

Chemical Information:

Name: 3-Cyclobutene-1,2-dione, 3,4-dihydroxy-
CAS No.: 2892-51-5 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_202819 Lot No.: MKBG2633V
NTP_CID No.: 6144 MW: 114.06 g/mol

Dates of Analysis:

LC/UV: 31 March 2017

LC/MS: 24 January 2017

Purity and Identity Results:

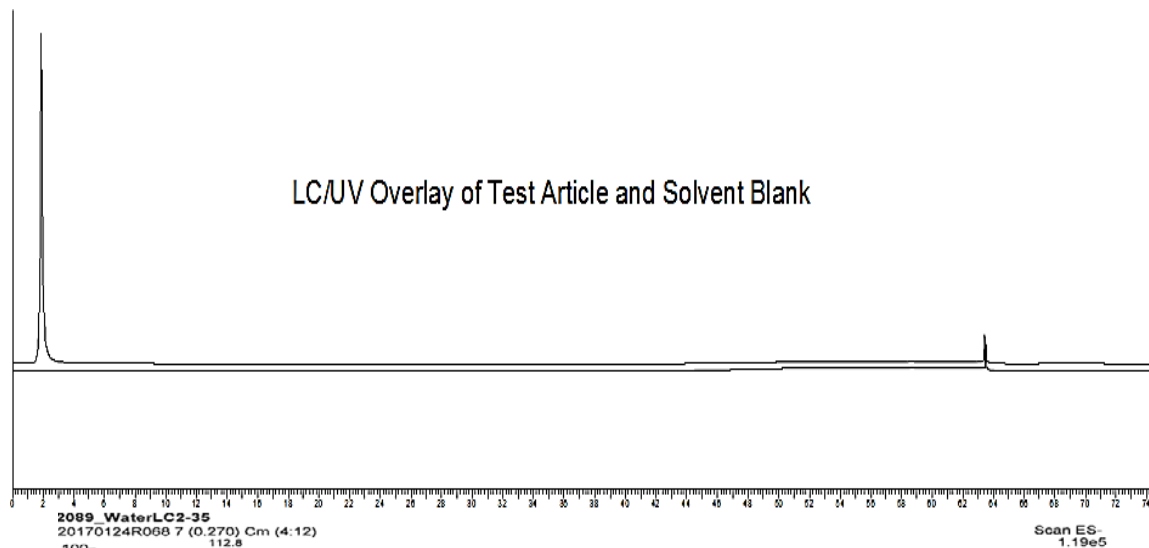
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
3-Cyclobutene-1,2-dione, 3,4-dihydroxy-	1.88	100.00

^a Peaks comprising $\geq 0.5\%$ of total area.

Instrument Parameters:

Instrument / Ionization	Shimadzu UPLC; Micromass Quattro II / ESI-
Solvent	Water
Column	Grace Alltima C18, 5 μ m, 250 mm x 4.6 mm ID
Injection Volume / Detection	10 μ L / 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 – 720 amu
Acquisition Software	LC/UV – LabSolutions, v 5.71.SP1 LC/MS – MassLynx 4.0

LC/UV Overlay of Test Article and Solvent Blank



(M-H)-

Major Component Mass Spectrum

