

### Chemical Information:

Name:	2-Nitro-4-thiocyananiline	Dates of Analysis:
CAS No.:	54029-45-7	Supplier: Sigma-Aldrich
Tox21_ID No.:	Tox21_202844	Lot No.: 04519LE
NTP_CID No.:	6222	MW: 195.20 g/mol
		LC/UV: 31 March 2017
		LC/MS: 10 January 2017

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Unknown	6.69	1.22
2-Nitro-4-thiocyananiline	7.55	83.71
Unknown	27.13	14.12

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

### Instrument Parameters:

Instrument / Ionization	Shimadzu UPLC; Micromass Quattro II / ESI+
Solvent	Methanol
Column	Grace Alltima C18, 5 $\mu$ m, 250 mm x 4.6 mm ID
Injection Volume / Detection	10 $\mu$ L / 225 nm
Mobile Phase	Water (A) / Acetonitrile (B)
Program / Flow Rate	50/50 A/B for 40 minutes; 0/100 in 10 minutes, hold 10 minutes; 50/50 for 15 minutes / 1.0 mL/minute
Cone / Corona	50 V / 3.0 kV
Source Temperature	125°C
Probe Temperature	350°C
Scan Range	20 – 1300 amu
Acquisition Software	LC/UV – LabSolutions, v 5.71.SP1; LC/MS – MassLynx 4.0

