

### Chemical Information:

Name: Thiocarbanilide  
CAS No.: 102-08-9  
Tox21\_ID No.: Tox21\_200269  
NTP\_CID No.: 1345

Supplier: Sigma Aldrich  
Lot No.: 12814PE  
MW: 228.31 g/mol

Date of Analysis: 10 December 2009

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	17.5	2.8
Thiocarbanilide	19.0	97.2

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

### LC/MS Instrument Parameters:

Instrument / Ionization	Micromass Quattro II with Shimadzu HPLC / ESI+
Solvent	Methanol
Column	Grace HP C18-AQ, 5 $\mu$ m, 250 mm x 2.1 mm ID
Injection Volume	20 $\mu$ L
Mobile Phase	95/5 (A) and 5/95 (B) Water/acetonitrile 2 mM ammonium formate, pH 3; acetonitrile (C)
Program / Flow Rate	100/0/0 A/B/C for 1 minute; 5/95/0 at 20 minutes, hold 2 minutes; 0/0/100 at 25 minutes, hold 3 minutes / 0.2 mL/minute
Cone / Capillary	25 V / 3.0 kV
Source Temperature	125°C
Desolve Temperature	325°C
Scan Range	100 – 1100 amu
Acquisition Software	MassLynx, v 4.0

