KnowItAll
Mass Spectrometry
Training

Vendor Neutral Data Processing Solution for Spectral Analyses

WILEY

KnowItAll™

"Interchanging Structures Between KnowItAll and NIST Search and Basics on Using MS Interpreter"

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Handouts for Videos:
Website: Little Mass Spec and Sailing
https://littlemsandsailing.com/

NOTE: Series of other training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

Link to Training

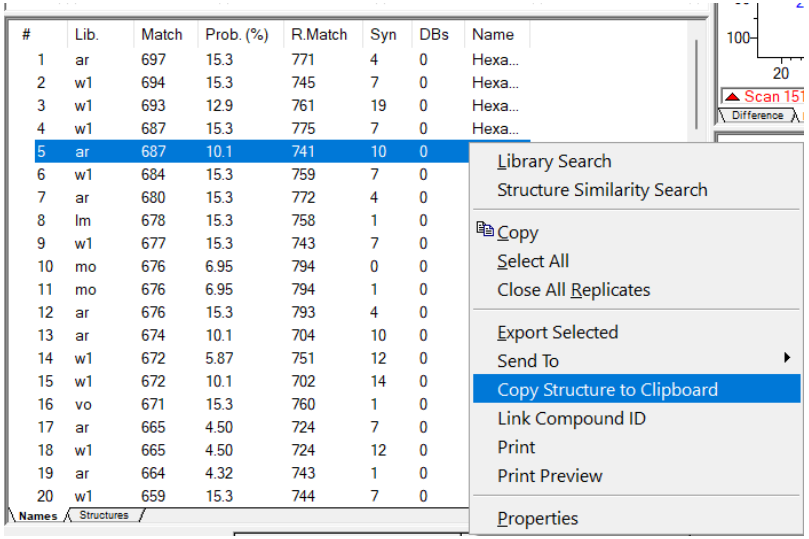
Sept 11, 2022

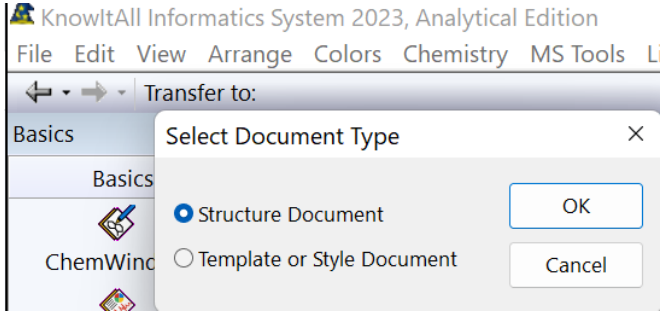
Three Ways to Send Structures from NIST Search to KnowItall ChemWindow

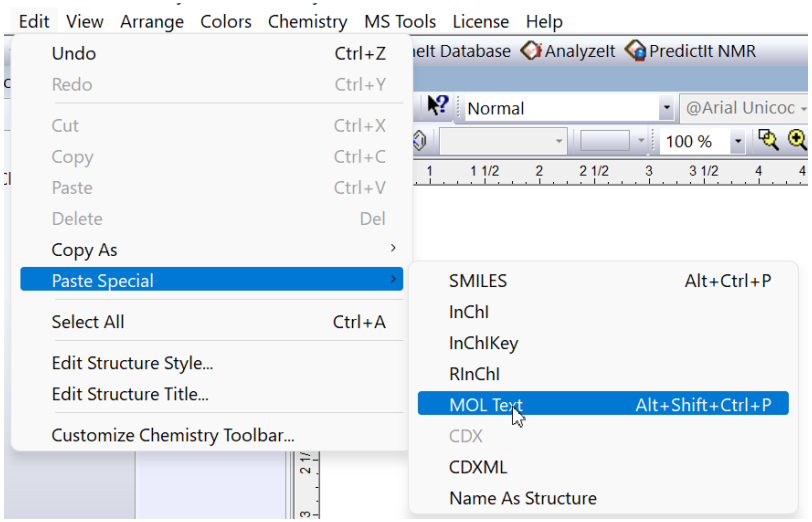
- "Copy structure to clipboard" function in NIST search and "paste special" in ChemWindow
- "Default App" setup within Microsoft Windows using ChemWindow as default
- "Autoimp.str" file within NIST20/MSSEARCH folder

First Method to Send Structures from NIST Search to KnowItall ChemWindow

- Find any entry in any list that has a structure
- Left click on entry to highlight
- Right click and Copy Structure to Clipboard
- NOT Copy!
- Open KnowItAll ChemWindow Function
- Left Click on File/New and select “Structure Document”
- Program will open up new tab at bottom of page and insert structure
- Next do “Paste Special” and “MOL text”
- Note the normal paste option in menu is grayed out

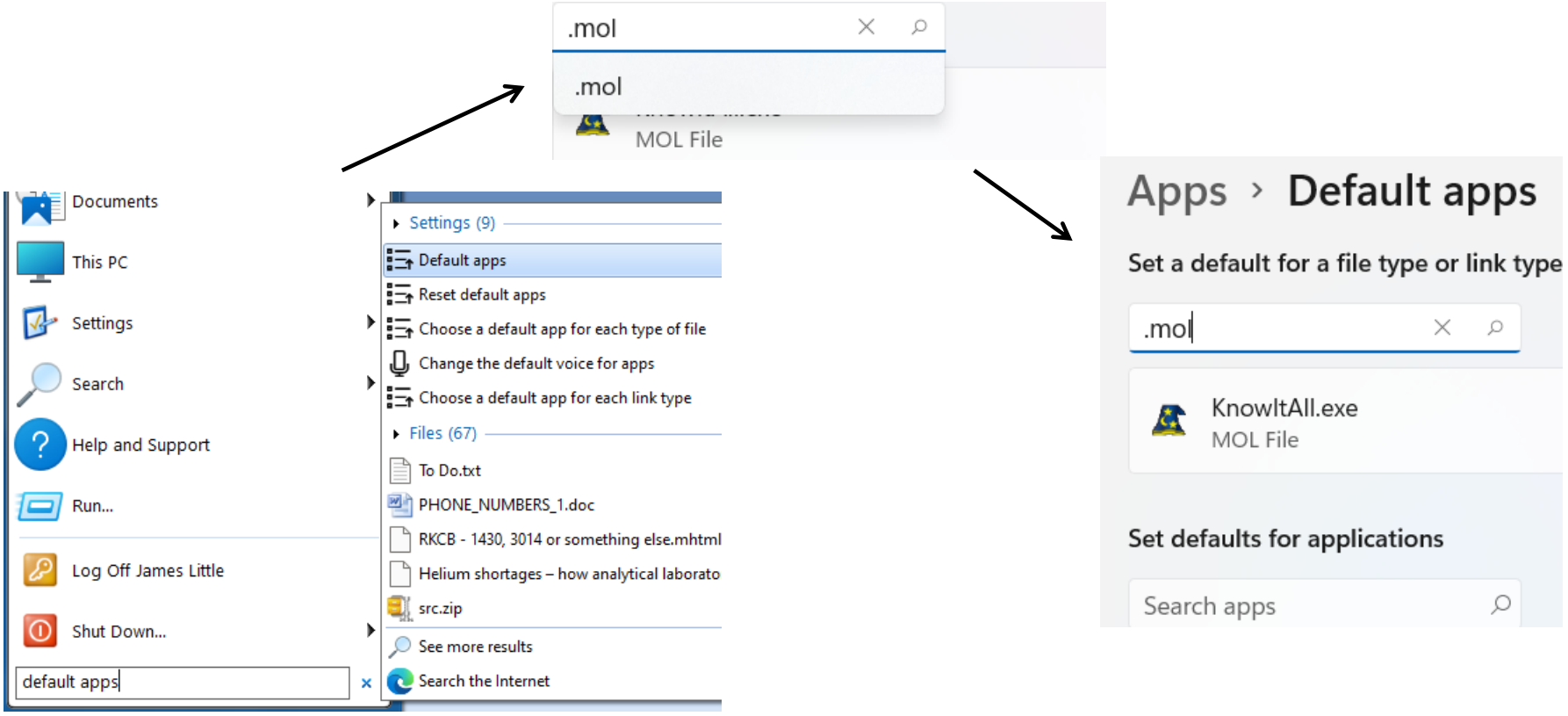






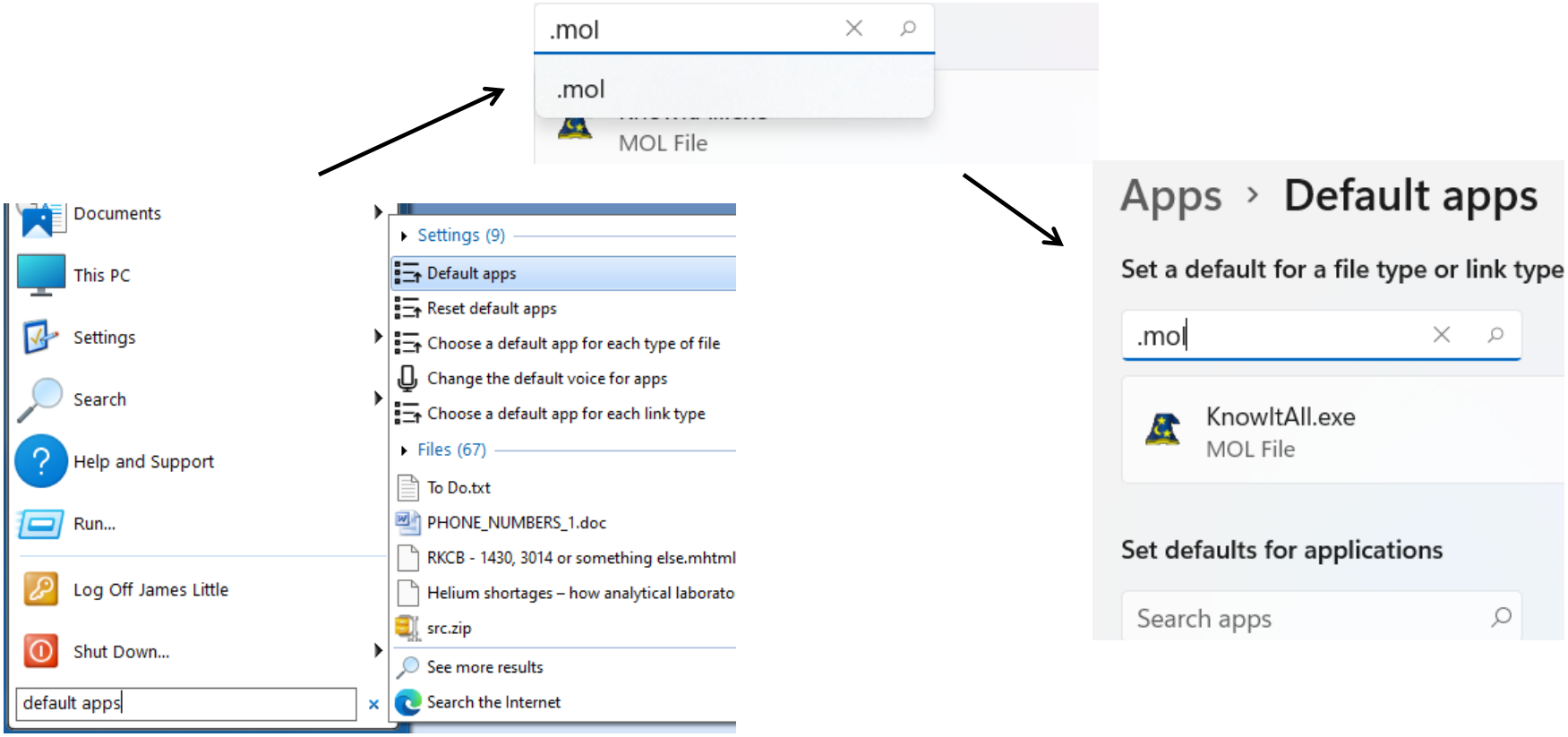
Second Method to Send Structures from NIST Search to KnowItall ChemWindow

- Change which program in Microsoft Windows associates with *.mol type files
- Go to bottom windows bar and type in “default apps”
- Menu will open and user can associate *.mol type with a selected application
- Select KnowItAll.exe



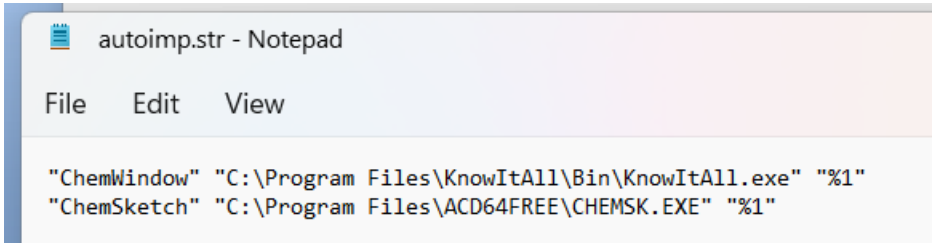
Using NIST MS Interpreter to Determine Fragmentation in EI Spectra

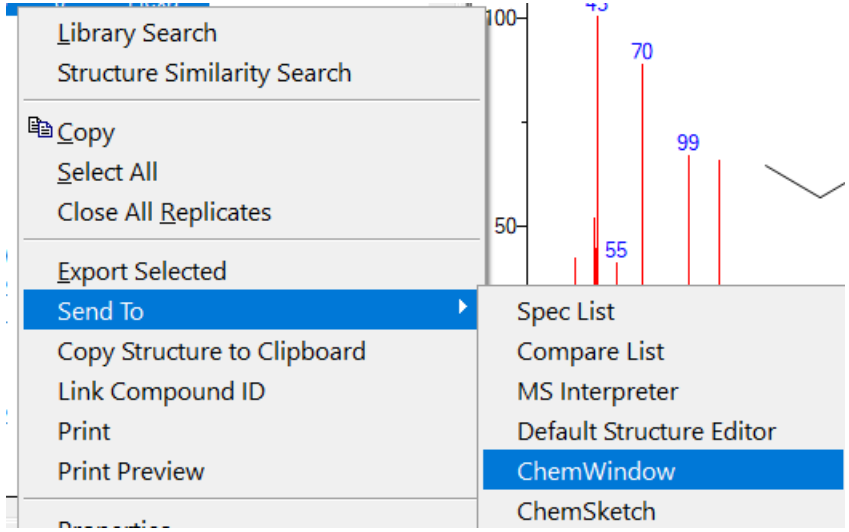
- Send spectrum of proposed unknown to NIST Search
- Send spectrum from NIST search list to MS Interpreter
- Paste in proposed structure from ChemWindow
- All ions in black show proposed substructure for ions observed and isotope ratios



Third Method to Send Structures from NIST Search to KnowItall ChemWindow

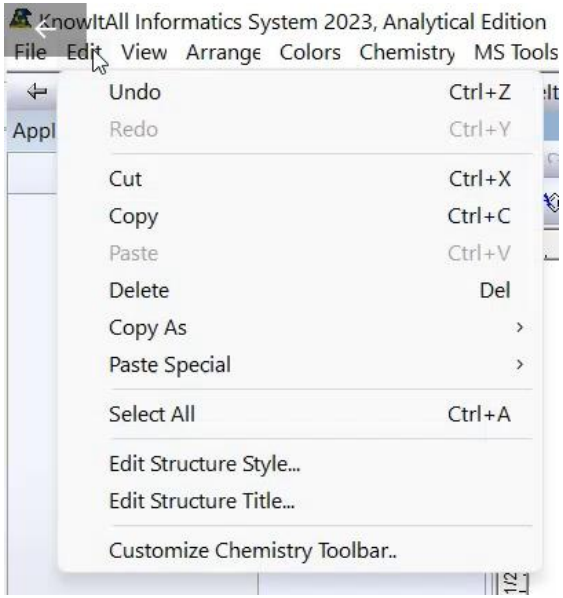
- Use Autoimp.str program found in NIST forlder with the NIST executable and libraries
- Might need to create using Notepad
- Described in page 68 of the NIST Users manual, see *link*
- Edit it with Windows Notepad program and save in the NIST folder
- First argument in parenthesis is name displayed in NIST Search Menu
- Second argument in parenthesis is the full windows location of file
- Third argument in parenthesis indicates, “%1”, indicates it will be in *.mol format
- When you left click and select and entry then right click actual program will be displayed as an option
- One can use a variety of drawing programs such as ChemSketch in addition to ChemWindw

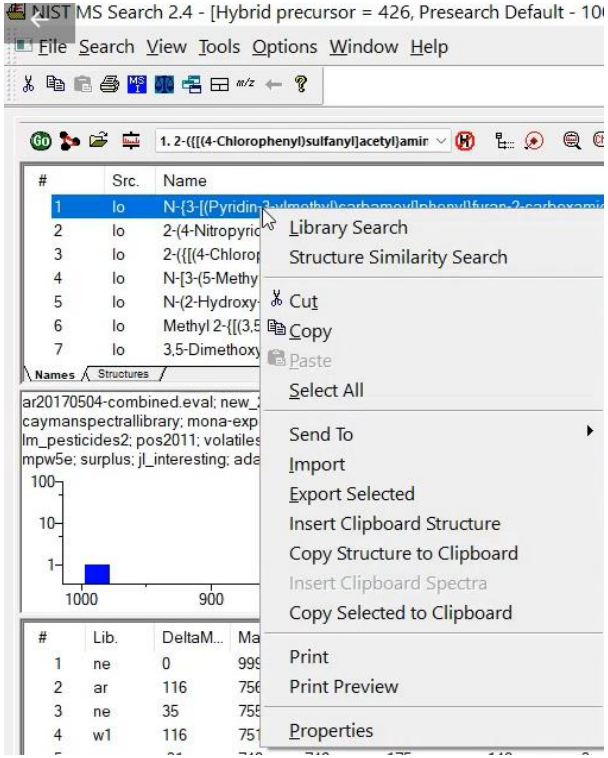


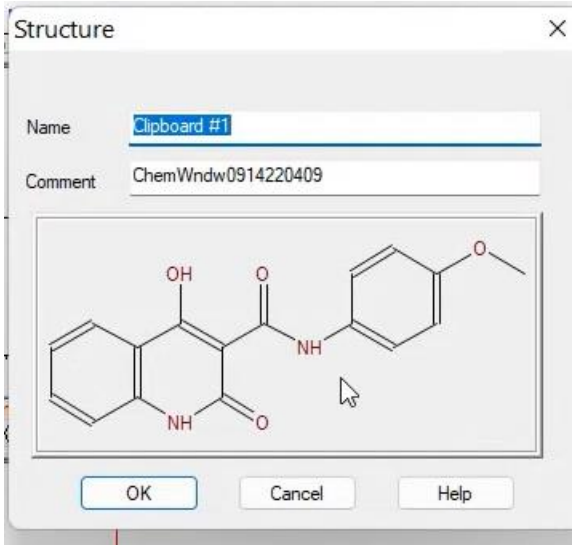


Can Also Send Structures from ChemWindow to NIST Search

- Go to ChemWindow and select a structure with arrow key
- Select Copy, NOT Copy As, the latter causes some difficulties
- Click in top window, the Search List, for in NIST Search program
- Left click on box, then right click and “Insert Clipboard Structure”
- ***DON’T*** use copy to insert! Might paste in other unwanted things from clipboard
- Can change name of the title on spectrum before accepting with “OK”

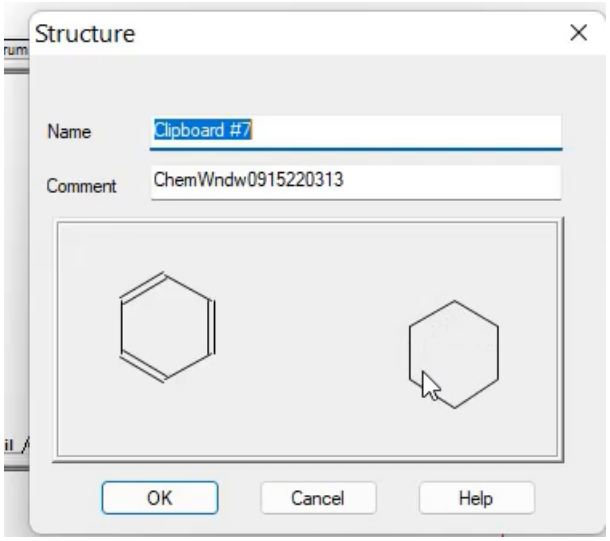






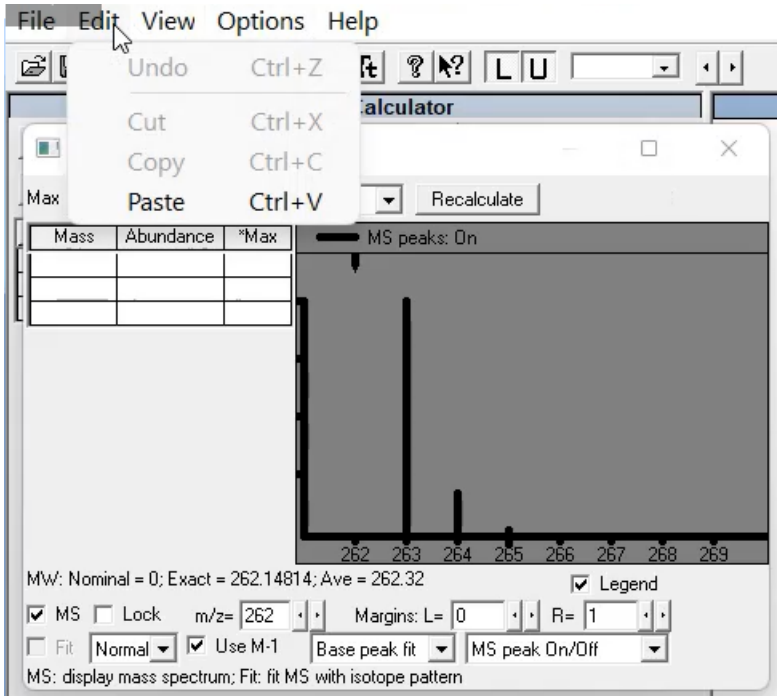
Small Problems When Sending Structures from ChemWindow to NIST Search

- If more than one structure is present in ChemWindow
- Even when selecting one by boxing with the arrow
- ***All*** structures in ChemWindow will be imported
- If aromatic structure such as benzene is depicted with the “circle in middle”
- Benzene and other aromatics will be imported as reduced form,, *e.g.* cyclohexane
- Thus, be sure to draw aromatics with alternating double bonds!



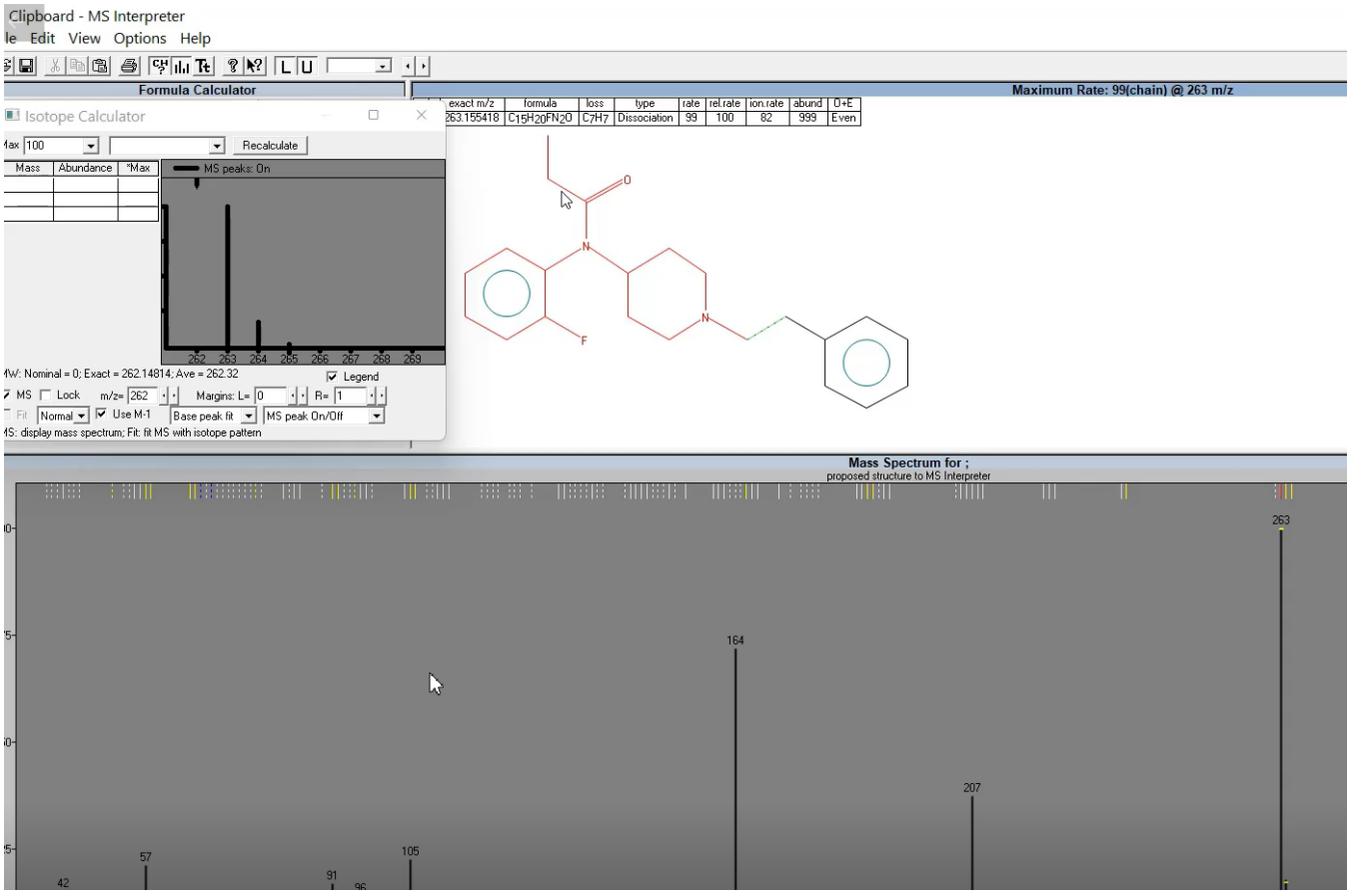
Advanced Topic: Using MS Interpreter to Understand EI Fragmentation (1 of 3)

- One transfers the spectrum of interest from KnowItAll as shown in ***previous*** video
- Draw the structure to correlate with fragmentation in ChemWindow
- Select structure with Select arrow in ChemWindow then “box it”
- Copy into with Edit/Copy to put in Windows clipboard
- Left click in Structure box which will be empty
- Then Edit/Paste



Advanced Topic: Using MS Interpreter to Understand EI Fragmentation (2 of 3)

- The structure will now be displayed in structure box
- Ions in black can be explained by program
- Part of molecule explained is in red
- Ions in white cannot be explained



Advanced Topic: Using MS Interpreter to Understand EI Fragmentation (3 of 3)

- The use of MS Interpreter can be found in links shown below
- Will take a little effort on user to become proficient

Links to References (click on them)

-video tutorial
-handout for video tutorial
-other useful references

Conclusions

- Very easy to send structures from NIST search program to KnowItAll ChemWindow
- Three different methods can be employed
- Structures can be sent from ChemWindow to NIST search, some minor limitations in aromatic ring structures
- Structures can be pasted with spectrum to ***NIST MS interpreter*** to aid in fragmentation interpretation (basic description plus ***links to training***}

NOTE: **Be sure to see my other videos for Mass Spec KnowItAll training on my personal website**

Link to Training