

Chemical Information:

Name: 4-Nitro-1,3-benzenediamine
CAS No.: 5131-58-8
Tox21_ID No.: Tox21_200992
NTP_CID No.: 387

Date of Analysis: 29 April 2009

Supplier: Sigma Aldrich
Lot No.: S110305KB-4
MW: 153.14 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
4-Nitro-1,3-benzenediamine	13.71	95.2
unknown	17.32	4.8

^a Peaks comprising ≥ 0.5% of total area.

LC/MS Instrument Parameters:

Instrument / Ionization	Micromass Quattro II with Shimadzu HPLC / APCI+
Solvent	Methanol
Column	Grace HP C18-AQ, 5 µm, 250 mm x 4.6 mm ID
Injection Volume	50 µL
Mobile Phase	Water (A) / methanol (B)
Program / Flow Rate	95/5 A/B for 1 minute; 10/90 in 20 minutes, hold 0.1 minute / 1 mL/minute
Cone / Corona	25 V / 2.5 kV
Source Temperature	125°C
Probe Temperature	300°C
Scan Range	85 – 750 amu
Acquisition Software	MassLynx, v 4.0

