

# Chemical Information:

Name: 5-Methyl-3-isoxazoline  
CAS No.: 1072-67-9 Supplier: Sigma Aldrich  
Tox21\_ID No.: Tox21\_201149 Lot No.: 04609JJ  
NTP\_CID No.: 5006 MW: 98.10 g/mol

Date of Analysis: 13 August 2015

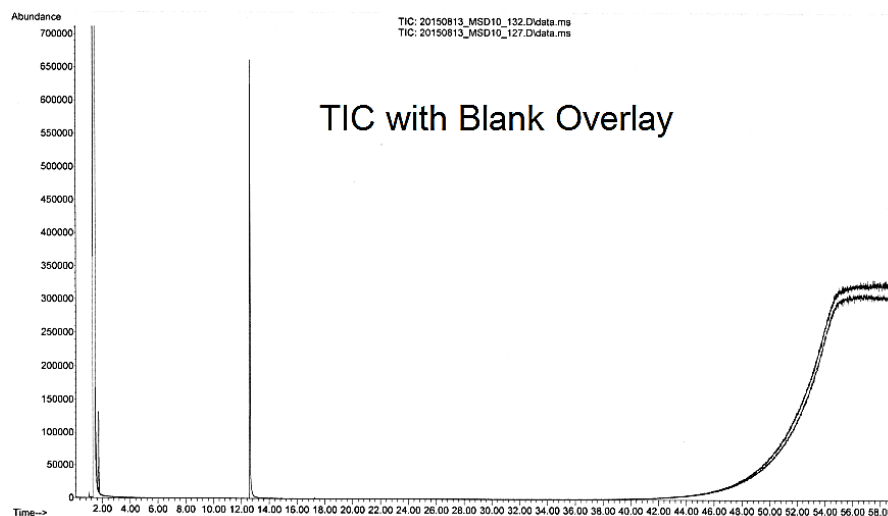
# Purity and Identity Results:

| Peak Identity          | Retention Time (min) | Purity (% Total Area) <sup>a</sup> |
|------------------------|----------------------|------------------------------------|
| 5-Methyl-3-isoxazoline | 12.62                | 99.58                              |

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

# GC/MS Instrument Parameters:

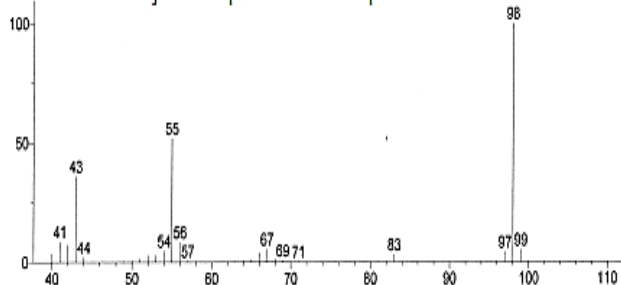
|                         |   |
|-------------------------|---|
| Instrument / Ionization | Gas Chromatograph with Mass Spectrometer / Electron Impact              |
| Solvent                 | Ethanol   |
| Column                  | Rtx-5 MS, 30 m x 0.25 mm ID, 1- $\mu$ m film thickness                  |
| Carrier Gas             | Helium at 2.0 mL/min  |
| Oven Program            | 50°C, hold 0 min; ramp @ 5°C/min to 320°C, hold 5 min                   |
| Source Temperature      | 230°C   |
| Auxiliary Temperature   | 250°C   |
| Scan Range              | 40 – 550 amu  |
| Injector Temperature    | 250°C   |
| Injection Volume / Mode | 1 $\mu$ L / Splitless   |
| Data Analysis Software  | MSD ChemStation, ver D.03.00.611, NIST Library ver 2.0d, build Dec 2005 |



Unknown: Scan 2151 (12.625 min): 20150813\_MSD10\_132.D\data.ms (-2123)  
Compound in Library Factor = 473

Hit 1: 3-Isloxazoline, 5-methyl-  
C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>O; MF: 98; RMF: 939; Prob 88.7%; CAS: 1072-67-9; Lib: replib; ID: 14939.

# Major Component Mass Spectrum



# NIST Reference Mass Spectrum

