

### Chemical Information:

Name: Benzenesulfonic acid, C10-16-alkyl derivatives  
CAS No.: 68584-22-5  
Tox21\_ID No.: Tox21\_202760  
NTP\_CID No.: 3305

Supplier: TCI America  
Lot No.: OGL02  
MW: 326.49 g/mol

Dates of Analysis:

LC/UV: 31 March 2017

LC/MS: 20 January 2017

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	1.26	0.71
Benzenesulfonic acid, C10-16-alkyl derivatives	2.48	98.91

<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

