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Electronic Supplementary Information

Dual-linker Ir-Zr-MOF Shows Improved Porosity to Enhance Aqueous Sulfide Photooxidation

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1. ^{1}H NMR Analysis of the digested 1

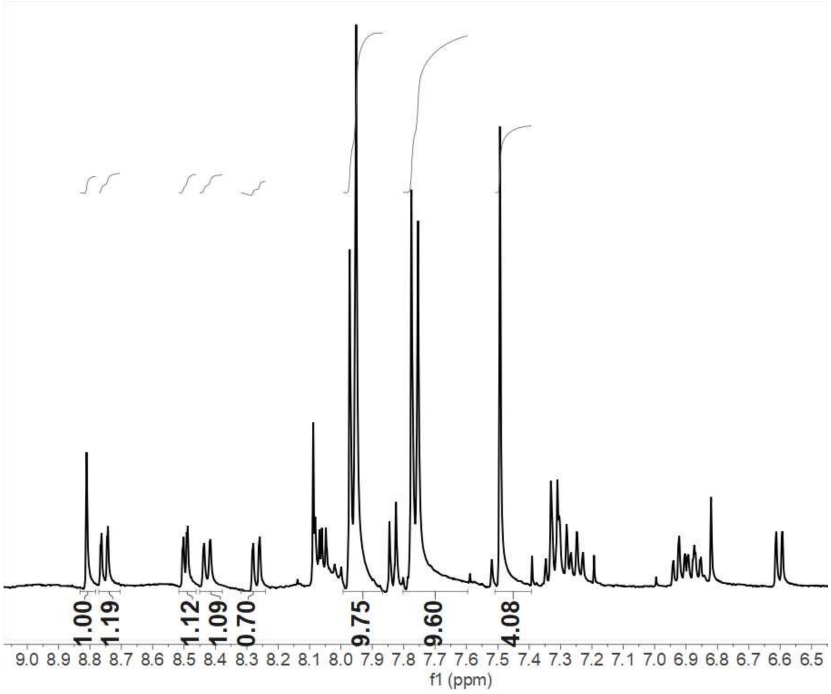

Fig. S1 ^{1}H NMR spectra of the digested **1** with TFA in DMSO- d_6. The relative content of the two linkers was analyzed by their integration of H5 of Irphen and H1 of H_2SDC, giving a mole ratio of around (9.75/2):1.00=4.9/1.

2. IR Analysis

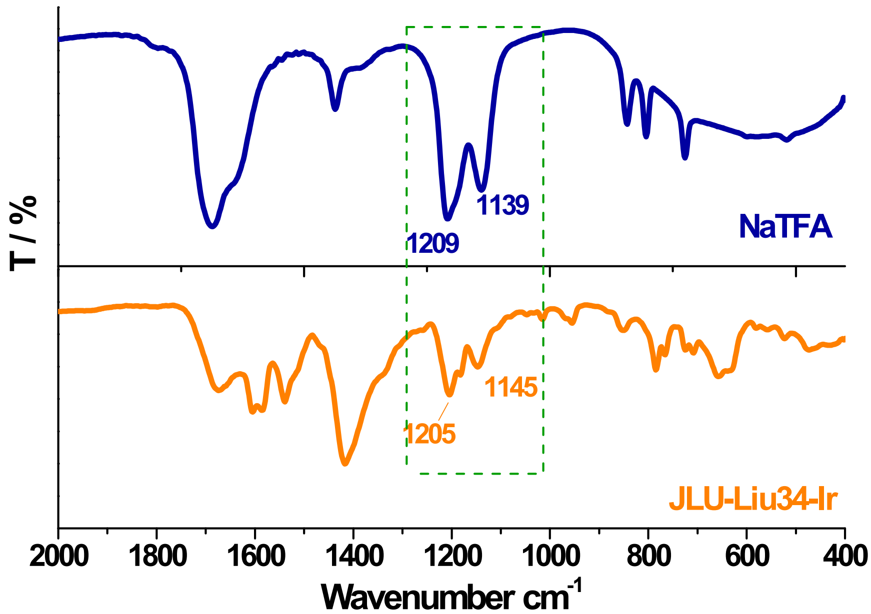

Fig. S2 IR spectra in scale of 2000-400 cm^{-1} for **1** and NaTFA, the labeled peaks associate with F-C-F vibration.

3. EDS-MAPPING Analysis

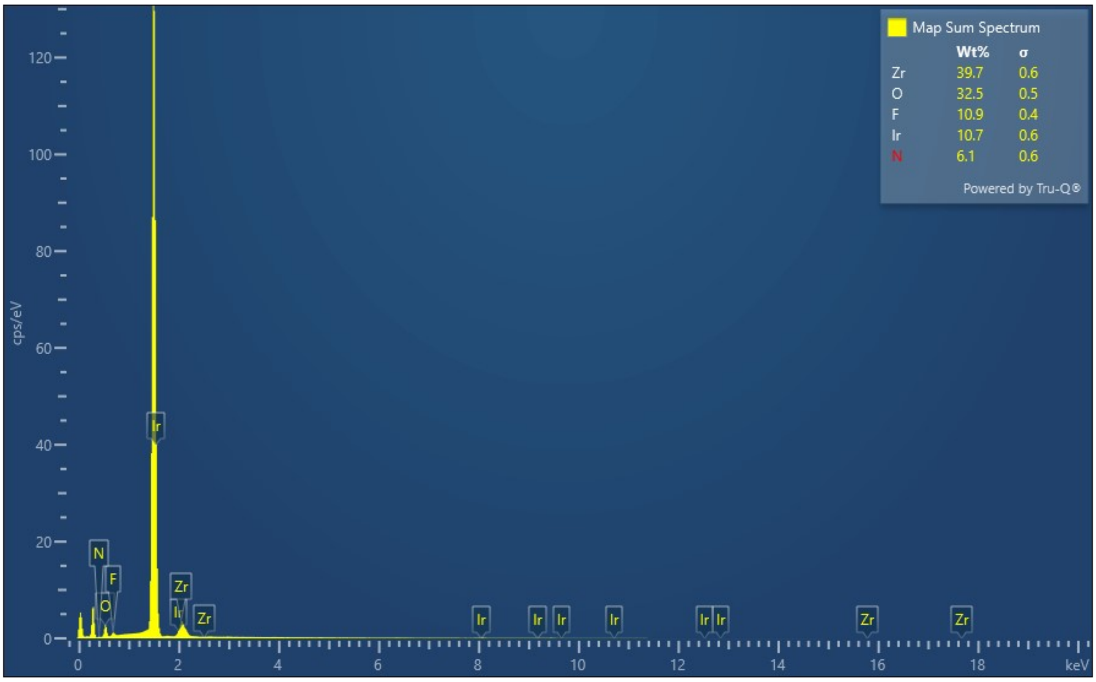

Fig. S3 EDS Spectra for **1**. Analysis revealed the mole ration of Zr/Ir/F = (39.7/91.2):(10.7/192.2):(10.9/19) = 6/0.78/8.01

4.TG Analysis

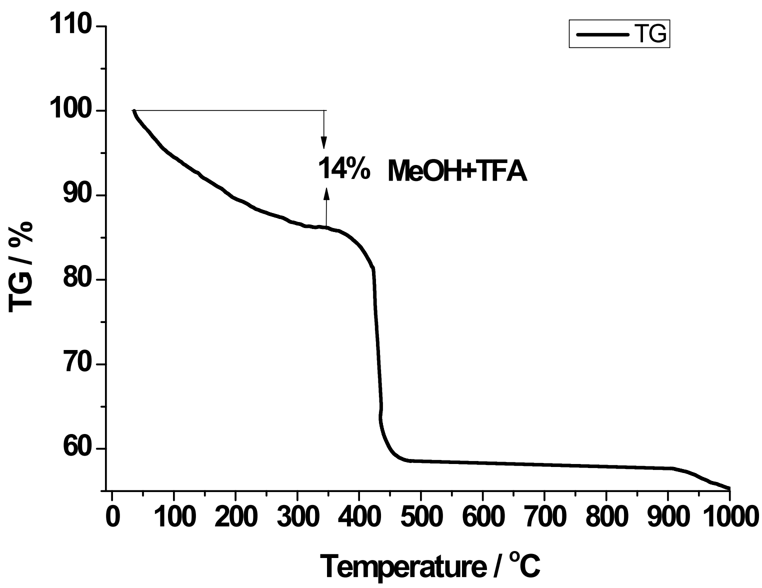

Fig. S4 TG curve for **1**, TG analysis reveals it contained 14% guest content.

5. [1]H NMR Test of Irphen released from 1

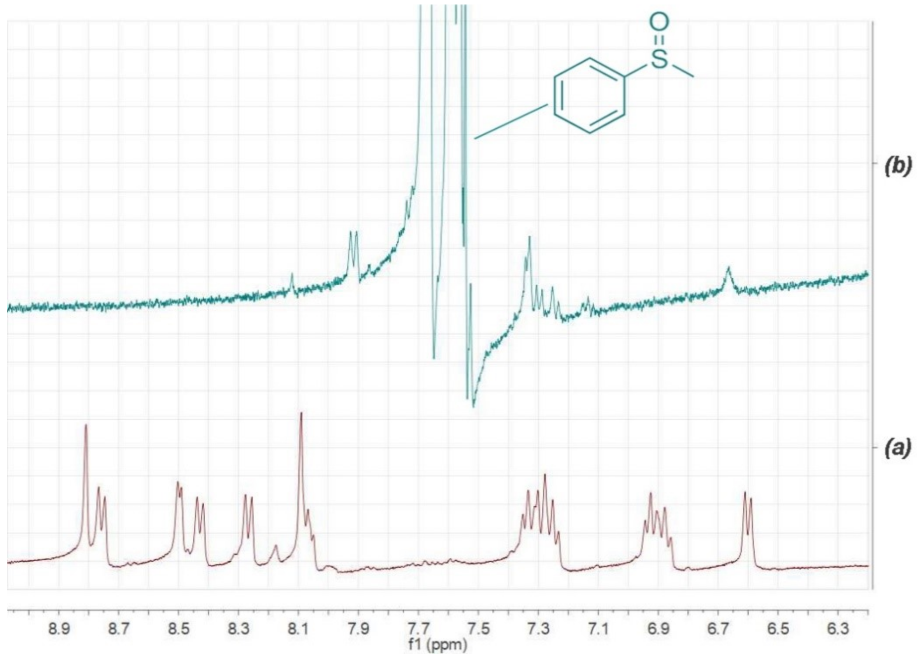

Fig. S5 Contrast [1]H NMR spectra for condensed solution after Methylphenyl sulfide photo oxidation by **1** (a) and pure Irphen (b) in d_6-DMSO.

6. [1]H NMR analysis of sulfoxide selectivity for the crude product

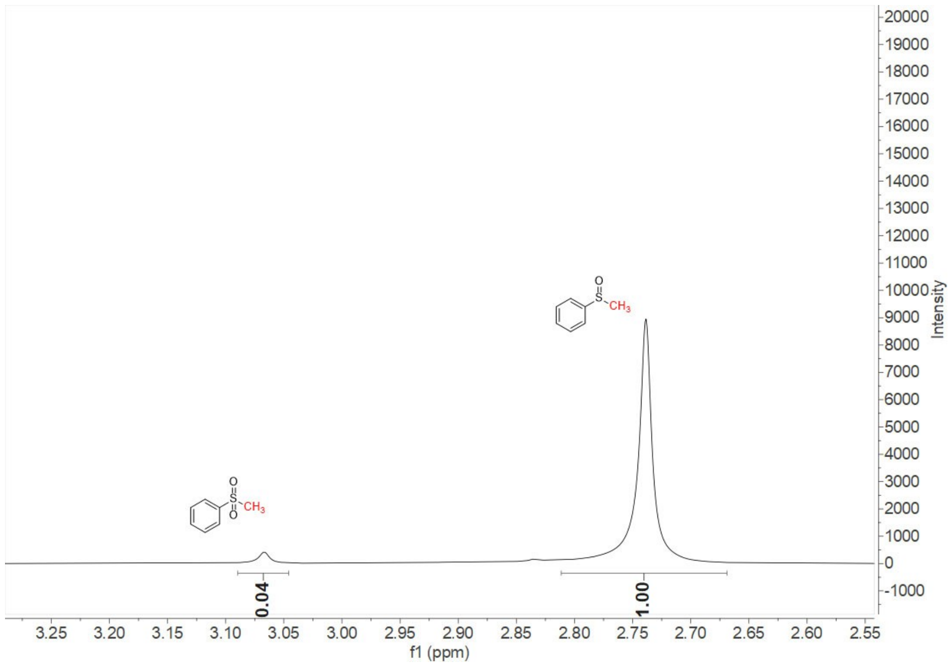

Fig. S6 The ratio analysis of Methyl phenyl sulfone and Methyl phenyl sulfoxide was based on integration of the methyl signal, affording a Methylphenylsulfoxide selectivity of 96% (1/1.04).

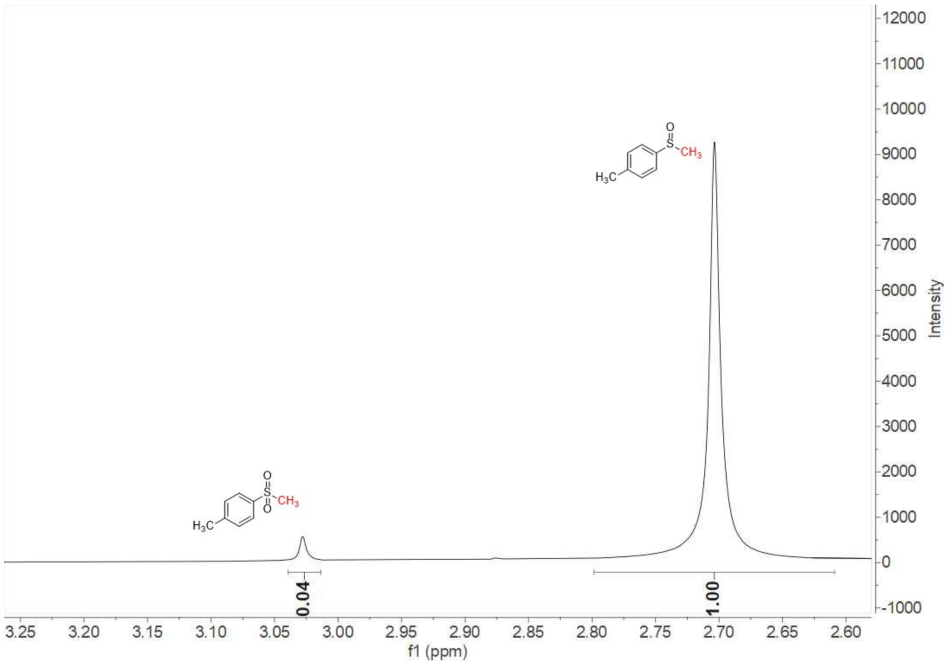

Fig. S7 The ratio analysis of Methyl 4-Tolyl sulfone and Methyl 4-Tolyl sulfoxide was based on integration of the methyl signal, affording a Methyl 4-Tolyl sulfoxide selectivity of 96% (1/1.04).

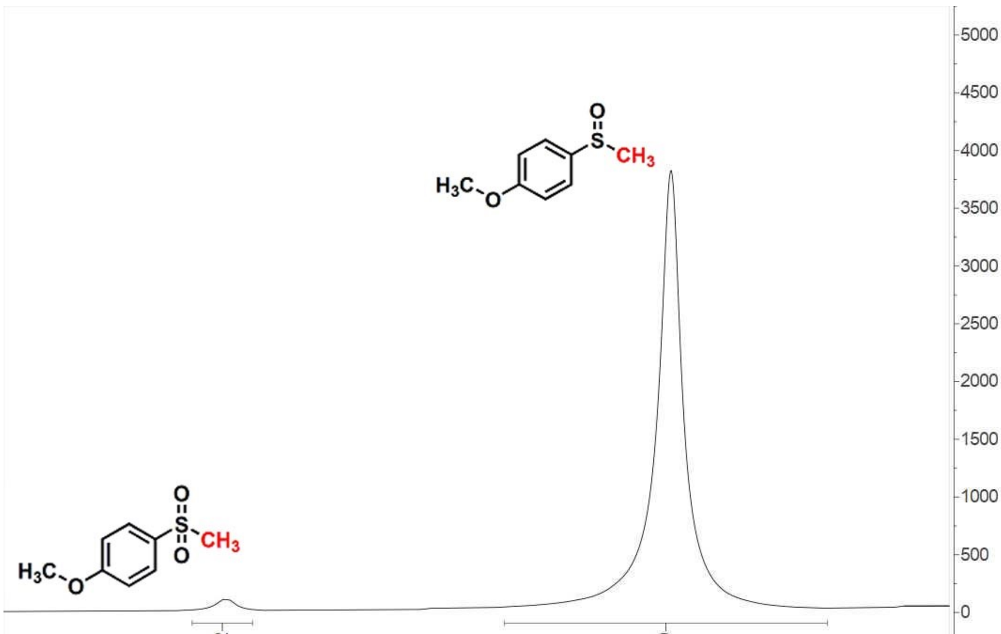

Fig. S8 The ratio analysis of 1-Methoxy-4-(methylsulfonyl)benzene and 1-Methoxy-4-(methylsulfinyl)benzene was based on integration of the methyl signal, affording a 1-Methoxy-4-(methylsulfinyl)benzene of 98% (1/1.02).

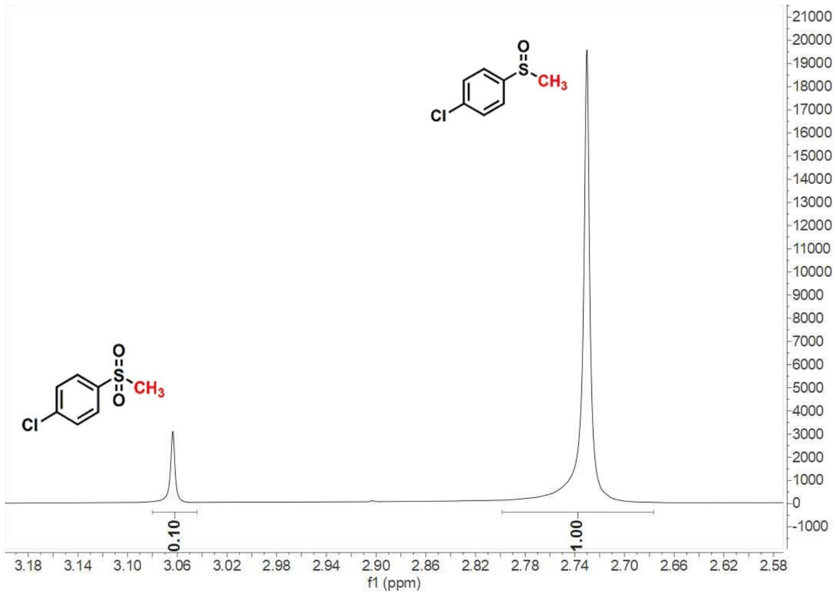

Fig. S9 The ratio analysis of 4-Chlorophenyl Methyl Sulfone and 1-Chloro-4-(methylsulfinyl)benzene was based on integration of the methyl signal, affording a 1-Chloro-4-(methylsulfinyl)benzene selectivity of 91% (1/1.1).

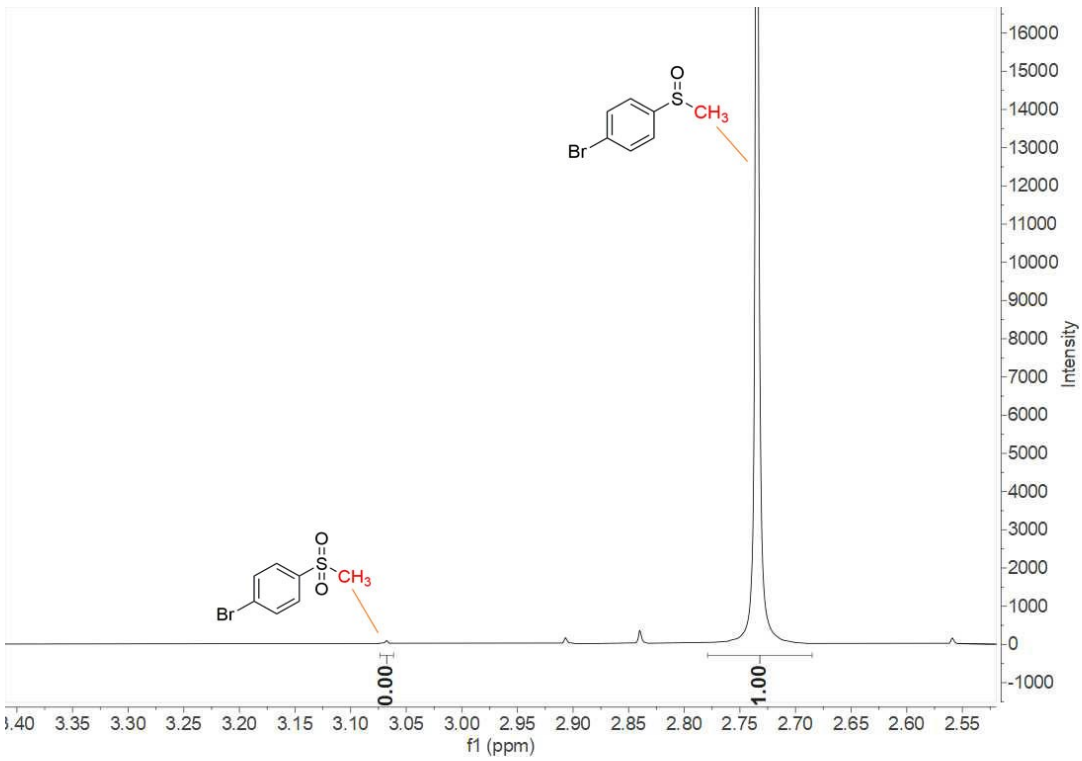

Fig. S10 The ratio analysis of 4-Bromophenyl Methyl Sulfone and 1-Bromo-4-(methylsulfinyl)benzene was based on integration of the methyl signal, affording a 1-Bromo-4-(methylsulfinyl)benzene selectivity ＞99%.

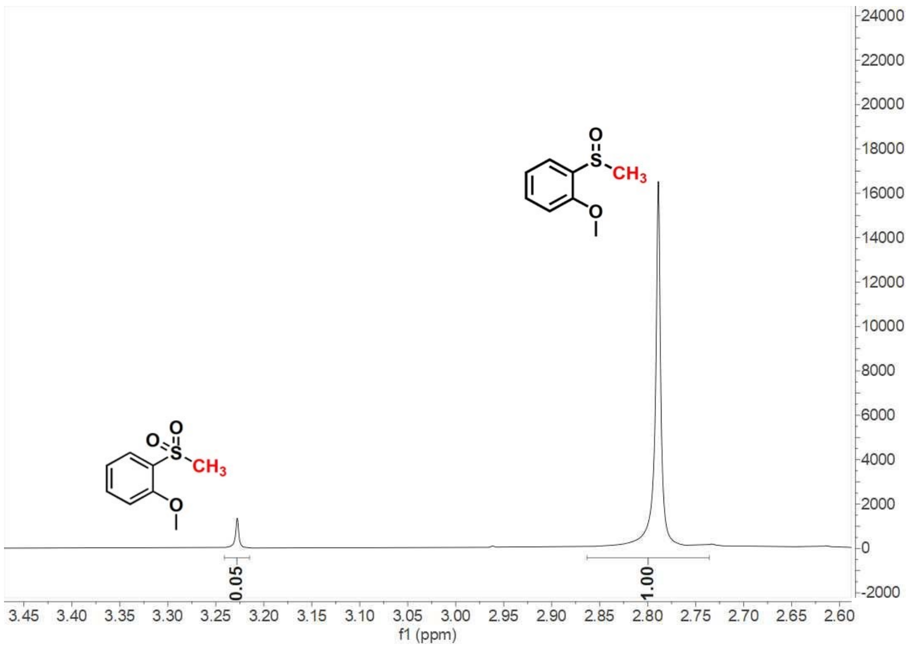

Fig. S11 The ratio analysis of 1-methoxy-2-(methylsulfonyl)benzene and 1-methoxy-2-(methylsulfinyl)benzene was based on integration of the methyl signal, affording a 1-methoxy-2-(methylsulfinyl)benzene selectivity of 95% (1/1.05).

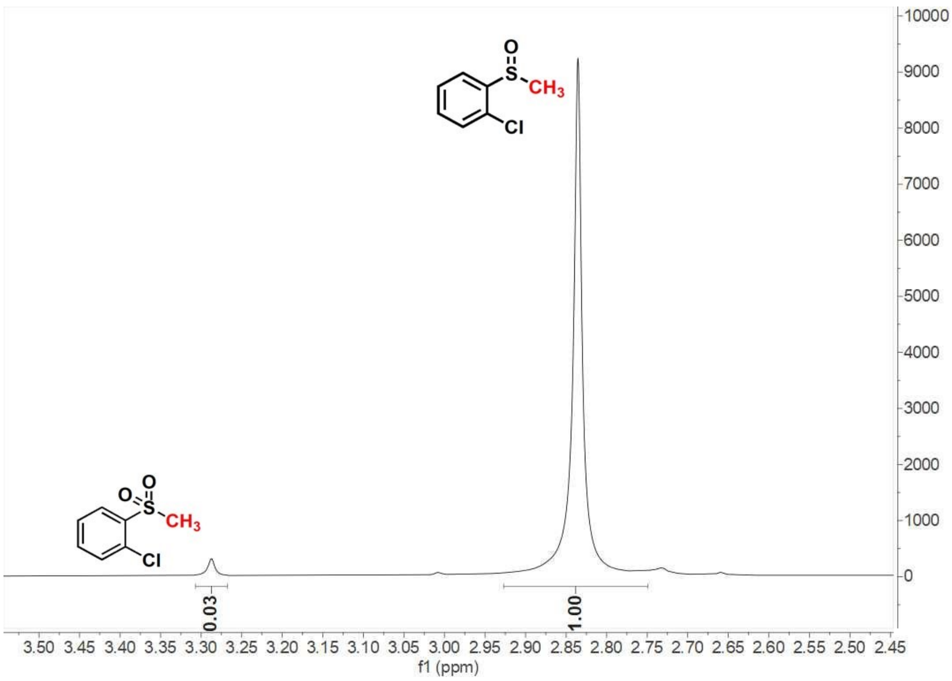

Fig. S12 The ratio analysis of 1-chloro-2-(methylsulfonyl)benzene and 1-chloro-2-(methylsulfinyl)benzene was based on integration of the methyl signal, affording a 1-chloro-2-(methylsulfinyl)benzene selectivity of 97% (1/1.03).

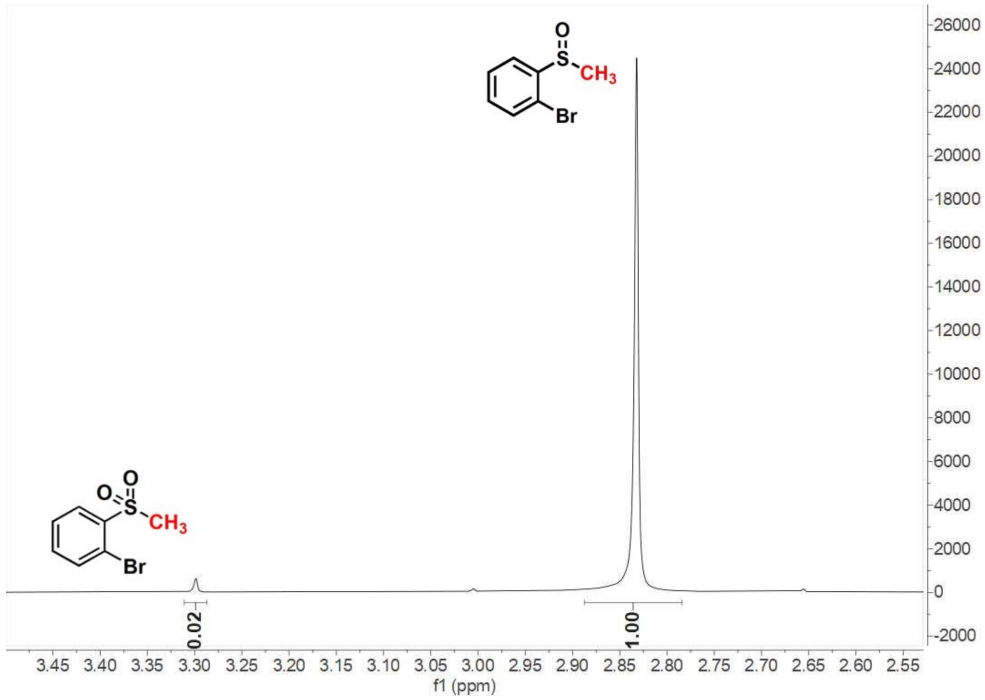

Fig. S13 The ratio analysis of 1-bromo-2-(methylsulfonyl)benzene and 1-bromo-2-(methylsulfinyl)benzene was based on integration of the methyl signal, affording a 1-bromo-2-(methylsulfinyl)benzene selectivity of 98% (1/1.02).

7. ^{1}H NMR spectra for the sulfoxide product

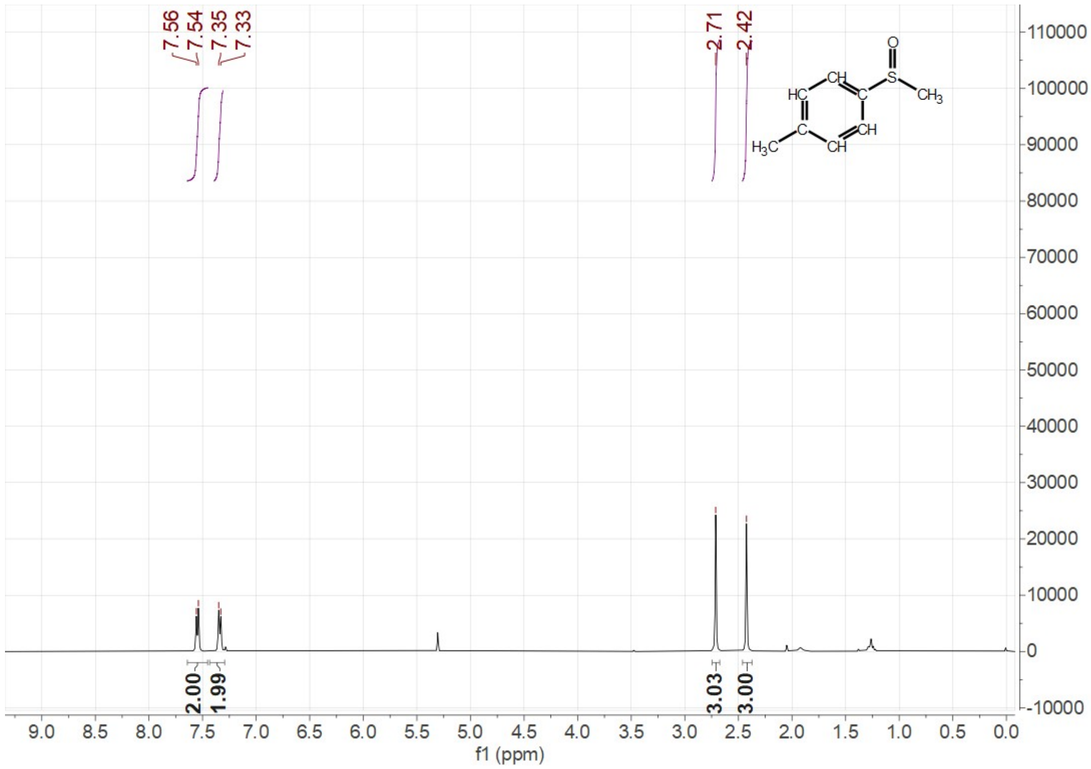

Fig.S14 ^{1}H NMR spectra of 1-methyl-4-(methylsulfinyl)benzene in $DCCl_3$.

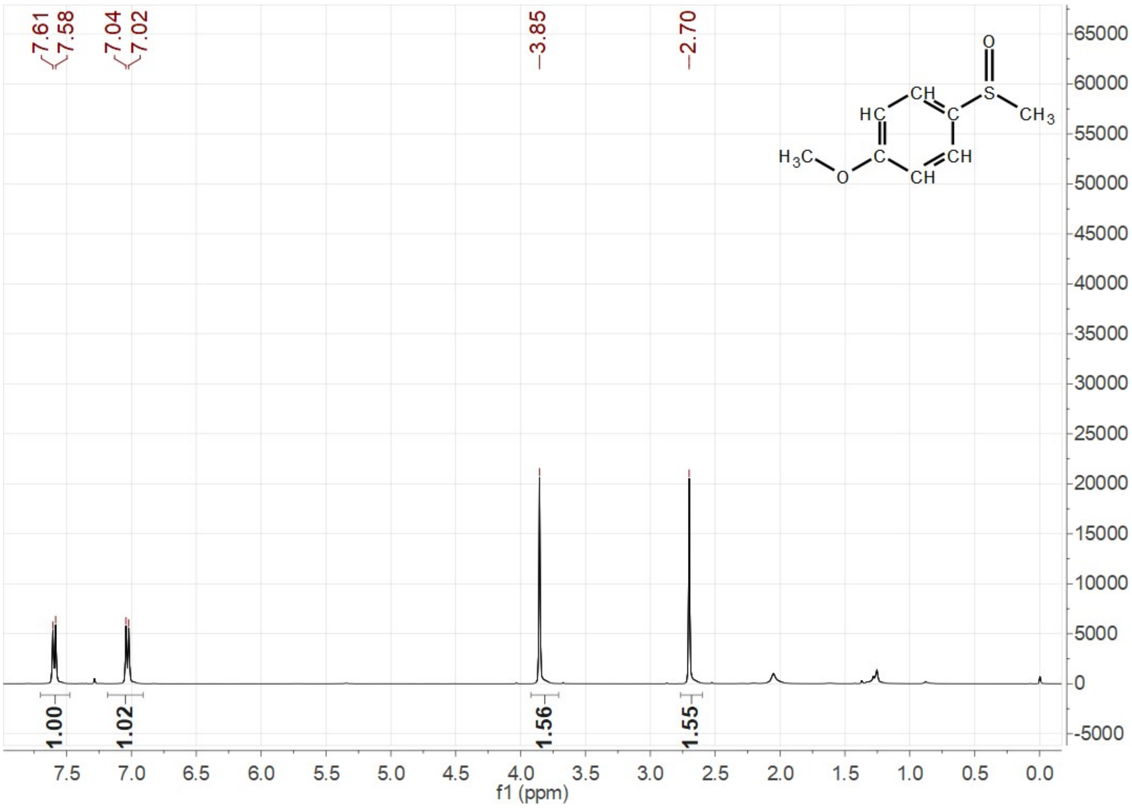

Fig. S15 ^{1}H NMR spectra of 1-methoxy-4-(methylsulfinyl)benzene $DCCl_3$.

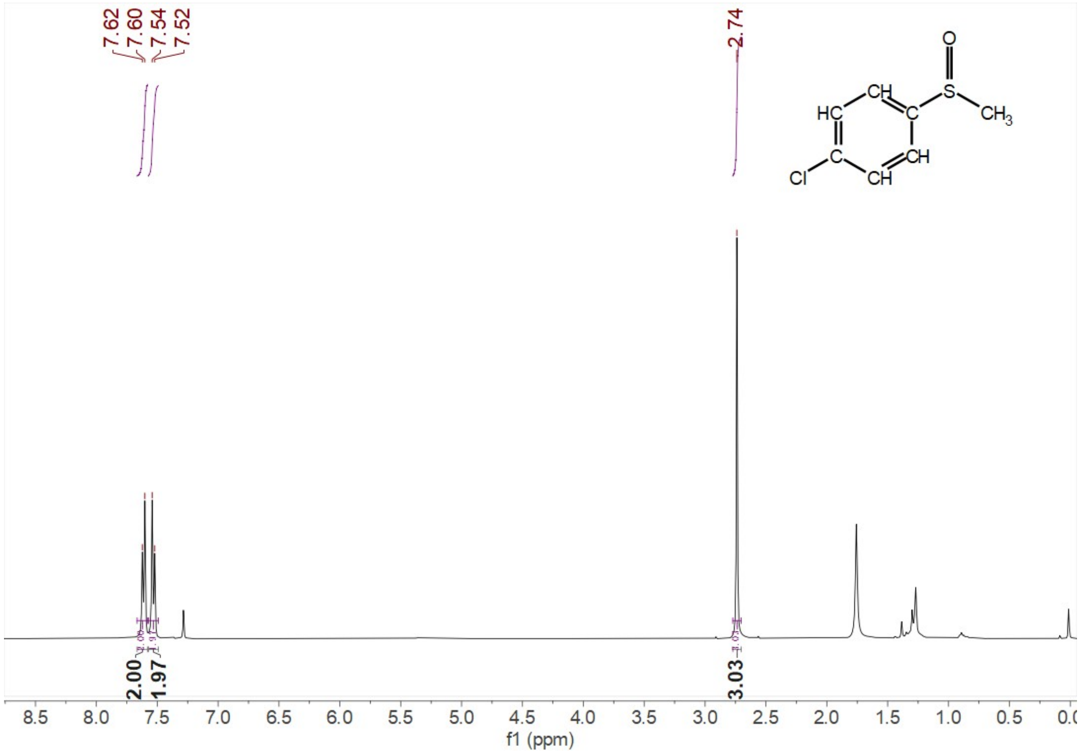

Fig. S16 ^{1}H NMR spectra of 1-chloro-4-(methylsulfinyl)benzene in $DCCl_3$.

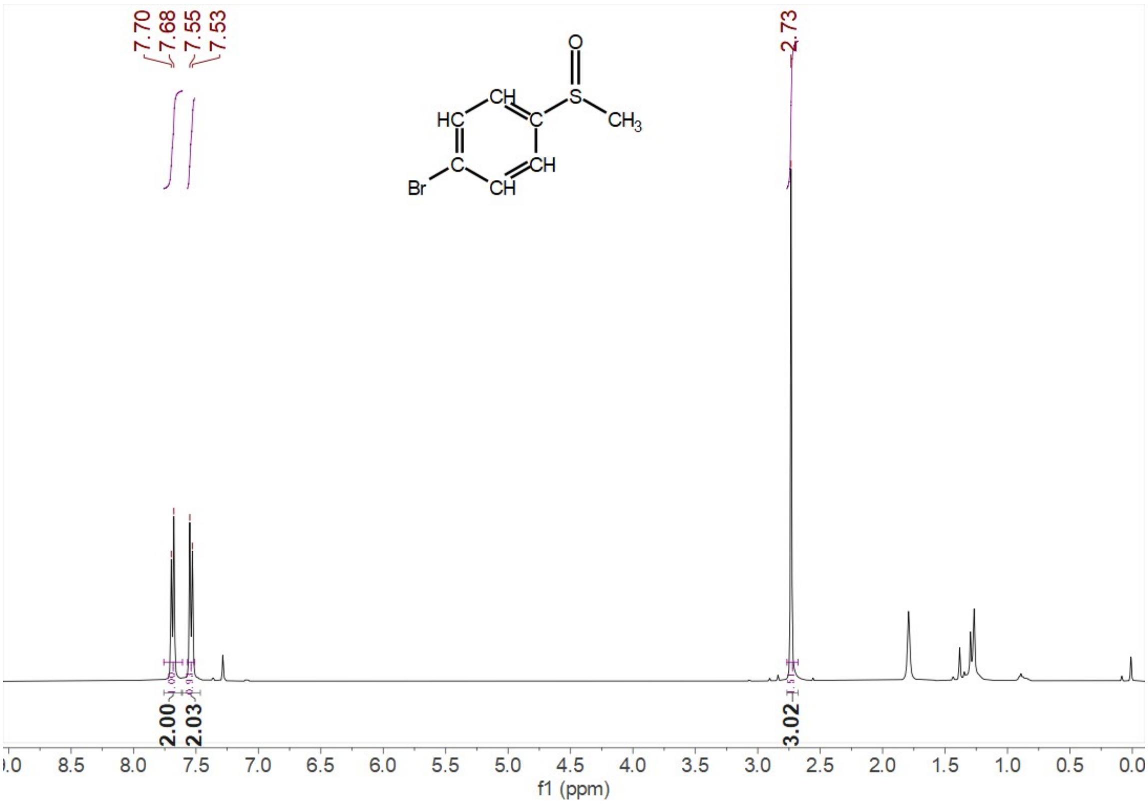

Fig. S17 ^{1}H NMR spectra of 1-bromo-4-(methylsulfinyl)benzene in $DCCl_3$.

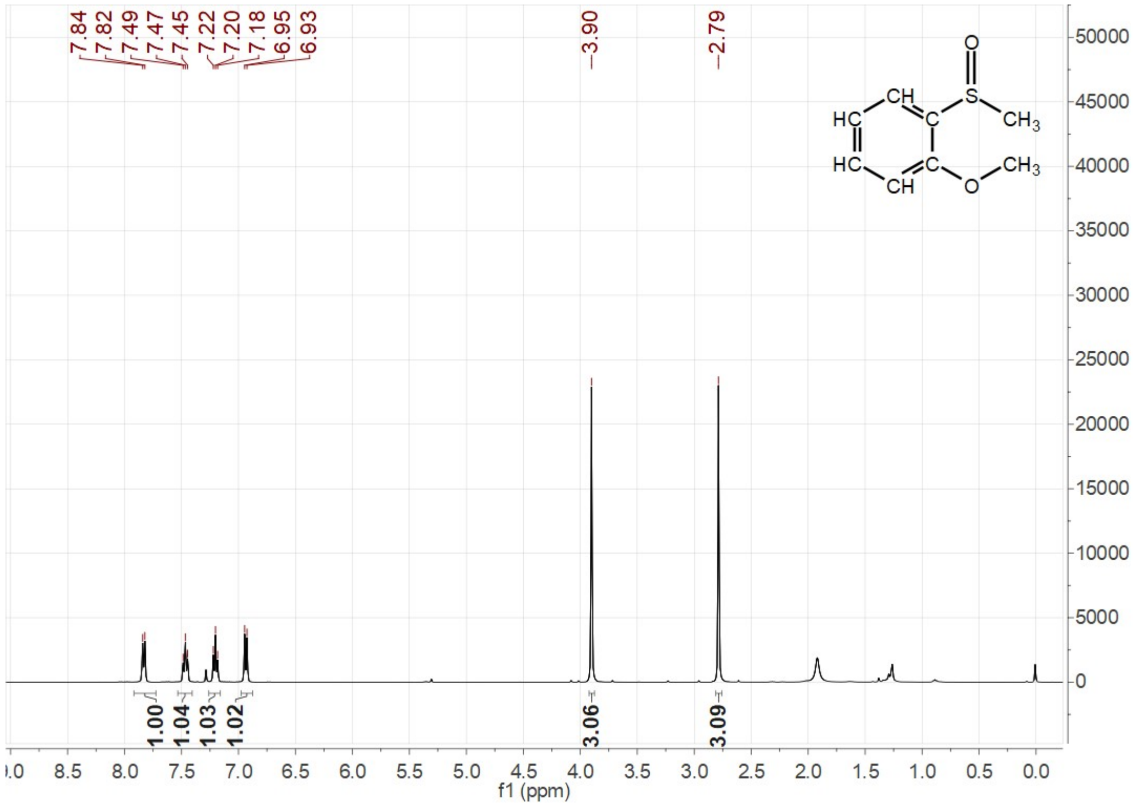

Fig. S18 ^{1}H NMR spectra of 1-methoxy-2-(methylsulfinyl)benzene in $DCCl_3$.

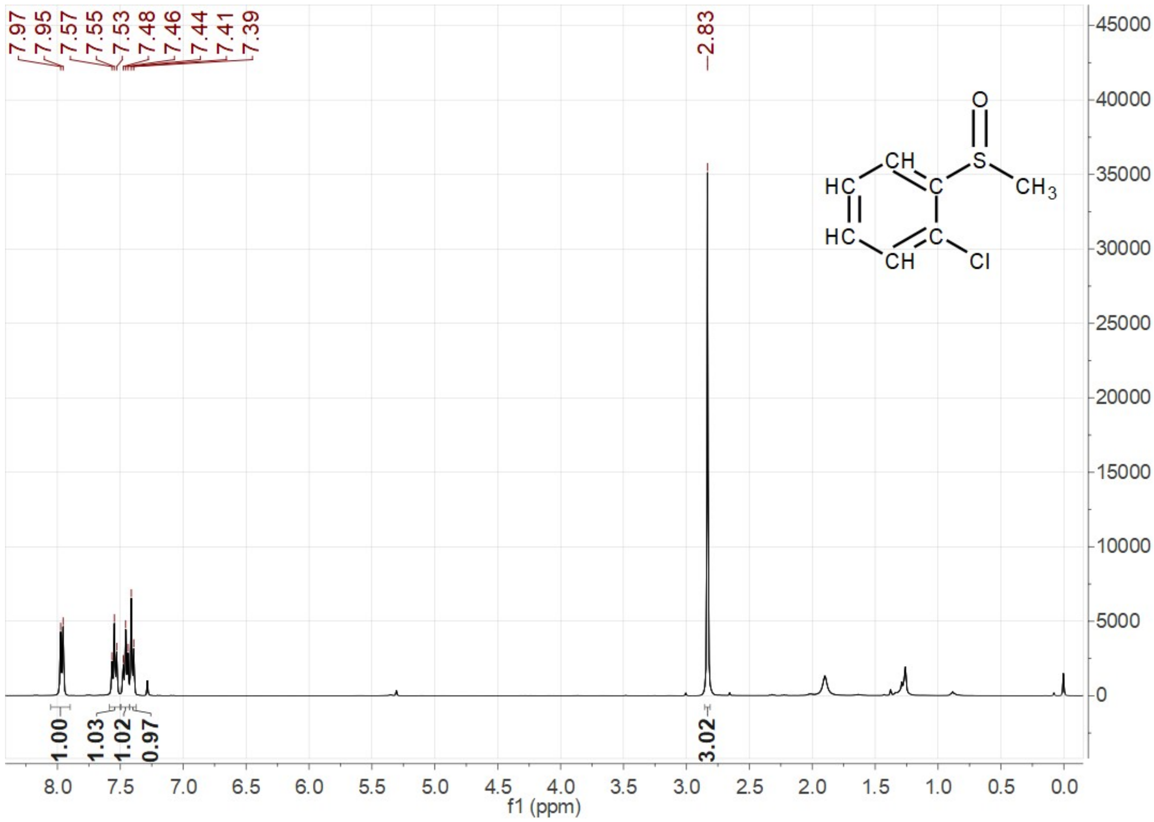

Fig. S19 ^{1}H NMR spectra of 1-chloro-2-(methylsulfinyl)benzene in $DCCl_3$.

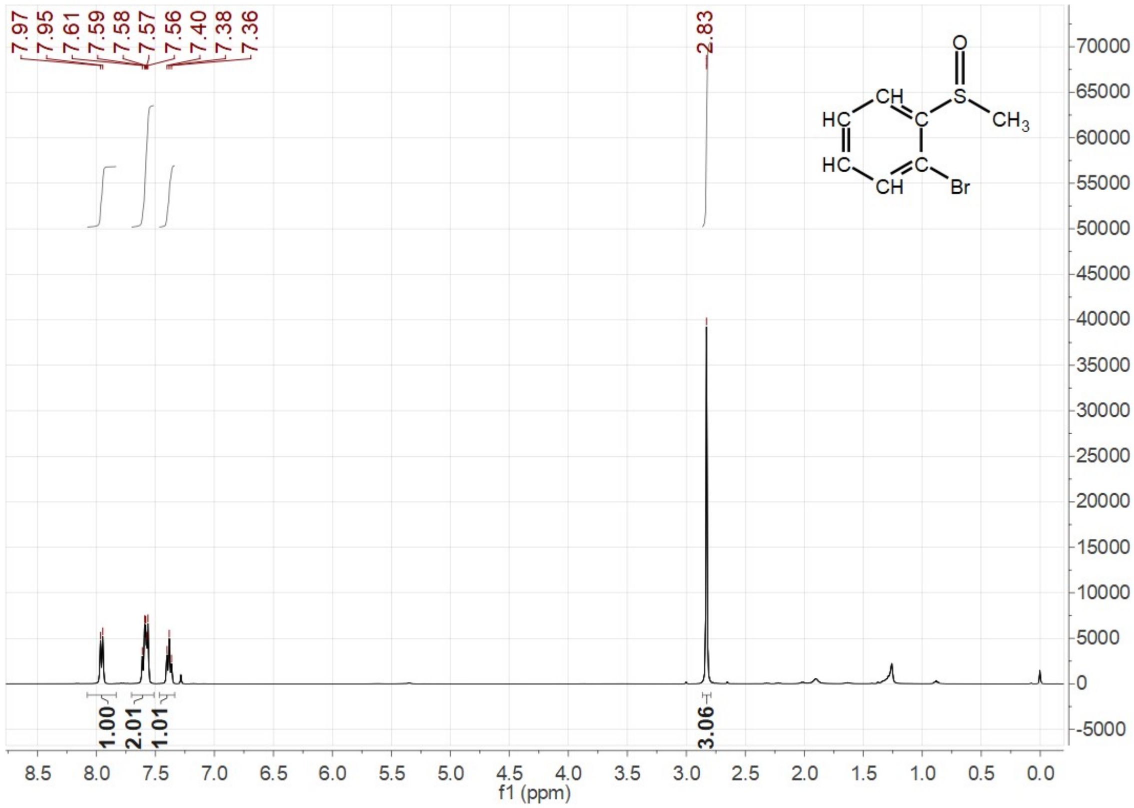

Fig. S20 [1]H NMR spectra 1-bromo-2-(methylsulfinyl)benzene in $DCCl_3$.