

### Chemical Information:

Name: 1,2-Propanediol, 3-mercapto-  
CAS No.: 96-27-5 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_202881 Lot No.: BCBF0682V  
NTP\_CID No.: 6315 MW: 108.16 g/mol

Date of Analysis: 16 December 2016

### Purity and Identity Results:

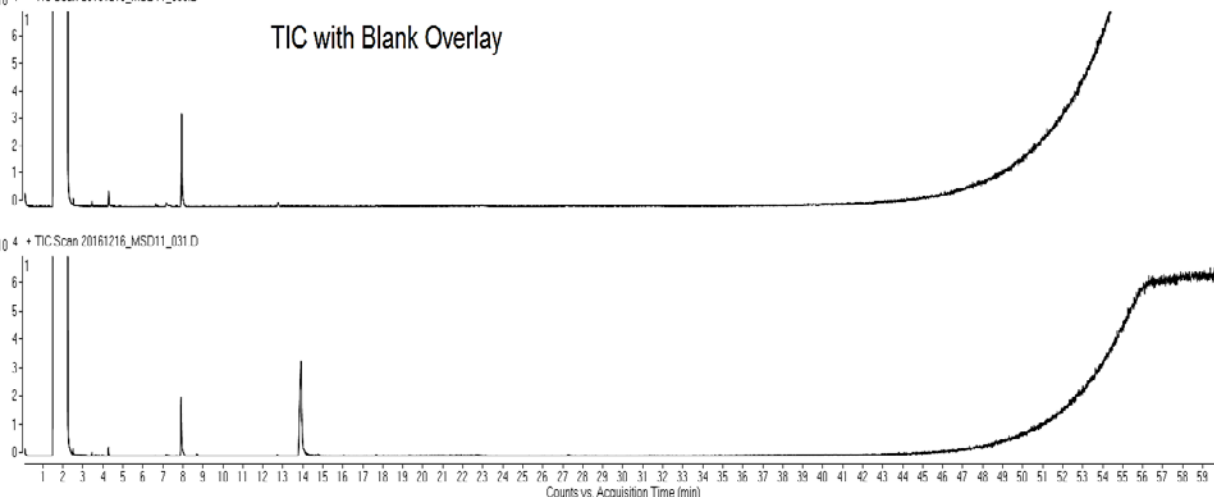
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
1,2-Propanediol, 3-mercapto-	13.91	100.00

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

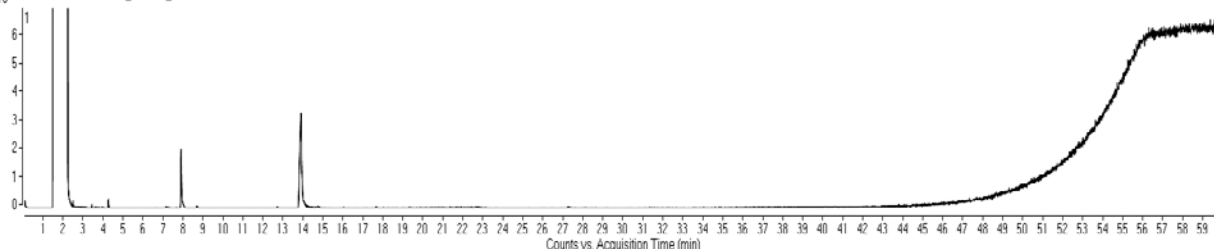
### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- $\mu$ m film thickness
Carrier Gas	Helium at 1.5 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 315°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	50 – 400 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Splitless
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / MassHunter Qualitative Analysis B.07.00 Build 7.0.7024.0 / NIST Library Version 2.2f Build 2014

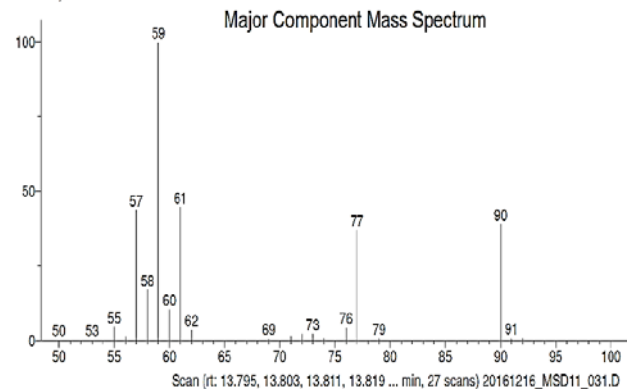
x10 4 + TIC Scan 20161216\_MSD11\_003.D



x10 4 + TIC Scan 20161216\_MSD11\_031.D



Unknown; InLib=168



Hit 1 : Monothiolglycerol

C3H8O2S; MF: 841; RMF: 841; Prob 93.3%; CAS: 96-27-5; Lib: mainlib; ID: 26219.

