

Chemical Information:

Name: 2,4,6-Trichloropyrimidine
CAS No.: 3764-01-0 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_202916 Lot No.: BCBD6569V
NTP_CID No.: 6529 MW: 183.42 g/mol

Date of Analysis: 14 December 2016

Purity and Identity Results:

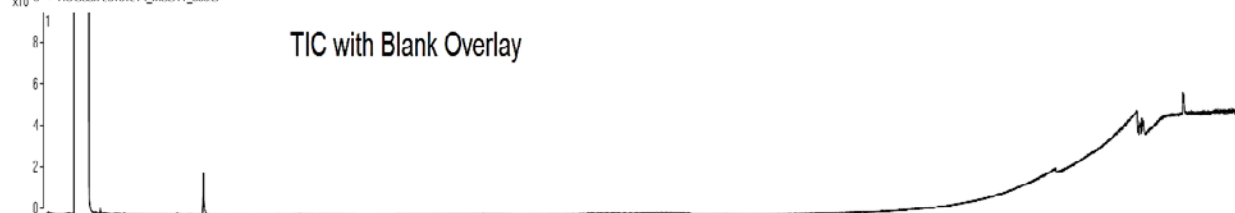
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
2,4,6-Trichloropyrimidine	18.64	99.83

^a Peaks comprising ≥ 0.5% of total area.

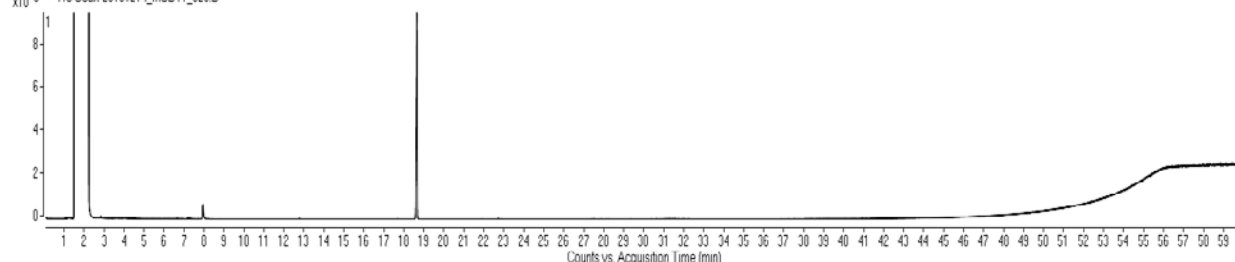
GC/MS Instrument Parameters:

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

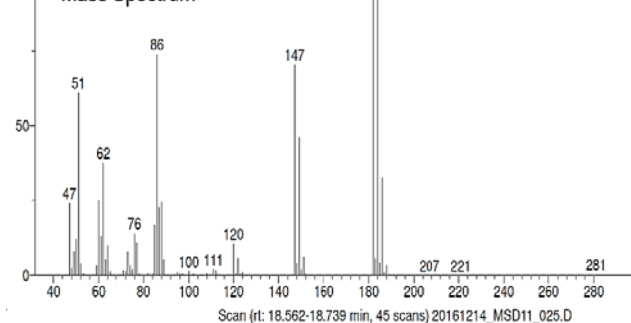
x10⁵ • TIC Scan 20161214_MSD11_003.D



x10⁵ • TIC Scan 20161214_MSD11_025.D



Major Component Mass Spectrum



Hit 1: Pyrimidine, 2,4,6-trichloro-
C4HClN2; MF: 679; RMF: 862; Prob 93.8%; CAS: 3764-01-0; Lib: replib; ID: 23138.

NIST Reference Mass Spectrum

