

Chemical Information:

Name: 4-Nitrobenzyl bromide
CAS No.: 100-11-8
Tox21_ID No.: Tox21_202713
NTP_CID No.: 6005

Date of Analysis: 14 December 2016

Supplier: Sigma-Aldrich
Lot No.: 14225PQV
MW: 216.03 g/mol

Purity and Identity Results:

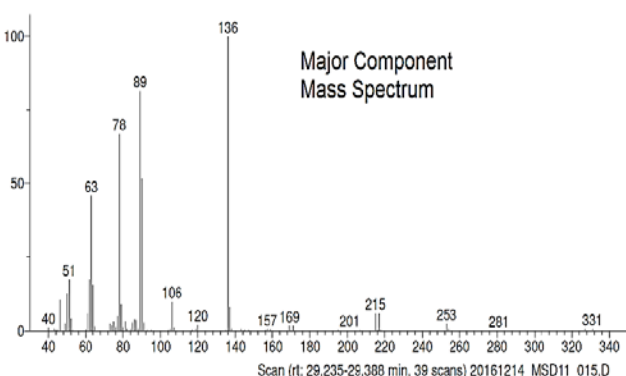
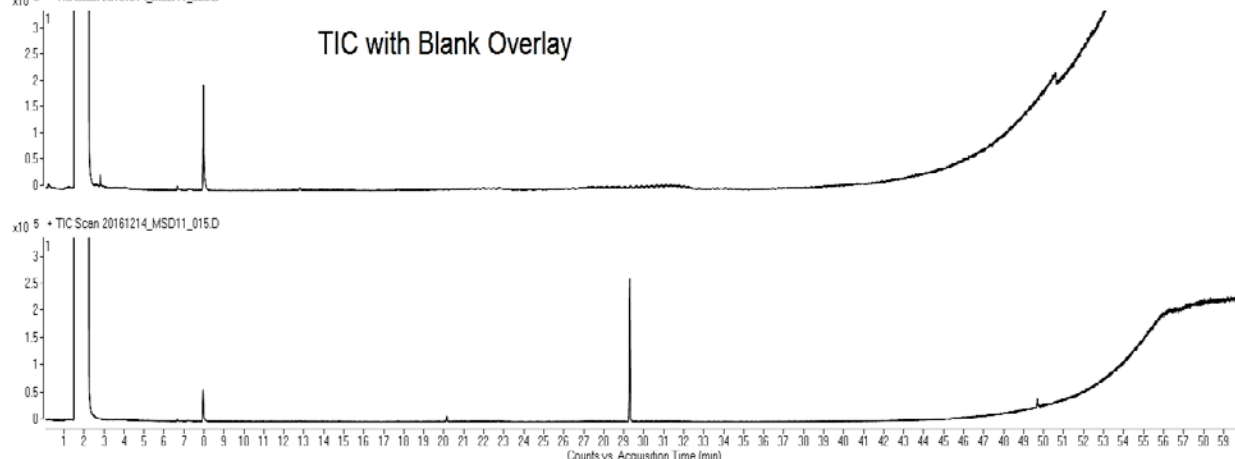
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	20.14	3.16
4-Nitrobenzyl bromide	29.30	90.02
4,4'-Dinitrobibenzyl	49.69	6.82

^a Peaks comprising ≥ 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-μm 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 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 380 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / 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

x10⁵ • TIC Scan 20161214_MSD11_003.D



Hit 1: Benzene, 1-(bromomethyl)-4-nitro-
C₇H₆BrNO₂; MF: 853; RMF: 865; Prob 75.8%; CAS: 100-11-8; Lib: replib; ID: 18532.

