

Chemical Information:

Name: Butane, 1-isocyanato-
CAS No.: 111-36-4 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_200437 Lot No.: 09114KH
NTP_CID No.: 2664 MW: 99.13 g/mol

Date of Analysis: 16 April 2010

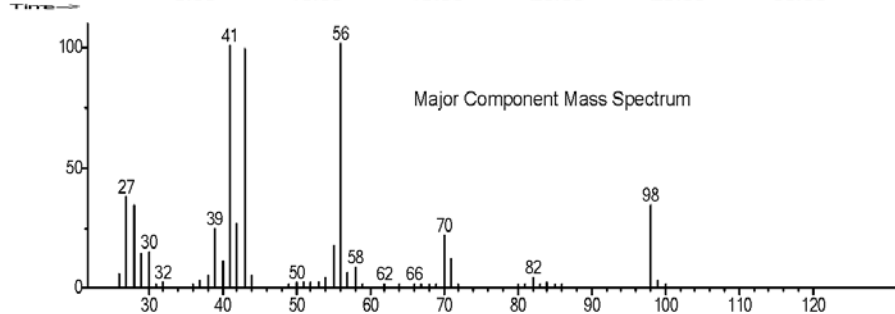
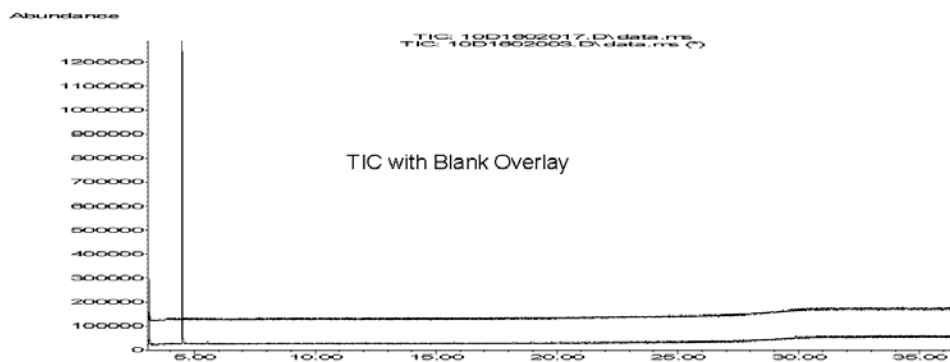
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Butane, 1-isocyanato-	4.49	100.00

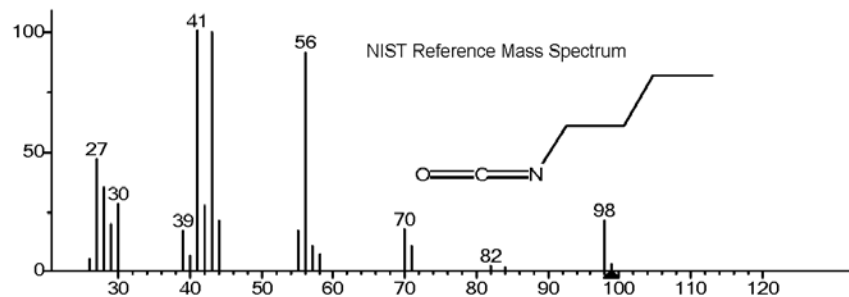
^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane (~ 1 mg/mL)
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	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	MSD ChemStation v E.02.00.SP2, and NIST Library v 2.0, build 7/23/2008



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(replib) Butane, 1-isocyanato-