

# Chemical Information:

Name: Hexane, 3-methyl-

Date of Analysis: 16 December 2016

CAS No.: 589-34-4

Supplier: Sigma-Aldrich

Tox21\_ID No.: Tox21\_202850

Lot No.: MKBD3451V

NTP\_CID No.: 6240

MW: 100.20 g/mol

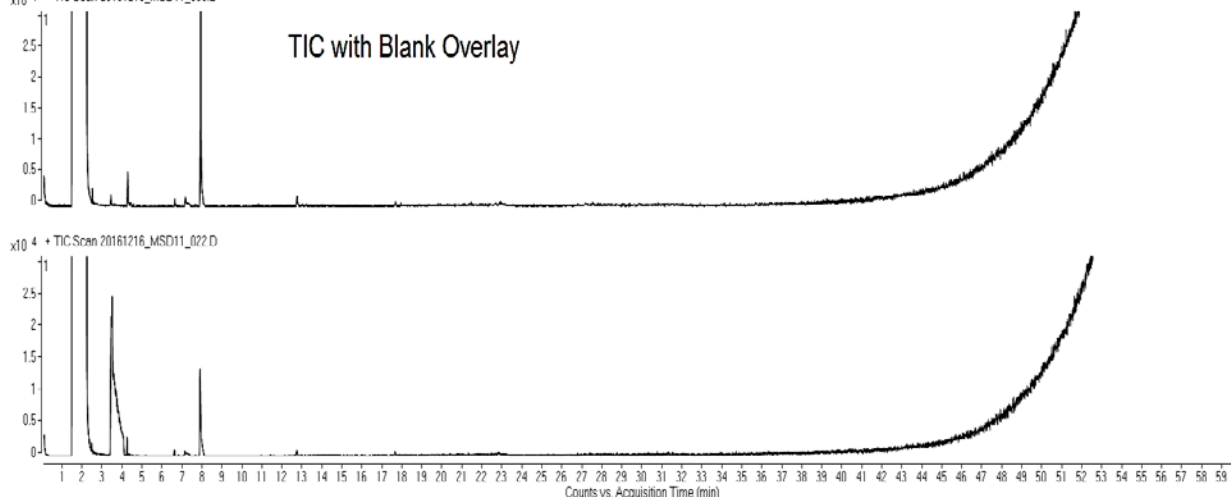
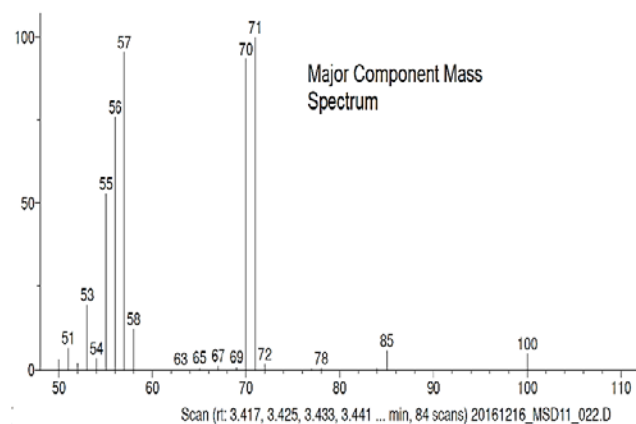
## Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Hexane, 3-methyl-	3.51	100.00

<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	Acetone
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- $\mu$ m 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	50 – 400 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 2.2f Build 2014

x10<sup>4</sup> + TIC:Scan 20161216\_MSD11\_003.D

x10<sup>4</sup> + TIC:Scan 20161216\_MSD11\_022.D

Hit 1 : Hexane, 3-methyl-  
C7H16, MF: 878, RMF: 881; Prob 71.1%; CAS: 589-34-4; Lib: replib; ID: 1745.
