

Chemical Information:

Name: Butanoic acid, 3-oxo-, methyl ester Date of Analysis: 6 March 2015
CAS No.: 105-45-3 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_200162 Lot No.: 26698PJ
NTP_CID No.: 2623 MW: 157.55 g/mol

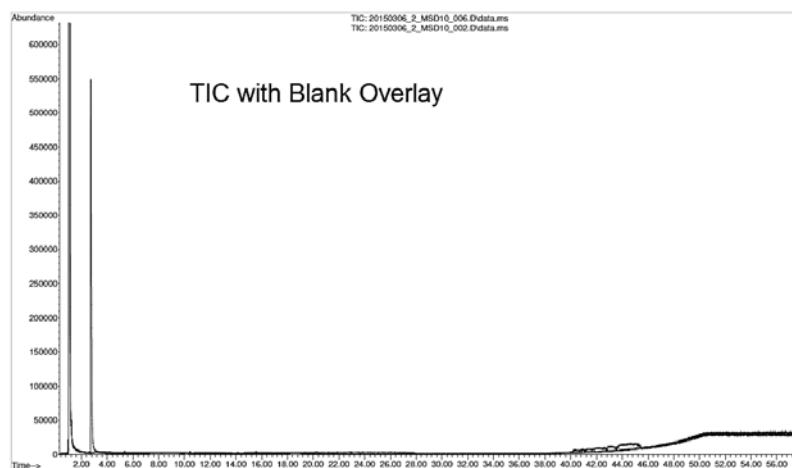
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Butanoic acid, 3-oxo-, methyl ester	2.736	100.0

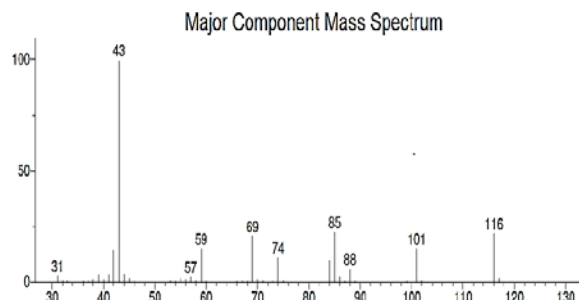
^a Peaks comprising $\geq 0.5\%$ of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph / Mass Spectrometer / Electron Impact
Solvent	Ethanol
Column	J&W DB-1, 30 m x 0.25 mm ID, 0.25- μ m film thickness
Carrier Gas	Helium at 1.5 mL/min
Oven Program	50°C, hold 0 min; ramp @ 5°C/min to 300°C, hold 10 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Splitless
Run Time	60.0 minutes
Data Analysis Software	MSD ChemStation, ver D.03.00.611, NIST Library ver 2.0d, build Dec 2005



Unknown: Scan 497 (2.772 min): 20150306_2_MSD10_006.D\data.ms (-377)
Compound in Library Factor = 237



Hit 1: Butanoic acid, 3-oxo-, methyl ester
C5H8O3; MF: 879; RMF: 886; Prob 94.3%; CAS: 105-45-3; Lib: mainlib; ID: 6073.

