

Chemical Information:

Name: Terephthalic acid
CAS No.: 100-21-0
Tox21_ID No.: Tox21_201659
NTP_CID No.: 1320

Supplier: Sigma Aldrich
Lot No.: 16525LB
MW: 166.13 g/mol

Date of Analysis: 29 March 2010

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Terephthalic acid	16.3	100

^a Peaks comprising ≥ 0.5% of total area.

LC/MS Instrument Parameters:

Instrument / Ionization	Micromass Quattro II with Shimadzu HPLC / ESI-
Solvent	Methanol
Column	Grace HP C18-AQ, 5 µm, 250 mm x 2.1 mm ID
Injection Volume	20 µL
Mobile Phase	95/5/0.1% (A) and 5/95/0.1% (B) Water/acetonitrile/acetic acid; acetonitrile (C)
Program / Flow Rate	100/0/0 A/B/C for 1 min; 0/100/0 at 35 min, hold 2 min; 0/0/100 at 37.1 min, hold 3 min; 100/0/0 at 40 min, hold 5 min / 0.2 mL/min
Cone / Capillary	25 V / 3.5 kV
Source Temperature	125°C
Desolve Temperature	325°C
Scan Range	100 – 1200 amu
Acquisition Software	MassLynx, v 4.0

