

James Little August 29, 2023 38 years Eastman Chemical Company 7 years Mass Spec Interpretation Services <u>https://littlemsandsailing.wpcomstaging.com/</u>

Link to GCMS Schematic Above

Link to University Logos

#### Free NIST GC-MS Software Lab for Universities

Part 1: Very Basic Theory of GCMS Analyses

Part 2: Installation of Software Part 3: Library Searches Part 4: Processing GCMS Data with AMDIS Part 5: Understanding EI Fragmentation with MS Interpreter Part 6: Structure Searches with Input from ChemSketch Part 7: Creating a User Library Part 8: Advanced Processing with NIST Software



Link to Training Website

# **NIST MS Interpreter**

For over 20 years, MS Interpreter has been a freely available software tool for quickly examining the possible origin of EI mass spectra for GC/MS.

After input of a structure and a spectrum, it assigns peaks to plausible molecular substructures based on a set of thermochemical estimates and fragmentation mechanisms based on a proposed chemical structure. A calculated rate for every bond dissociation shows its reactivity with values from 0 to 120.

## *No* Manual for MS Interpreter, Only Index Help within Application



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## Standard Settings, Initial Ones Work Well





Fragment options	
<ul> <li>Show fragments</li> <li>Show unspecified clear</li> <li>Show fragments with r</li> <li>Mark Isotope Peaks</li> <li>Display fragments for peaks not lower than:</li> </ul>	avage no peak % max 0 💌
Rate threshold	40
Sort by ( mz C relative rate C abundance	Tic coloring ▼ Ring opening ▼ H-transfer ▼ Protonated ▼ Molecular ion ▼ Unspecified
Cancel	ОК

#### **Problem with MS Interpreter Not Opening**

-problem when opening MS Interpreter from NIST MS Search

-error message saying server busy

-close AMDIS and NIST search

-solution was to go to the Demo installation and open MS search folder

-delete all Mspcal\*.ini type files

-the necessary ini files for MS Interpreter will be created -apparently the ini files were corrupt

-MS Interpreter Program is actually MSPcalc.exe when run



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#### **MS Interpreter Basics**

-Any ion in black can be assigned a substructure by program, white is not explained

-The substructure in red is assigned by program

-More than one structure can be assigned for ion, so click on ion to see 1,2,3,... etc. -

-Hash marks in yellow above ion clusters are theoretical and thus user can compare to observed -Size of windows can be changed • • mz=49 (1/2) •

-Spectrum area can be changed to see small ions, right click and unzoom to go back to full scale display

-User can left click and circle to manually create their own fragments for a structure

