

Chemical Information:

Name: 5-Methyl-2-furancarboxylic acid
CAS No.: 1917-15-3 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_202200 Lot No.: MKBB7838
NTP_CID No.: 5003 MW: 126.11 g/mol

Date of Analysis: 18 July 2016

Purity and Identity Results:

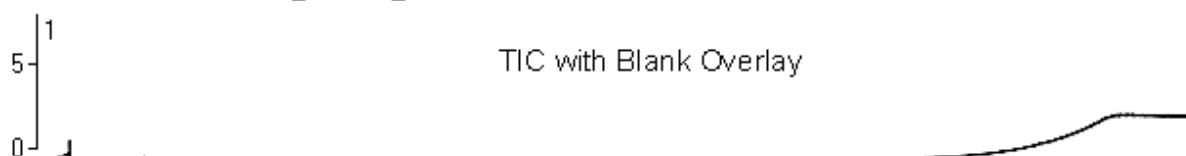
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
5-Methyl-2-furancarboxylic acid	18.03	100.00

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

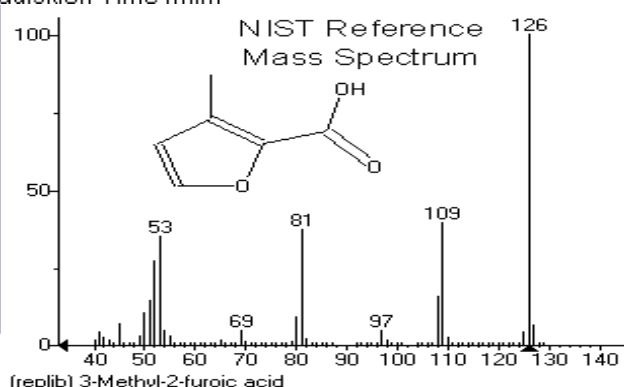
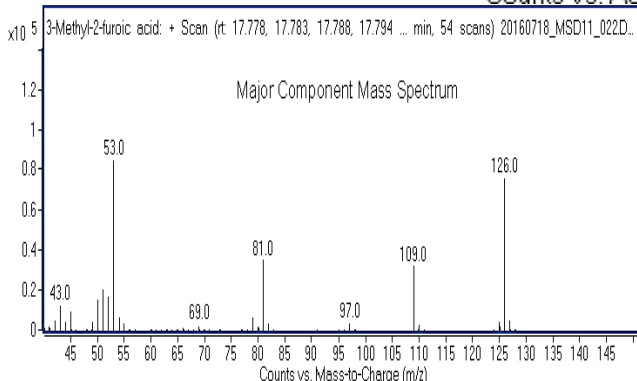
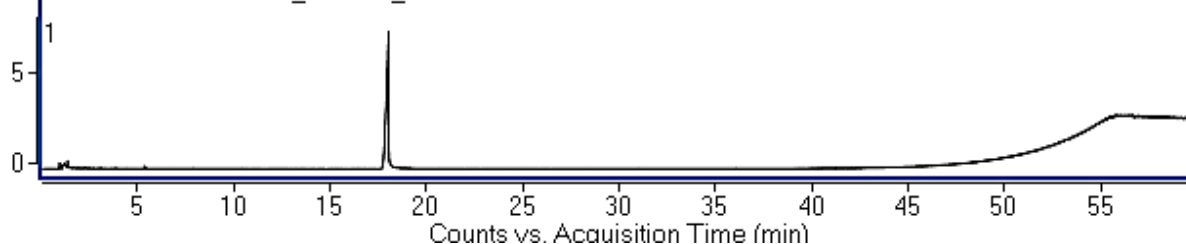
GC/MS Instrument Parameters:

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- μ m film thickness
Carrier Gas	Helium at 2.0 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	40 – 475 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Split (5:1)
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 5 + TIC Scan 20160718_MSD11_007.D



x10 5 + TIC Scan 20160718_MSD11_022.D



Reference is for 3-methyl-2-furancarboxylic acid. A reference for the 5-methyl substitution was not available in the NIST or SDBS databases. Identification as 5-methyl-2-furancarboxylic acid is supported by the difference in the relative abundance of the m/z 53 ion (C₄H₅).