

Chemical Information:

Name: 1,2-Benzenedicarboxylic acid, 4-sulfo-
CAS No.: 89-08-7 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_202553 Lot No.: 02397LJ
NTP_CID No.: 2568 MW: 246.19 g/mol

Dates of Analysis:
LC/UV: 31 March 2017
LC/MS: 10 January 2017

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
1,2-Benzenedicarboxylic acid, 4-sulfo-	1.67	99.95

^a Peaks comprising ≥ 0.5% of total area.

Instrument Parameters:

Instrument / Ionization	Shimadzu UPLC; Micromass Quattro II / ESI-
Solvent	Methanol
Column	Grace Alltima C18, 5 µm, 250 mm x 4.6 mm ID
Injection Volume / Detection	10 µL / 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

