

### Chemical Information:

Name: 1-Propanaminium, 3-chloro-2-hydroxy-N,N,N-trimethyl-, chloride  
 CAS No.: 3327-22-8 Supplier: Pfaltz & Bauer Dates of Analysis:  
 Tox21\_ID No.: Tox21\_202563 Lot No.: 789 LC/UV: 31 March 2017  
 NTP\_CID No.: 3047 MW: 188.10 g/mol LC/MS: 20 January 2017

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	1.30	7.52
unknown	1.39	4.29
1-Propanaminium, 3-chloro-2-hydroxy-N,N,N-trimethyl-, chloride	3.21	79.88
unknown	3.50	6.44
unknown	8.17	1.86

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

### Instrument Parameters:

Instrument / Ionization	Shimadzu UPLC; Micromass Quattro II / ESI+
Solvent	Water
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 – 1280 amu
Acquisition Software	LC/UV – LabSolutions, v 5.71.SP1 LC/MS – MassLynx 4.0

