

### Chemical Information:

Name: Methylpyruvate  
CAS No.: 600-22-6  
Tox21\_ID No.: Tox21\_202853  
NTP\_CID No.: 6248

Supplier: Sigma Aldrich  
Lot No.: MKBD7767V  
MW: 102.09 g/mol

Date of Analysis: 21 March 2017

### Purity and Identity Results:

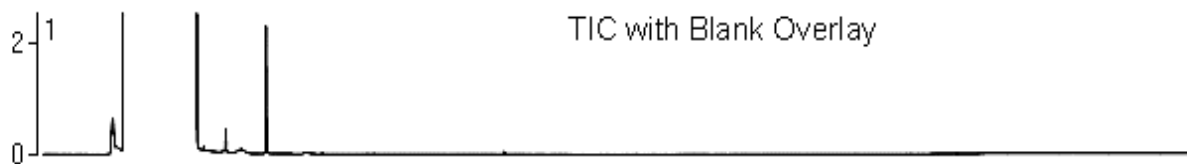
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Unknown	7.30	1.84
Methylpyruvate	8.14	98.16

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

### GC/MS Instrument Parameters:

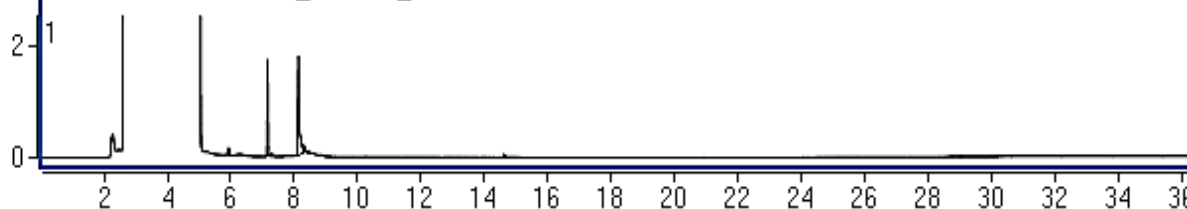
Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1- $\mu$ m film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	10 – 120 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / 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 2.2 Build 2014

x10<sup>6</sup> + TIC Scan 20170321\_MSD11\_003.D



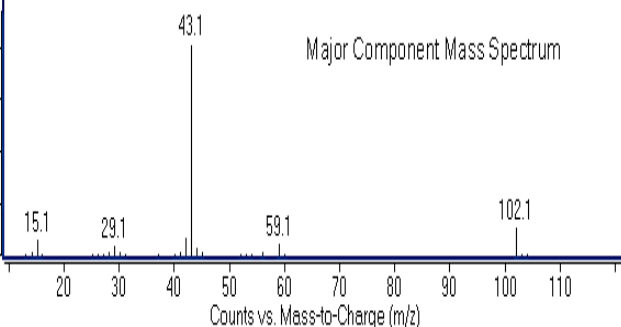
TIC with Blank Overlay

x10<sup>6</sup> + TIC Scan 20170321\_MSD11\_004.D

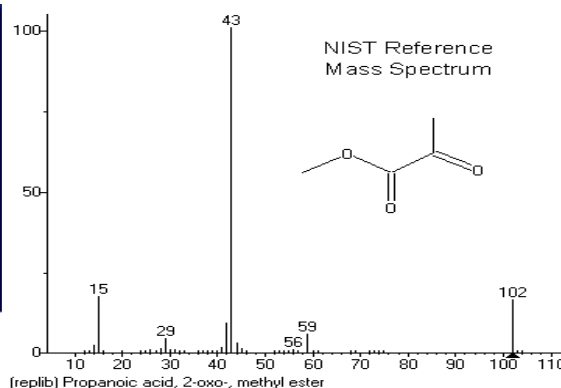


Counts vs. Acquisition Time (min)

x10<sup>5</sup> Propanoic acid, 2-oxo-, methyl ester: + Scan (rt: 8.099, 8.100, 8.102, 8.104 ... min, 85 scan...)



Major Component Mass Spectrum



NIST Reference Mass Spectrum

(replib) Propanoic acid, 2-oxo-, methyl ester