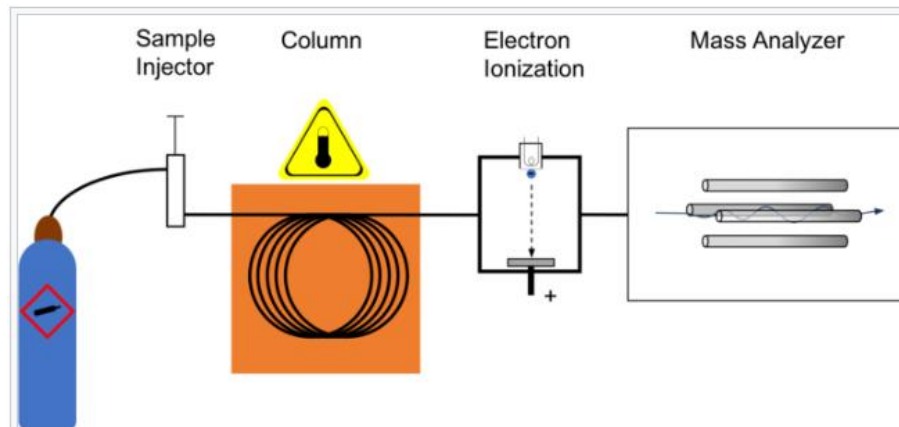**Fr*ee* NIST GC-MS Softwar*e* Lab for Universiti*es*:**

Part 7: Creating a User Library

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

A "Little" Mass Spec and Sailing
Organic Mass Spectrometry, NMR, Sailing, Tesla, Duplicate Bridge

Mass Spec Interpretation Services
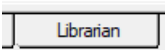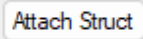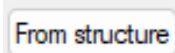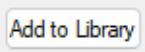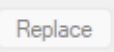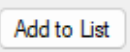
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Link to Training Website

Addition Process

➢ Obtain a good background subtracted spectrum from AMDIS (use the little blue triangles!)

➢ Send to MS Search to see if in the library

➢ If not, open librarian tab at bottom of screen [Librarian]

➢ Open ACD software (ChemSketch) and draw structure

➢ Create a name in ChemSketch

➢ Lasso the structure and copy

➢ Open librarian tab and click on ed button [ed]

➢ Edit the peaks to remove any unwanted ones, use left mouse while holding shift key on keyboard for range or left mouse button while hold Ctrl key on keyboard for individual ions

➢ While ions highlighted, MUST use Delete Key *on KEYBOARD* to delete the ions, *no button within software* [Delete]

➢ Paste structure in from ChemSketch [Attach Struct]
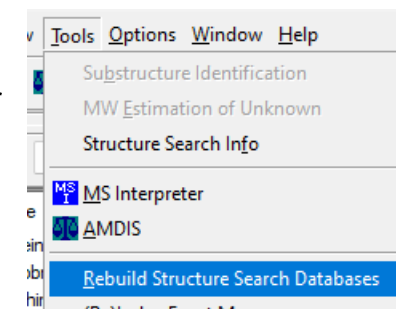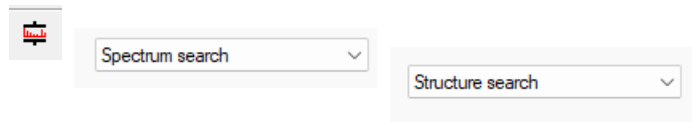
➢ Click on From Structure button to automatically calculate molecular formula and weight and add to field [From structure]

➢ Go back to ChemSketch and lasso the name and copy

➢ Right click on name field within Librarian and paste in the ChemSketch name

➢ Add any comments of interest

➢ Then ADD to list with button (could just Add to library) [Add to Library] [Replace] [Add to List]

➢ Now you can send to MS interpreter from within librarian to check fragmentation

➢ If satisfied, use add to library button in menu bar within MS Search Librarian Tab

➢ To make structure search work correctly after adding a new entry with structure, go to Tools/Rebuilt Structure Search Databases in Lib search tab

➢ Go to Lib Search/Library Search Options Icon/Librarian Tab and add your library to the Spectrum and Structure Search

[Spectrum search] [Structure search]

Tools Options Window Help
Substructure Identification
MW Estimation of Unknown
Structure Search Info
MS Interpreter
AMDIS
Rebuild Structure Search Databases

Adding Structure to MS Interpreter

-Can draw structure in ChemSketch and paste directly into MS interpreter window
-Might have to click on structure window and Ctrl V keyboard sequence to overwrite another
structure already present