

### Chemical Information:

Name: Heptadecane, 1-bromo-  
CAS No.: 3508-00-7 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_202825 Lot No.: 1272422  
NTP\_CID No.: 6164 MW: 319.36 g/mol

Date of Analysis: 04 January 2017

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Unknown	31.73	0.57
Unknown	37.89	0.71
Heptadecane,1-bromo-	39.74	98.39

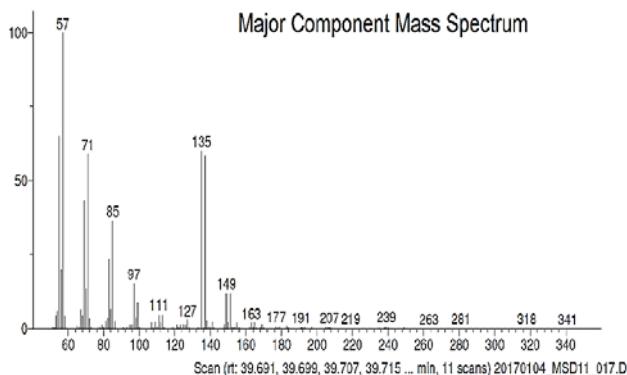
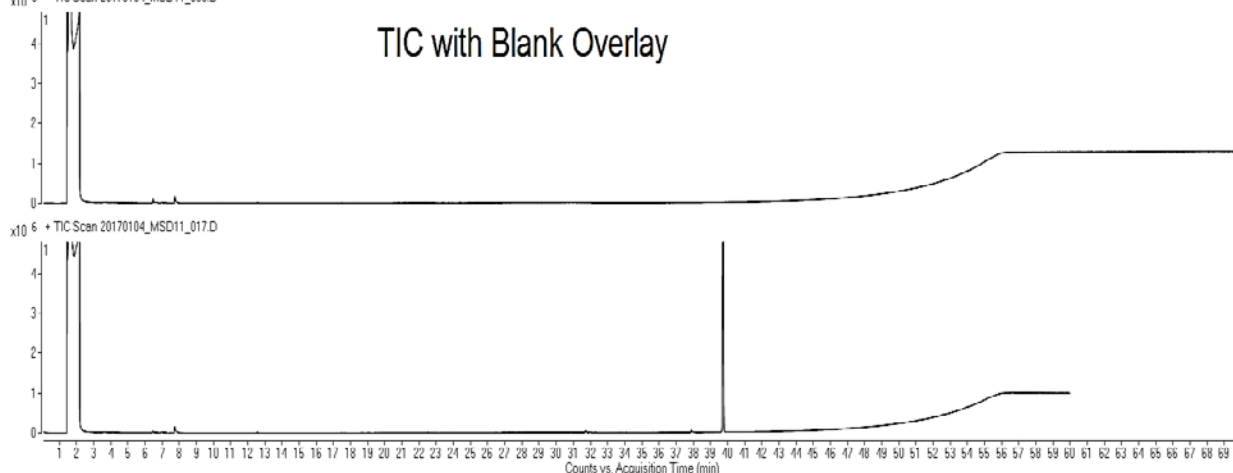
<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- $\mu$ m film thickness
Carrier Gas	Helium at 1.5 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 315°C, hold 15 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	50 – 400 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Splitless
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / MassHunter Qualitative Analysis B.07.00 Build 7.0.7024.0 / NIST Library Version 2.2f Build 2014

x10<sup>6</sup> • TIC Scan 20170104\_MSD11\_003.D

### TIC with Blank Overlay



Hit 1: Pentadecane, 1-bromo-  
C<sub>15</sub>H<sub>31</sub>Br; MF: 946; RMF: 969; Prob 35.1%; CAS: 629-72-1; Lib: mainlib; ID: 21746.

