Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Bovine serum albumin-cobalt(II) Schiff base complex hybrid: an efficient artificial metalloenzyme for enantioselective sulfoxidation using hydrogen peroxide

Table S1 Selected bond lengths (Å) and angles (º) for complexes CoL

Symmetry code: (A) −x+1, −y+1, −z.

Co1—Cl1	**2.4106 (8)**	**Co1—O2**	**2.1268 (15)**	**Co1—O1**	**2.1401 (15)**
Co2—Cl1A	**2.5858 (9)**	**Co2—O2**	**1.8776 (15)**	**Co2—O1**	**1.8843 (14)**
Co2—N1	**1.8771 (18)**	**Co2—N2**	**1.8818 (18)**		
O2A—Co1—Cl1A	**95.63 (4)**	**O2A—Co1—Cl1**	**84.37 (4)**	**O2A—Co1—O1A**	**71.03 (6)**
O2A—Co1—O1	**108.97 (6)**	**O1A—Co1—Cl1**	**84.00 (4)**	**O1—Co1—Cl1**	**96.00 (4)**
O2—Co2—Cl1A	**84.78 (5)**	**O2—Co2—O1**	**82.43 (6)**	**O2—Co2—N2**	**94.55 (7)**
O1—Co2—Cl1A	**84.56 (5)**	**N1—Co2—Cl1A**	**94.15 (6)**	**N1—Co2—O2**	**176.29 (7)**
N1—Co2—O1	**93.94 (7)**	**N1—Co2—N2**	**89.13 (8)**	**N2—Co2—Cl1A**	**99.28 (6)**
N2—Co2—O1	**174.92 (7)**	**N2—Co2—O1**			

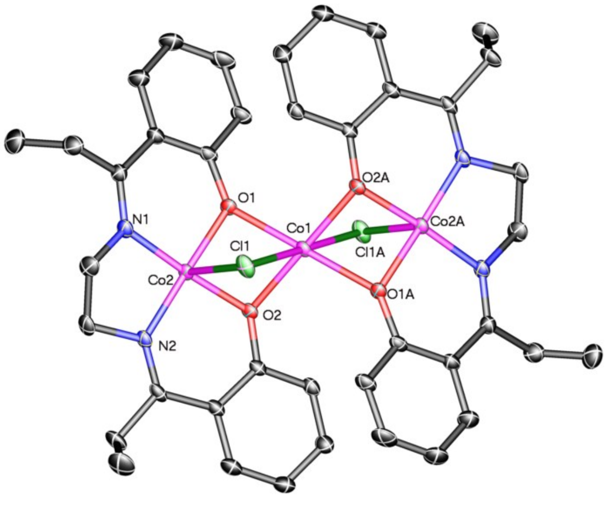


Fig. S1 The local coordination environments of complex CoL.

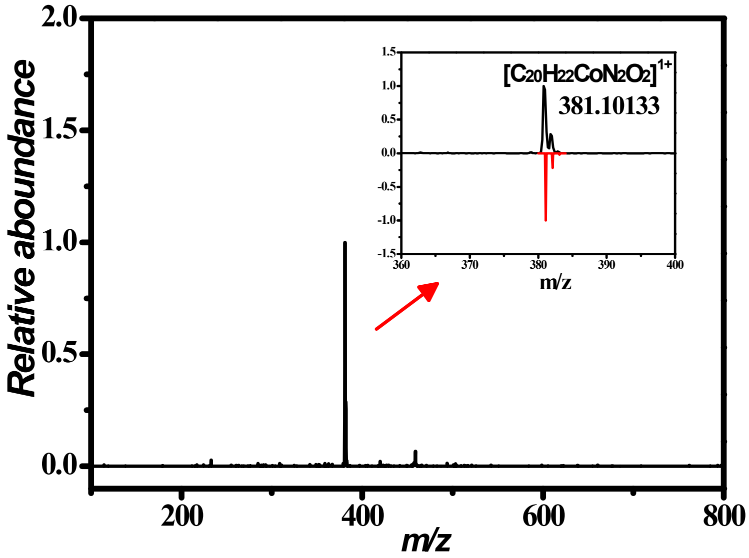


Fig. S2 The ESI mass spectrum of CoL in the scale of *m/z* = 100-800.

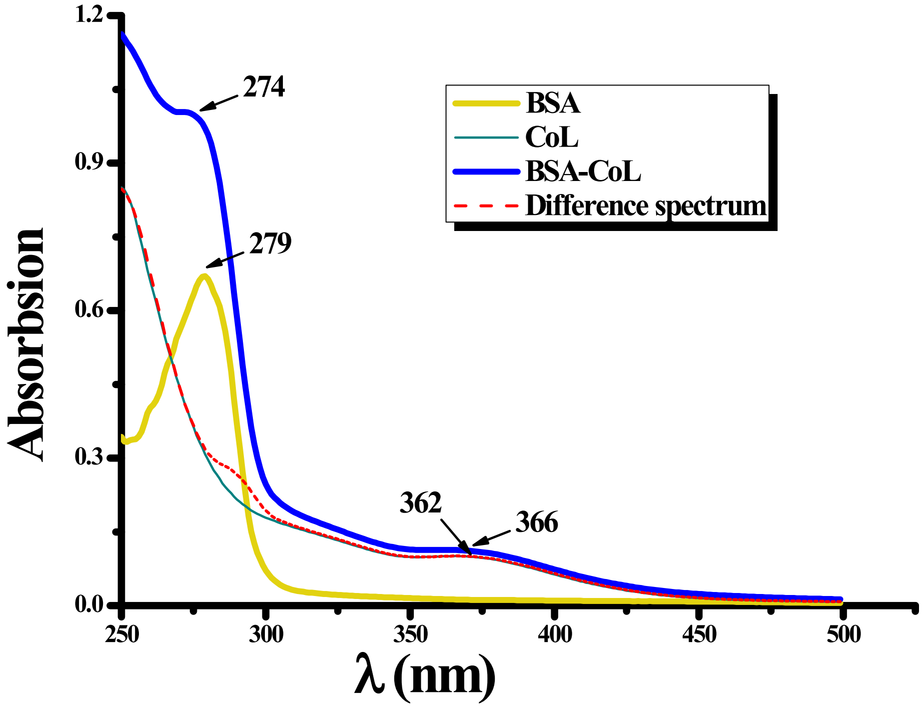


Fig. S3 UV-visible spectra of 10 μM BSA (yellow solid line), 10 μM complex CoL (green solid line), 10 μM hybrid BSA-CoL (blue solid line) and difference spectrum of BSA-CoL minus BSA (red dashed line) in PBS (pH 7.45, 0.05 M).

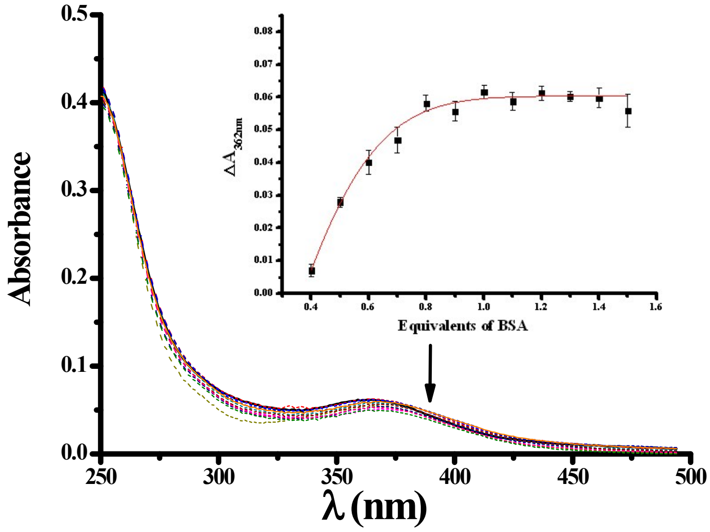
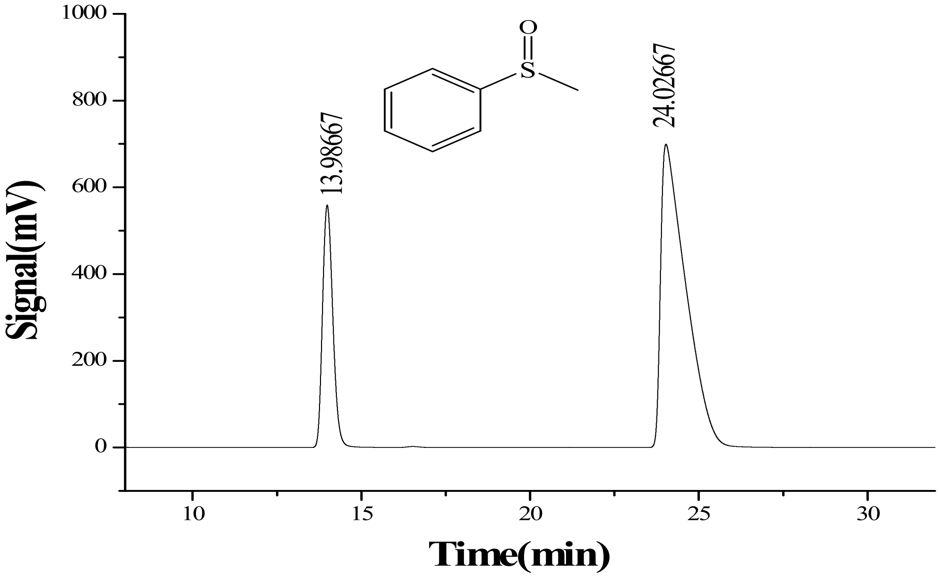


Fig. S4 UV-visible titration of CoL by BSA. Evolution of the UV-visible spectrum of 4.5 μM solution of CoL in 0.05 M PBS, pH 7.45, upon addition of increasing amounts of BSA (0 to 1.5 molar equivalents). Insert: difference between the absorbance value at 362 nm of the BSA-CoL solution and that of the cofactor alone, $\Delta A_{362nm} = A_0 - A_s$ plotted against the BSA/CoL ratio.

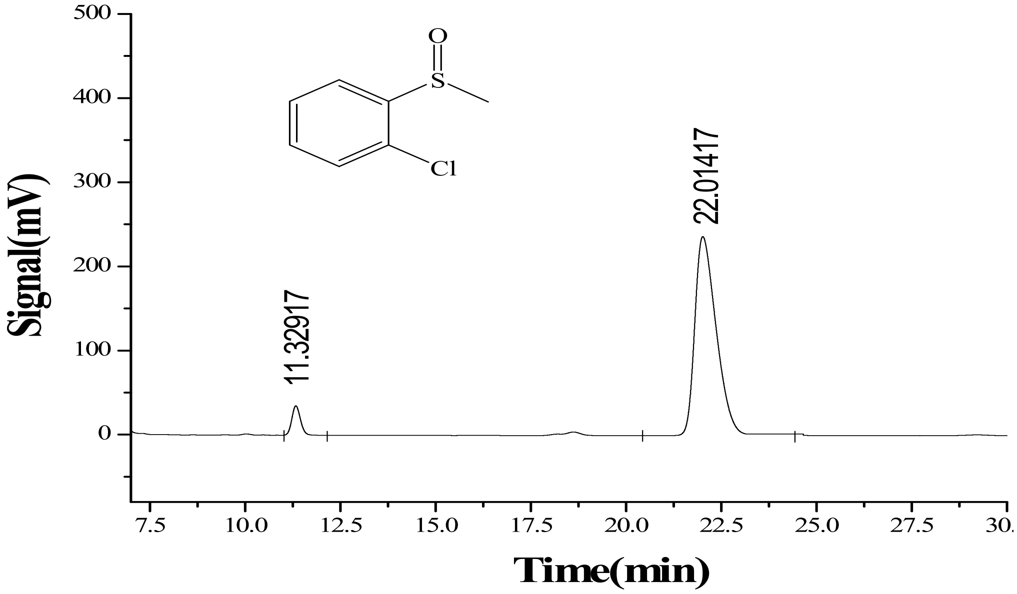
HPLC chromatogram of sulfoxides

Methyl phenyl sulfoxide



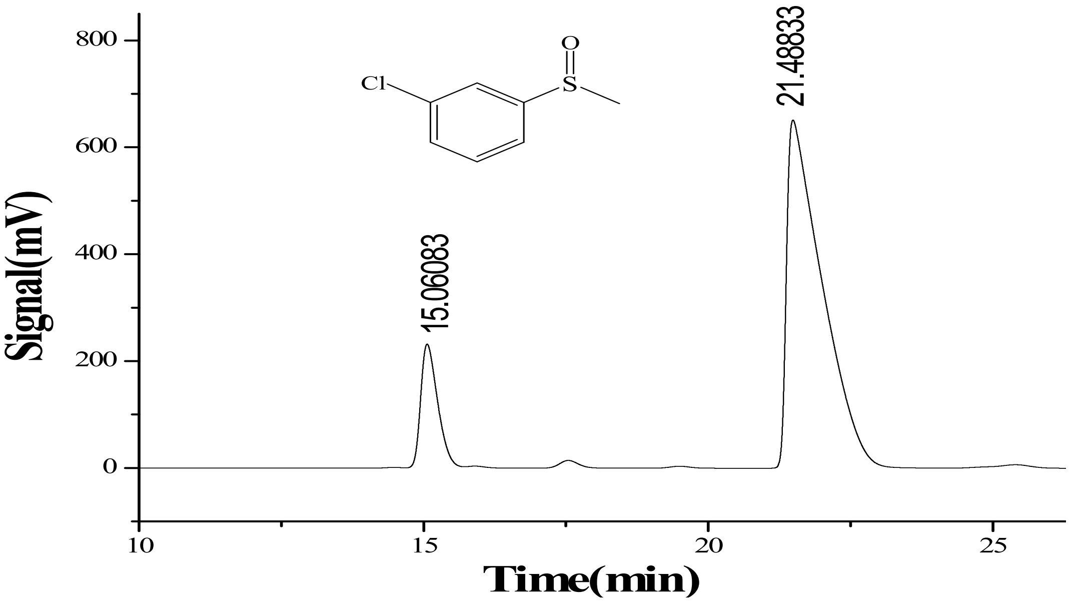
Peak	Ret.Time (min)	Area	Area%
1	13.987	11888.19	24.72
2	24.027	36208.63	75.28 (R)

2-Chlorophenyl methyl sulfoxide



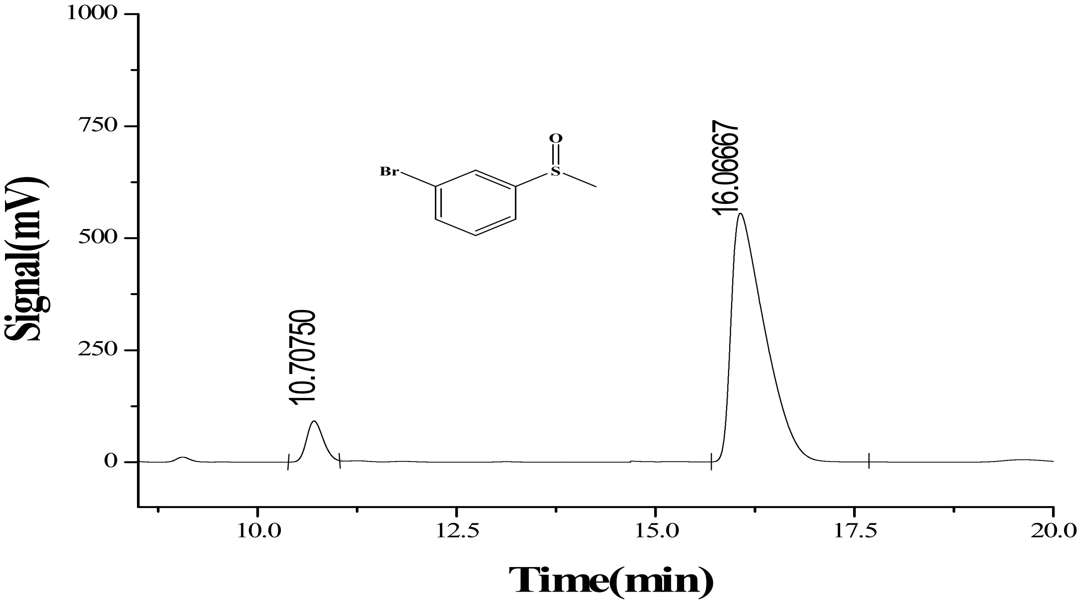
Peak	Ret.Time (min)	Area	Area%
1	11.329	554.17	5.758
2	22.014	9069.67	94.242 (R)

3-Chlorophenyl methyl sulfoxide



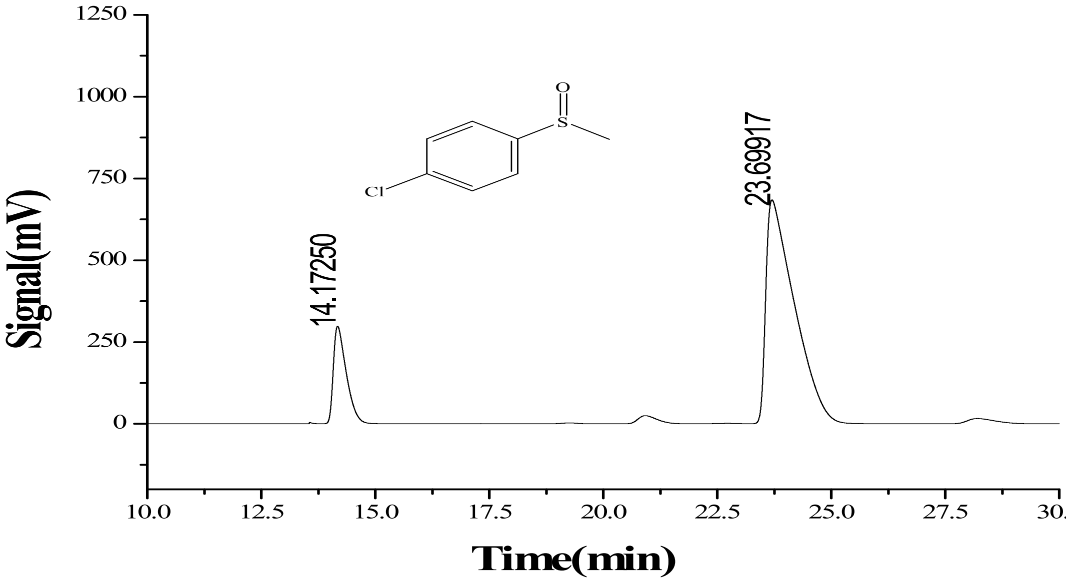
Peak	Ret.Time (min)	Area	Area%
1	15.061	4740.51	14.370
2	21.488	28248.18	85.630 (R)

3-Bromophenyl methyl sulfoxide



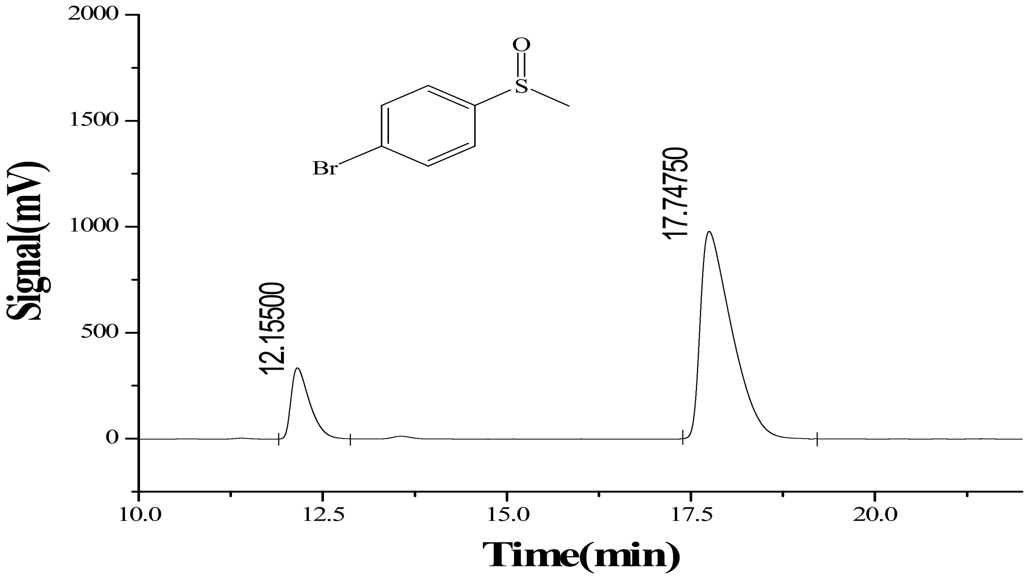
Peak	Ret.Time (min)	Area	Area%
1	10.708	1390.09	7.861
2	16.067	16293.04	92.139 (R)

4-Chlorophenyl methyl sulfoxide



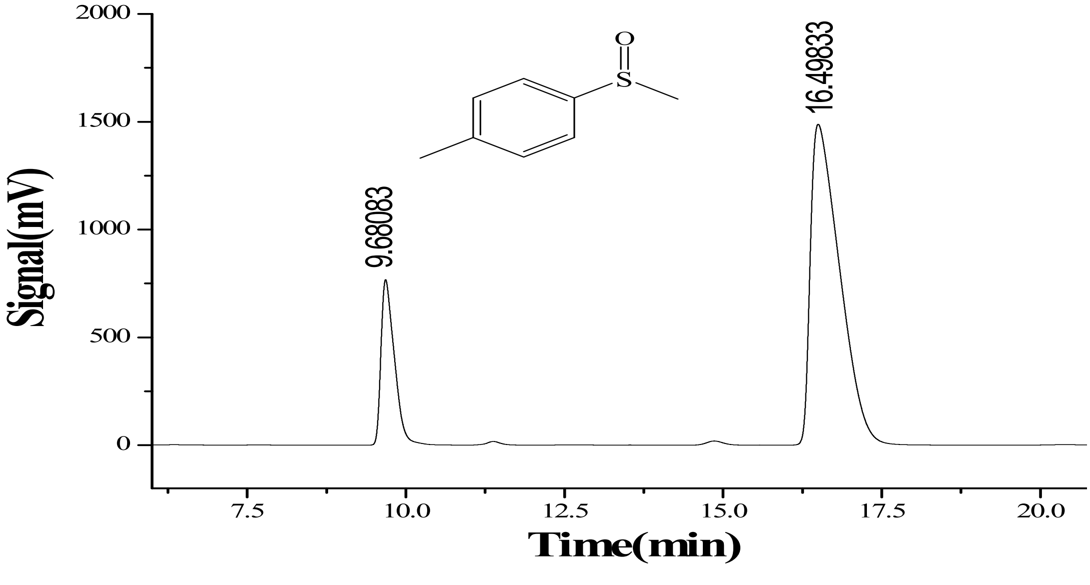
Peak	Ret.Time (min)	Area	Area%
1	14.173	5893.86	16.508
2	23.699	29809.32	83.492 (R)

4-Bromophenyl methyl sulfoxide



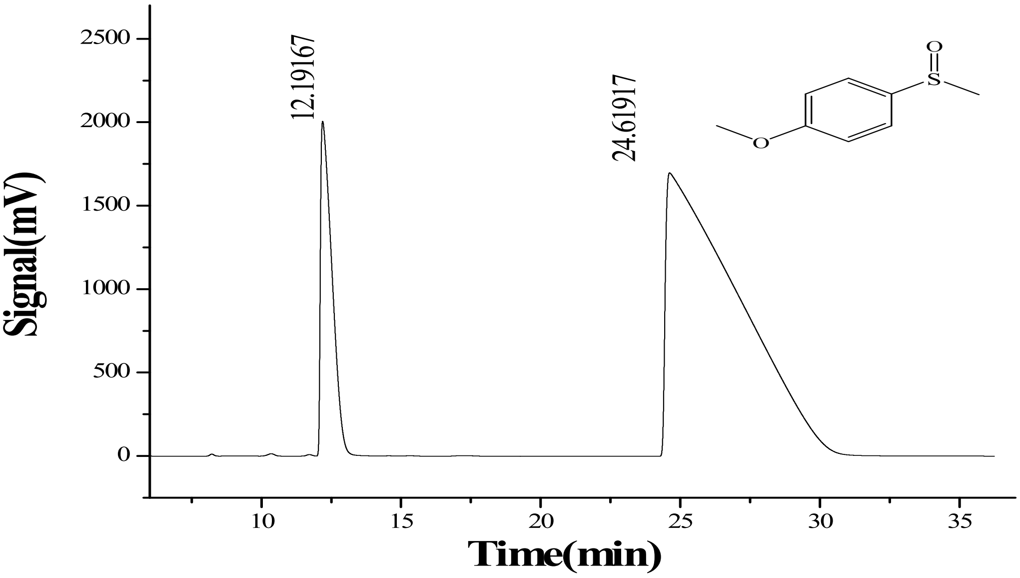
Peak	Ret.Time (min)	Area	Area%
1	12.155	5926.47	16.896
2	17.748	29150.65	83.104 (R)

4-Methylphenyl methyl sulfoxide



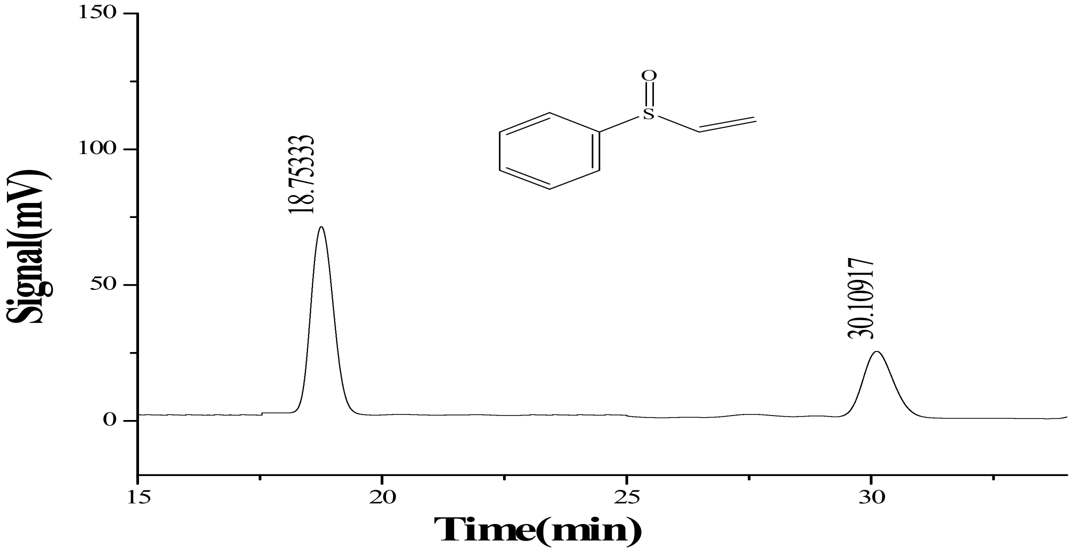
Peak	Ret.Time (min)	Area	Area%
1	9.681	11334.11	19.178
2	16.499	47765.70	80.822 (R)

4-Methoxyphenyl methyl sulfoxide



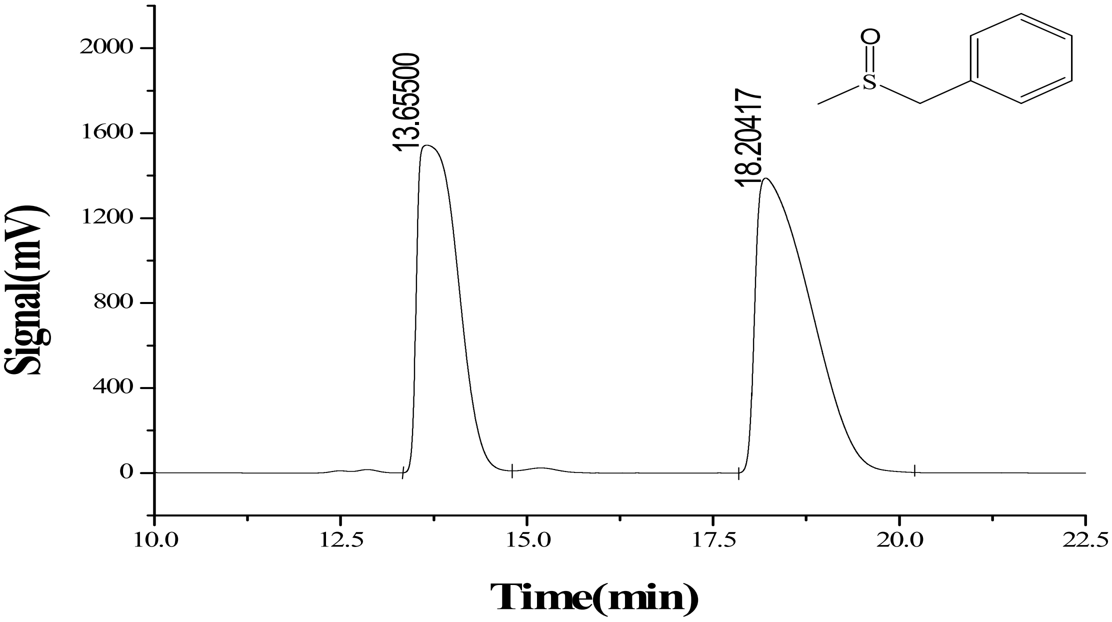
Peak	Ret.Time (min)	Area	Area%
1	12.192	57197.60	15.709
2	24.619	306914.00	84.291 (R)

Vinyl Phenyl Sulfoxide



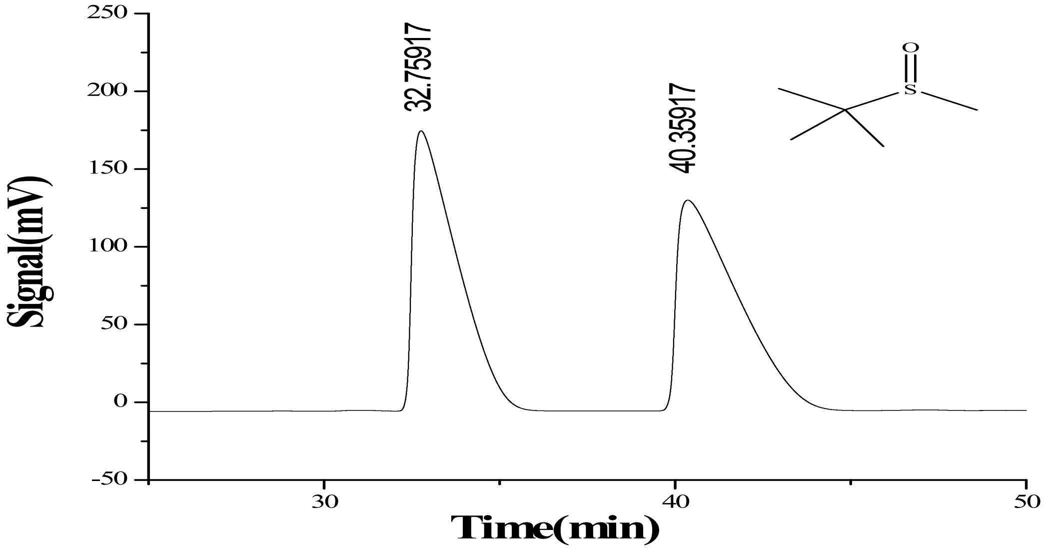
Peak	Ret.Time (min)	Area	Area%
1	18.753	2196.69	67.571 (S)
2	30.109	1054.26	32.429

Methyl Benzyl Sulfoxide



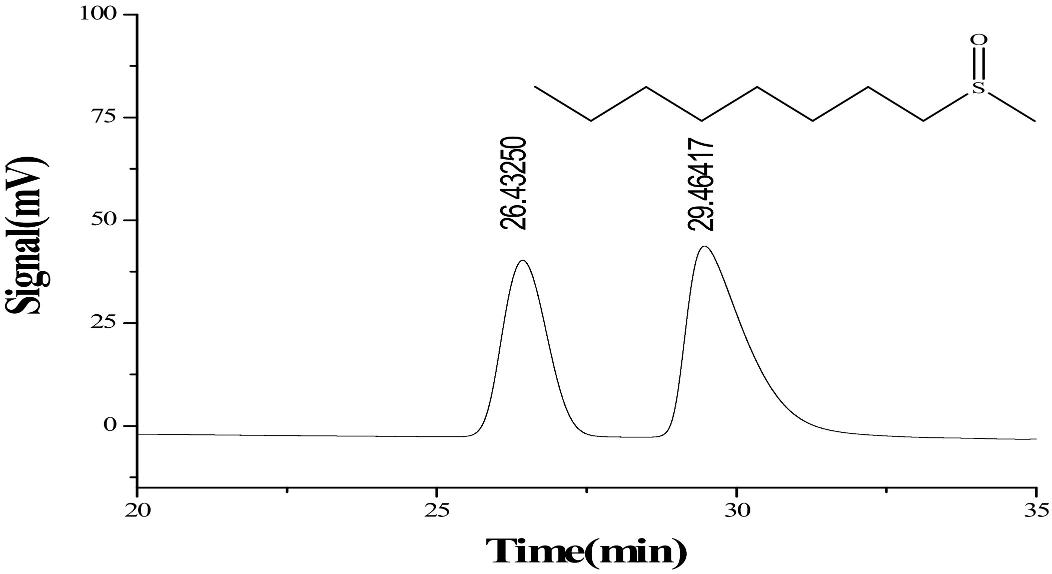
Peak	Ret.Time (min)	Area	Area%
1	13.655	58111.96	45.118
2	18.204	70687.06	54.882 (R)

Methyl *tert*-Butyl Sulfoxide



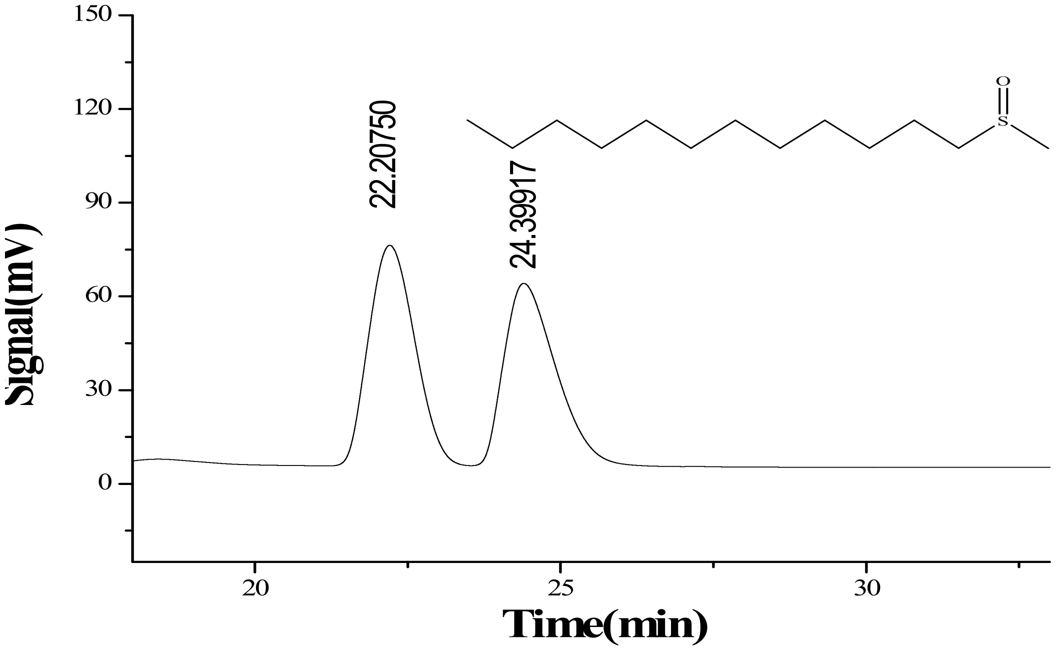
Peak	Ret.Time (min)	Area	Area%
1	32.759	15930.64	49.4
2	40.359	16335.03	50.6

Methyl *n*-Octyl Sulfoxide



Peak	Ret.Time (min)	Area	Area%
1	26.433	2240.20	40.387
2	29.464	3307.97	59.613 (R)

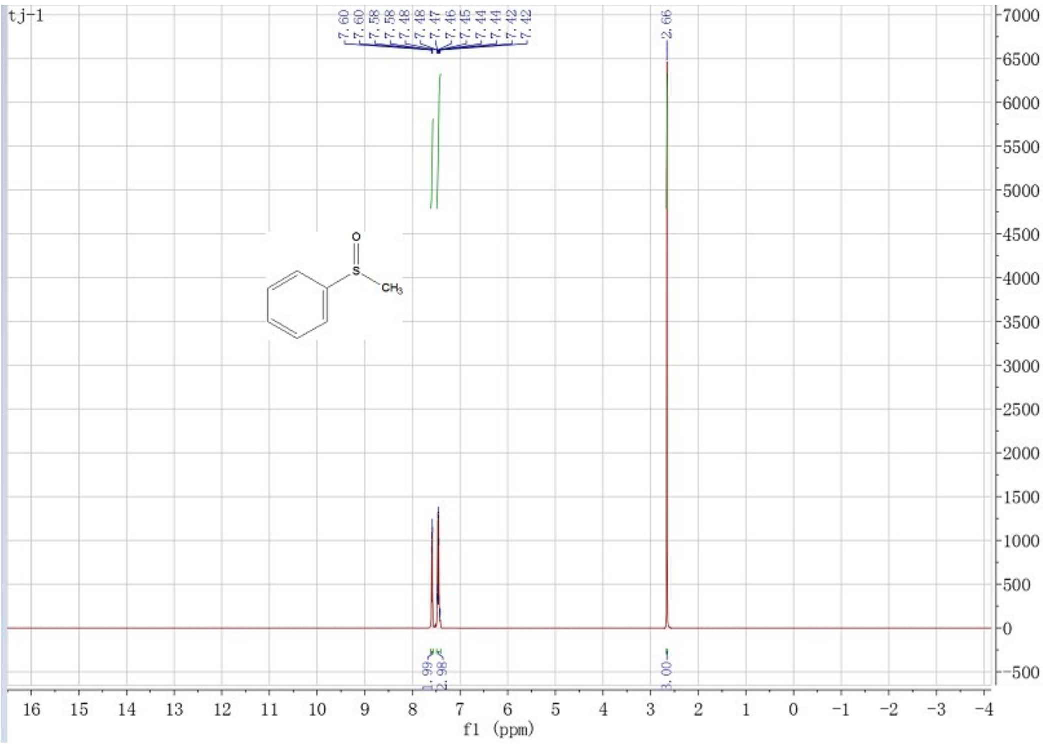
Methyl *n*-Dodecyl methyl Sulfoxide

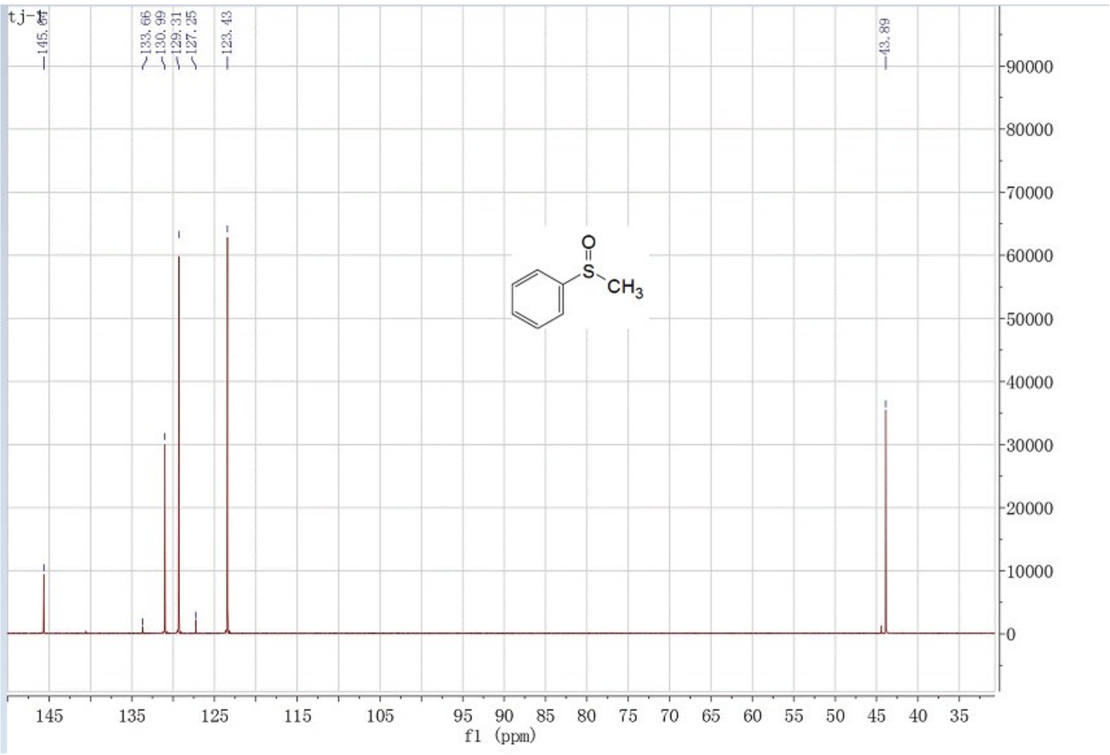


Peak	Ret.Time (min)	Area	Area%
1	22.208	3700.05	50.78
2	24.399	3445.59	49.22

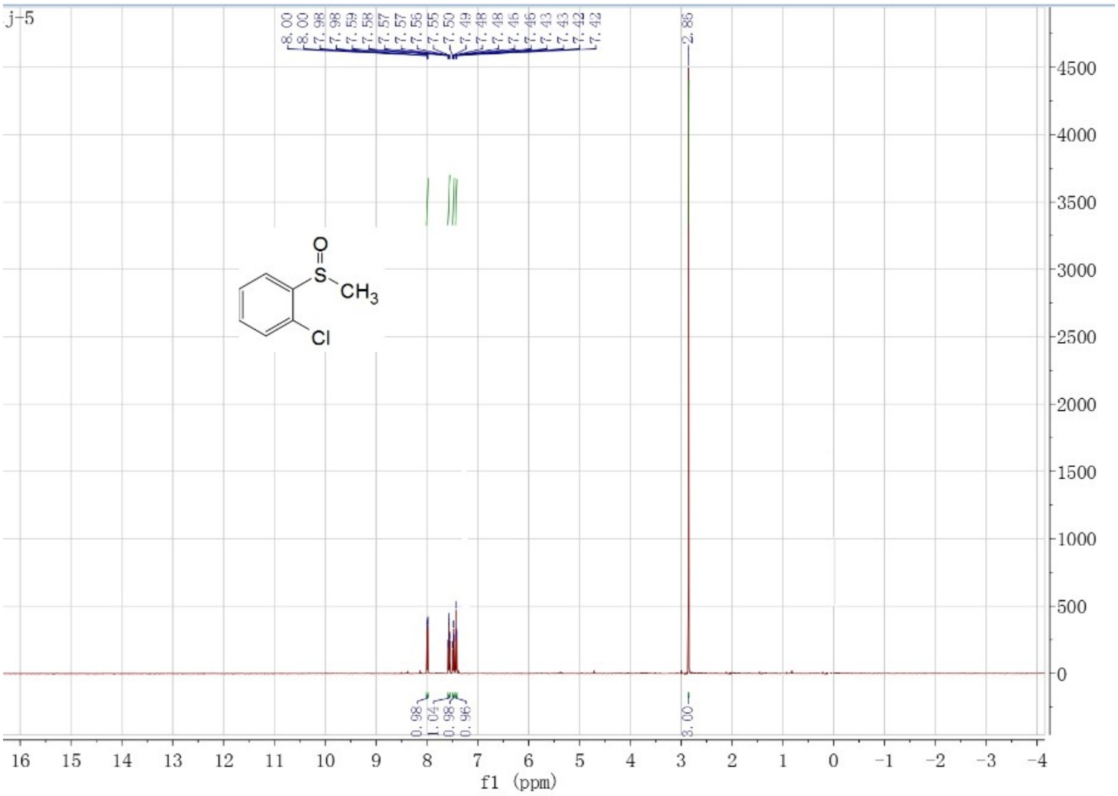
^1H NMR and ^{13}C NMR of sulfoxides:

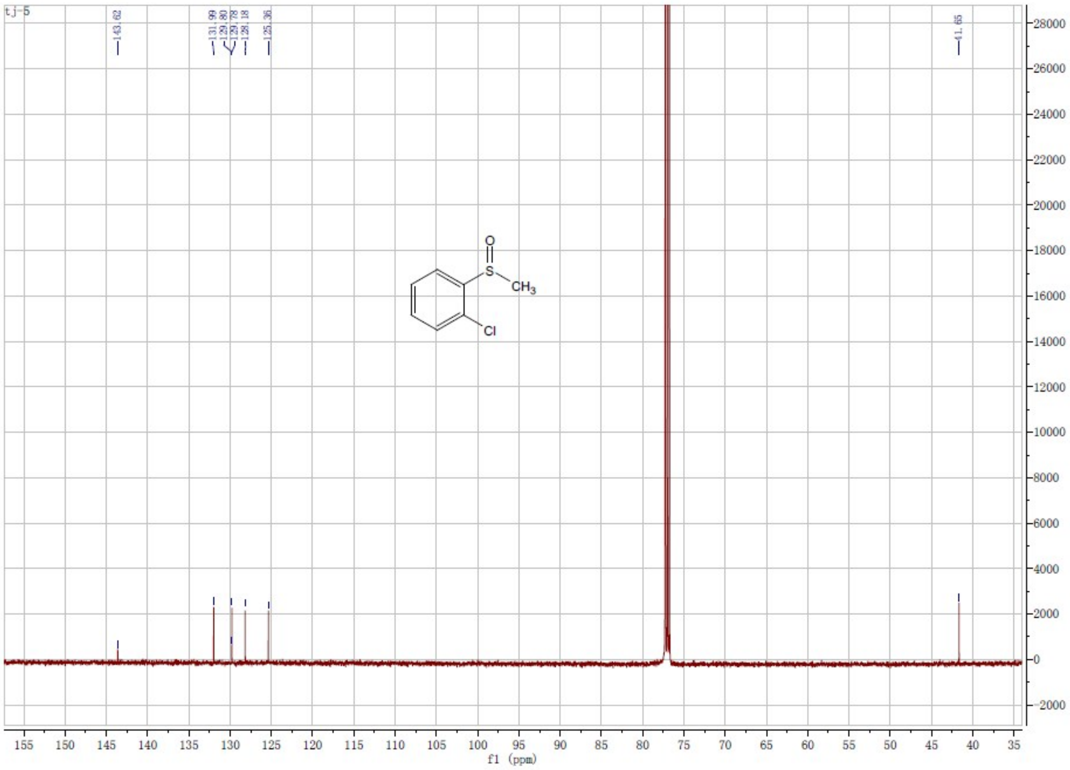
Methyl phenyl sulfoxide



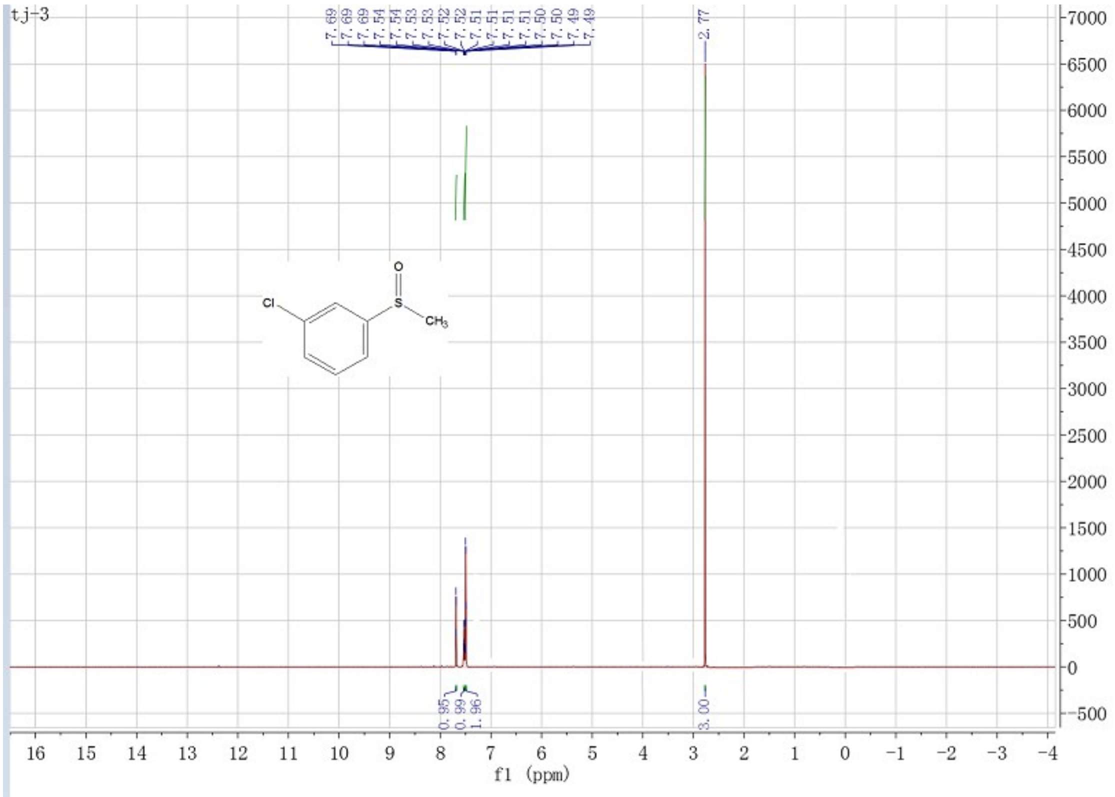


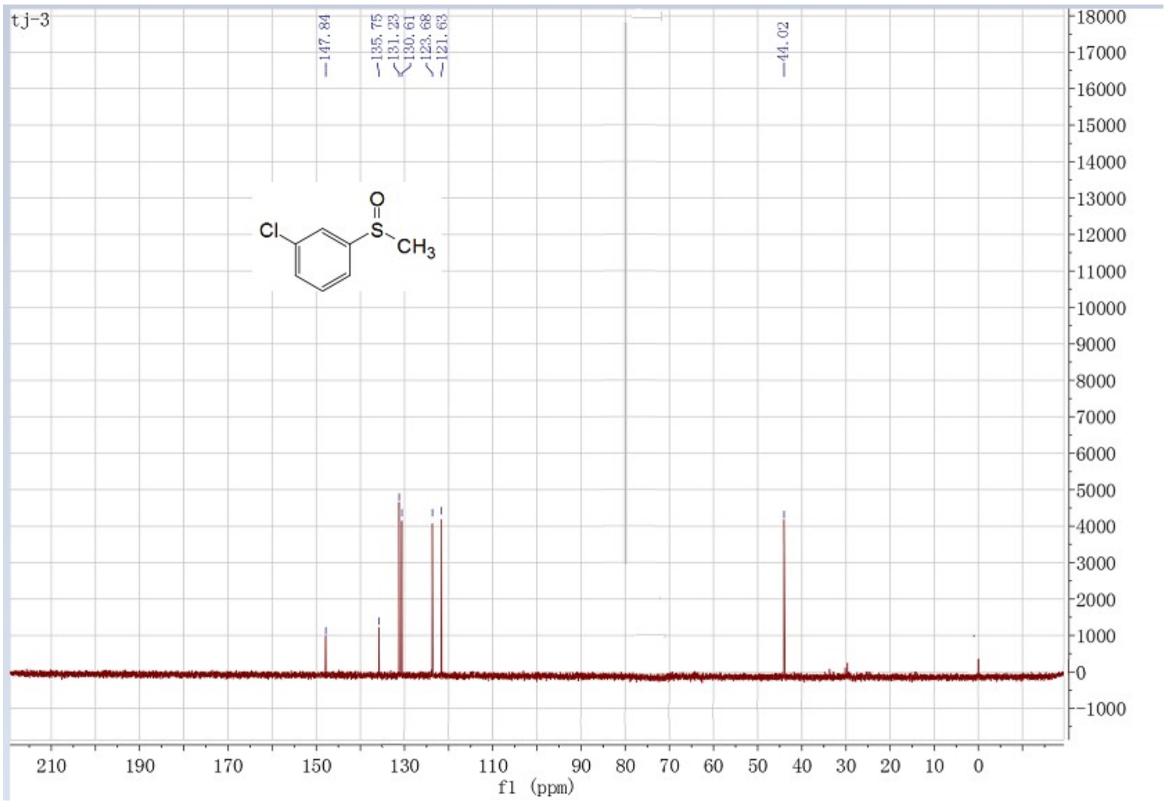
2-Chlorophenyl methyl sulfoxide



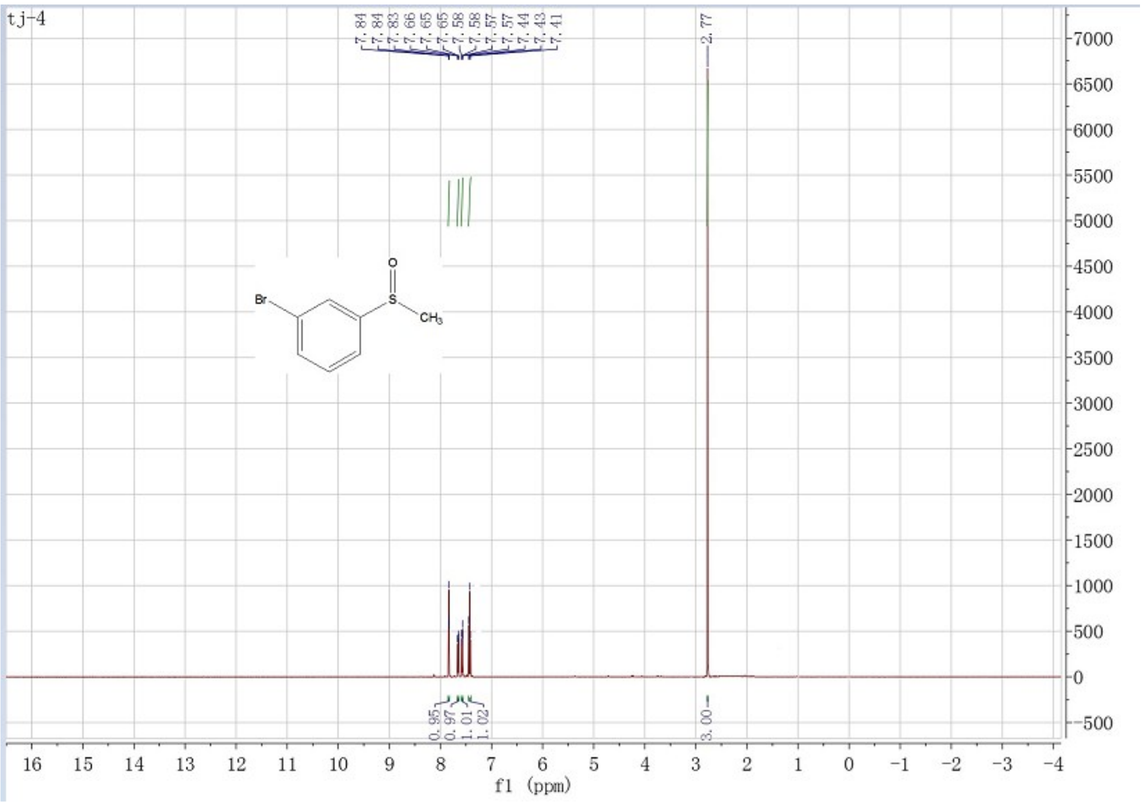


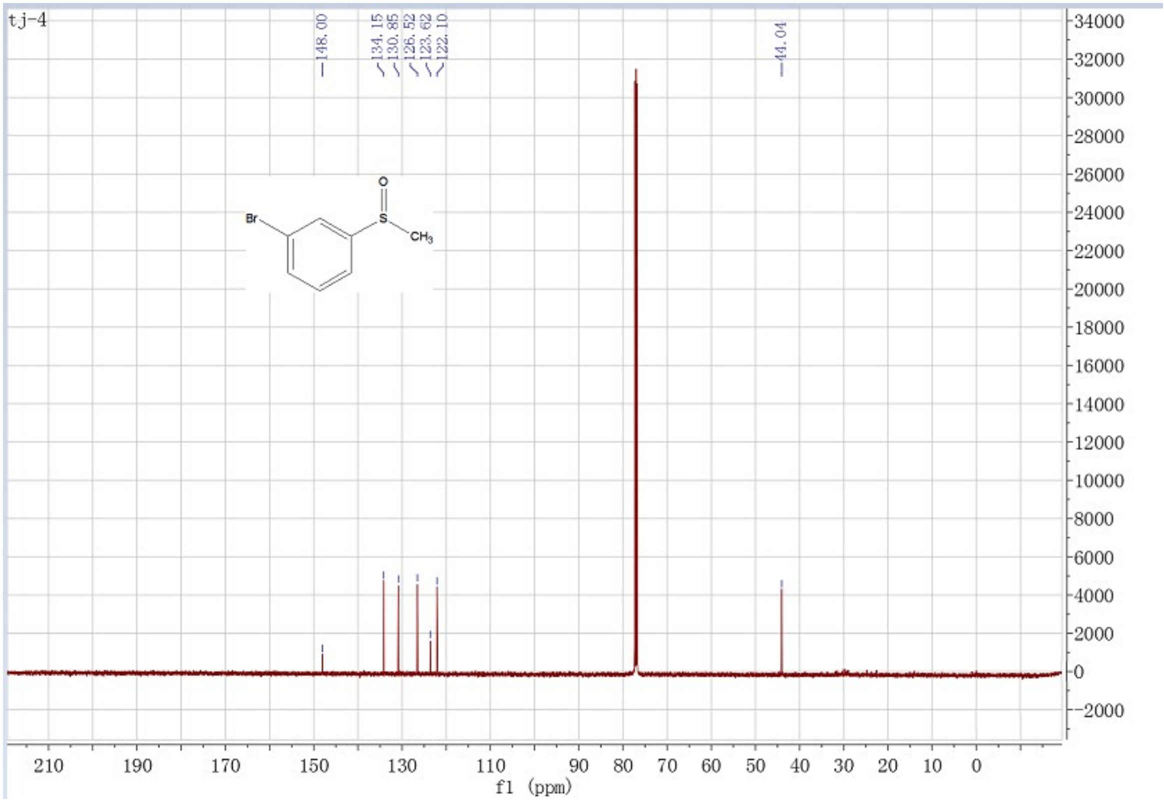
3-Chlorophenyl methyl sulfoxide



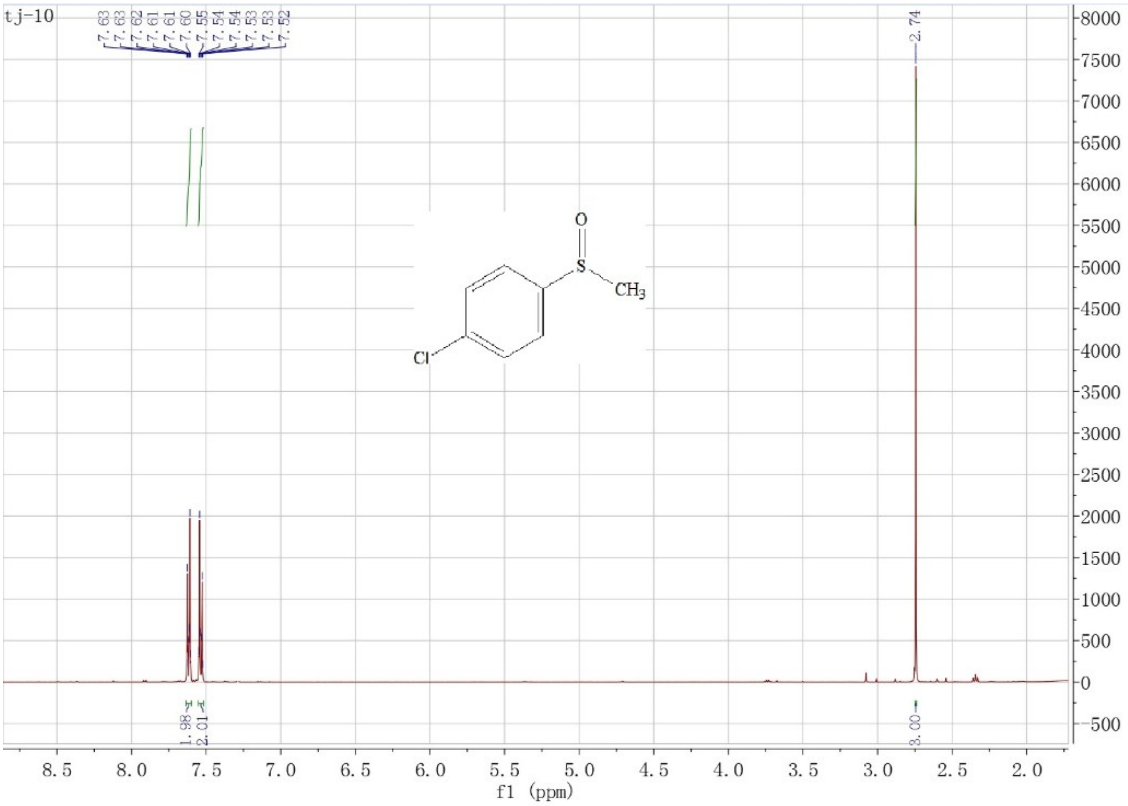


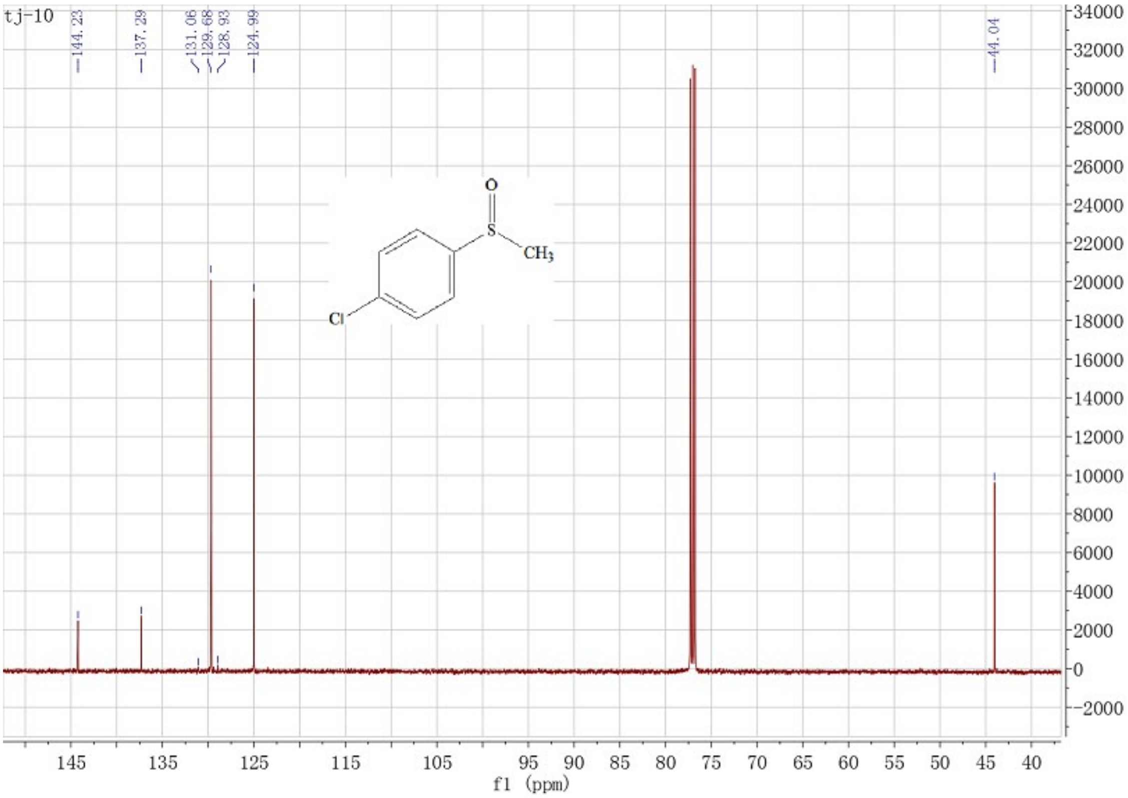
3-Bromophenyl methyl sulfoxide



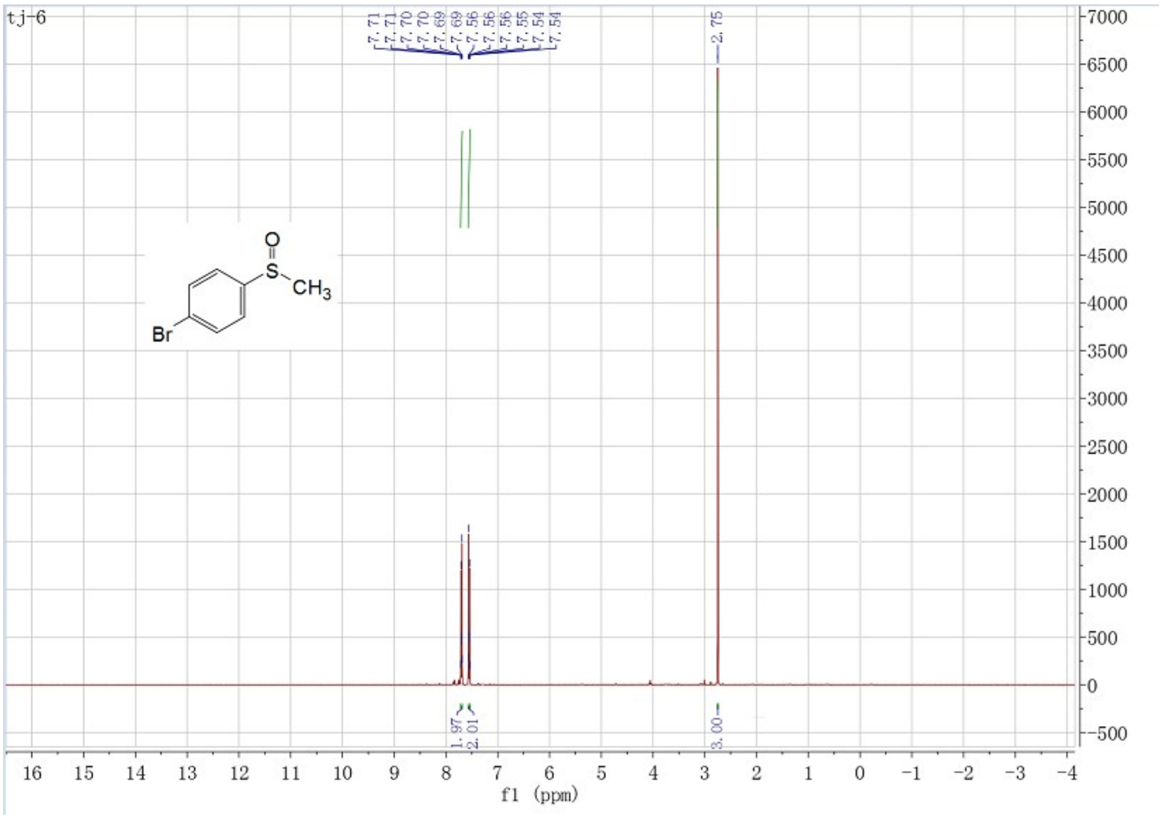


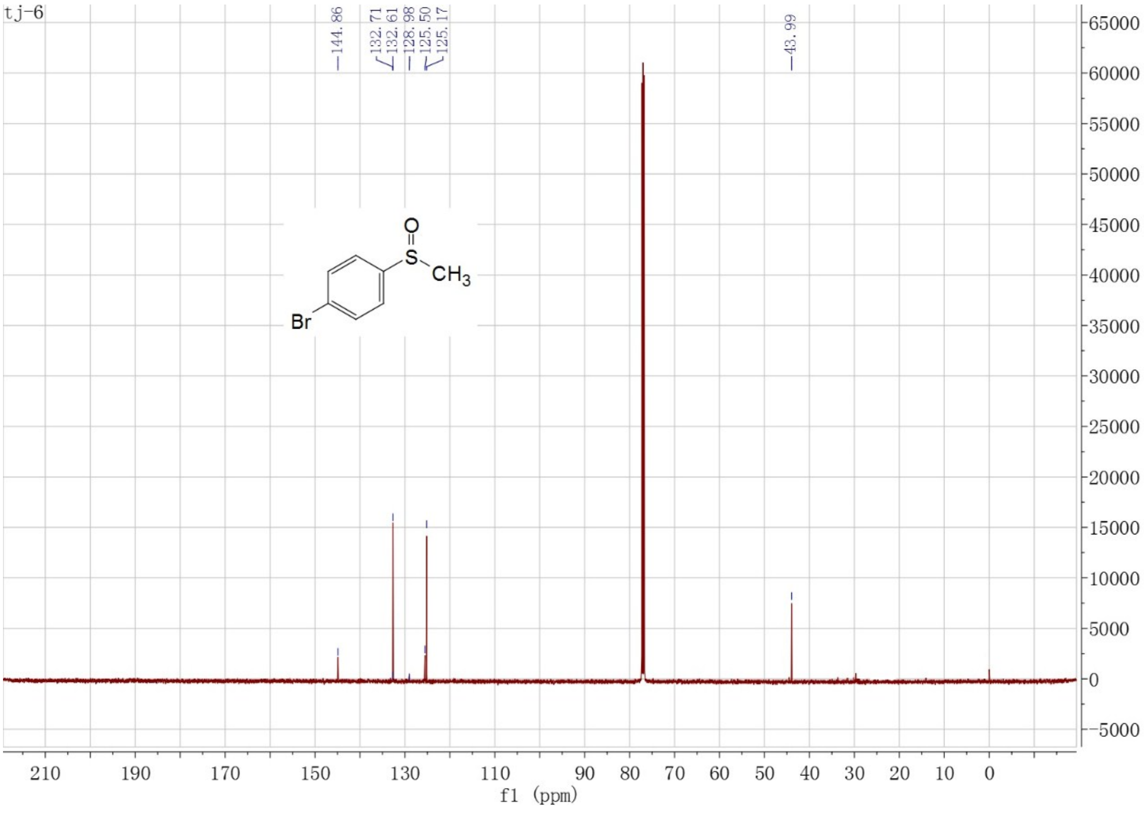
4-Chlorophenyl methyl sulfoxide



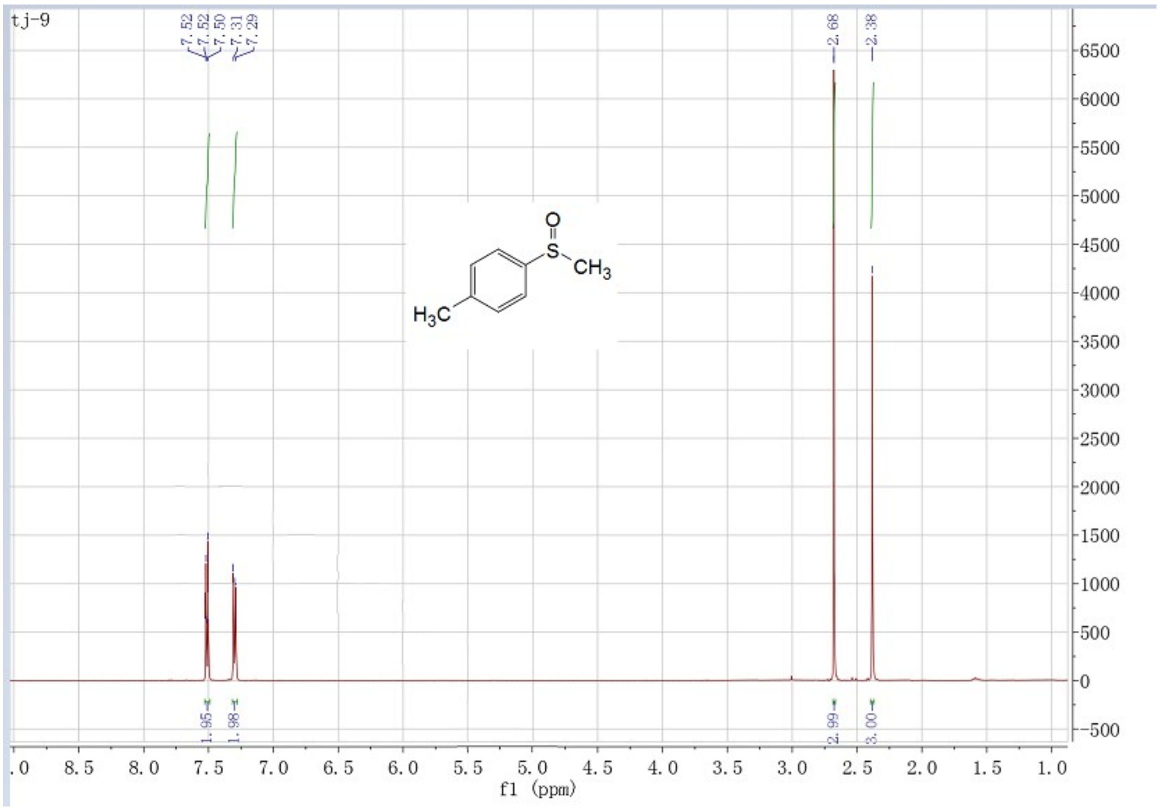


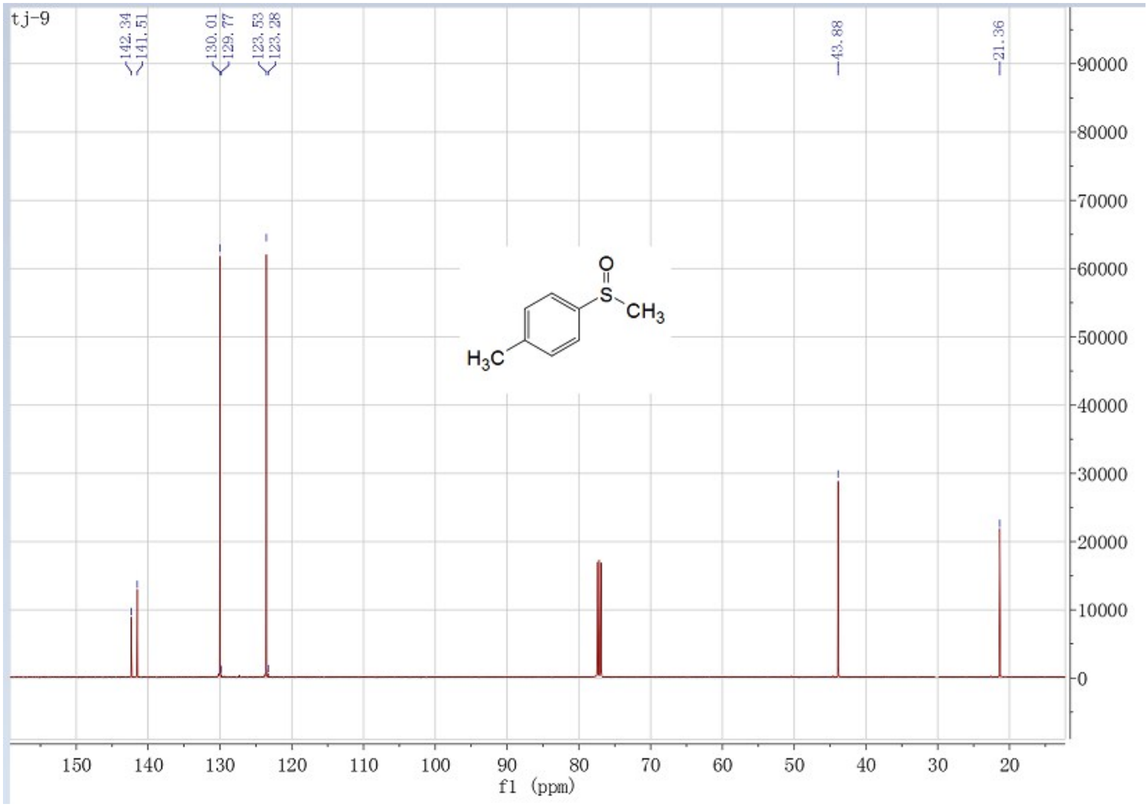
4-Bromophenyl methyl sulfoxide



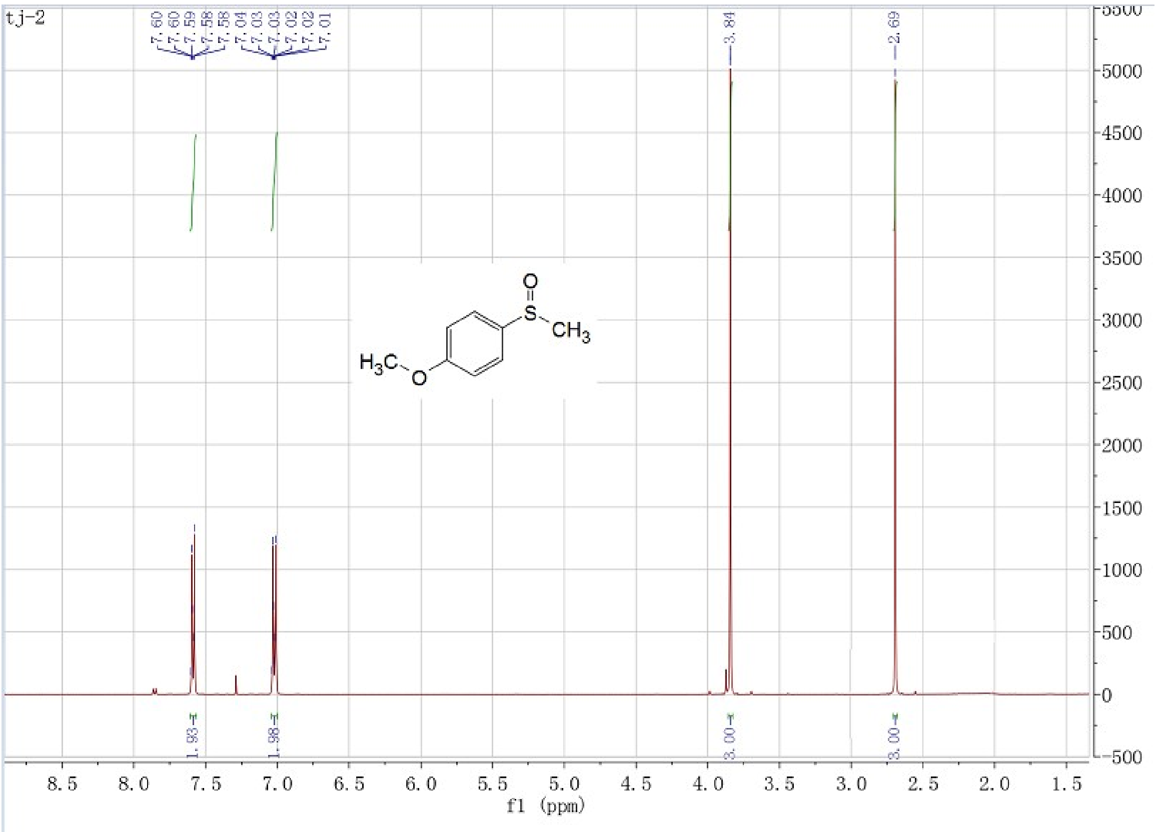


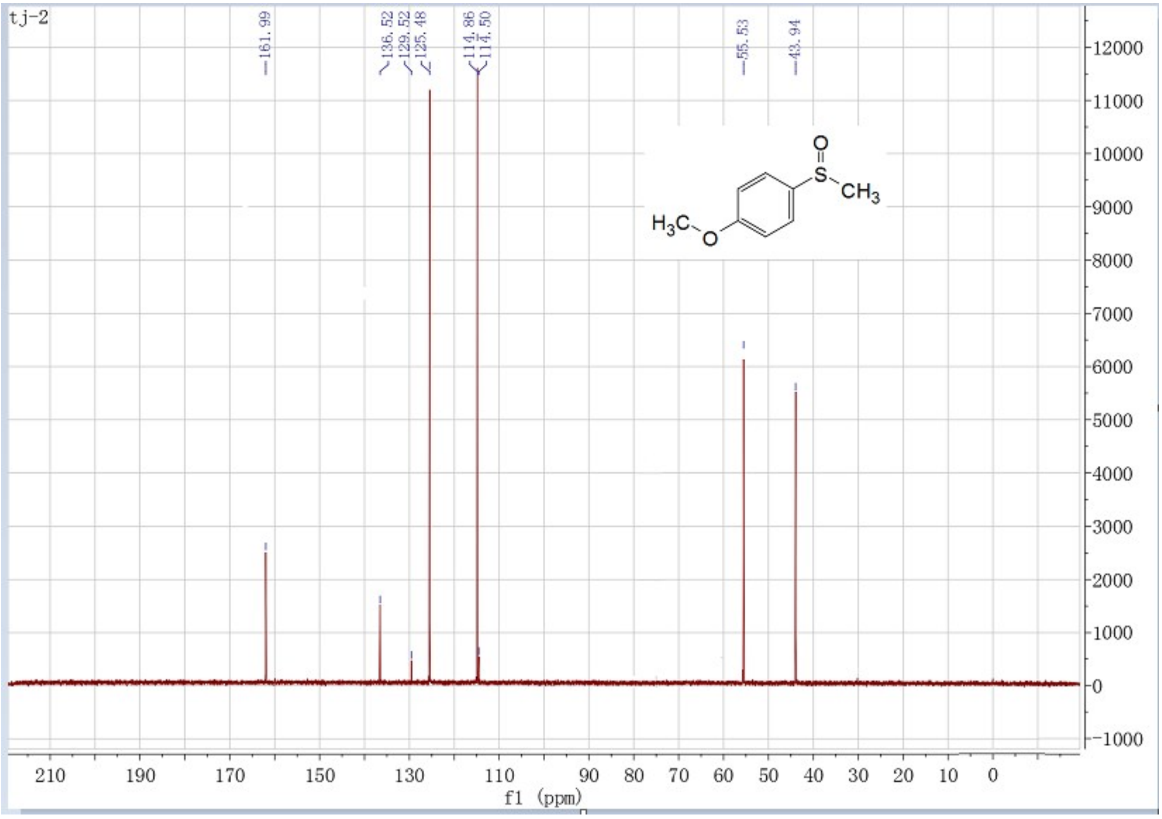
4-Methylphenyl methyl sulfoxide



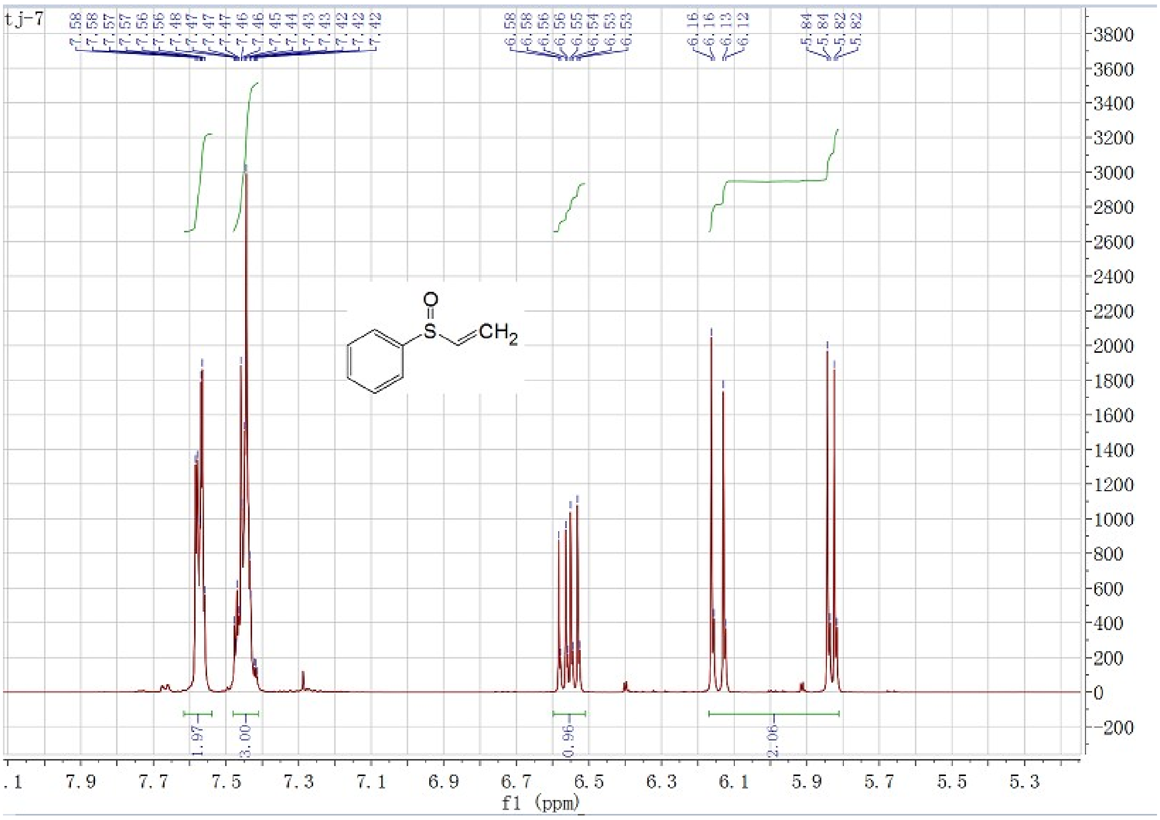


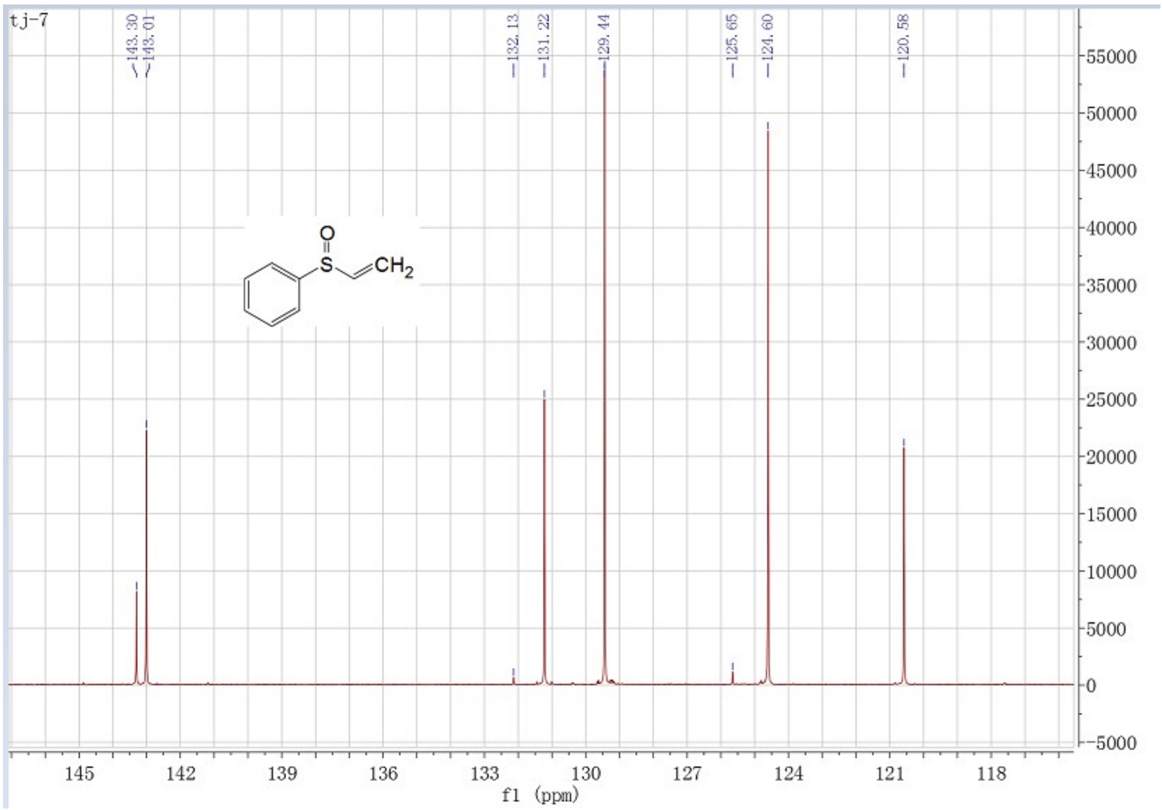
4-Methoxyphenyl methyl sulfoxide



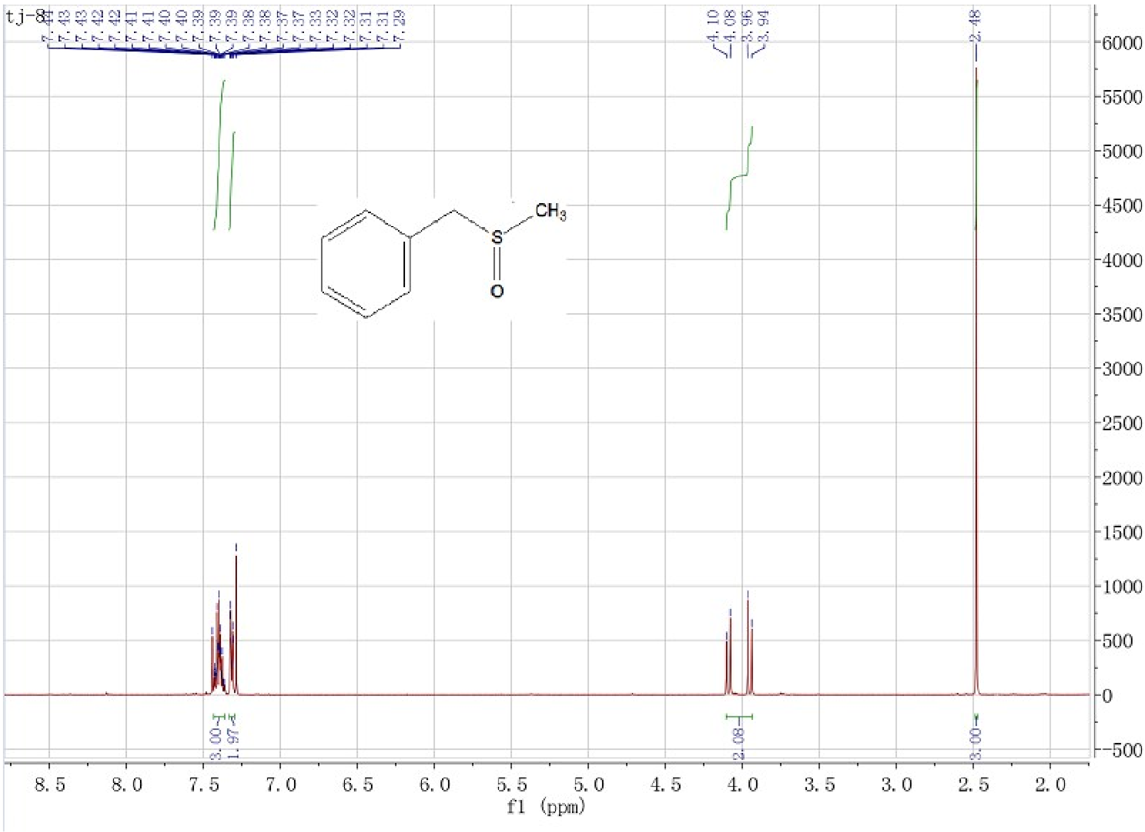


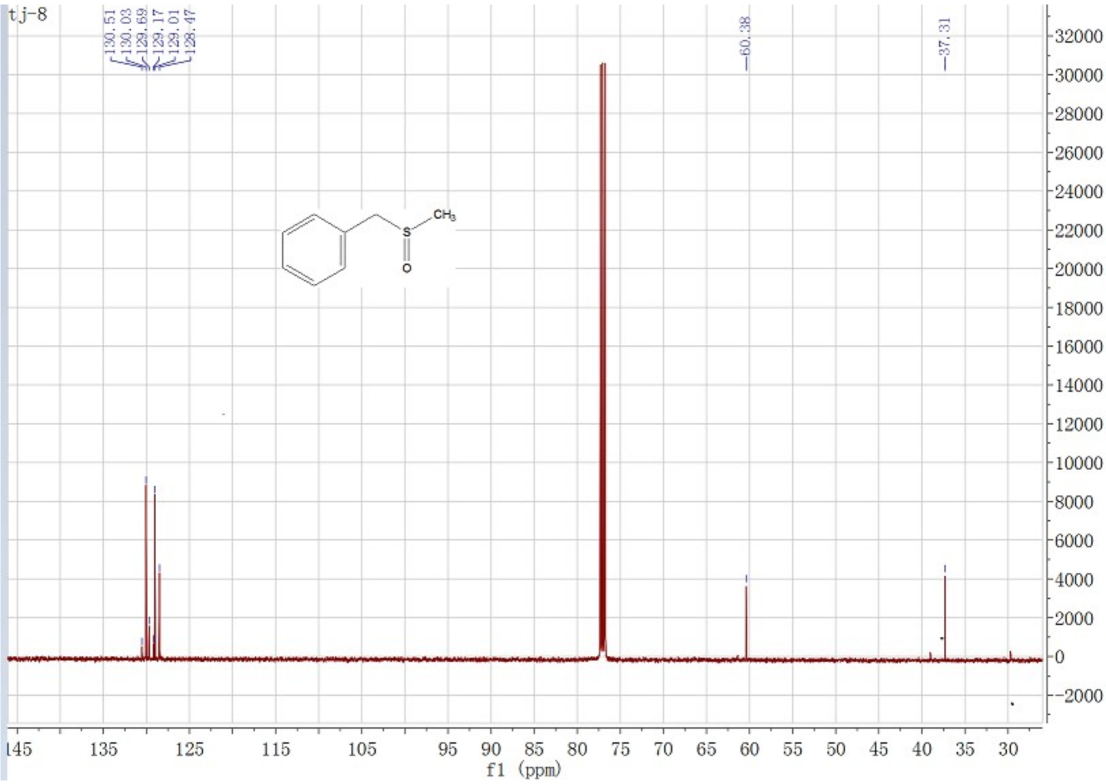
Vinyl Phenyl Sulfoxide



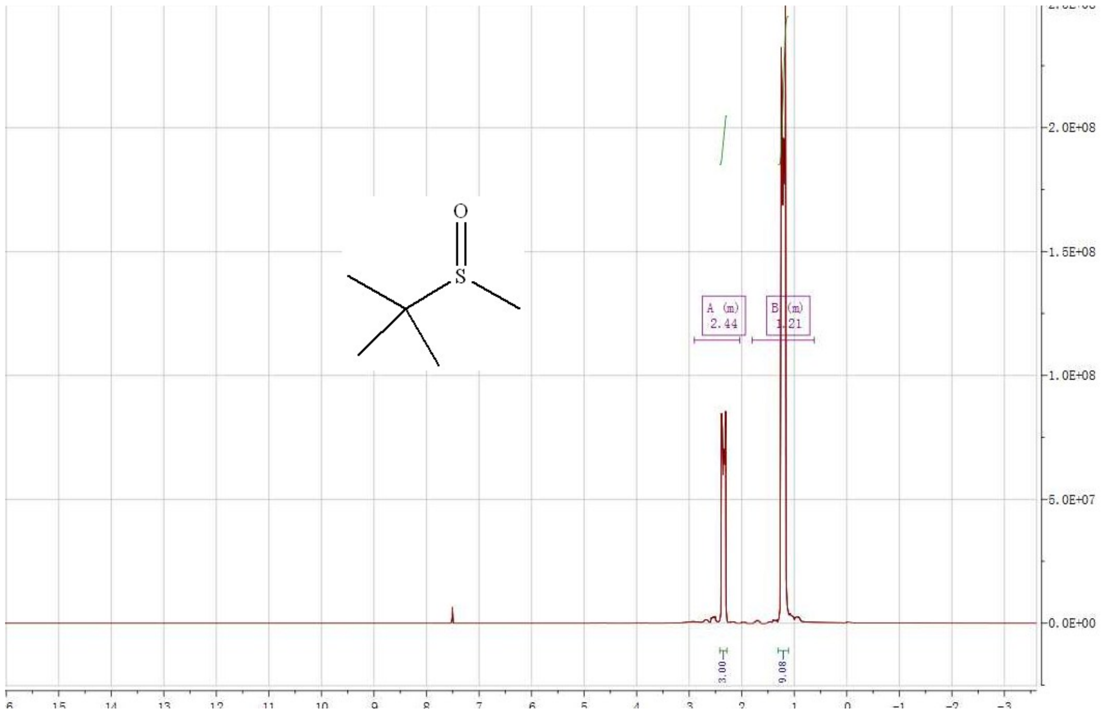


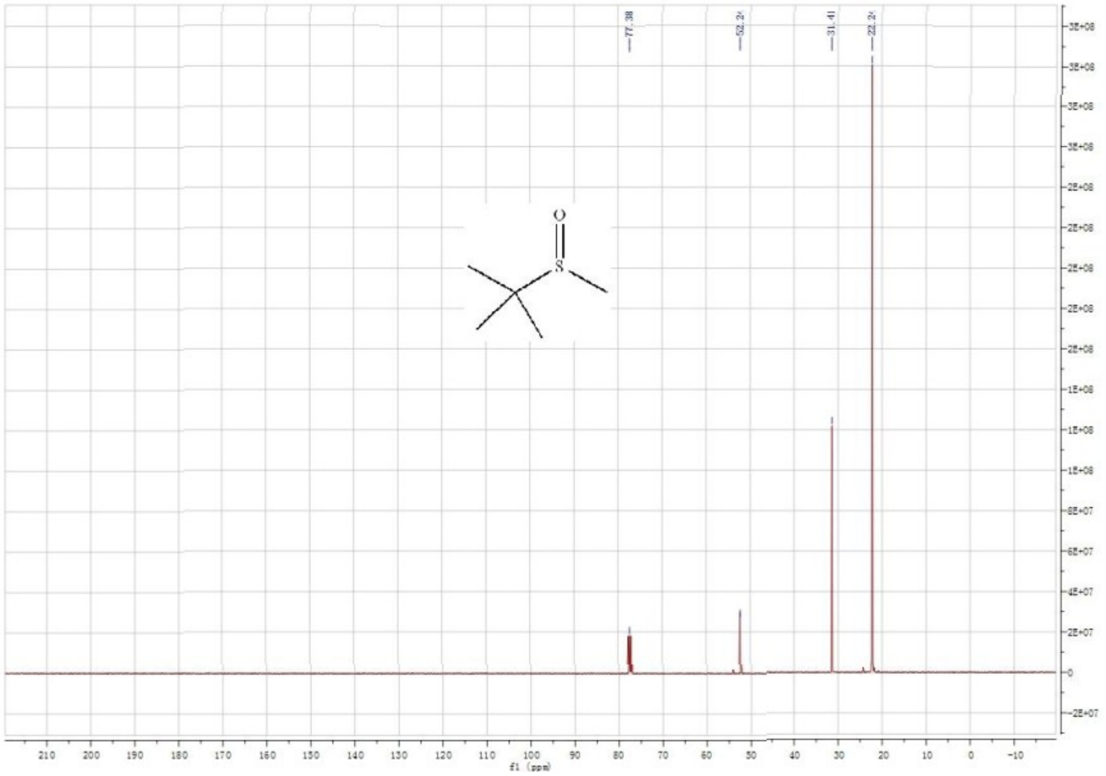
Methyl Benzyl Sulfoxide



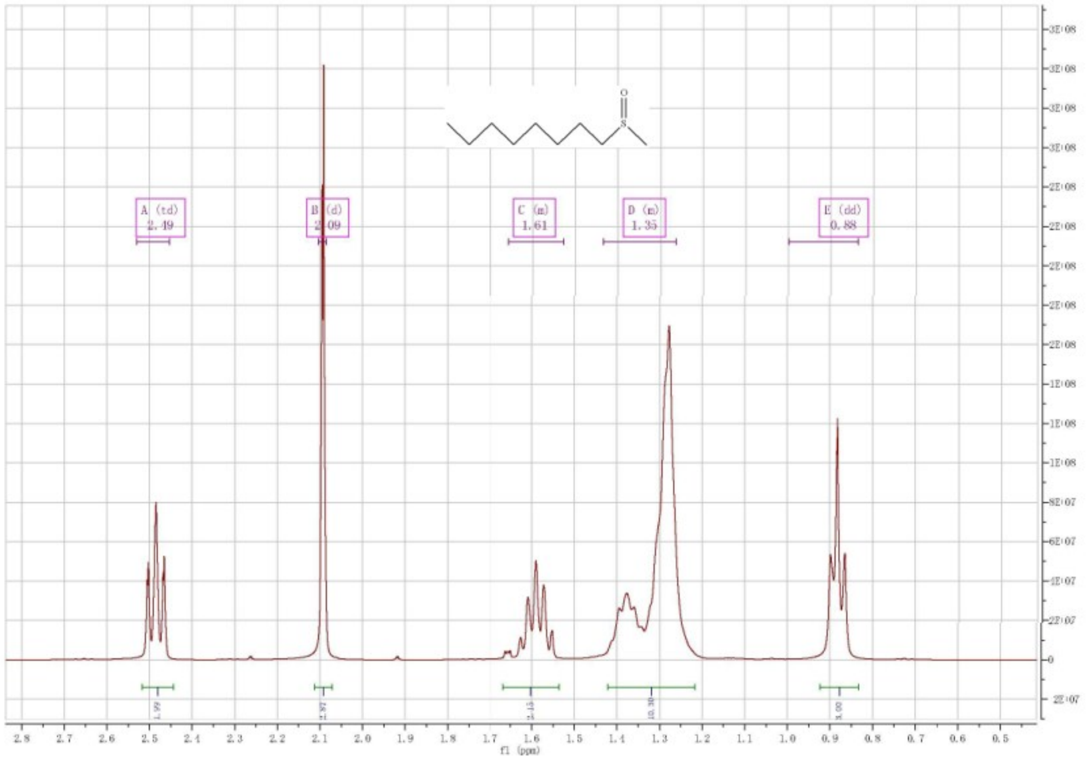


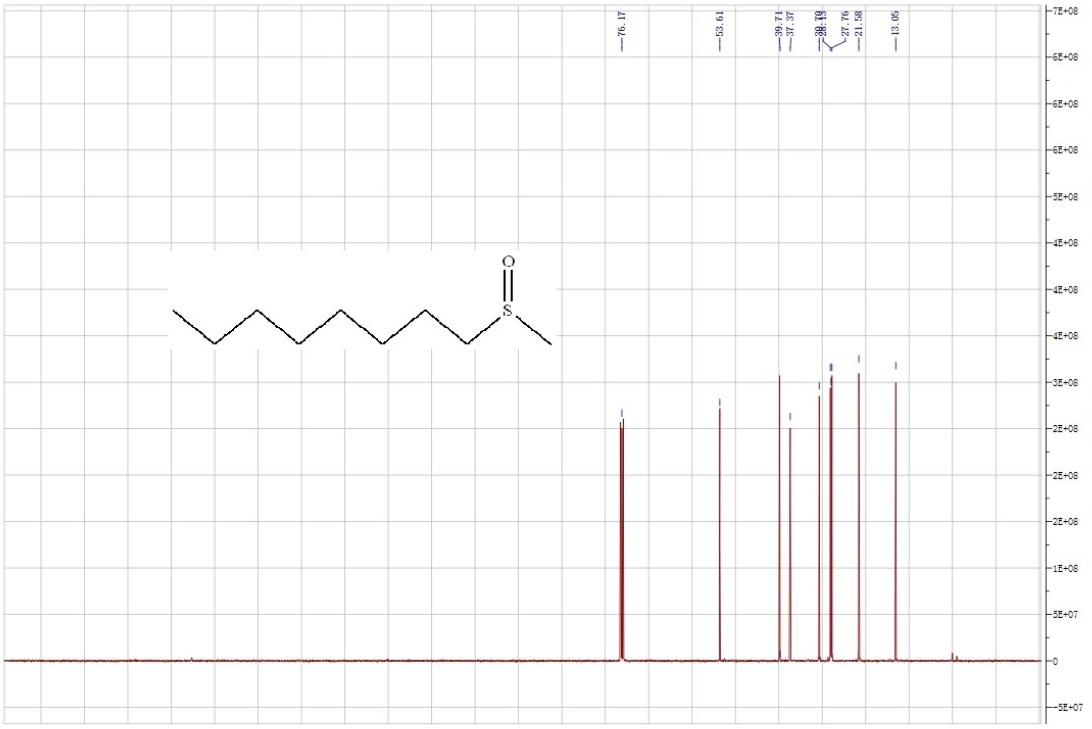
Methyl *tert*-Butyl Sulfoxide





Methyl *n*-Octyl Sulfoxide





Methyl *n*-Dodecyl methyl Sulfoxide