

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”

James Little
Mass Spec Interpretation Services

Handouts for Videos:

Website: Little Mass Spec and Sailing

<https://littlemsandsailing.wordpress.com>

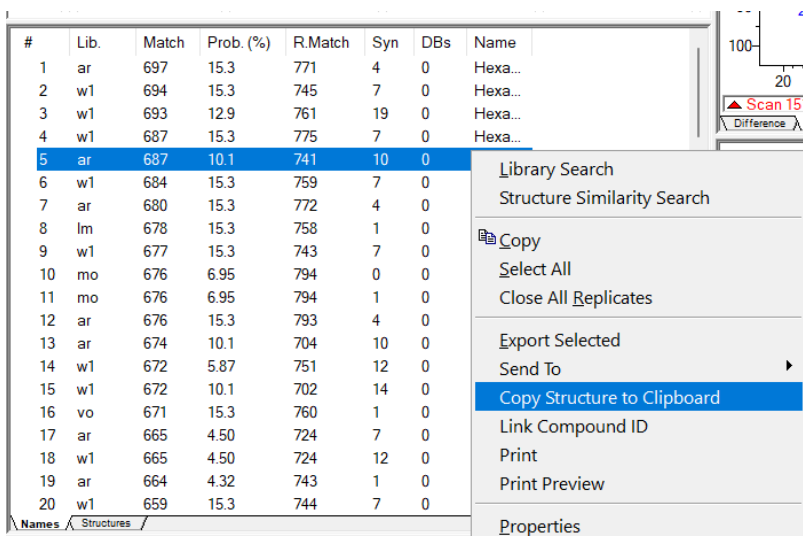
NOTE: Series of other training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

Three Ways to Send Structures from NIST Search to KnowItall ChemWindow

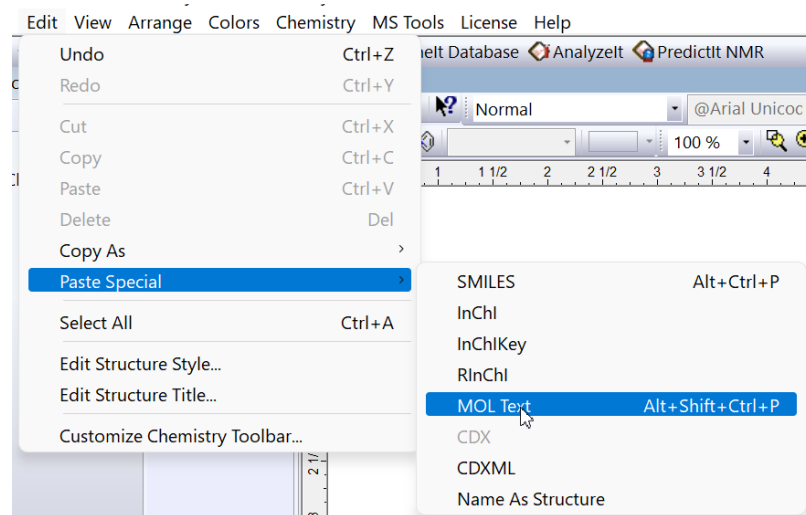
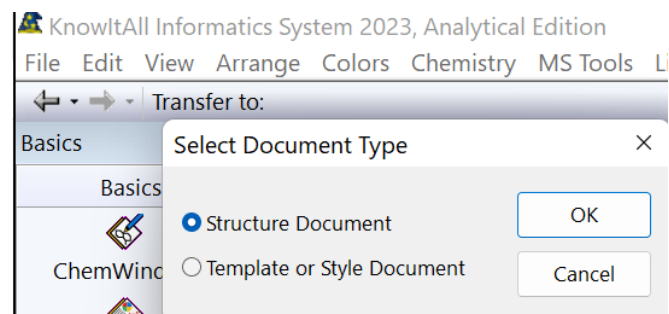
- “Copy structure to clipboard” function in NIST search and “paste special” in ChemWindow
- “Default App” setup within Microsoft Windows using ChemWindow as default
- “Autoimp.str” file within NIST20/MSSEARCH folder

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

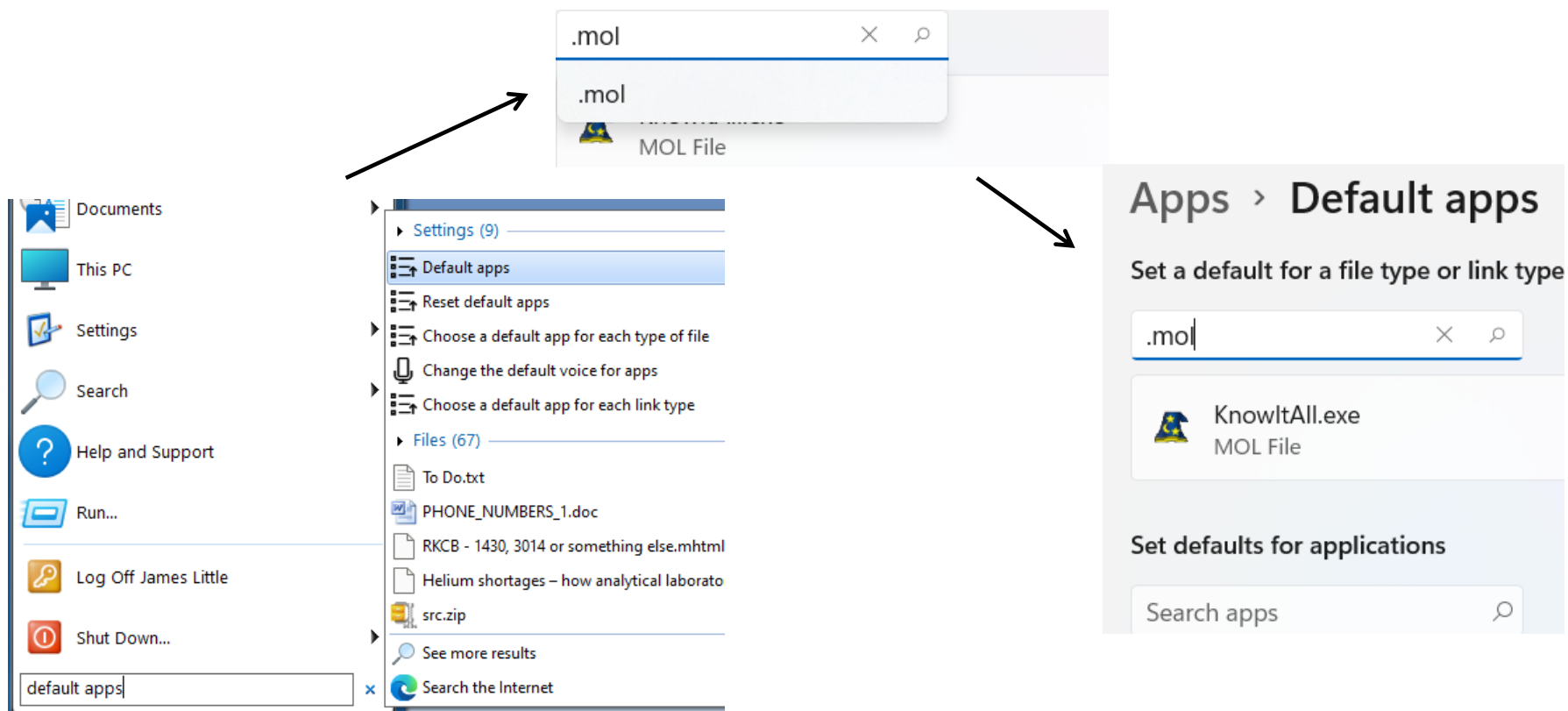


#	Lib.	Match	Prob. (%)	R.Match	Syn	DBs	Name
1	ar	697	15.3	771	4	0	Hexa...
2	w1	694	15.3	745	7	0	Hexa...
3	w1	693	12.9	761	19	0	Hexa...
4	w1	687	15.3	775	7	0	Hexa...
5	ar	687	10.1	741	10	0	
6	w1	684	15.3	759	7	0	
7	ar	680	15.3	772	4	0	
8	lm	678	15.3	758	1	0	
9	w1	677	15.3	743	7	0	
10	mo	676	6.95	794	0	0	
11	mo	676	6.95	794	1	0	
12	ar	676	15.3	793	4	0	
13	ar	674	10.1	704	10	0	
14	w1	672	5.87	751	12	0	
15	w1	672	10.1	702	14	0	
16	vo	671	15.3	760	1	0	
17	ar	665	4.50	724	7	0	
18	w1	665	4.50	724	12	0	
19	ar	664	4.32	743	1	0	
20	w1	659	15.3	744	7	0	



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

The image shows a sequence of steps in Windows Settings to set a default application for a specific file type. On the left, the Start menu is open with 'default apps' typed into the search bar. The 'Settings (9)' application is selected, and the 'Default apps' section is expanded. On the right, the 'Default apps' settings window is shown with '.mol' entered in the search field. The 'KnowItAll.exe' application is listed as the default for 'MOL File'.

Documents

This PC

Settings

Search

Help and Support

Run...

Log Off James Little

Shut Down...

default apps

Settings (9)

Default apps

Reset default apps

Choose a default app for each type of file

Change the default voice for apps

Choose a default app for each link type

Files (67)

To Do.txt

PHONE_NUMBERS_1.doc

RKCB - 1430, 3014 or something else.mhtml

Helium shortages - how analytical laborato

src.zip

See more results

Search the Internet

Apps > Default apps

Set a default for a file type or link type

.mol

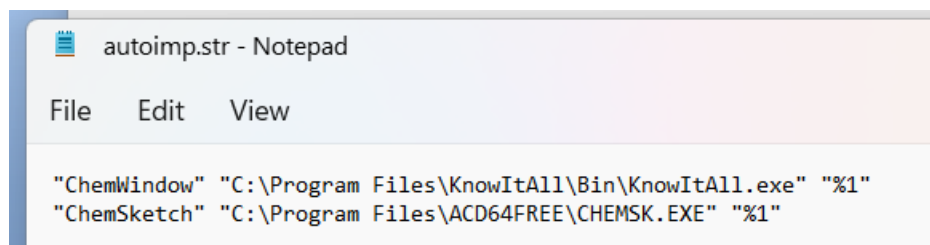
KnowItAll.exe
MOL File

Set defaults for applications

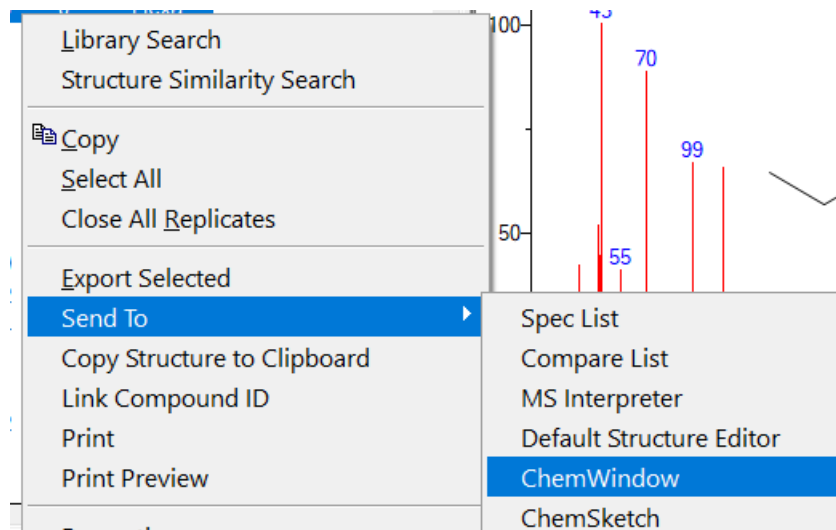
Search apps

Third Method to Send Structures from NIST Search to KnowItAll ChemWindow

- Use Autoimp.str program found in NIST folder 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 ChemWindow

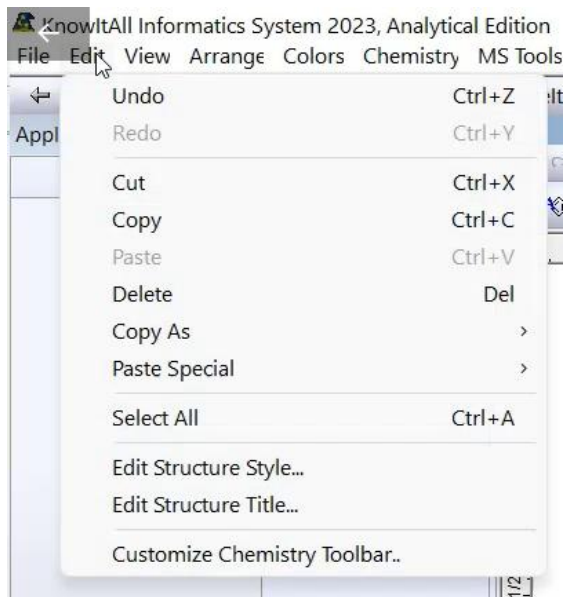


```
autoimp.str - Notepad
File Edit View
"ChemWindow" "C:\Program Files\KnowItAll\Bin\KnowItAll.exe" "%1"
"ChemSketch" "C:\Program Files\ACD64FREE\CHEMSK.EXE" "%1"
```



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”



The screenshot shows the NIST MS Search 2.4 interface. The 'Search List' window is open, displaying a table of search results. The first entry is selected:

#	Src	Name
1	lo	N-[3-((Pyridin-2-ylmethyl)carbamoyl)propyl]acetamide
2	lo	2-(4-Nitrophenyl)propanoic acid
3	lo	2-((4-Chlorophenyl)sulfonyl)acetamide
4	lo	N-[3-(5-Methyl-2-hydroxyphenyl)propyl]acetamide
5	lo	N-(2-Hydroxyphenyl)acetamide
6	lo	Methyl 2-((3,5-dimethoxyphenyl)amino)acetate
7	lo	3,5-Dimethoxyphenylamine

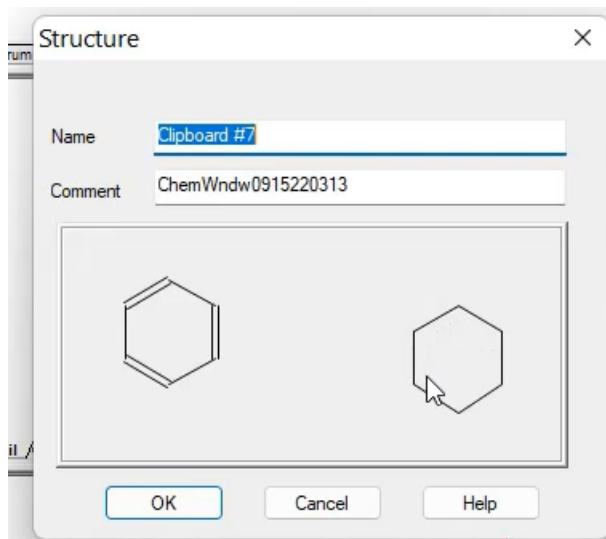
Below the search list is a mass spectrum plot showing relative intensity versus m/z. The x-axis ranges from 100 to 900, and the y-axis ranges from 1 to 100. A single prominent peak is visible at m/z 100.

The screenshot shows the 'Structure' dialog box in NIST MS Search. The 'Name' field contains 'Clipboard #1' and the 'Comment' field contains 'ChemWndw0914220409'. The 'Structure' field displays a chemical structure of a substituted benzamide derivative. The structure consists of a benzamide core with a hydroxyl group and a methyl group on the benzene ring, and a methoxy group on the amide nitrogen's phenyl ring.

Buttons: OK, Cancel, Help

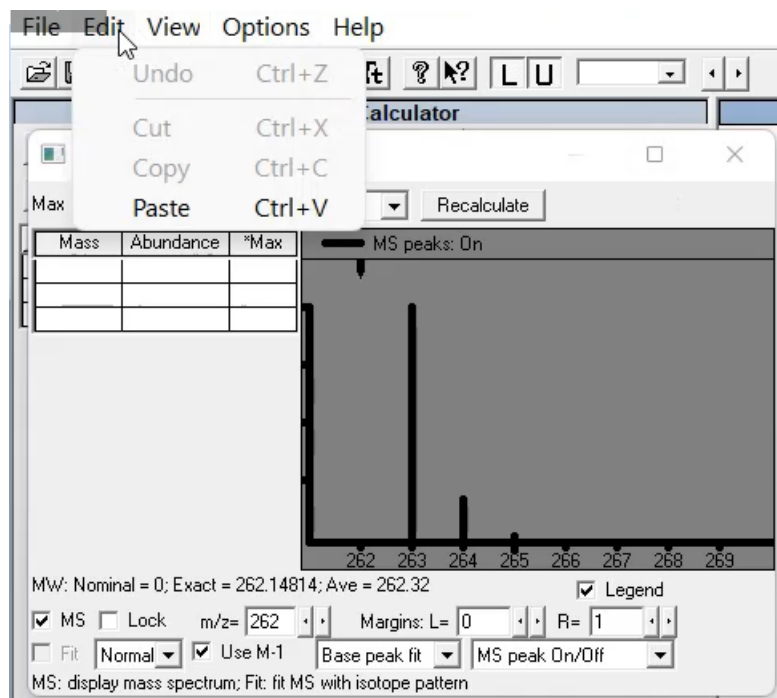
Small Problems When Sending Structures from ChemWindow to NIST Search

- 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!



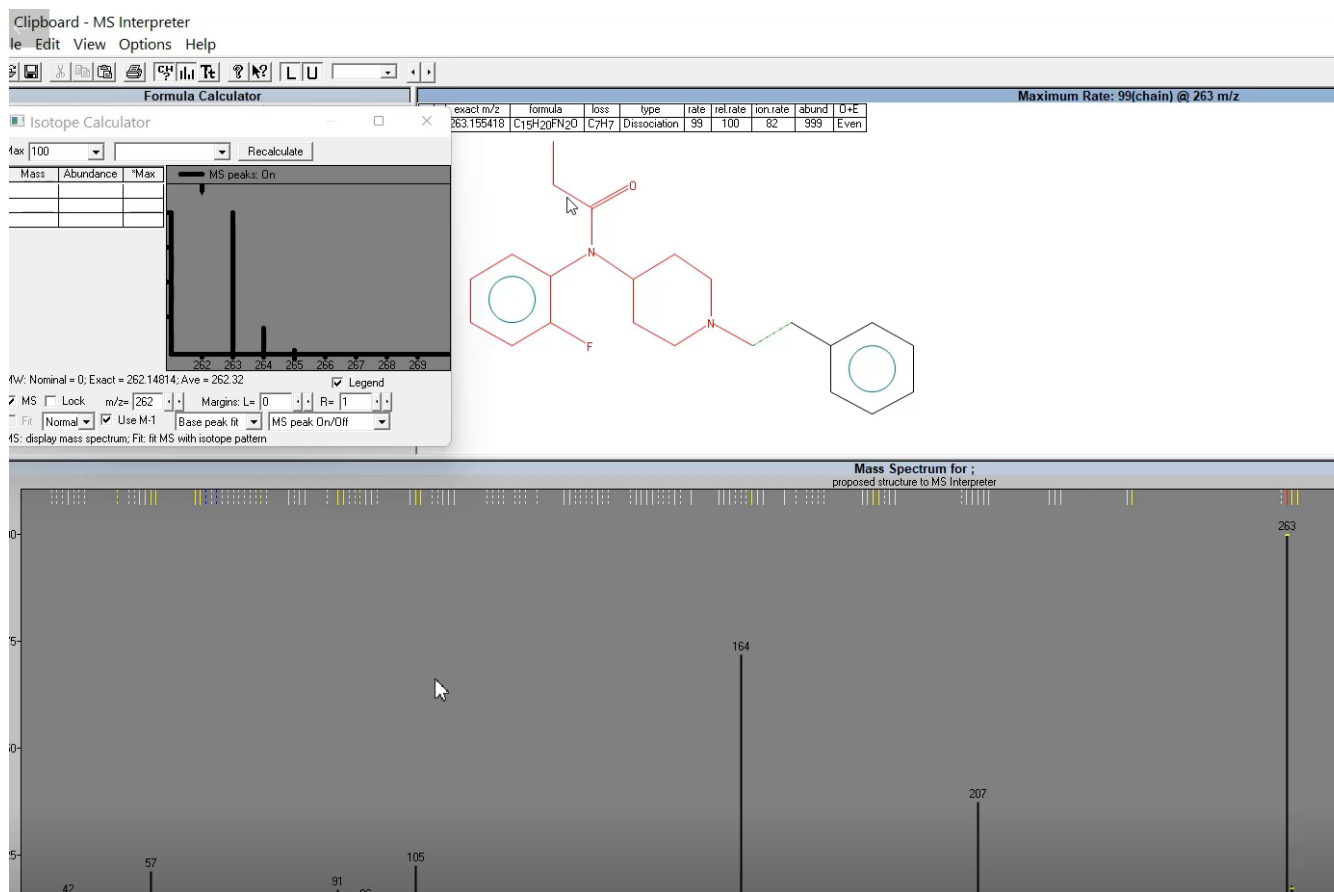
Advanced Topic: Using MS Interpreter to Understand EI Fragmentation (1 of 3)

- 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