

### Chemical Information:

Name: Ferrocene

CAS No.: 102-54-5

Tox21\_ID No.: Tox21\_202514

NTP\_CID No.: 806

Supplier: Sigma-Aldrich

Lot No.: 11224LC

MW: 186.03 g/mol

Dates of Analysis:

LC/UV: 25 January 2017

LC/MS: 05 January 2017

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Ferrocene	34.77	100.00

<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

