# **Supplementary Materials**

#### 1. Experimental Data

**Table S1.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with H<sub>2</sub>O<sub>2</sub> catalyzed by camphor-10-sulfonic acid <sup>a</sup>.

	S_CH <sub>3</sub> Camphor-10-sulfonic a 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O, 25°C, 2	cid, 4.0h → SCH <sub>3</sub>	
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	99.6	99.3
2	1.0	99.8	99.0
3	2.0	99.7	97.7
4	3.0	99.7	97.8
5	4.0	99.9	97.5
6	5.0	99.9	98.3

<sup>a</sup> Reaction conditions: catalyst camphor-10-sulfonic acid (0.25 mmol, 58.1 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S2.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by camphor-10-sulfonic acid <sup>a</sup>.

	S_CH <sub>3</sub> Camphor-10-sulfonic at 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O, 25°C, 2	cid, 4.0h → CH <sub>3</sub>	
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	39.8	39.8
2	0.4	38.6	38.6
3	0.3	43.6	43.6
4	0.2	46.4	46.4

<sup>a</sup> Reaction conditions: catalyst camphor-10-sulfonic acid (0.025 mmol, 5.8 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S3.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by camphor-10-sulfonic acid in pH 1.30 <sup>a</sup>.

	S_CH <sub>3</sub> Camphor-10-sulfonic ac 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O, 25°C, 24	tid, 4.0h → CH <sub>3</sub>	
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	99.8	98.3
2	1.0	99.7	98.0
3	2.0	99.7	97.0
4	3.0	99.8	97.4
5	4.0	99.8	97.4
6	5.0	99.9	97.6

<sup>a</sup> Reaction conditions: 30%  $H_2O_2$  (1.15 equ.), catalyst and solvent (2.0 mL pH 1.30 aqueous solution of camphor-10-sulfonic acid), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

	S-CH <sub>3</sub> Methanesu 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O		°`CH <sub>3</sub>
Entry	Catalyst Loading (%)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.0	36.5	36.5
2	2.5	39.0	39.0
3	5.0	48.9	48.9
4	7.5	53.8	53.6
5	10.0	66.0	65.6
6	12.5	68.2	67.8
7	15.0	77.6	77.1
8	17.5	84.3	83.7
9	20.0	90.0	89.2
10	22.5	97.4	96.6
11	25.0	99.1	98.5

**Table S4.** Effect of catalyst loading on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by methanesulfonic acid <sup>a</sup>.

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30% H<sub>2</sub>O<sub>2</sub> (1.15 mmol, 130 µL), solvent (2.0 mL H<sub>2</sub>O), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S5.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by methanesulfonic acid <sup>a</sup>.

	S CH <sub>3</sub> Methanesulfonic acid 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O, 25°C, 24		
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	99.7	98.8
2	1.0	99.8	98.4
3	2.0	99.9	98.0
4	3.0	99.8	97.7
5	4.0	99.9	97.5
6	5.0	99.9	97.7

<sup>a</sup> Reaction conditions: catalyst methanesulfonic acid (0.25 mmol, 24.0 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S6.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by methanesulfonic acid <sup>a</sup>.

	SCH <sub>3</sub> Methanesulfonic acid, 30%H2O2, H2O, 25°C, 24		
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	42.3	42.3
2	0.4	46.0	46.0
3	0.3	46.4	46.4
4	0.2	51.6	51.6

<sup>a</sup> Reaction conditions: catalyst methanesulfonic acid (0.025 mmol, 2.4 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

	S-CH <sub>3</sub> <u><i>p</i>-Toluenesu 30%H<sub>2</sub>O<sub>2</sub>, H<sub>2</sub>O</u>		`CH₃
Entry	Catalyst Loading (%)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.0	39.1	39.1
2	2.5	45.8	45.8
3	5.0	47.8	47.8
4	7.5	57.2	56.9
5	10.0	64.4	64.1
6	12.5	75.5	75.1
7	15.0	82.5	82.0
8	17.5	88.2	87.6
9	20.0	96.1	95.5
10	22.5	99.4	98.6
11	25.0	<b>99.</b> 7	<b>98.8</b>

**Table S7.** Effect of catalyst loading on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by *p*-toluenesulfonic acid <sup>a</sup>.

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<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30%  $H_2O_2$  (1.15 mmol, 130  $\mu$ L), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S8.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by *p*-toluenesulfonic acid <sup>a</sup>.

	CH <sub>3</sub> <u><i>p</i>-Toluenesulfonic acid</u> 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O, 25°C, 24	I.oh → CH <sub>3</sub>	
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	99.7	98.8
2	1.0	99.8	98.5
3	2.0	99.9	98.1
4	3.0	99.9	97.9
5	4.0	99.9	98.1
6	5.0	99.9	98.1

<sup>a</sup> Reaction conditions: catalyst *p*-toluenesulfonic acid (0.25 mmol, 43.1 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S9.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by *p*-toluenesulfonic acid <sup>a</sup>.

	S CH <sub>3</sub> <u><i>p</i>-Toluenesulfonic acid</u> 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O, 25°C, 24	.0h → CH <sub>3</sub>	
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	45.9	45.9
2	0.4	44.4	44.4
3	0.3	51.9	51.9
4	0.2	53.4	53.4

<sup>a</sup> Reaction conditions: catalyst *p*-toluenesulfonic acid (0.025 mmol, 4.3 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h. <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

	CH <sub>3</sub> Methand 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O		`CH₃
Entry	Catalyst Loading (%)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.0	39.1	39.1
2	100.0	58.7	58.5
3	150.0	63.4	63.2
4	200.0	79.3	78.9
5	250.0	85.8	85.4
6	300.0	89.8	89.4
7	350.0	97.3	96.8
8	400.0	99.1	98.6
9	450.0	99.3	97.4
10	500.0	99.3	95.9

**Table S10.** Effect of catalyst loading on the oxidation of methyl phenyl sulfide with H<sub>2</sub>O<sub>2</sub> catalyzed by methanoic acid <sup>a</sup>.

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30% H<sub>2</sub>O<sub>2</sub> (1.15 mmol, 130 µL), solvent (2.0 mL H<sub>2</sub>O), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S11.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by methanoic acid <sup>a</sup>.

	S CH <sub>3</sub> <u>Methanoic acid,</u> <u>30%H₂O₂</u> , H₂O, 25℃, 24	4.0h → CH <sub>3</sub>	
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.50	99.4	98.1
2	0.75	99.6	98.0
3	1.00	99.6	98.3
4	1.25	99.7	98.3
5	1.50	99.7	98.1
6	1.75	99.8	97.9
7	2.00	99.8	98.5

<sup>a</sup> Reaction conditions: catalyst methanoic acid (4.00 mmol, 184.1 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

	S CH <sub>3</sub> Methanoic acid, 30%H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O, 25°C, 2	4.0h	
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	41.9	41.9
2	0.4	39.4	39.4
3	0.3	46.9	46.9
4	0.2	48.4	48.4

**Table S12.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by methanoic acid <sup>a</sup>.

<sup>a</sup> Reaction conditions: catalyst methanoic acid (1.00 mmol, 46.0 mg), 30%  $H_2O_2$  (1.15 equ.), solvent (2.0 mL  $H_2O$ ), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S13.** Effect of catalyst loading on the oxidation of methyl phenyl sulfide with H<sub>2</sub>O<sub>2</sub> catalyzed by acetic acid <sup>a</sup>.

	S_CH <sub>3</sub> <u>Acetic acid,</u> H <sub>2</sub> O, 25°		CH3
Entry	Catalyst Loading (%)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.0	41.5	41.5
2	100.0	54.9	54.7
3	150.0	61.9	61.8
4	200.0	66.8	66.7
5	250.0	70.8	70.7
6	300.0	75.2	75.0
7	350.0	86.8	86.6
8	400.0	93.8	93.6
9	450.0	95.3	95.1
10	500.0	96.6	96.4
11	550.0	99.1	98.9
12	600.0	99.1	98.9

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30% H<sub>2</sub>O<sub>2</sub> (1.15 mmol, 130 µL), solvent (2.0 mL H<sub>2</sub>O), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

	S CH <sub>3</sub> Acetic acid, 30%H <sub>2</sub> O <sub>2</sub> H <sub>2</sub> O, 25°C, 24.0h		
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.50	99.2	98.9
2	0.75	98.6	98.3
3	1.00	98.5	98.1
4	1.25	99.3	98.9
5	1.50	99.5	99.0
6	1.75	99.7	99.1
7	2.00	99.6	99.0
8	2.25	99.6	98.8
9	2.50	99.1	98.5
10	2.75	98.9	98.1
11	3.00	99.1	97.8

**Table S14.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by acetic acid <sup>a</sup>.

<sup>a</sup> Reaction conditions: catalyst acetic acid (5.50 mmol, 330.0 mg), 30% H<sub>2</sub>O<sub>2</sub> (1.15 equ.), solvent (2.0 mL H<sub>2</sub>O), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S15.** Effect of the substrate amount on the oxidation of methyl phenyl sulfide with  $H_2O_2$  catalyzed by acetic acid <sup>a</sup>.

	S-CH <sub>3</sub> Acetic acid, 30%H <sub>2</sub> O <sub>2</sub> H <sub>2</sub> O, 25°C, 24.0h		
Entry	Substrate Concentration (mmol/mL)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	0.5	46.8	46.8
2	0.4	47.2	47.2
3	0.3	47.6	47.6
4	0.2	58.1	58.1

<sup>a</sup> Reaction conditions: catalyst acetic acid (1.00 mmol, 60.1 mg), 30% H<sub>2</sub>O<sub>2</sub> (1.15 equ.), solvent (2.0 mL H<sub>2</sub>O), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

	°	ethanesulfonic acid, $_{2}O_{2}$ , H $_{2}O$ , 25°C, 24.0h	SCH3
Entry	pH Value	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	2.00	43.7	43.6
2	1.90	49.8	49.6
3	1.80	57.9	57.6
4	1.70	67.5	67.2
5	1.60	72.7	72.3
6	1.50	78.2	77.4
7	1.40	98.0	97.2
8	1.30	99.8	<b>98.</b> 7
9	1.20	99.7	98.4
10	1.10	99.5	97.9
11	1.00	99.3	96.4

**Table S16.** Effect of pH value on the oxidation of methyl phenyl sulfide with H<sub>2</sub>O<sub>2</sub> catalyzed by methanesulfonic acid <sup>a</sup>.

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30%  $H_2O_2$  (1.15 mmol, 130  $\mu$ L), catalyst and solvent (2.0 mL aqueous solution of methanesulfonic acid), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

<b>Table S17.</b> Effect of pH value on the oxidation of methyl phenyl sulfide with H <sub>2</sub> O <sub>2</sub> catalyzed
by <i>p</i> -toluenesulfonic acid <sup>a</sup> .

	· ·	oluenesulfonic acid, ₂O₂, H₂O, 25°C, 24.0h ➤	CH3
Entry	pH Value	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	2.00	53.7	53.5
2	1.90	55.8	55.6
3	1.80	57.5	57.2
4	1.70	67.0	66.6
5	1.60	75.5	75.0
6	1.50	85.6	85.0
7	1.40	96.8	96.0
8	1.30	99.7	98.5
9	1.20	99.8	98.2
10	1.10	99.6	96.8
11	1.00	99.5	93.9

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30%  $H_2O_2$  (1.15 mmol, 130  $\mu$ L), catalyst and solvent (2.0 mL aqueous solution of *p*-toluenesulfonic acid), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

S.	·	noic acid, 30%H₂O₂, ₂O, 25°C, 24.0h	CH3
Entry	pH Value	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	2.00	49.3	49.1
2	1.90	50.3	50.2
3	1.80	53.8	53.3
4	1.70	57.1	56.6
5	1.60	71.3	70.8
6	1.50	74.9	74.3
7	1.40	98.4	97.9
8	1.30	99.6	99.1
9	1.20	99.6	98.7
10	1.10	99.8	98.1
11	1.00	99.2	97.3

**Table S18.** Effect of pH value on the oxidation of methyl phenyl sulfide with H<sub>2</sub>O<sub>2</sub> catalyzed by methanoic acid <sup>a</sup>.

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30% H<sub>2</sub>O<sub>2</sub> (1.15 mmol, 130 µL), catalyst and solvent (2.0 mL aqueous solution of methanoic acid), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

**Table S19.** Effect of pH value on the oxidation of methyl phenyl sulfide with H<sub>2</sub>O<sub>2</sub> catalyzed by sulfuric acid <sup>a</sup>.

	S.C	· · · · · · · · · · · · · · · · · · ·	ric acid, 30%H <sub>2</sub> O <sub>2</sub> , <sub>2</sub> O, 25°C, 24.0h	► U S CH <sub>3</sub>
	Entry	pH Value	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
	1	2.00	52.5	52.2
	2	1.90	53.5	53.3
	3	1.80	56.9	56.7
	4	1.70	59.1	58.8
	5	1.60	73.3	72.8
	6	1.50	76.1	75.6
	7	1.40	98.5	97.9
	8	1.30	<b>99.</b> 7	98.6
	9	1.20	99.6	97.8
	10	1.10	99.7	98.2
-	11	1.00	99.2	97.1

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30%  $H_2O_2$  (1.15 mmol, 130  $\mu$ L), catalyst and solvent (2.0 mL aqueous solution of sulfuric acid), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

S	CH <sub>3</sub> Hydroc	chloric acid, 30%H₂O₂, I₂O, 25°C, 24.0h	CH3
Entry	pH Value	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	2.00	48.1	47.9
2	1.90	52.8	52.6
3	1.80	61.5	61.1
4	1.70	64.5	64.1
5	1.60	68.3	68.0
6	1.50	88.9	88.0
7	1.40	99.2	98.3
8	1.30	<b>99.</b> 7	<b>98.8</b>
9	1.20	99.6	98.4
10	1.10	99.3	97.1
11	1.00	99.3	97.3

**Table S20.** Effect of pH value on the oxidation of methyl phenyl sulfide with H<sub>2</sub>O<sub>2</sub> catalyzed by hydrochloric acid <sup>a</sup>.

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30%  $H_2O_2$  (1.15 mmol, 130  $\mu$ L), catalyst and solvent (2.0 mL aqueous solution of hydrochloric acid), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

<b>Table S21.</b> Effect of pH value on the oxidation of methyl phenyl sulfide with H <sub>2</sub> O <sub>2</sub> catalyzed
by trifluoroacetic acid <sup>a</sup> .

S.	-	pacetic acid, 30%H₂O₂, ₂O, 25°C, 24.0h	CH3
Entry	pH Value	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	2.00	52.9	52.7
2	1.90	60.8	60.6
3	1.80	66.1	65.8
4	1.70	66.2	65.9
5	1.60	78.0	77.5
6	1.50	89.0	88.2
7	1.40	97.7	96.6
8	1.30	98.8	97.7
9	1.20	99.0	96.4
10	1.10	95.1	92.0
11	1.00	95.1	85.3

<sup>a</sup> Reaction conditions: substrate (1.0 mmol, 124.2 mg), 30%  $H_2O_2$  (1.15 mmol, 130  $\mu$ L), catalyst and solvent (2.0 mL aqueous solution of trifluoroacetic acid), 25 °C, 24.0 h; <sup>b</sup> Conversion and selectivity were determined by GC with *p*-xylene as internal standard, product was determined by comparison with the authentic sample.

## 2. <sup>1</sup>H-NMR Spectra of Product Sulfoxides

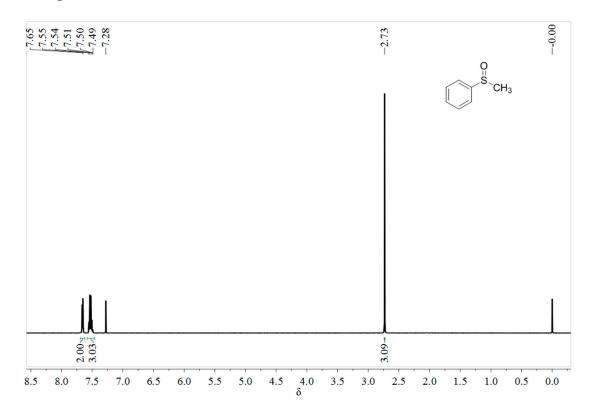
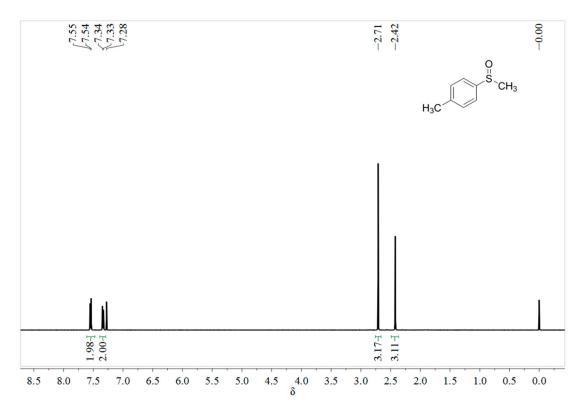
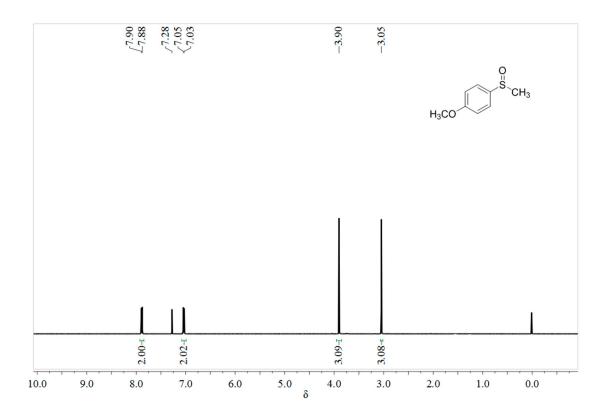


Figure S1. <sup>1</sup>H-NMR spectrum of methyl phenyl sulfoxide.



**Figure S2.** <sup>1</sup>H-NMR spectrum of methyl (4-methylphenyl) sulfoxide.



**Figure S3.** <sup>1</sup>H-NMR spectrum of methyl (4-methoxylphenyl) sulfoxide.

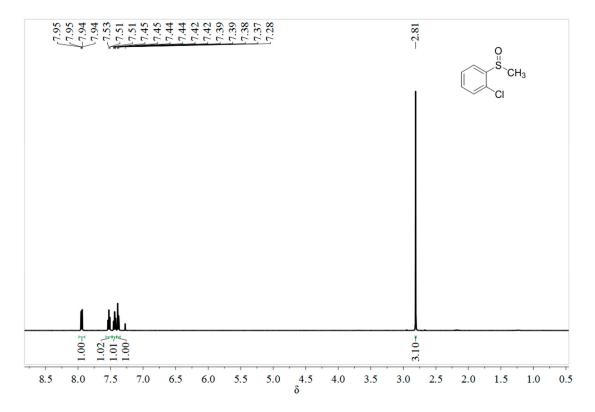


Figure S4. <sup>1</sup>H-NMR spectrum of methyl (2-chlorophenyl) sulfoxide.

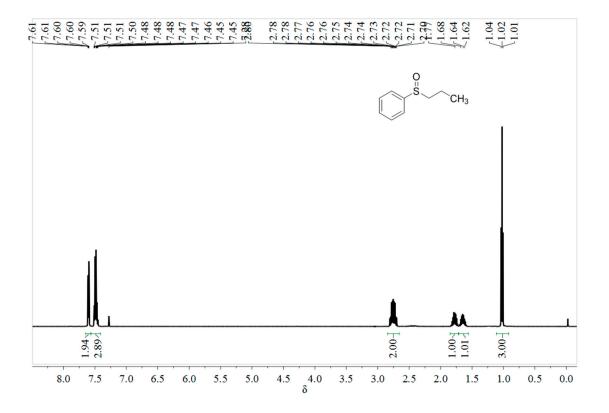
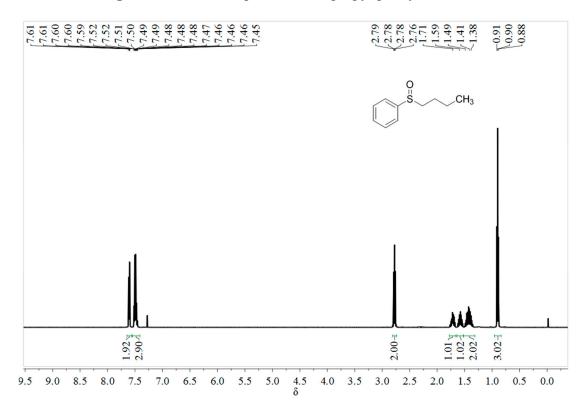


Figure S5. <sup>1</sup>H-NMR spectrum of *n*-propyl phenyl sulfoxide.



**Figure S6.** <sup>1</sup>H-NMR spectrum of *n*-butyl phenyl sulfoxide.

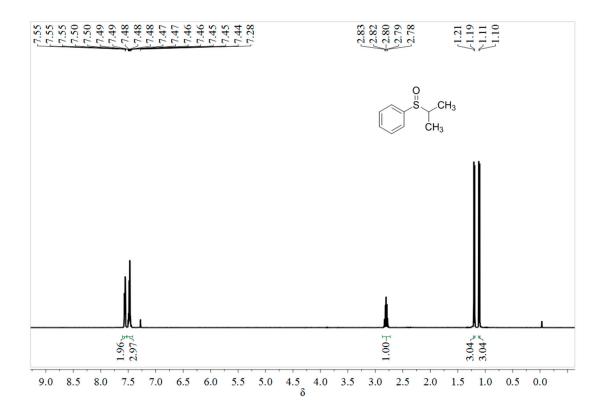


Figure S7. <sup>1</sup>H-NMR spectrum of isopropyl phenyl sulfoxide.

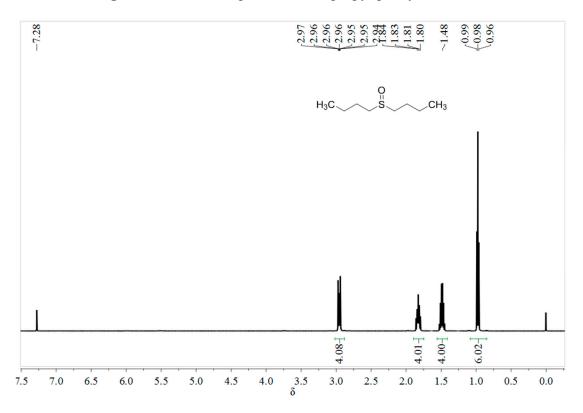


Figure S8. <sup>1</sup>H-NMR spectrum of *n*-butyl sulfoxide.

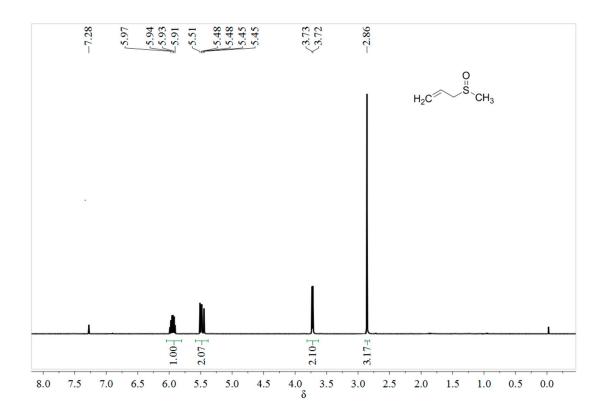
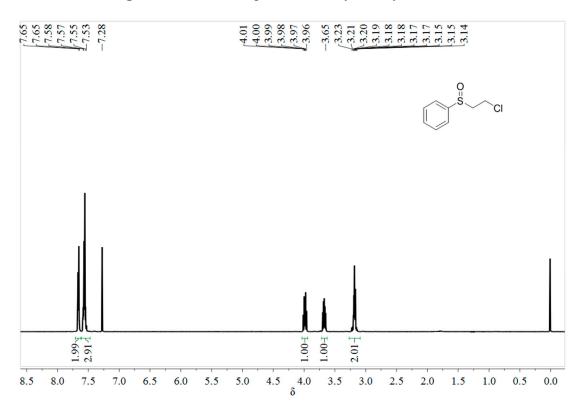
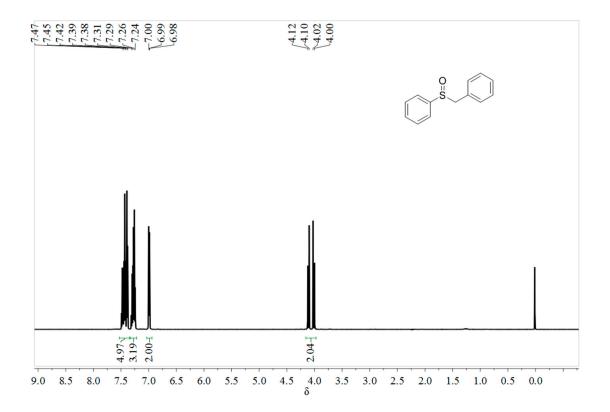


Figure S9. <sup>1</sup>H-NMR spectrum of allyl methyl sulfoxide.



**Figure S10.** <sup>1</sup>H-NMR spectrum of 2-chloroethyl phenyl sulfoxide.



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

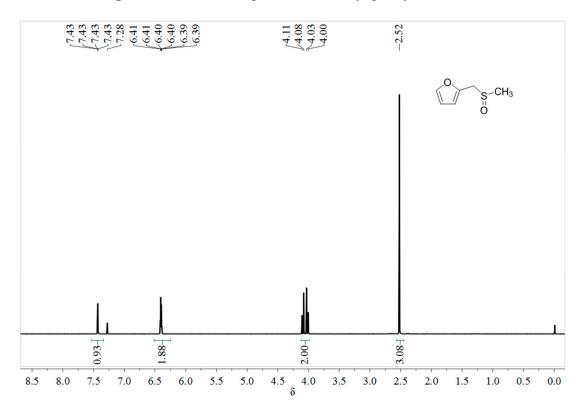
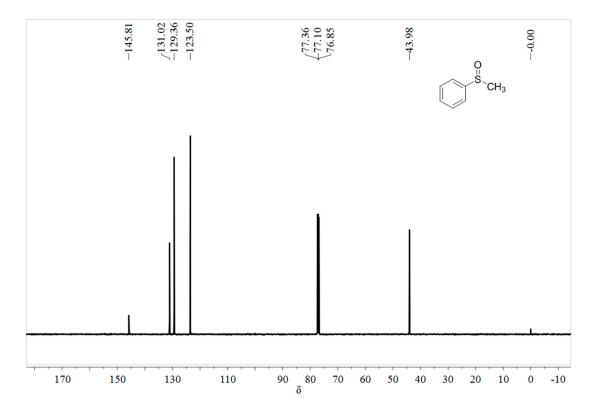


Figure S12. <sup>1</sup>H-NMR spectrum of furfuryl methyl sulfoxide.

# 3. <sup>13</sup>C-NMR Spectra of Product Sulfoxides



**Figure S13.**<sup>13</sup>C-NMR spectrum of methyl phenyl sulfoxide.

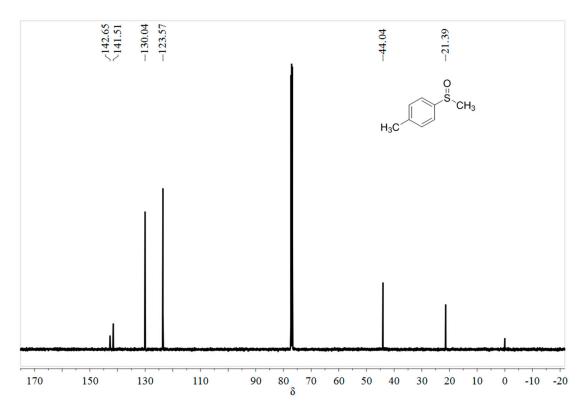


Figure S14. <sup>13</sup>C-NMR spectrum of methyl (4-methylphenyl) sulfoxide.

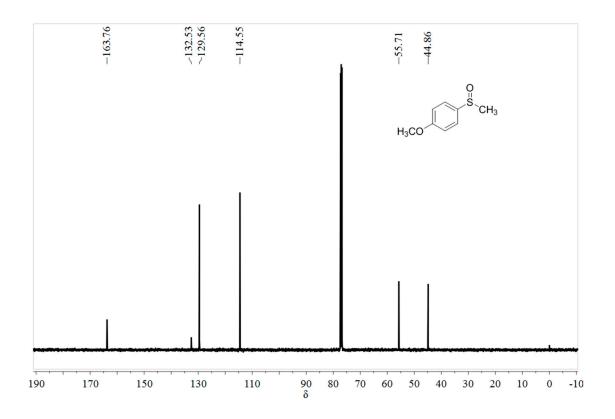


Figure S15. <sup>13</sup>C-NMR spectrum of methyl (4-methoxylphenyl) sulfoxide.

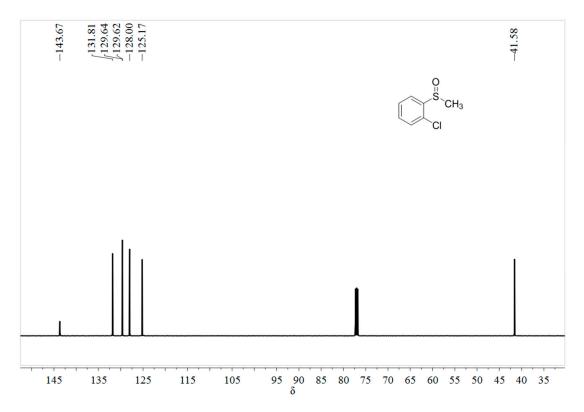
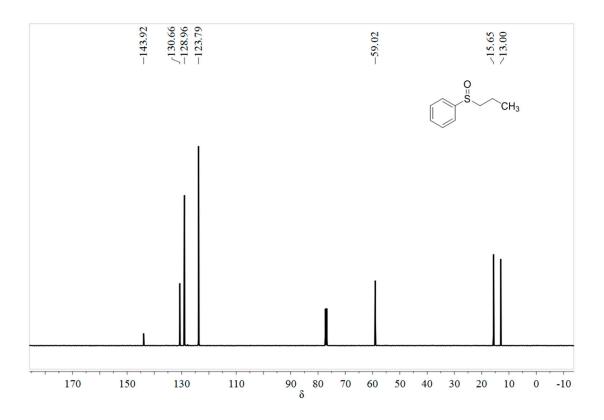
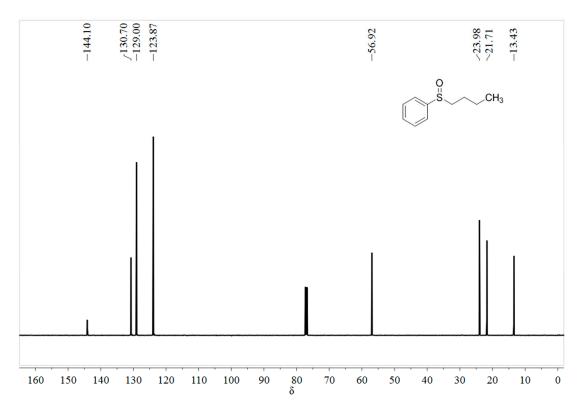


Figure S16. <sup>13</sup>C-NMR spectrum of methyl (2-chlorophenyl) sulfoxide.



**Figure S17.** <sup>13</sup>C-NMR spectrum of *n*-propyl phenyl sulfoxide.



**Figure S18.** <sup>13</sup>C-NMR spectrum of *n*-butyl phenyl sulfoxide.

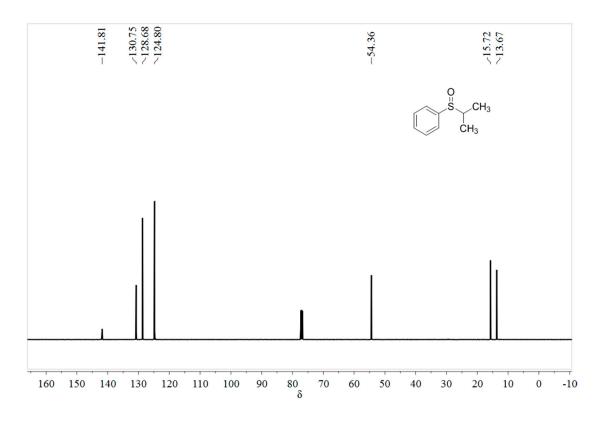


Figure S19. <sup>13</sup>C-NMR spectrum of isopropyl phenyl sulfoxide.

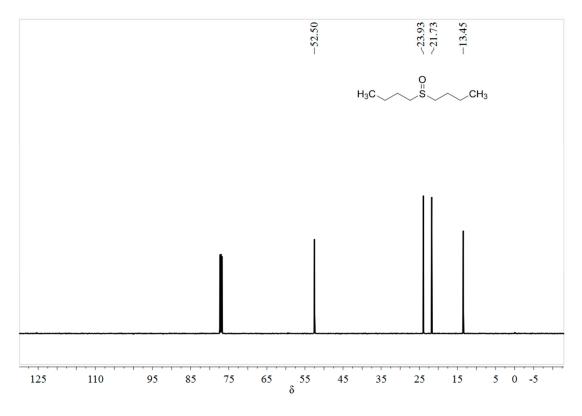


Figure S20. <sup>13</sup>C-NMR spectrum of *n*-butyl sulfoxide.

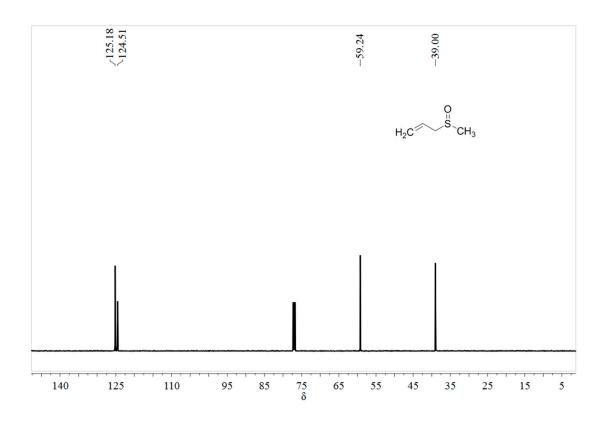


Figure S21. <sup>13</sup>C-NMR spectrum of allyl methyl sulfoxide.

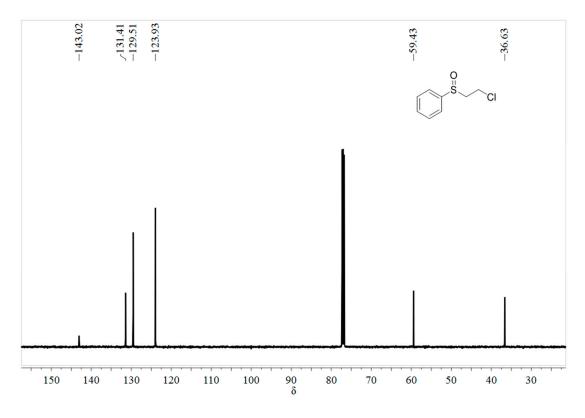


Figure S22. <sup>13</sup>C-NMR spectrum of 2-chloroethyl phenyl sulfoxide.

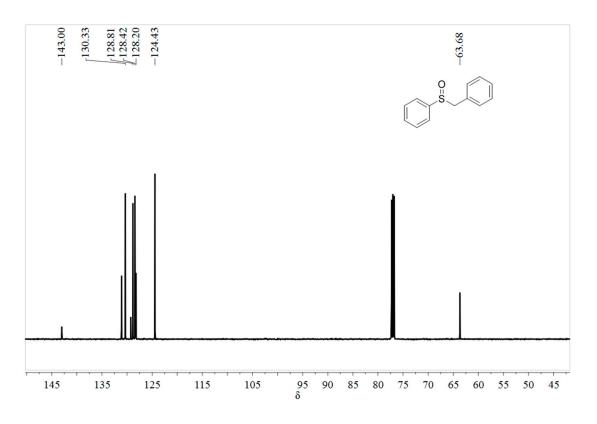


Figure S23. <sup>13</sup>C-NMR spectrum of benzyl phenyl sulfoxide.

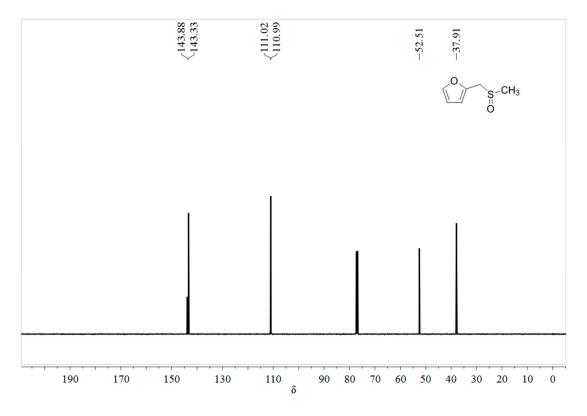


Figure S24. <sup>13</sup>C-NMR spectrum of furfuryl methyl sulfoxide.

# 4. NMR Data of Product Sulfoxides

			1
Table S22.	NMK	Data of Product Sulfoxi	des.

No.	Molecule Structures	<sup>1</sup> H- Data	<sup>13</sup> C- Data
1	CH3	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.65 (d, 2H), 7.54–7.49 (m, 3H), 2.73 ppm (s, 3H)	<ul> <li><sup>13</sup>C-NMR (400 MHz, CDCl<sub>3</sub>): δ = 145.81,</li> <li>131.02, 129.36, 123.50,</li> <li>43.98 ppm</li> </ul>
2	H <sub>3</sub> C	<sup>1</sup> H-NMR (400MHz, CDCl <sub>3</sub> ): δ = 7.55 (d, 2H), 7.34 (d, 2H), 2.71 (s, 3H), 2.42 ppm (s, 3H)	<ul> <li><sup>13</sup>C-NMR (400 MHz, CDCl<sub>3</sub>): δ =142.65,</li> <li>141.51, 130.04, 123.57,</li> <li>44.04, 21.39 ppm</li> </ul>
3	H <sub>3</sub> CO	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.90 (d, 2H), 7.05 (d, 2H), 3.90 (s, 3H), 3.05 ppm (s, 3H)	<sup>13</sup> C-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 163.76, 132.53, 129.56, 114.55, 55.71, 44.86 ppm
4	CI	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.95 (d, 1H), 7.51 (t, 1H), 7.45 (t, 1H), 7.39 (d, 1H), 2.81 ppm (s, 3H)	<ul> <li><sup>13</sup>C-NMR (400 MHz, CDCl<sub>3</sub>): δ = 143.67,</li> <li>131.81, 129.64, 129.62,</li> <li>128.00, 125.17, 41.58 ppm</li> </ul>
5	CH <sub>3</sub>	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.61 (d, 2H), 7.51-7.45 (m, 3H), 2.78–2.70 (m, 2H), 1.77–1.62 (m, 2H), 1.02 ppm (t, 3H)	<sup>13</sup> C-NMR (400 MHz, CDCl <sub>3</sub> ): δ =143.92, 130.66, 128.96, 123.79, 59.02, 15.65, 13.00 ppm
6	CH3	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.61 (d, 2H), 7.52–7.45 (m, 3H), 2.78 (t, 2H), 1.76–1.68 (m, 1H), 1.62–1.54 (m, 1H), 1.50–1.34 (m, 2H), 0.90 ppm (t, 3H)	<ul> <li><sup>13</sup>C-NMR (400 MHz, CDCl<sub>3</sub>): δ =144.10, 130.70, 129.00, 123.87, 56.92,</li> <li>23.98, 21.71, 13.43 ppm</li> </ul>
7	CH <sub>3</sub>	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.55 (d, 2H), 7.50–7.44 (m, 3H), 2.83–2.78 (m, 1H), 1.21 (d, 3H), 1.11 ppm (d, 3H)	<ul> <li><sup>13</sup>C-NMR (400 MHz, CDCl<sub>3</sub>): δ =141.81,</li> <li>130.75, 128.68, 124.80,</li> <li>54.36, 15.72, 13.67 ppm</li> </ul>
8	H <sub>3</sub> C CH <sub>3</sub>	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): $\delta = 2.97-2.94$ (m, 4H), 1.86–1.80 (m, 4H), 1.52–1.45 (m, 4H), 0.98 ppm (t, 6H)	<sup>13</sup> C-NMR (400 MHz, CDCl <sub>3</sub> ): δ =52.50, 23.93, 21.73, 13.45 ppm
9	H <sub>2</sub> C <sup>S</sup> CH <sub>3</sub>	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): $\delta = 5.97-5.91$ (m, 1H), 5.51–5.45 (m, 2H), 3.73 (d, 2H), 2.86 ppm (s, 3H)	<sup>13</sup> C-NMR (400 MHz, CDCl <sub>3</sub> ): δ =125.18, 124.51, 59.24, 39.00 ppm

No.	<b>Molecule Structures</b>	<sup>1</sup> H- Data	<sup>13</sup> C- Data
10	O S CI	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.67–7.65 (m, 2H), 7.59–7.53 (m, 3H), 4.01–3.96 (m, 1H), 3.70–3.65 (m, 1H), 3.23–3.14 ppm (m, 2H)	<sup>13</sup> C-NMR (400 MHz, CDCl <sub>3</sub> ): δ =143.02, 131.41, 129.51, 123.93, 59.43, 36.63 ppm
11	S 0	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): $\delta = 7.49-7.38$ (m, 5H), 7.32-7.24 (m, 3H), 7.00 (d, 2H), 4.12-4.00 ppm (m, 2H)	<ul> <li><sup>13</sup>C-NMR (400 MHz, CDCl<sub>3</sub>):</li> <li>δ =143.00, 131.09, 130.33,</li> <li>129.24, 128.81, 128.42,</li> <li>128.20, 124.43, 63.68 ppm</li> </ul>
12	C S C H <sub>3</sub> O	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ): δ = 7.43 (s, 1H), 6.41-6.39 (m, 2H), 4.11–4.00 (m, 2H), 2.52 ppm (s, 3H)	<sup>13</sup> C-NMR (400 MHz, CDCl <sub>3</sub> ): δ =143.88, 143.33, 111.02, 110.99, 52.51, 37.91 ppm

Table S22. Cont.

## 5. ESI-MS Spectra of Product Sulfoxides

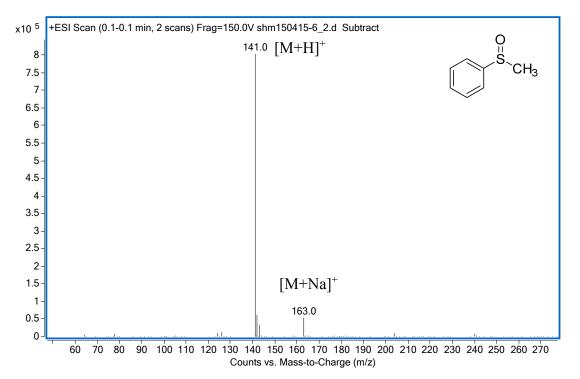


Figure S25. ESI-MS spectrum of methyl phenyl sulfoxide.

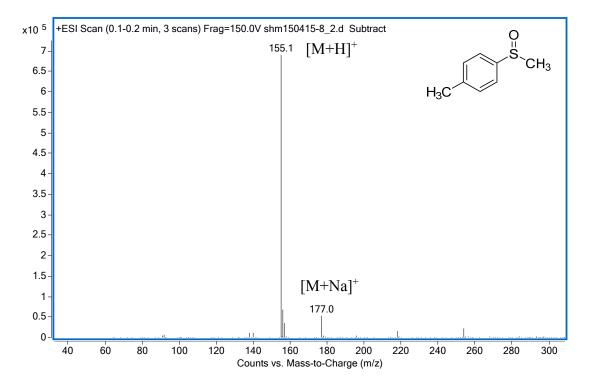


Figure S26. ESI-MS spectrum of methyl (4-methylphenyl) sulfoxide.

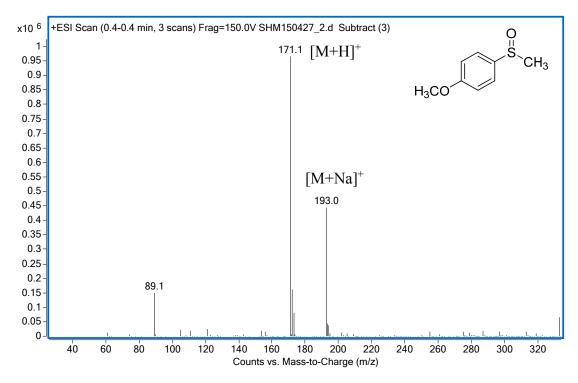


Figure S27. ESI-MS spectrum of methyl (4-methoxylphenyl) sulfoxide.

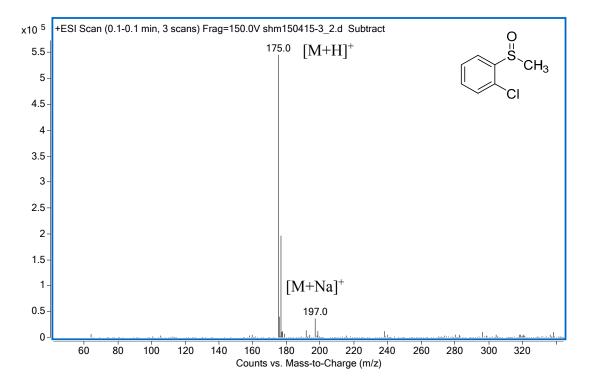


Figure S28. ESI-MS spectrum of methyl (2-chlorophenyl) sulfoxide.

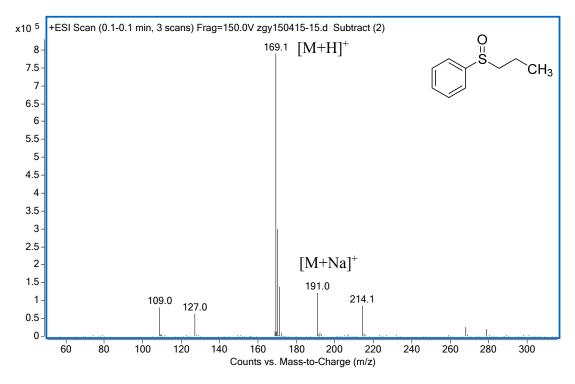


Figure S29. ESI-MS spectrum of *n*-propyl phenyl sulfoxide.

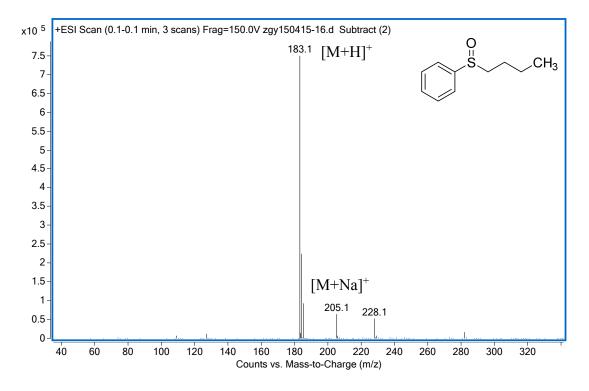


Figure S30. ESI-MS spectrum of *n*-butyl phenyl sulfoxide.

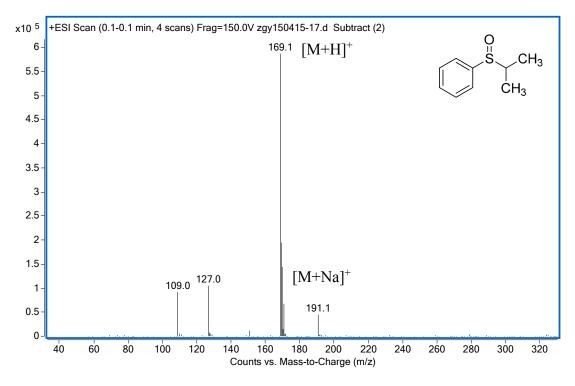
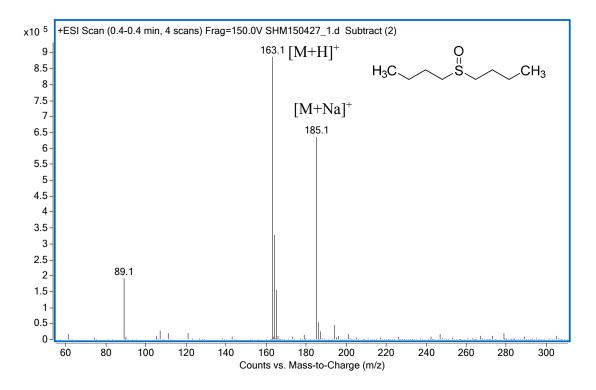
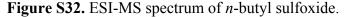


Figure S31. ESI-MS spectrum of isopropyl phenyl sulfoxide.





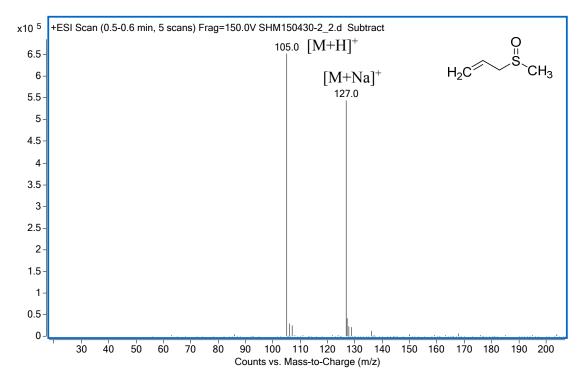


Figure S33. ESI-MS spectrum of allyl methyl sulfoxide.

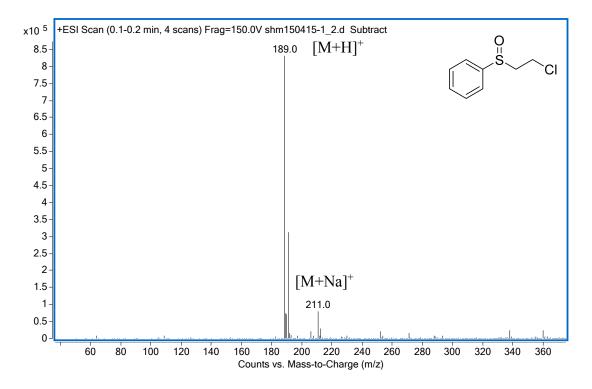


Figure S34. ESI-MS spectrum of 2-chloroethyl phenyl sulfoxide.

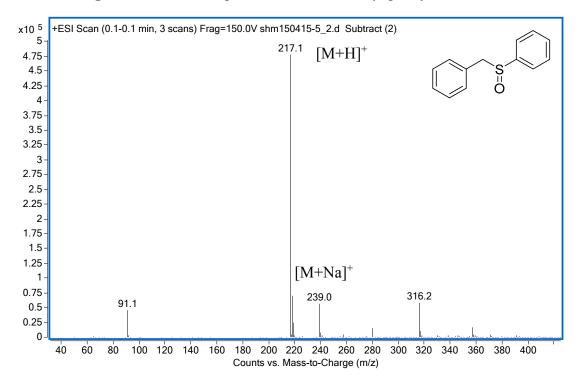


Figure S35. ESI-MS spectrum of benzyl phenyl sulfoxide.

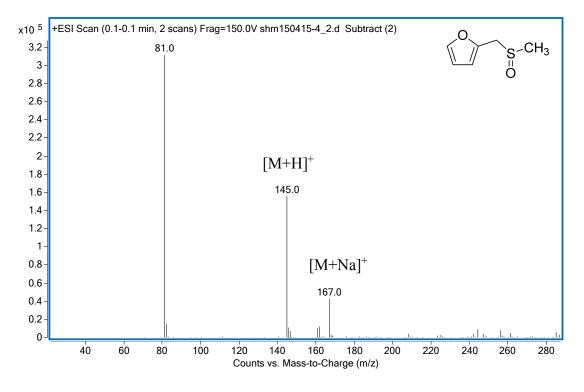


Figure S36. ESI-MS spectrum of furfuryl methyl sulfoxide.

6. Typical GC Spectra for the Product Sulfoxides

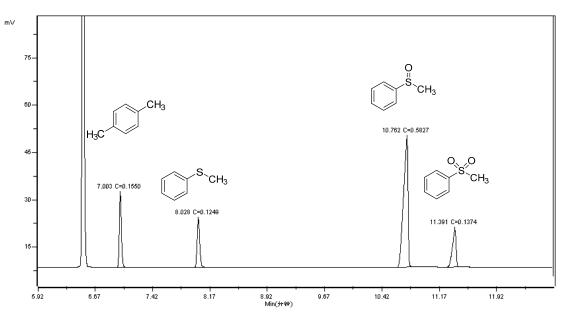


Figure S37. Typical qualitative spectrum.

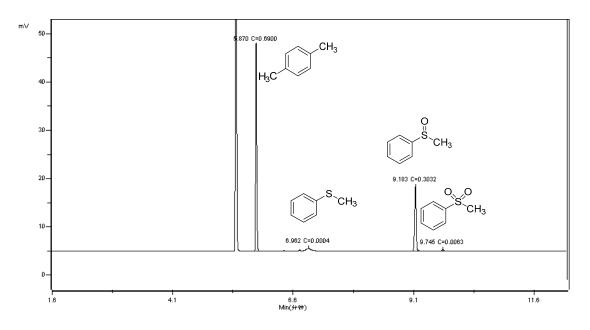


Figure S38. Typical quantitative spectrum.