

Chemical Information:

Name: Benzyl sulfide
CAS No.: 538-74-9
Tox21_ID No.: Tox21_200326
NTP_CID No.: 540

Supplier: Sigma-Aldrich
Lot No.: 10304KN
MW: 214.33 g/mol

Date of Analysis: 19 April 2007

Purity and Identity Results:

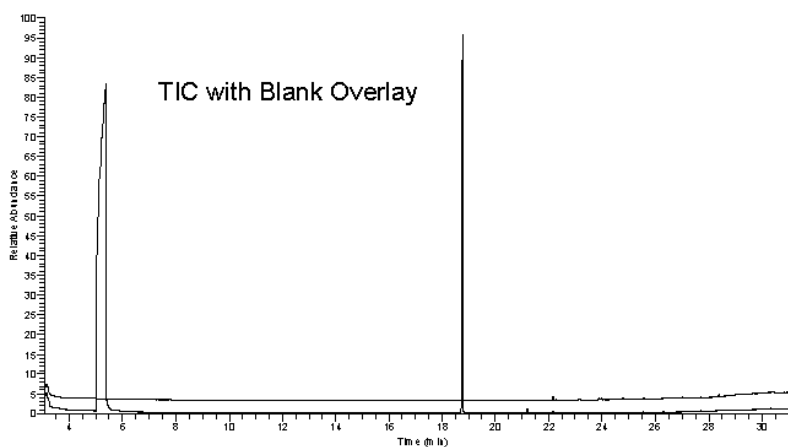
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.38	Not applicable
Benzyl sulfide	18.76	98.98
Unknown	21.20	1.02

^a Peaks comprising ≥ 0.5% of total area.

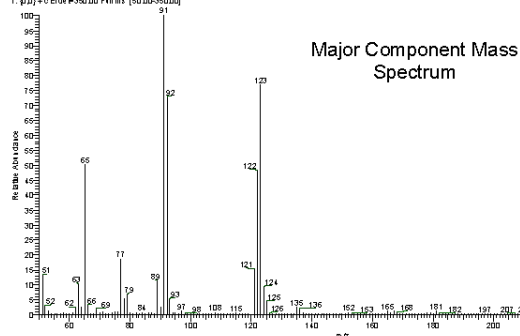
GC/MS Instrument Parameters:

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-μm 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 μL / 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 - 31.47 SM: 3G



07d1916 #1891 RT: 18.76 AC: 1 NL: 3.6466
T: (p2) +o Elide 350.00 F11111 (50.00-350.00)



NIST Reference Mass Spectrum

