

Chemical Information:

Name: Hexachloro-1,3-butadiene
CAS No.: 87-68-3 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201725 Lot No.: 10207MC
NTP_CID No.: 846 MW: 260.76 g/mol

Date of Analysis: 26 June 2007

Purity and Identity Results:

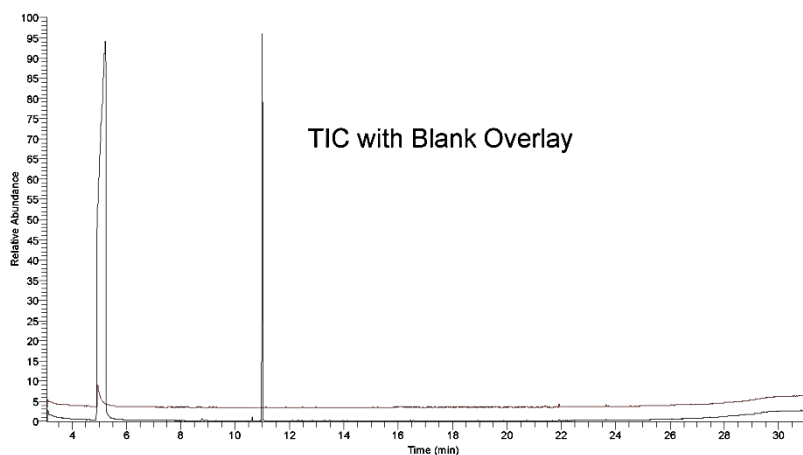
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.23	Not applicable
unknown	8.78	0.78
unknown	10.63	0.98
Hexachloro-1,3-butadiene	11.00	97.12

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

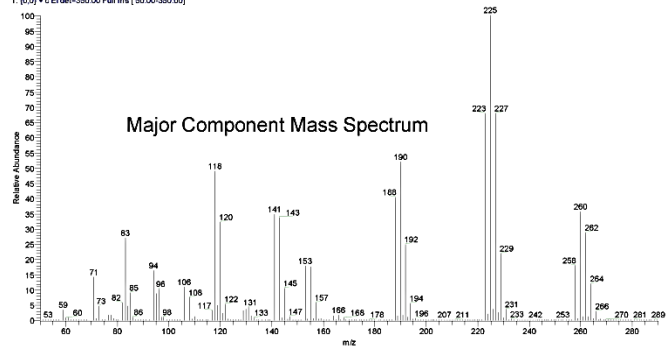
GC/MS Instrument Parameters:

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	50 – 350 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 - 31.49 SM 3G



07/26/15 #960 RT: 11.00 Av: 1 NL: 3.01E6
T: (0.0) * c: El det=350.00 Full ms [50.00-350.00]



NIST Reference Mass Spectrum

