

Chemical Information:

Name: Methylene bis(thiocyanate) Date of Analysis: 30 August 2007
CAS No.: 6317-18-6 Supplier: Tenneco (via Albright & Wilson Inc)
Tox21_ID No.: Tox21_202325 Lot No.: 2908
NTP_CID No.: 966 MW: 130.19 g/mol

Purity and Identity Results:

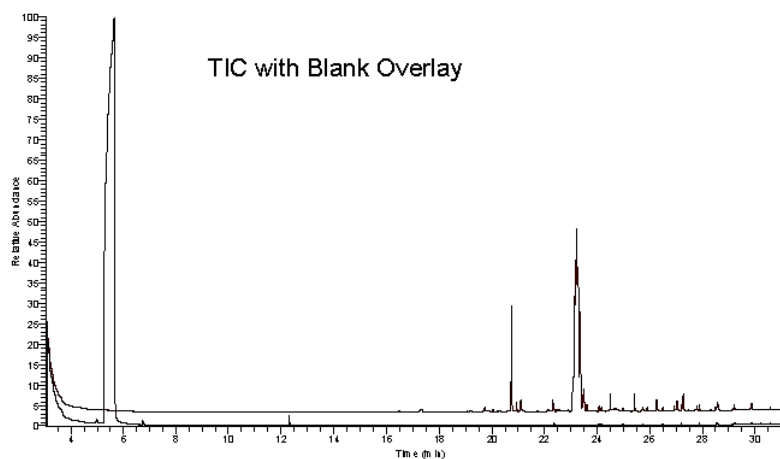
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.66	Not applicable
Methylene bis(thiocyanate)	12.29	100.00

^a Peaks comprising $\geq 0.5\%$ of total area.

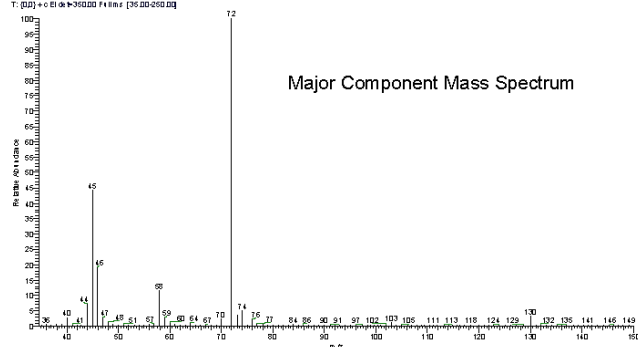
GC/MS Instrument Parameters:

Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- μ m film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	35 – 250 amu
Injector Temperature	250°C
Injection Volume / Mode	2 μ L / Splitless
Run Time	31.5 minutes
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 1.7, build 11/5/1999

RT: 3.05 - 31.50 SM: 3G



DTA2003 #2431 RT: 12.29 AUC: 1 MUL: 7.3285
T: (0.0) + c01 d1-315020 F1 m1 f [35.00-250.00]



NIST Reference
Mass Spectrum

