

Chemical Information:

Name: Benzothiazole
CAS No.: 95-16-9
Tox21_ID No.: Tox21_201853
NTP_CID No.: 530

Supplier: Sigma-Aldrich
Lot No.: 03811KC
MW: 135.19 g/mol

Date of Analysis: 27 March 2007

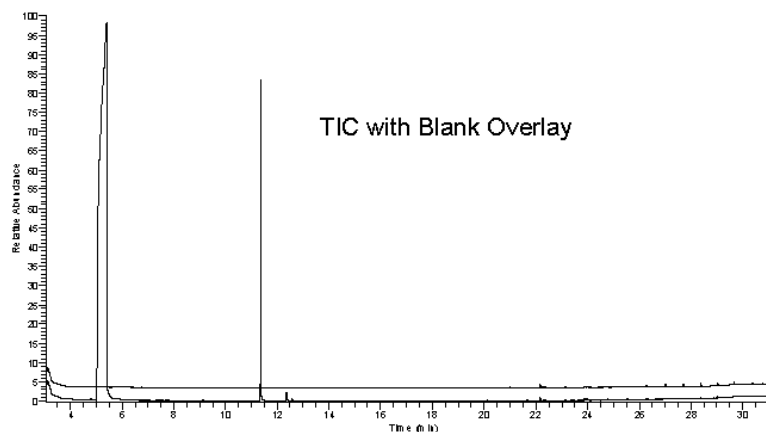
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.40	Not applicable
Benzothiazole	11.36	97.56
unknown	12.36	2.44

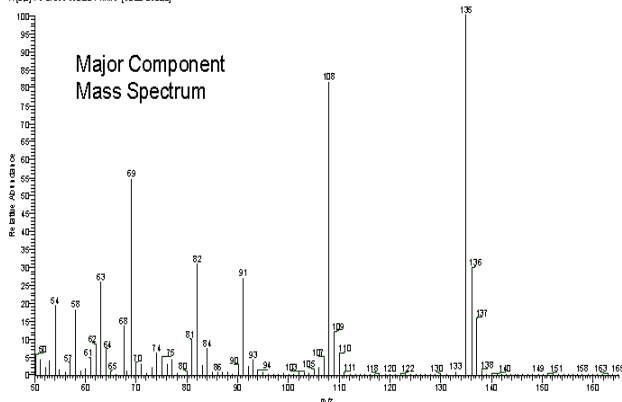
^a Peaks comprising $\geq 0.5\%$ of total area.

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 – 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



Major Component Mass Spectrum



NIST Reference Mass Spectrum

