

Chemical Information:

Name: 2-Octyl-3-isothiazolone
CAS No.: 26530-20-1 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201459 Lot No.: 2172X
NTP_CID No.: 280 MW: 213.34 g/mol

Date of Analysis: 05 October 2007

Purity and Identity Results:

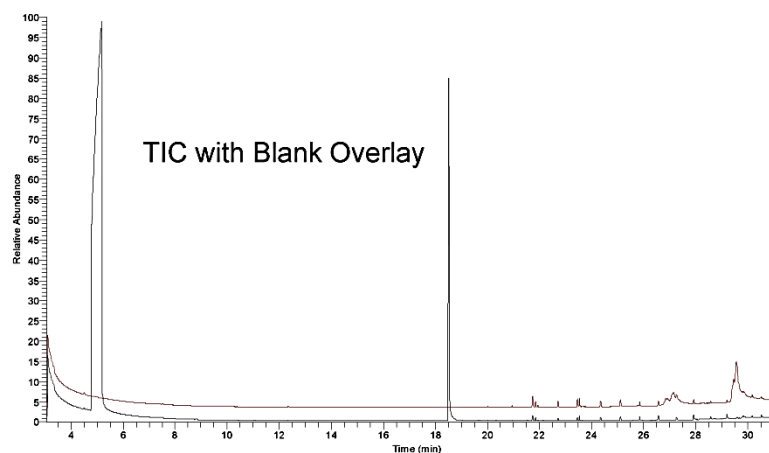
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.18	Not applicable
2-Octyl-3-isothiazolone	18.51	99.77

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

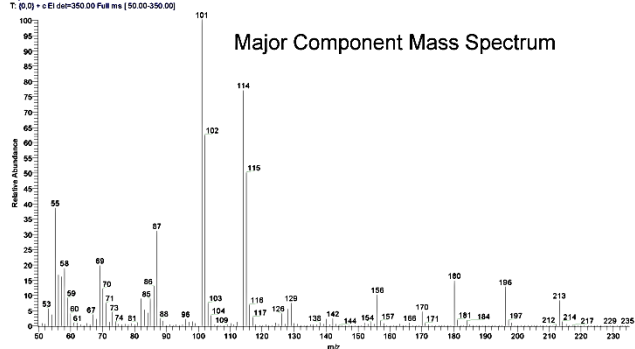
GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph / Mass Spectrometer / 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

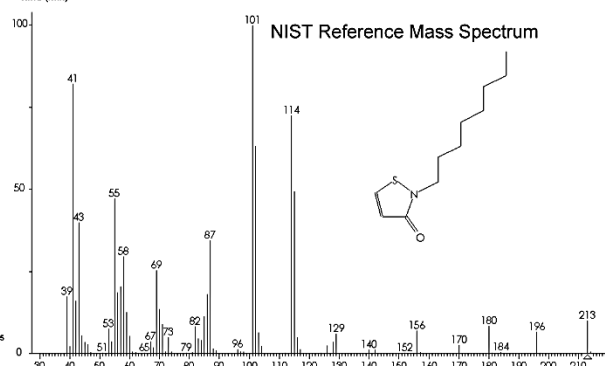
RT: 3.05 - 31.50 SM: 3G



07/05/09 #1850 RT: 18.50 AU: 1 NL: 2.5305
T: (0.0) + e El det=350.00 Full ms [50.00-350.00]



Major Component Mass Spectrum



NIST Reference Mass Spectrum

