

Chemical Information:

Name: Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, chloride
 CAS No.: 5039-78-1 Supplier: Sigma-Aldrich Dates of Analysis:
 Tox21_ID No.: Tox21_202564 Lot No.: MKBC8910 LC/UV: 31 March 2017
 NTP_CID No.: 3087 MW: 207.70 g/mol LC/MS: 20 January 2017

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	1.73	23.21
unknown	2.21	2.06
Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, chloride	3.13	65.92
unknown	4.28	5.62
unknown	6.63	2.88

^a 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

