

### Chemical Information:

Name: Tributoxyethyl phosphate  
CAS No.: 78-51-3 Supplier: Sigma Aldrich  
Tox21\_ID No.: Tox21\_201593 Lot No.: 09901EW  
NTP\_CID No.: 1364 MW: 398.47 g/mol

Date of Analysis: 10 May 2010

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>	Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	21.80	0.68	unknown	29.90	1.20
unknown	22.54	0.79	Tributoxyethyl phosphate	35.07	96.87

<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	Grace HP C18-AQ, 5 µm, 250 mm x 2.1 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 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 / 3.0 kV
Source Temperature	125°C
Desolve Temperature	325°C
Scan Range	65 – 1100 amu
Acquisition Software	MassLynx, v 4.0

