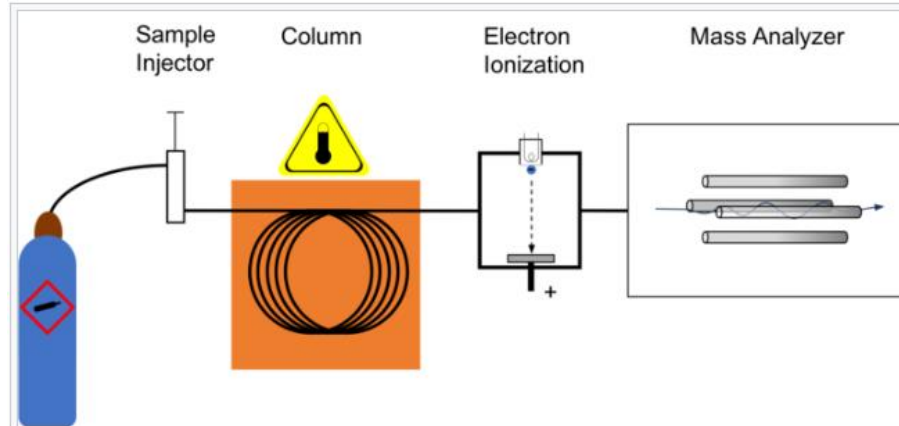**Fr*ee* NIST GC-MS Softwar*e* Lab for Univ*e*rsiti*e*s:**

Part 5: Understanding EI Fragmentation with MS Interpreter

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

Free NIST GC-MS Software Lab for Universities

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.

Link to NIST ASMS Poster 2019

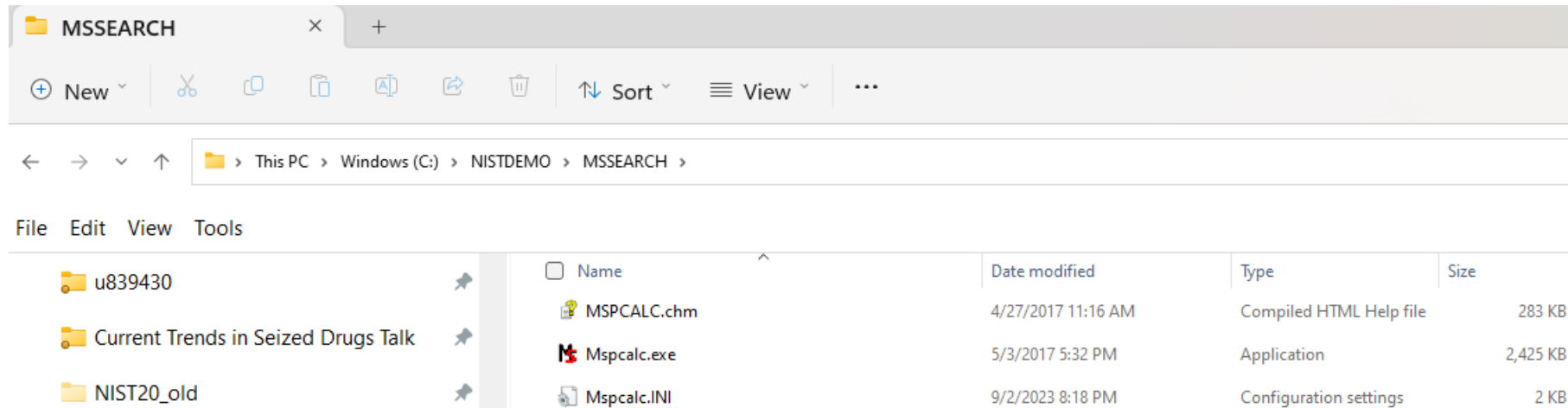# *No* Manual for MS Interpreter, Only Index Help within Application
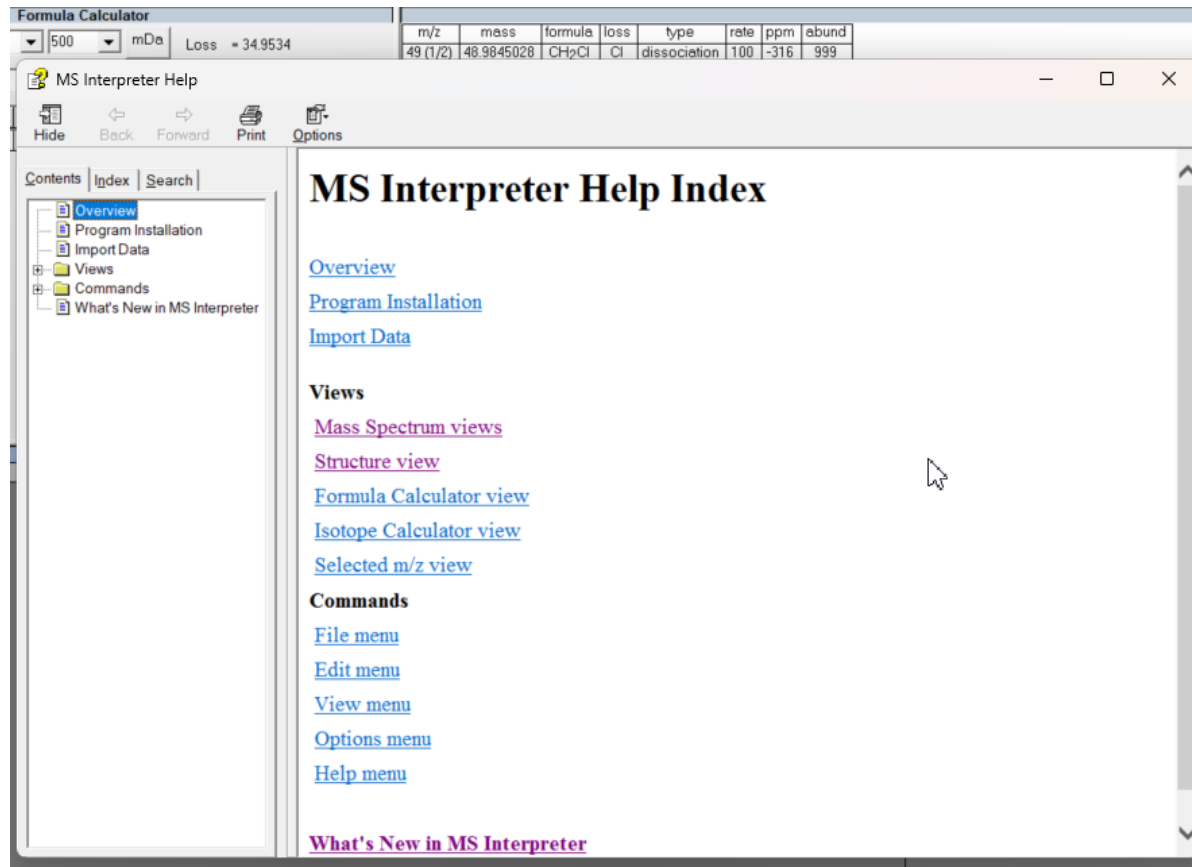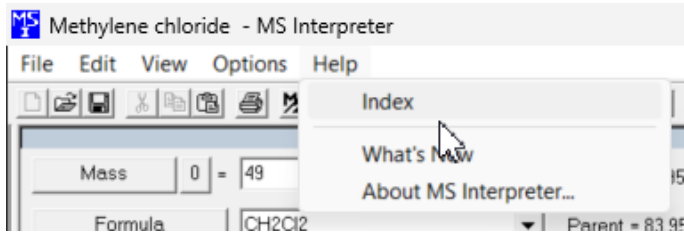
Standard Settings, Initial Ones Work Well
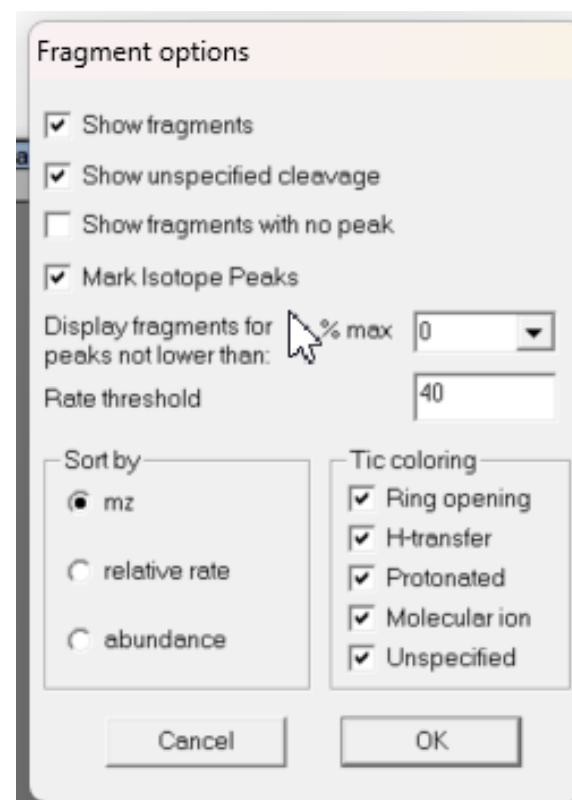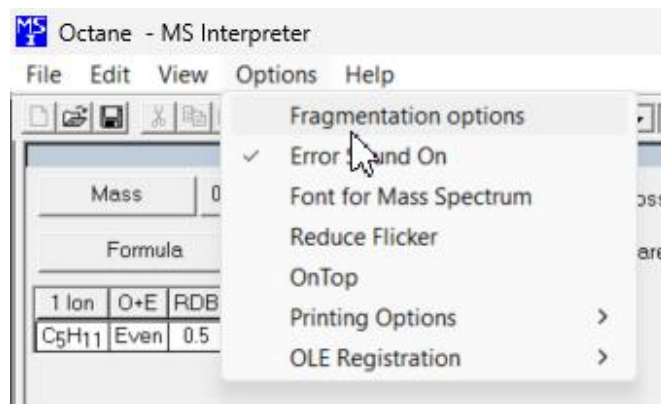
Problem with MS Interpreter Not Opening

-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

Server Busy

This action cannot be completed because the other program is busy. Choose 'Switch To' to activate the busy program and correct the problem.

Switch To...   Retry   Cancel

MSSEARCH

New   Sort   View   ...

This PC > Windows (C:) > NISTDEMO > MSSEARCH >

File   Edit   View   Tools

u839430

Current Trends in Seized Drugs Talk

NIST20_old

Name	Date modified	Type	Size
MSPCALC.chm	4/27/2017 11:16 AM	Compiled HTML Help file	283 KB
Mspcalc.exe	5/3/2017 5:32 PM	Application	2,425 KB
Mspcalc.INI	9/2/2023 8:18 PM	Configuration settings	2 KB

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
-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