

Chemical Information:

Name: Diacetone alcohol
CAS No.: 123-42-2
Tox21_ID No.: Tox21_201266
NTP_CID No.: 2434

Supplier: Sigma-Aldrich
Lot No.: 06626MH
MW: 116.16 g/mol

Date of Analysis: 29 July 2009

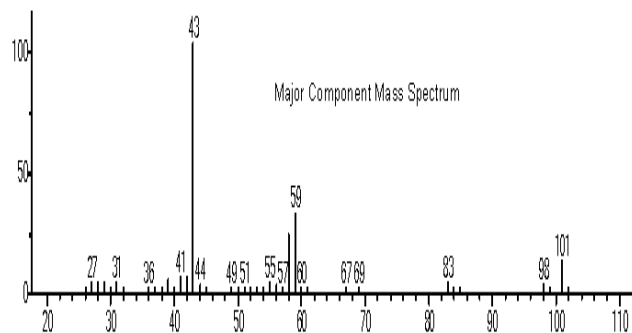
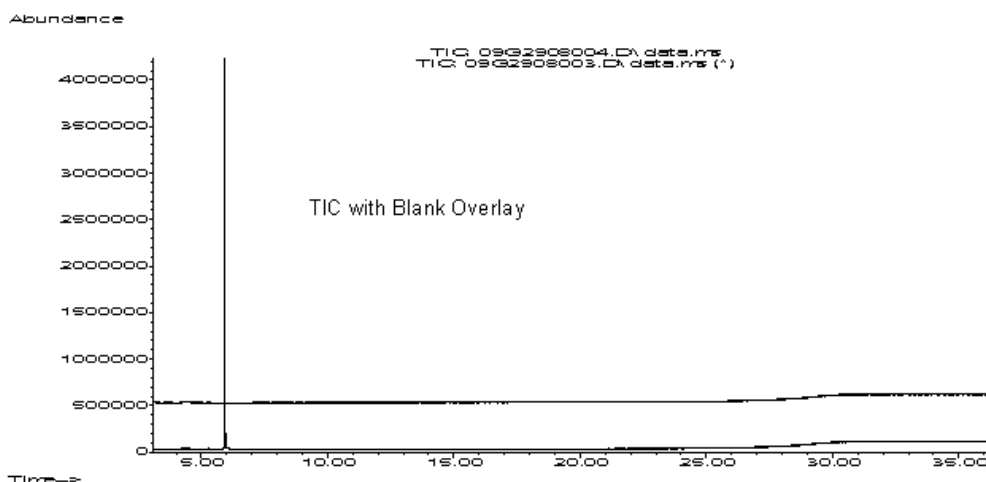
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Diacetone alcohol	5.92	100.00

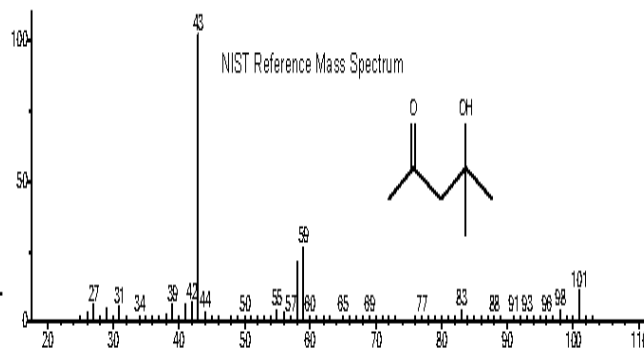
^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Chloroform (~ 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)
Run Time	36.5 minutes
Data Analysis Software	MSD ChemStation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/08/2008



(Text File) Scan 521 (5.918 min): 0962908004.D\data.ms



MW: 116 CAS# 123-42-2 (mainlib) 2-Pentanone, 4-hydroxy-4-methyl-