STYRENE EPOXIDATION : GC ANALYSIS
(catalyzed by 1)

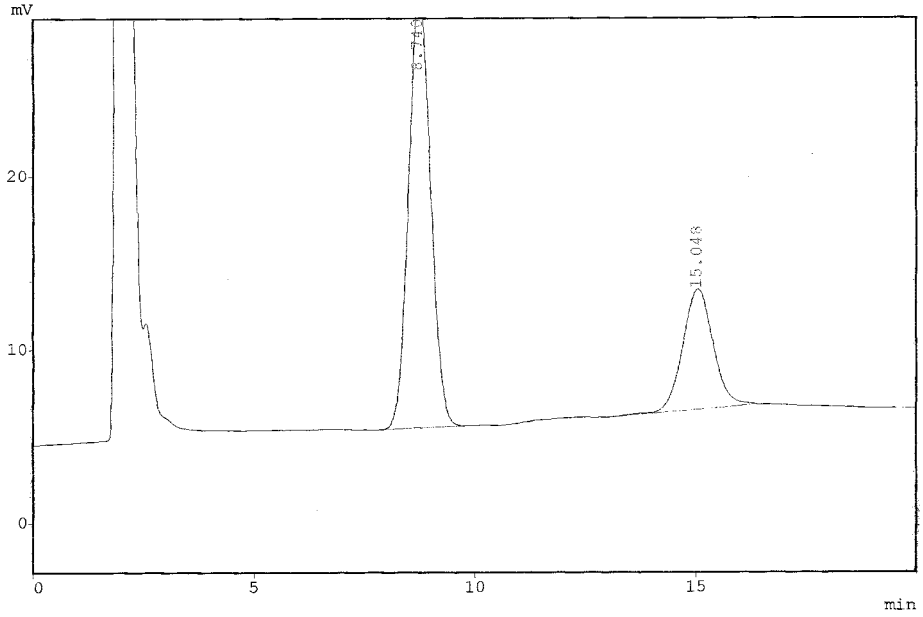
DETECTOR: FID
COLUMN: STAINLESS STEEL PACKED COLUMN (5%SE 30, 5m)
TEMP PROGRAM: 100° C -0min-5 °/min-175° C-5min.
INJECTOR PORT TEMP: 200° C
DETECTOR: 300° C
CARRIER GAS: NITROGEN

GAS CHROMATOGRAMS OF STANDARD SAMPLES TO DRAW THE CALIBRATION PLOT

A) 50 mg of Styrene oxide + 75 mg of PhBr (Internal Standard) in 10 ml Ether.

```
CLASS-GC10 Ver.=1.62  SYS=1 Ch=1 REPORT.NO=2  DATA=@CHRM1.D04 04/01/31 08:14:34
Sample          :
ID              :
Dilution Factor: 1
Type            : Unknown
Detector        : FID
Operator        :

*** Chromatogram ***  Filename:@CHRM1.C04
```



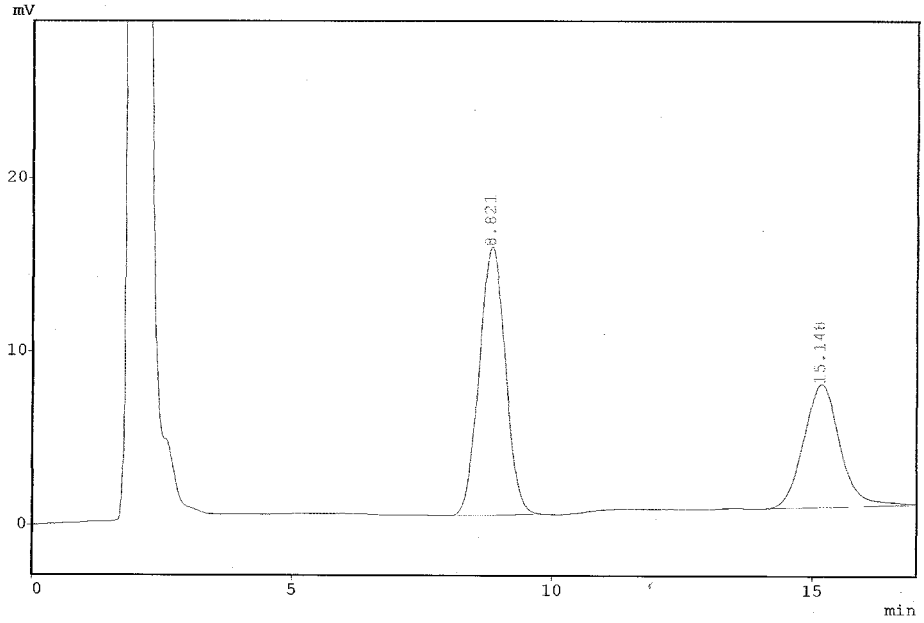

```
*** Peak Report ***
PKNO   TIME       AREA        HEIGHT   MK  IDNO     CONC         NAME
   1   8.740       870781       25029                72.4038
   2  15.048       331892        6934                27.5962
-------------------------------------------------------------------------------
                  1202673       31963               100.0000
```

Conc. of Styrene oxide / Conc. of PhBr = 0.38

B) 75 mg of Styrene oxide + 75 mg of PhBr in 10 ml Ether.

```
CLASS-GC10 Ver.=1.62  SYS=1 Ch=1 REPORT.NO=2  DATA=ST75R.D13 04/01/25 10:32:44
Sample          :
ID              :
Dilution Factor: 1
Type            : Unknown
Detector        : FID
Operator        :

*** Chromatogram ***  Filename:@CHRM1.C13
```



*** Peak Report ***

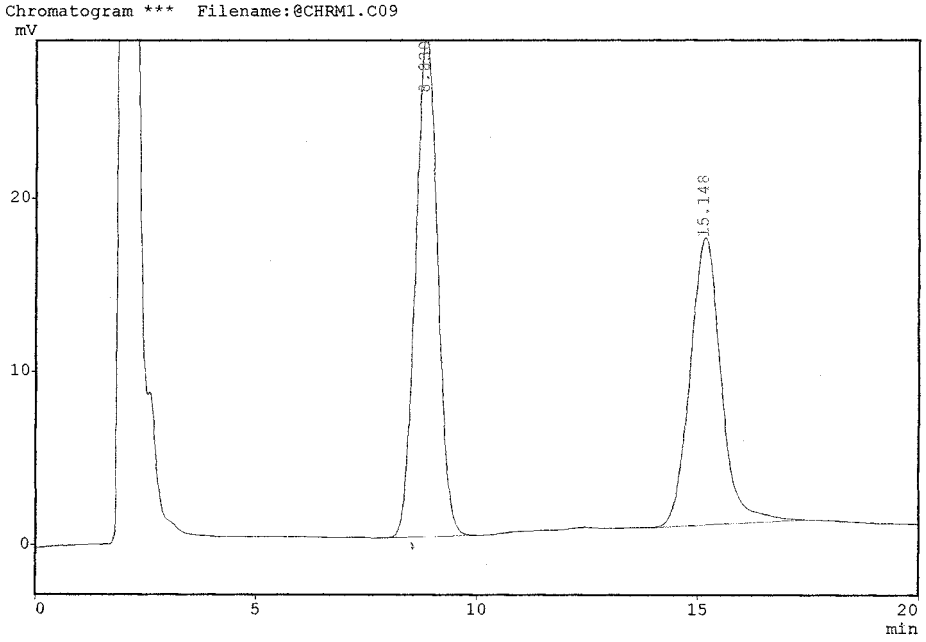
PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	8.821	541841	15468			61.1485	
2	15.148	344266	7078			38.8515	
		886107	22545			100.0000	

Conc. of Styrene oxide / Conc. of PhBr = 0.57

C) 100 mg of Styrene oxide + 75 mg of PhBr in 10 ml Ether.

```
CLASS-GC10 Ver.=1.62  SYS=1 Ch=1 REPORT.NO=6  DATA=ST100.D09 04/01/25 08:37:42
Sample          :
ID              :
Dilution Factor: 1
Type            : Unknown
Detector        : FID
Operator        :

*** Chromatogram ***  Filename:@CHRM1.C09
```



*** Peak Report ***

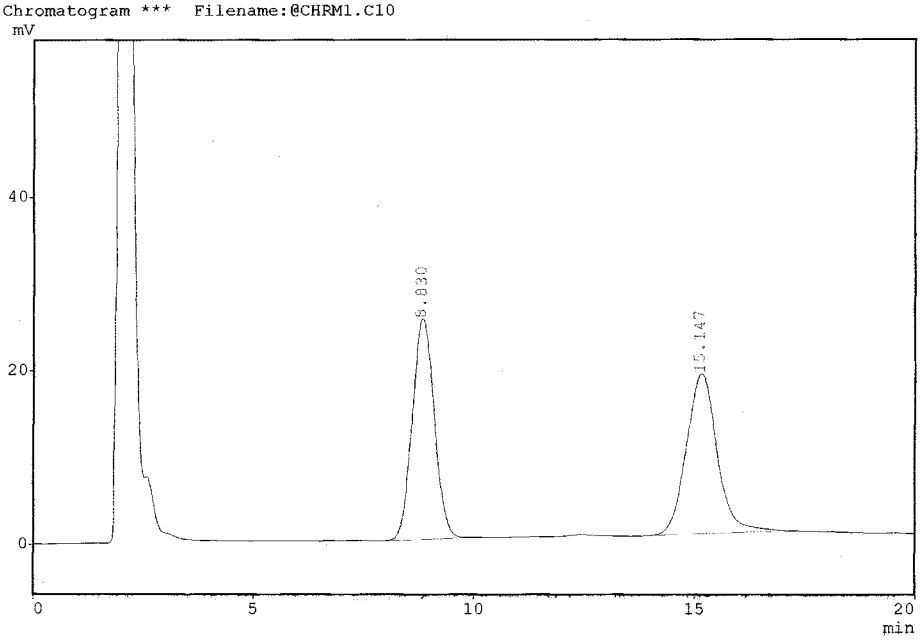
PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	8.830	1006086	28877			55.5075	
2	15.148	806437	16536			44.4925	
		1812523	45413			100.0000	

Conc. of Styrene oxide / Conc. of PhBr = 0.80

D) 125 mg of Styrene oxide + 75 mg of PhBr in 10 ml Ether.

```
CLASS-GC10 Ver.=1.62  SYS=1 Ch=1 REPORT.NO=5  DATA=ST125.D10 04/01/25 09:10:04
Sample          :
ID              :
Dilution Factor: 1
Type            : Unknown
Detector        : FID
Operator        :

*** Chromatogram ***  Filename:@CHRM1.C10
```




```
*** Peak Report ***
PKNO   TIME       AREA        HEIGHT   MK  IDNO      CONC          NAME
   1   8.830       883977       25428                  49.6549
   2  15.147       896266       18427                  50.3451
-------------------------------------------------------------------------------
                  1780243       43855                 100.0000
```

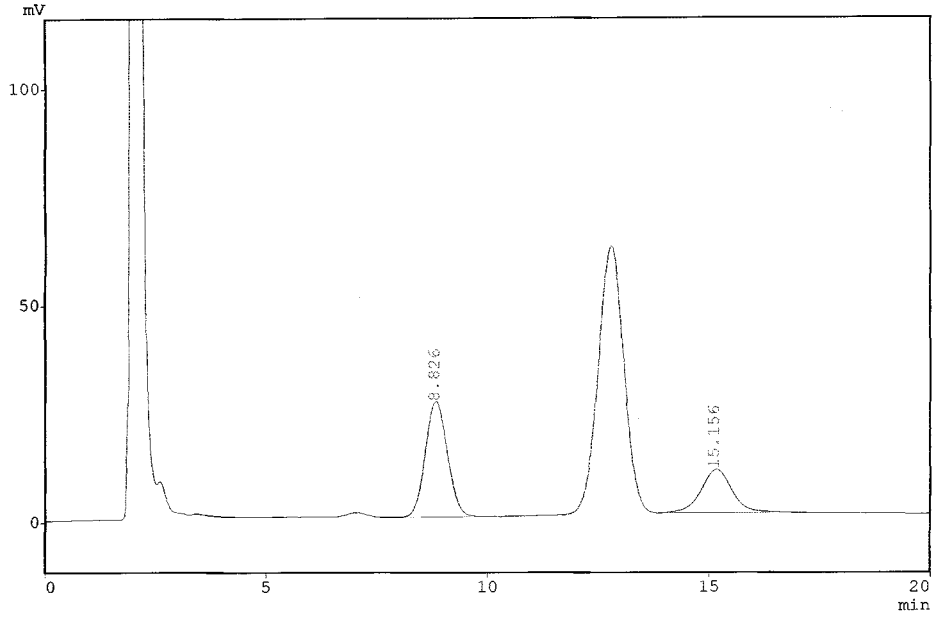
Conc. of Styrene oxide / Conc. of PhBr = 1.01

GAS CHROMATOGRAM OF EPOXIDATION PRODUCT

Reaction product (**Unknown concentration of styrene oxide**) + 75 mg PhBr in 10 ml Ether.

```
CLASS-GC10 Ver.=1.62  SYS=1 Ch=1 REPORT.NO=10 DATA=STSTA2.D07 04/01/25 07:41:26
Sample          :
ID              :
Dilution Factor: 1
Type            : Unknown
Detector        : FID
Operator        :

*** Chromatogram ***  Filename:@CHRM1.C07
```



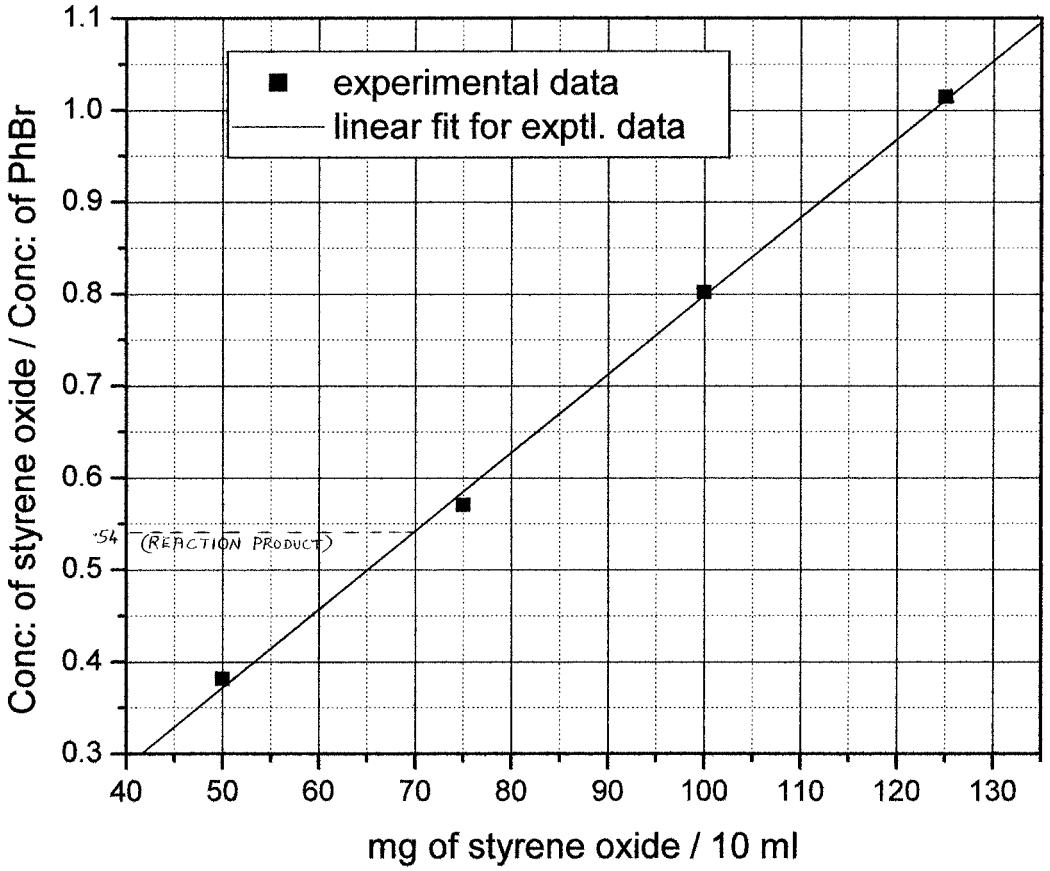

```
*** Peak Report ***
PKNO   TIME       AREA        HEIGHT   MK  IDNO      CONC          NAME
   1   8.826        922975       26552                  65.0001
   2  15.156        496985       10000                  34.9999
-------------------------------------------------------------------------------
                   1419960       36552                 100.0000
```

Conc. of Styrene oxide / Conc. of PhBr = 0.54

Supplementary Material (ESI) for New Journal of Chemistry

LINEAR FIT OF STANDARD DATA TO FIND OUT UNKNOWN CONCENTRATION OF STYRENE OXIDE.

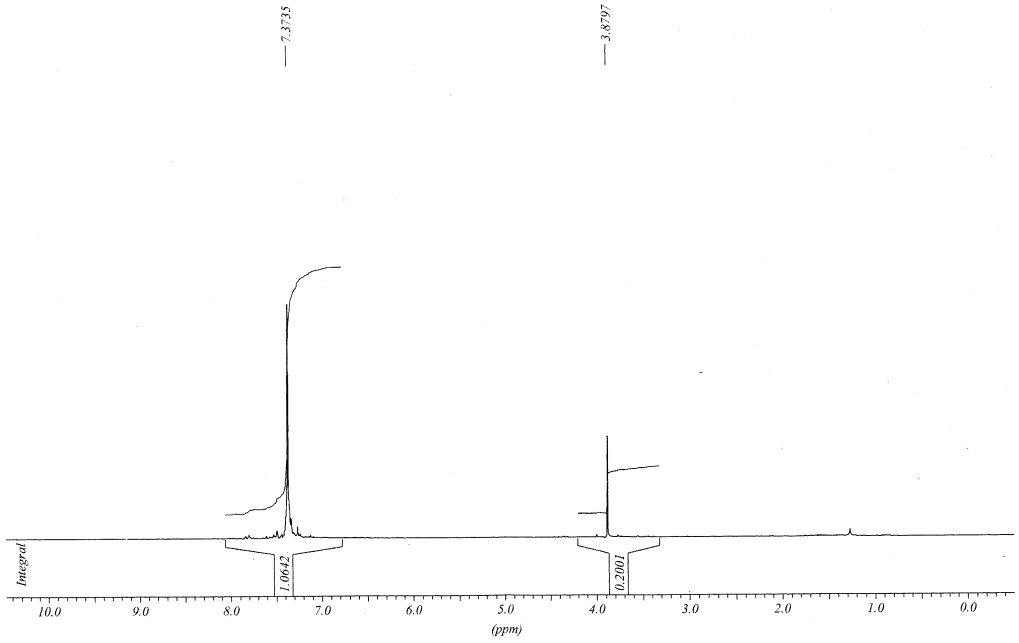
[CALIBRATION PLOT]



From the calibration plot, the concentration of styrene oxide formed in the reaction of styrene with PhIO, catalyzed by [$Mn^{IV}L_2$] 1 was found to be 70 mg.

Supplementary Material (ESI) for New Journal of Chemistry

NMR Spectrum of (E)-Stilbene oxide isolated from the reaction of (E)-Stilbene with iodosobenzene catalyzed by 1 in MeCN



This spectrum (in $CDCl_3$) shows $\delta \sim 3.85$, which is characteristics of (E)-stilbene oxide as reported earlier (reference 7 in the paper).