

### Chemical Information:

Name: Hexamethyl-p-rosaniline chloride (Gentian violet) Date of Analysis: 26 January 2010  
CAS No.: 548-62-9 Supplier: Sigma Aldrich  
Tox21\_ID No.: Tox21\_201762 Lot No.: 015K1229  
NTP\_CID No.: 851 MW: 407.98 g/mol

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Gentian violet	18.3	100

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

### LC/MS Instrument Parameters:

Instrument / Ionization	Micromass Quattro II with Shimadzu HPLC / ESI+
Solvent	Methanol
Column	Phenomenex Luna, 3 µm Phenyl-Hexyl, 150 mm x 2.0 mm ID
Injection Volume	20 µL
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 – 1200 amu
Acquisition Software	MassLynx, v 4.0

