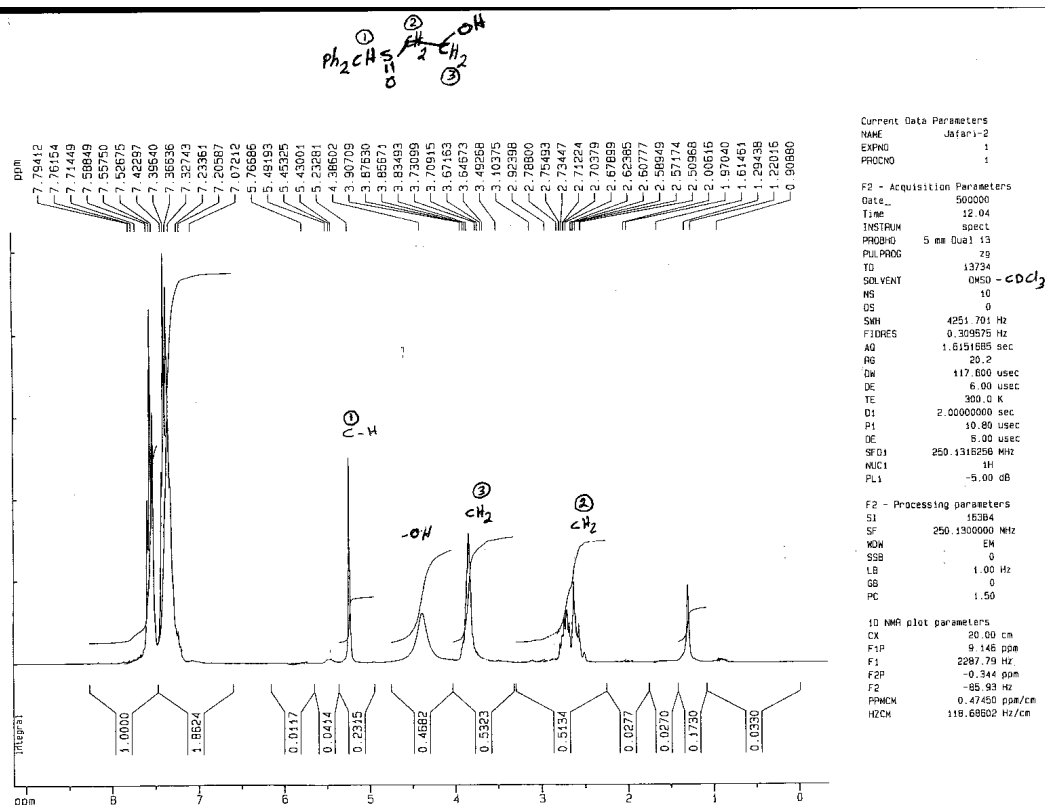
**2-Benzhydrylsulfanyl-ethanol [ $\text{Ph}_2\text{CHS(O)CH}_2\text{CH}_2\text{OH}$ ]:**

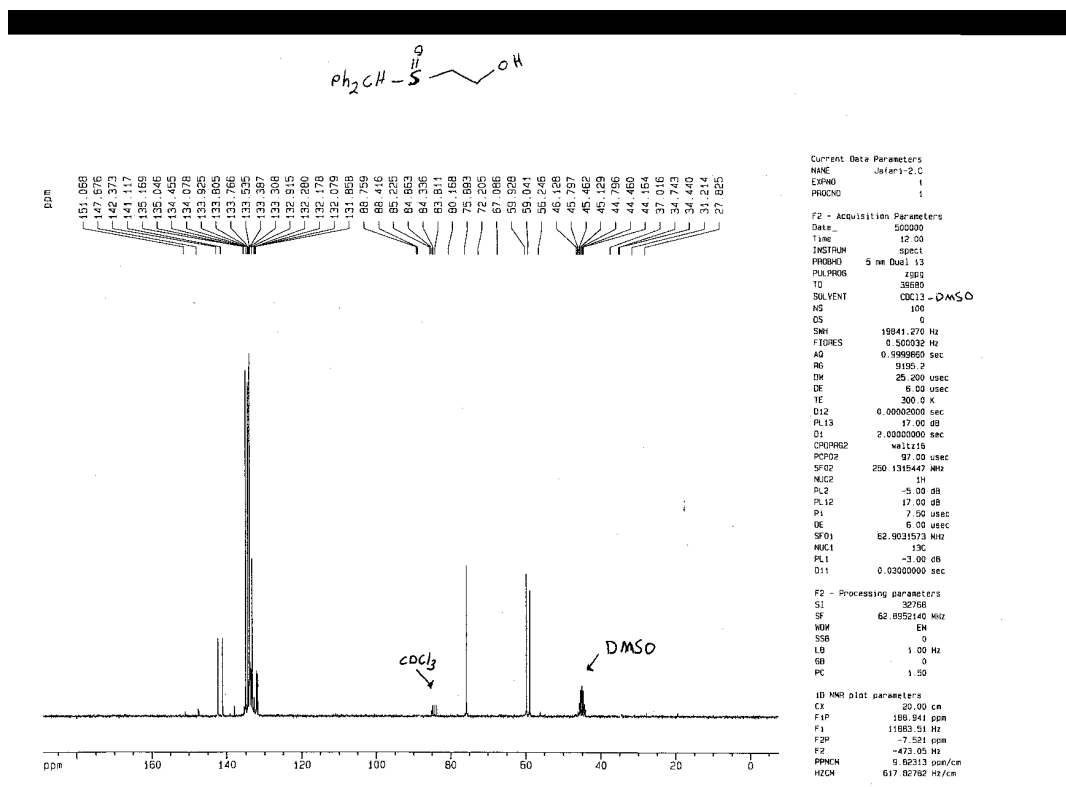
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 2.57–2.62 (m, 1H), 2.68–2.75 (m, 1H), 3.83–3.90 (m, 2H), 4.39 (s, 1H, OH), 5.23 (s, 1H), 7.33–7.42 (m, 6H), 7.52–7.59 (m, 4H).

$^{13}\text{C}$  NMR (63 MHz,  $\text{CDCl}_3$ ): 52.0, 52.9, 68.9, 126.3, 126.8, 126.9, 1127.4, 1128.0, 134.1, 135.4 ppm.

MS (EI, 70 ev),  $m/e$ :  $M^+$ =260.

Anal. Calcd for ( $\text{C}_{15}\text{H}_{16}\text{O}_2\text{S}$ ): C, 69.20; H, 6.19. Found: C, 69.12; H, 6.15.





## 2-Cyanoethyl Phenyl Sulfoxide [ $\text{PhS(O)CH}_2\text{CH}_2\text{CN}$ ].<sup>[1]</sup>

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 2.71–3.08 (m, 4 H), 7.53 (m, 5 H).

$^{13}\text{C}$  NMR ( $\text{CHCl}_3$ , 63 MHz): 18.1, 48.4, 118.2, 123.36, 129.24, 130.92, 145.51.

### General procedure for preparation of solid sulfoxides (Table 2, entries 2, 3, 5, 6):

A 10 mL flask was charged with 1 mL (8.0 mmol) of aqueous solution of  $\text{H}_2\text{O}_2$  (35%), 0.029 g (0.10 mmol) of SDS, and 2 mmol sulfide. To the resulting mixture, 20  $\mu\text{L}$  (0.2 mmol) of aqueous HCl solution was added and stirred at room temperature. The progress of the reaction was followed by TLC. As the reaction proceeded, the solid sulfoxides precipitated out. After complete disappearance of the reactant, 5 mL of water was added to the reaction mixture and the solid sulfoxide was filtered off and washed with water and dried under diminished pressure.

### Diphenyl Sulfoxide [ $\text{PhS(O)Ph}$ ].<sup>[1]</sup>

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 7.43–7.68 (m).

$^{13}\text{C}$  NMR ( $\text{CHCl}_3$ , 63 MHz):  $\delta$  = 124.8, 129.3, 131.1, 145.8.

**Benzyl Phenyl Sulfoxide [ $\text{PhCH}_2\text{S(O)Ph}$ ]:<sup>[1]</sup>**

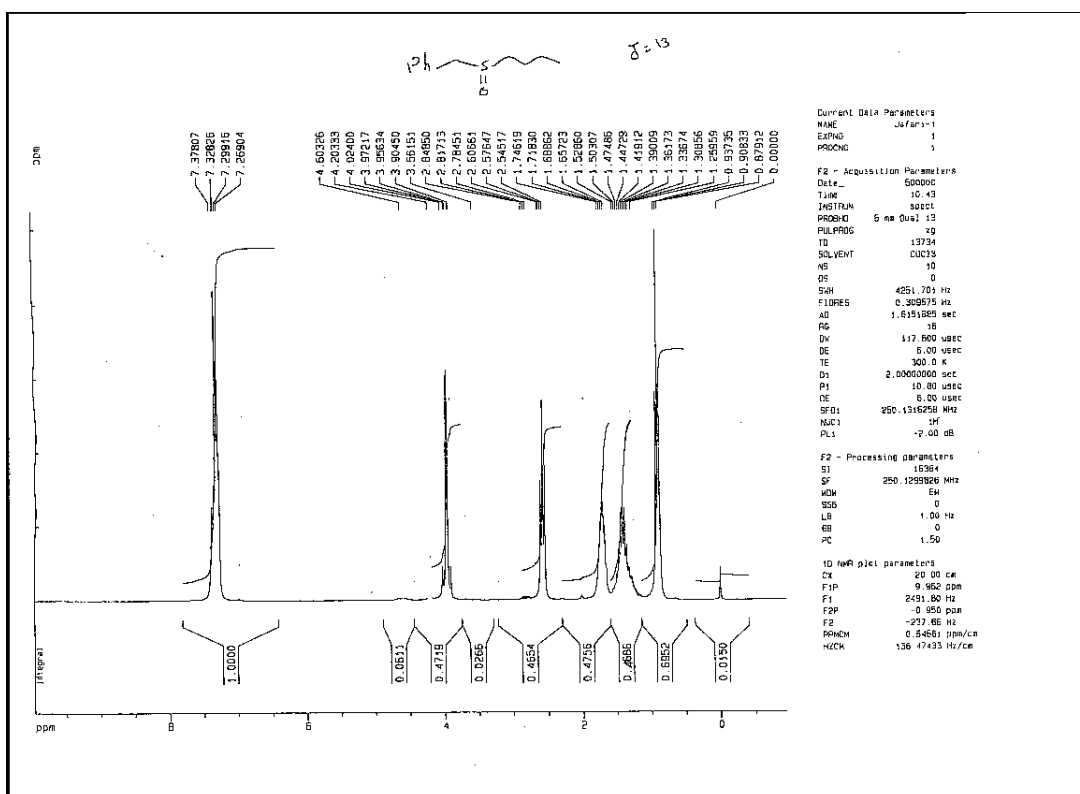
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 3.98 (d, 1 H,  $J$  = 14 Hz), 4.09 (d, 1 H,  $J$  = 14 Hz), 6.95–7.00 (m, 2 H), 7.22–7.28 (m, 3 H), 7.35–7.45 (m, 5 H).

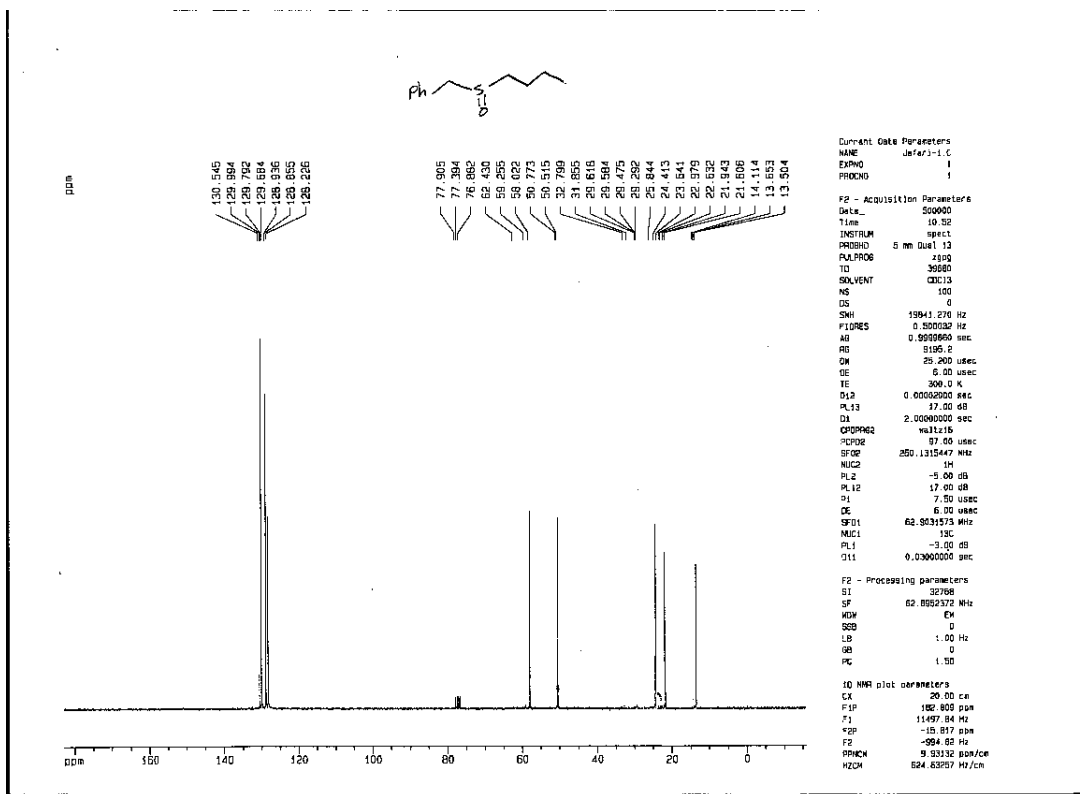
$^{13}\text{C}$  NMR ( $\text{CHCl}_3$ , 63 MHz):  $\delta$  = 63.2, 123.3, 127.9, 128.1, 128.5, 128.7, 129.9, 130.7, 142.3.

**Benzyl Butyl Sulfoxide [ $\text{PhCH}_2\text{S(O)CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ ]:**

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 0.91 (t, 3 H,  $J$  = 7.4 Hz), 1.42 (m, 2H), 1.71 (m, 2H), 2.61 (t, 2 H,  $J$ =15.5), 3.96 (dd, 2 H,  $J$  = 13 Hz), 7.28–7.45 (m, 5 H).

$^{13}\text{C}$  NMR ( $\text{CHCl}_3$ , 63 MHz):  $\delta$  = 13.5, 22.0, 24.4, 50.5, 58.0, 128.2, 128.9, 129.8, 129.9.





### Dibenzyl Sulfoxide [ $\text{PhCH}_2\text{S(O)CH}_2\text{Ph}$ ]:<sup>[2]</sup>

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 250 MHz):  $\delta$  = 3.85 (d, 2 H,  $J$  = 13 Hz), 3.92 (d, 2 H,  $J$  = 13 Hz), 7.25–7.38 (m, 10 H).

$^{13}\text{C}$  NMR ( $\text{CHCl}_3$ , 63 MHz):  $\delta$  = 57.1, 128.2, 128.8, 130.2, 130.0.

### References:

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- [2]. S. S. Kim, K. Nehru, S. S. Kim, D. W. Kim, H. C. Jung, *Synthesis*, **2002**, 2484.
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