

# Chemical Information:

Name: Benzaldehyde, 2-bromo-5-hydroxy-  
CAS No.: 2973-80-0 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_202820 Lot No.: MKBB5750  
NTP\_CID No.: 6146 MW: 201.02 g/mol

Date of Analysis: 04 January 2017

## Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Benzaldehyde, 2-bromo-5-hydroxy <sup>b</sup>	29.43	99.29

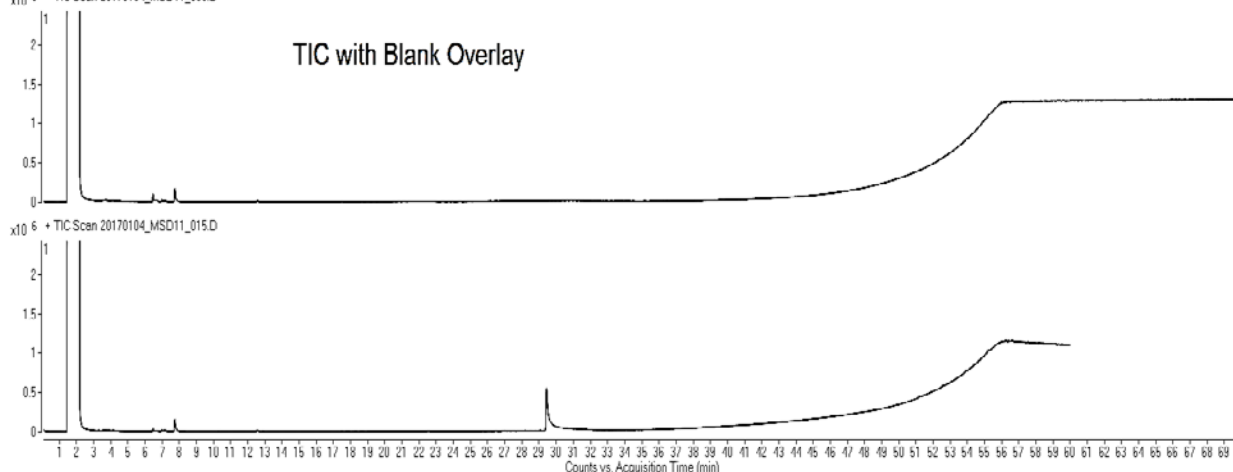
<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

<sup>b</sup> NIST reference was not available for test article; identification based on comparison to reference spectrum of benzaldehyde, 5-bromo-2-hydroxy (CAS# 1761-61-1).

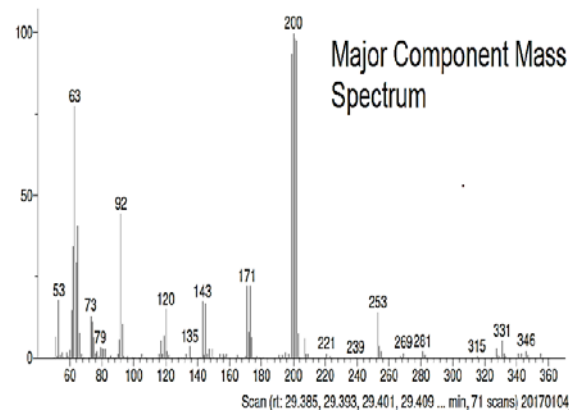
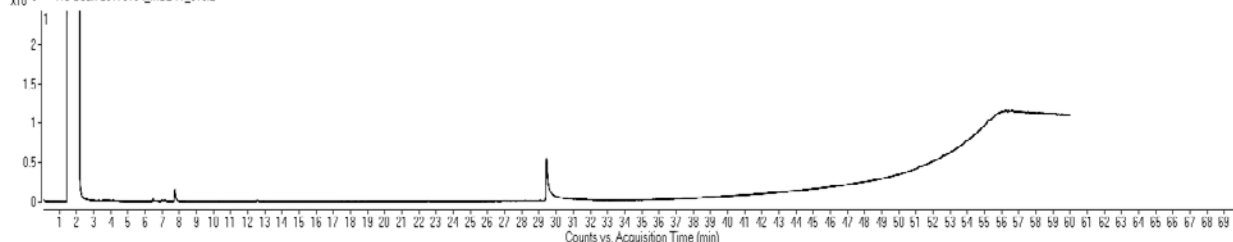
## GC/MS Instrument Parameters:

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



x10<sup>6</sup> • TIC Scan 20170104\_MSD11\_015.D



Hit 1: Benzaldehyde, 5-bromo-2-hydroxy-  
C7H5BrO2; MF: 751; RMF: 817; Prob 84.2%; CAS: 1761-61-1; Lib: replib; ID: 24323.

