

# Chemical Information:

Name: o-Nitrobenzoic acid  
CAS No.: 552-16-9  
Tox21\_ID No.: Tox21\_201020  
NTP\_CID No.: 1114

Supplier: Sigma-Aldrich  
Lot No.: 15320CE  
MW: 167.12 g/mol

Date of Analysis: 30 August 2010

# Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	10.19	1.64
o-Nitrobenzoic acid	17.13	97.91

<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
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	230°C
Auxiliary Temperature	250°C
Scan Range	15 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Splitless
Data Analysis Software	MSD ChemStation v D.03.00.SP1, and NIST Library v 2.0f, build 10/08/2008

