

### Chemical Information:

Name: 2-Bromobenzothiazole  
CAS No.: 2516-40-7  
Tox21\_ID No.: Tox21\_202134  
NTP\_CID No.: 4940

Date of Analysis: 13 October 2009

Supplier: Sigma-Aldrich  
Lot No.: 03703JJ  
MW: 214.08 g/mol

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	13.28	1.86
2-Bromobenzothiazole	14.70	96.28
unknown	17.27	0.97
unknown	18.04	0.89

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol (~ 1 mg/mL)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- $\mu$ 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 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Split (100:1)
Data Analysis Software	Xcalibur, ver 1.2 and NIST Library ver 2.0f, build 10/08/2008

