

### Chemical Information:

Name: Sodium bithionolate  
CAS No.: 6385-58-6  
Tox21\_ID No.: Tox21\_202791  
NTP\_CID No.: 4740

Supplier: TCI America  
Lot No.: QYHVL  
MW: 400.02 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) <sup>a</sup>
Sodium bithionolate	37.43	89.09
Unknown	46.08	1.06
Unknown	52.17	0.87
Unknown	54.27	5.72
Unknown	56.26	1.84

<sup>a</sup> 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 $\mu$ m, 250 mm x 4.6 mm ID
Injection Volume / Detection	10 $\mu$ 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

