

### Chemical Information:

Name: Butanedioic acid, sulfo-, 1,4-bis(2-ethylhexyl) ester, sodium salt  
Date of Analysis: 15 April 2010  
CAS No.: 577-11-7 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_201342 Lot No.: 1399756  
NTP\_CID No.: 2412 MW: 444.56 g/mol

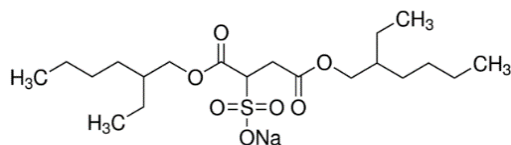
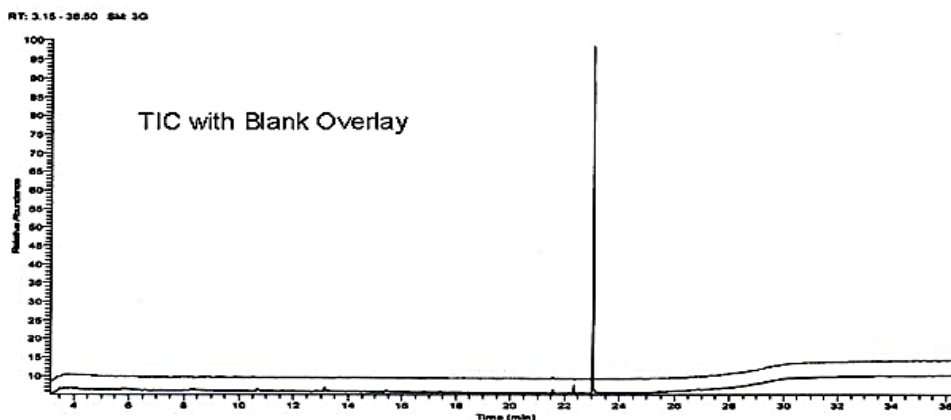
### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	22.37	2.21
Butanedioic acid, sulfo-, 1,4-bis(2-ethylhexyl) ester, sodium salt	23.04	97.79

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

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane (~ 1 mg/mL)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25-μm film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	Xcalibur ver 1.2, and NIST Library ver 2.0f, build 10/08/2008



m/z	Fragment	m/z	Fragment
211	C12H19O3	82	H2O3S
112	C8H16	71	C3H3O2
100	C6H12O	70	C3H2O2
99	C7H15	57	C4H9
85	C4H5O2	41	C2HO
83	C6H11	29	C2H5

