MS Interpreter for Accurate Mass Data: Correlating Structure to *m/z*
Video/Handout

James Little
Mass Spec Interpretation Services
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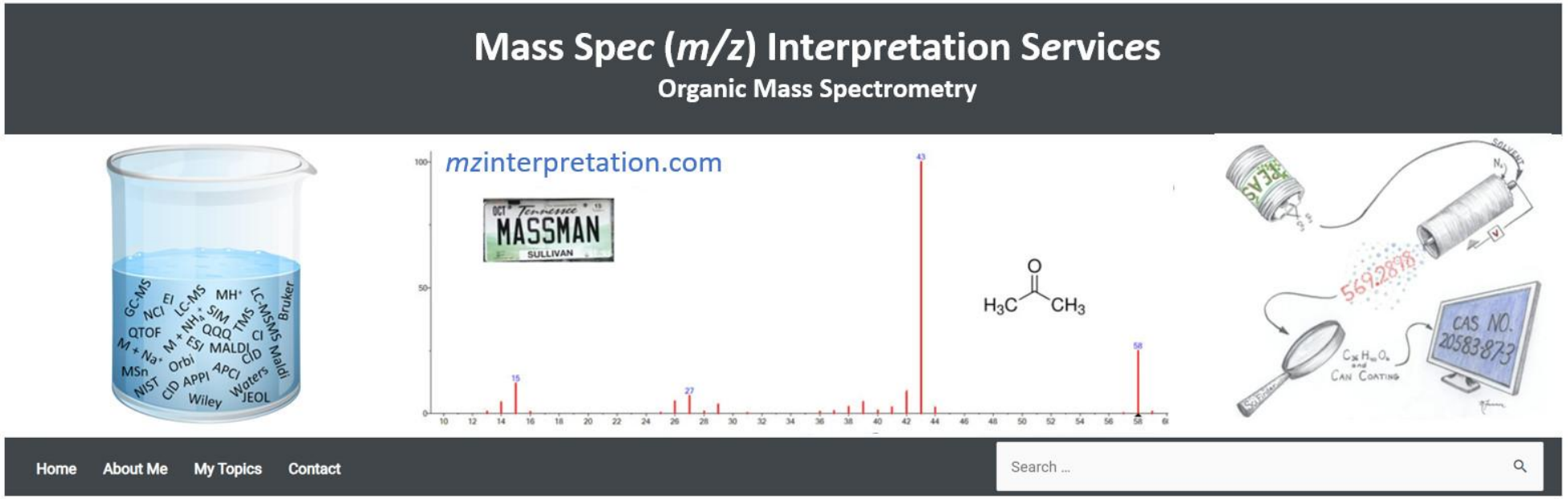
mzinterpretation.com

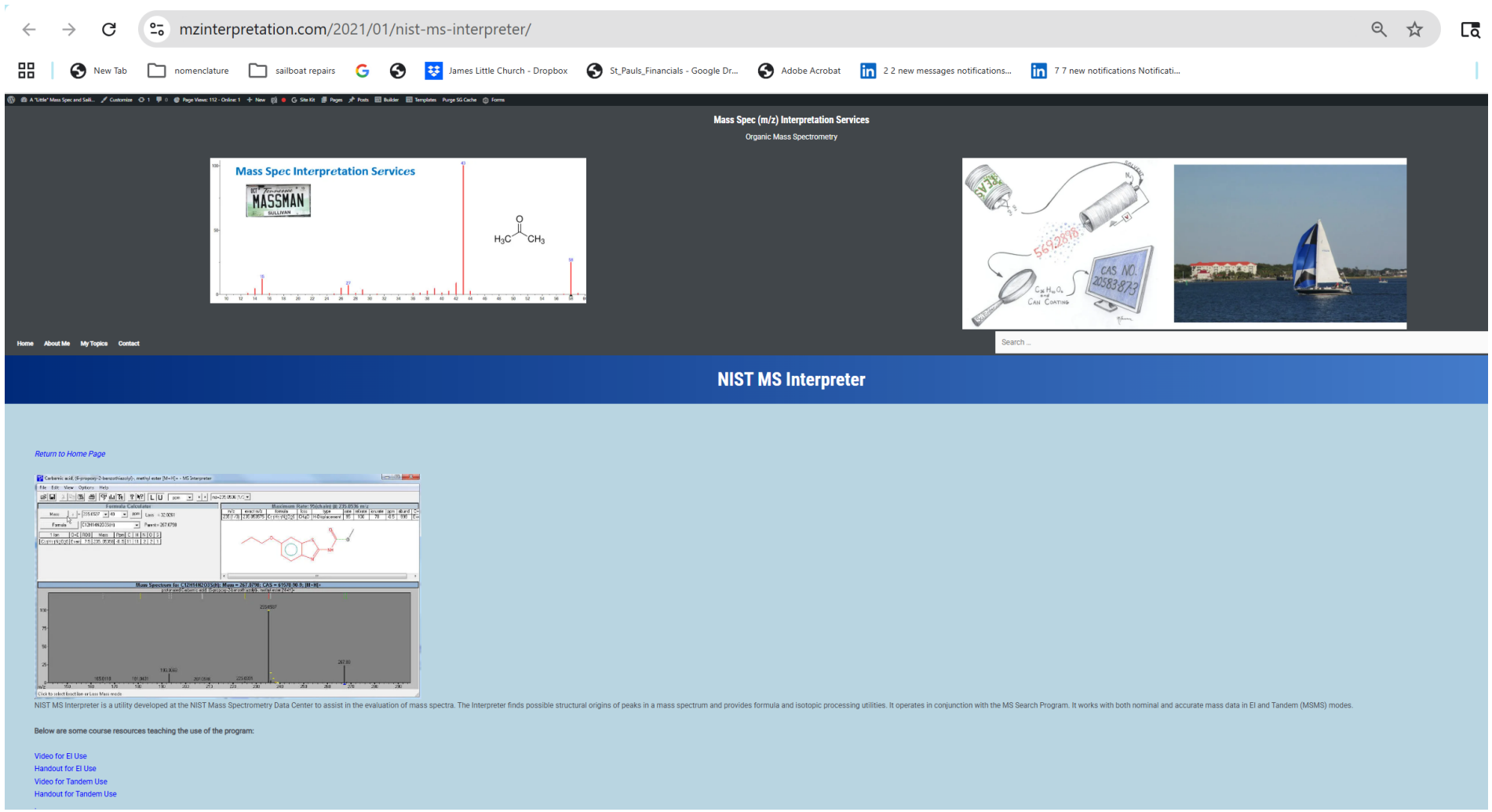
See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!



Only Basics of Using MS Interpreter in Video and Handout

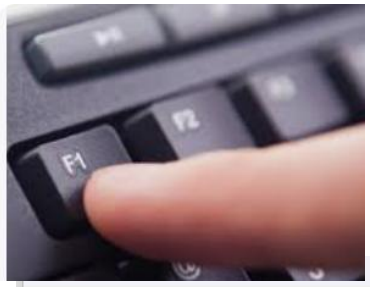
More ***Detailed Information*** on MS Interpreter on my website

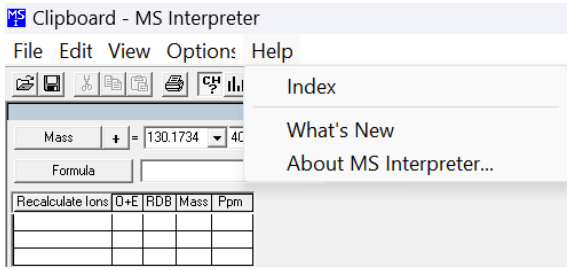
See Link

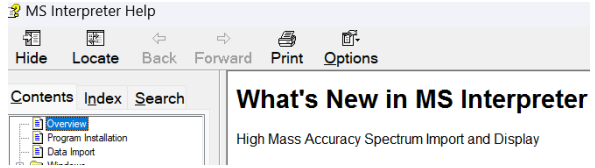


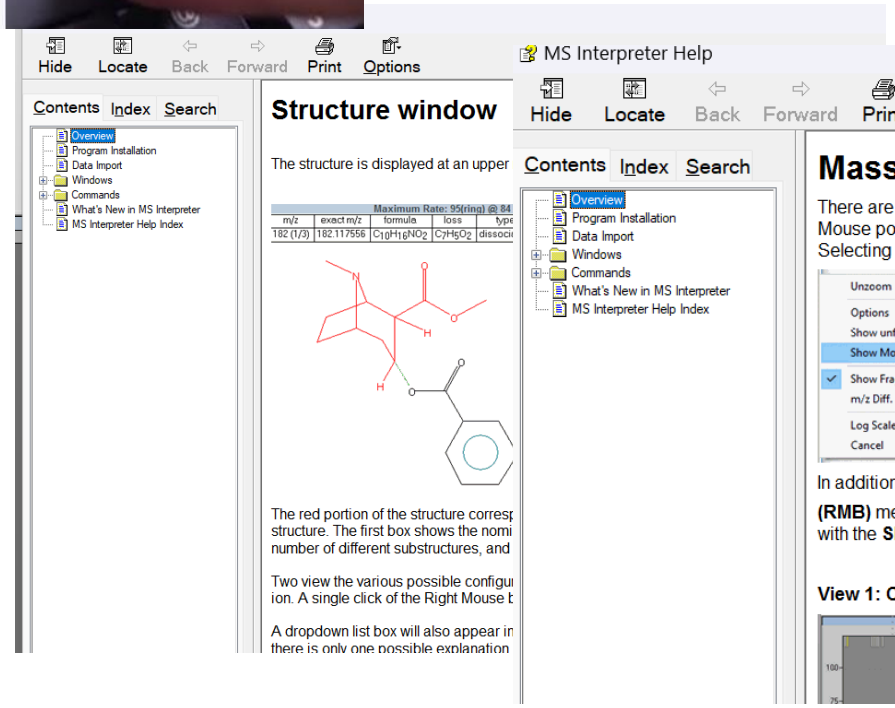
Help in Using MS Interpreter

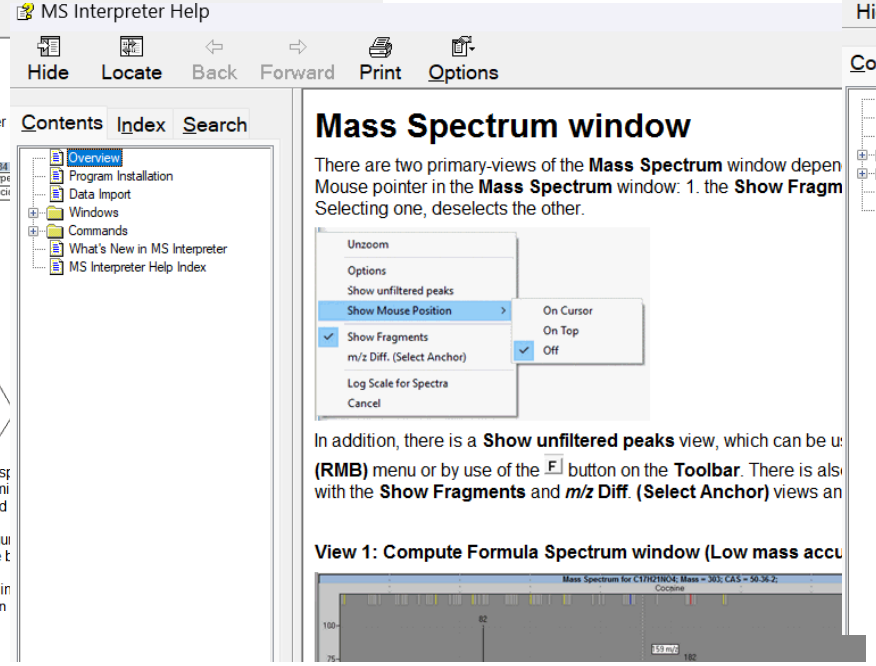
- **Use the Help on Menu Bar and see Whats New and Index**
- ***ALSO*, F1 on keyboard when *ANY* of the windows give addition information**

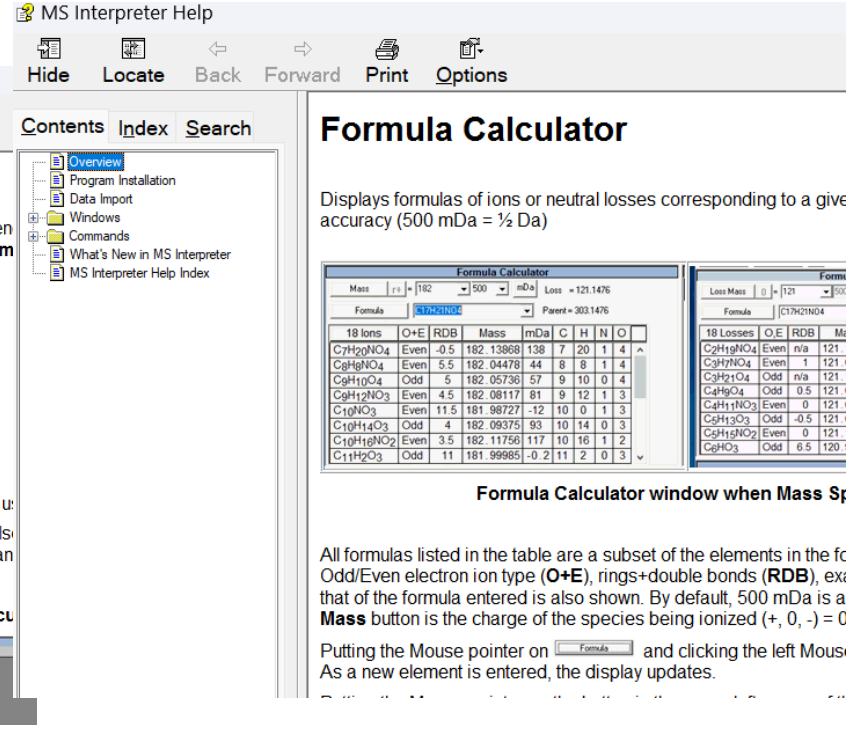






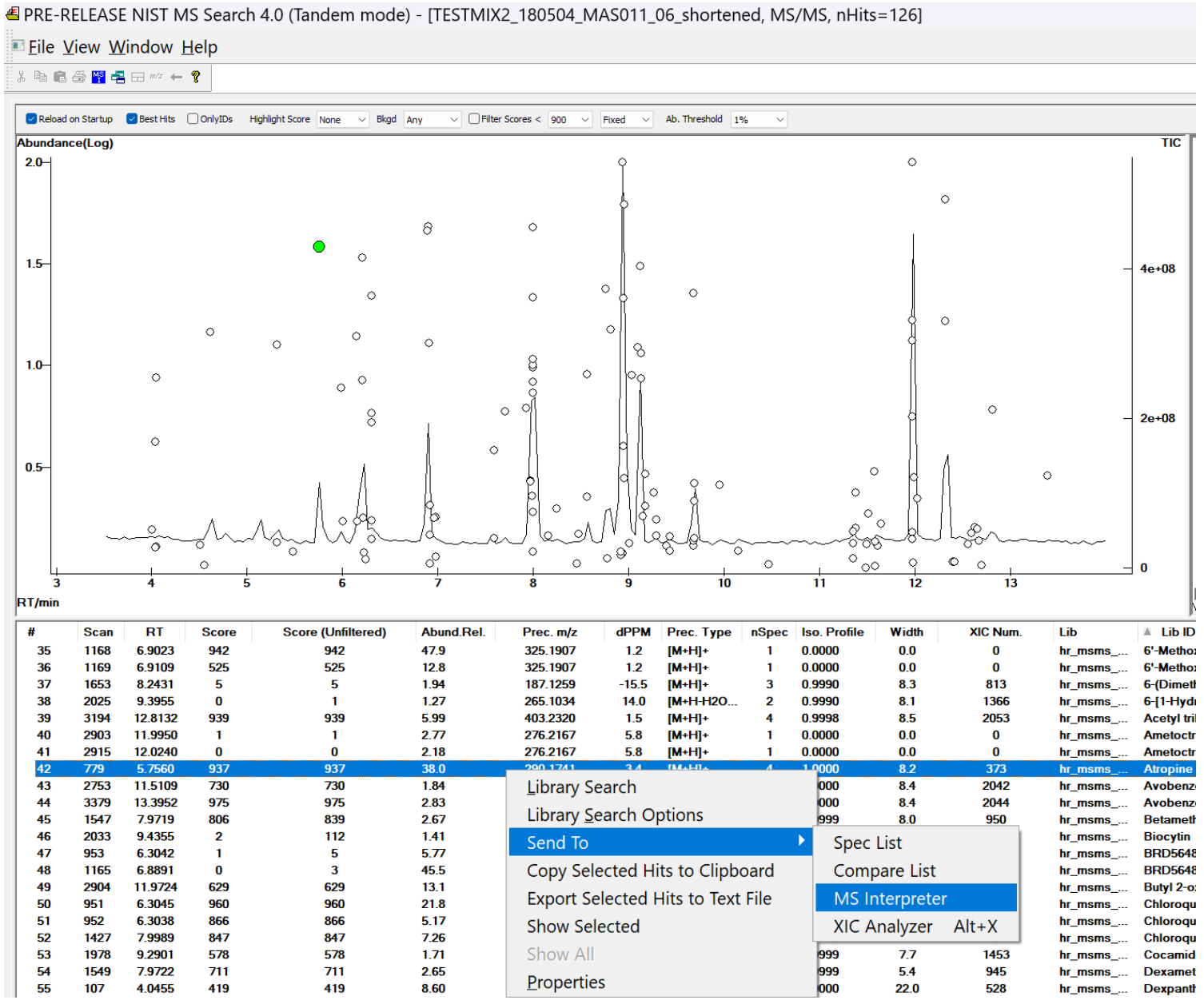






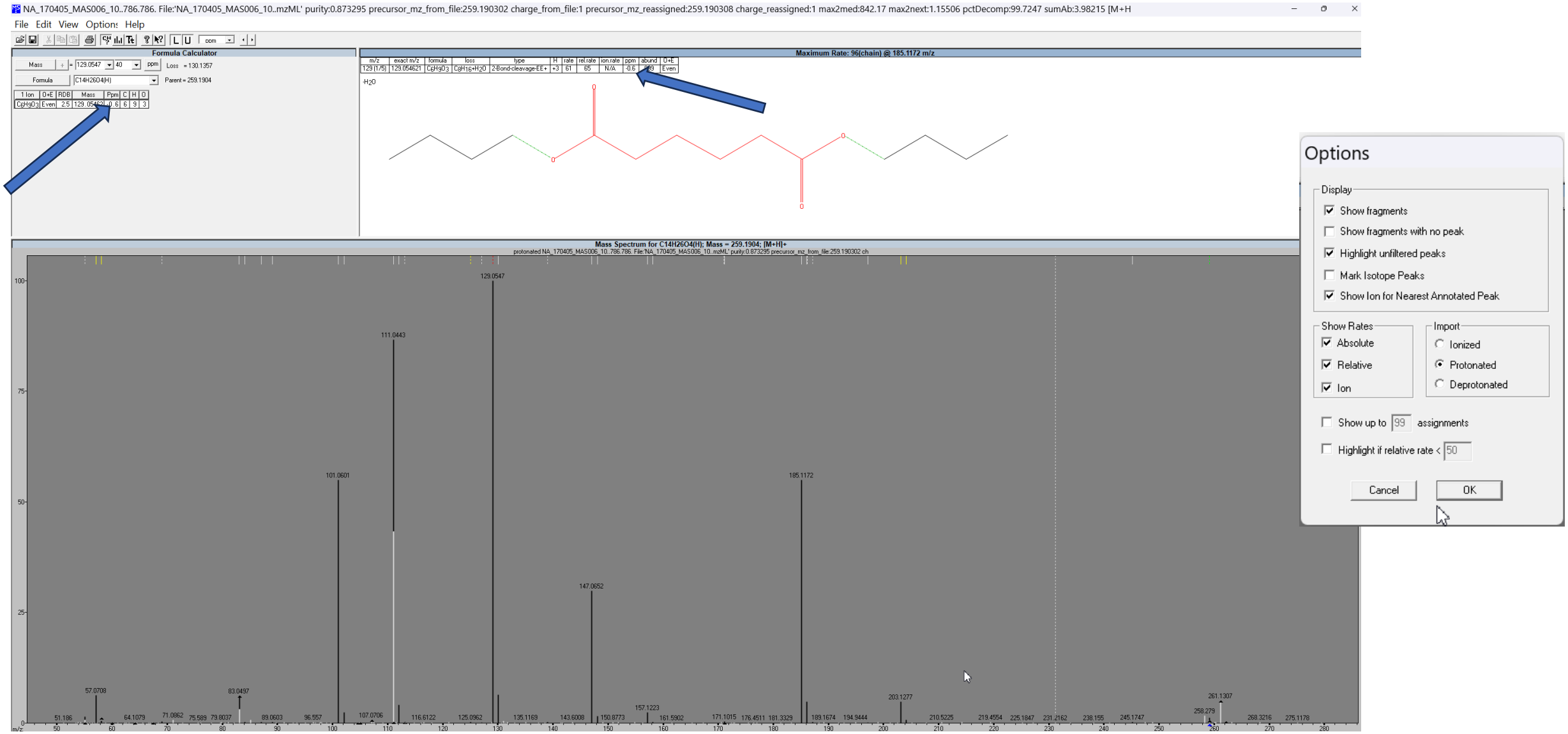
Can Send Any Result in Chromatogram Search Results List to MS Interpreter

When you right click in the list and “Send to MS Interpreter,” your unknown spectrum sent to MS Interpreter and paired with the structure from library identification in list



Left Click on Any Ion in the Spectrum to See Substructure and Associated ppm Accuracy

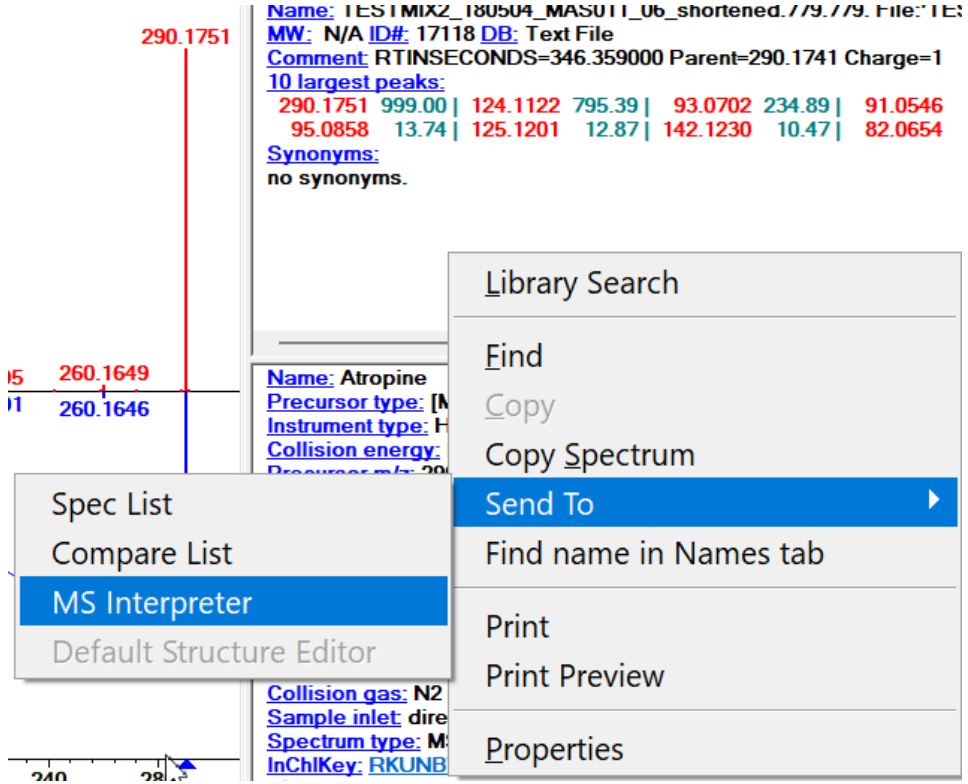
Note in Options, "Protonated" is Selected Automatically



Spectra sent from Text Box of Your “Head to Tail Plot” to MS Interpreter

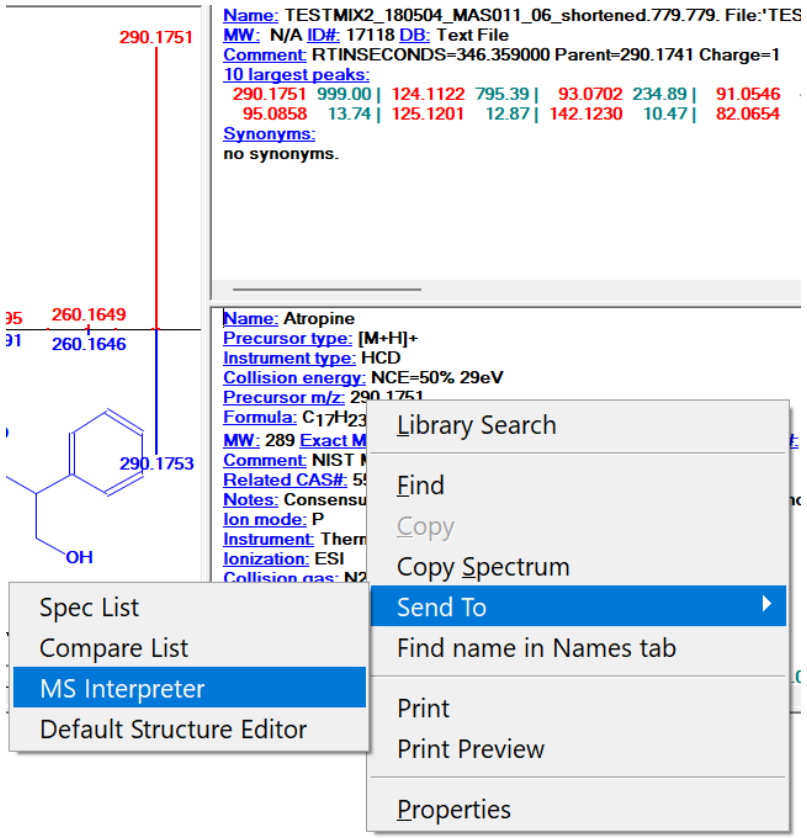
Sent from Text of Unknown with Right Click, Spectrum of Unknown Sent to MS Interpreter with ***No*** structure

*Note **Ionized Selected Automatically**, Change to Protonated in MS Interpreter Options!*

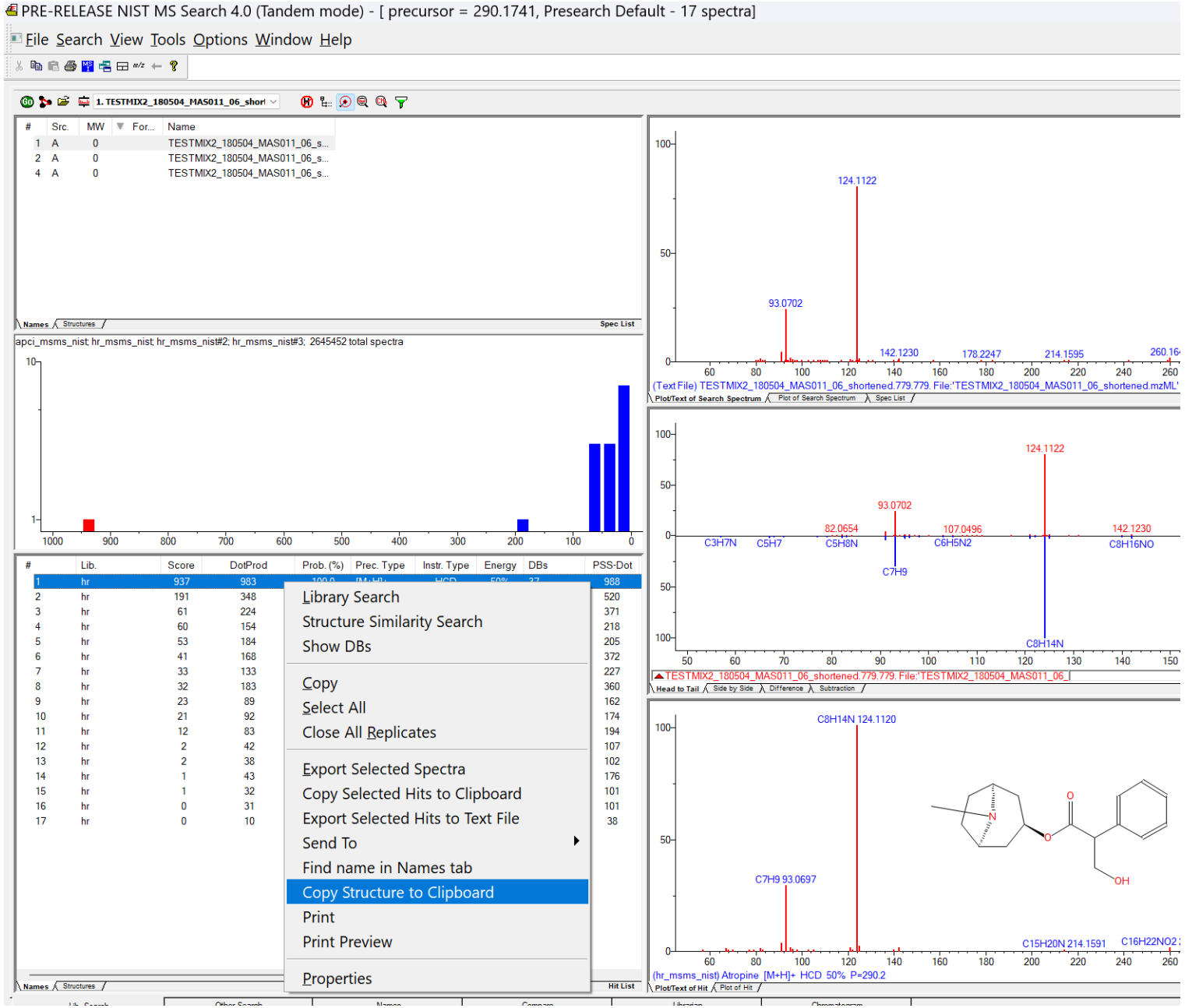


Sent from Text of Library Results with Right Click, Library Spectrum and Associated Structure Sent to MS Interpreter

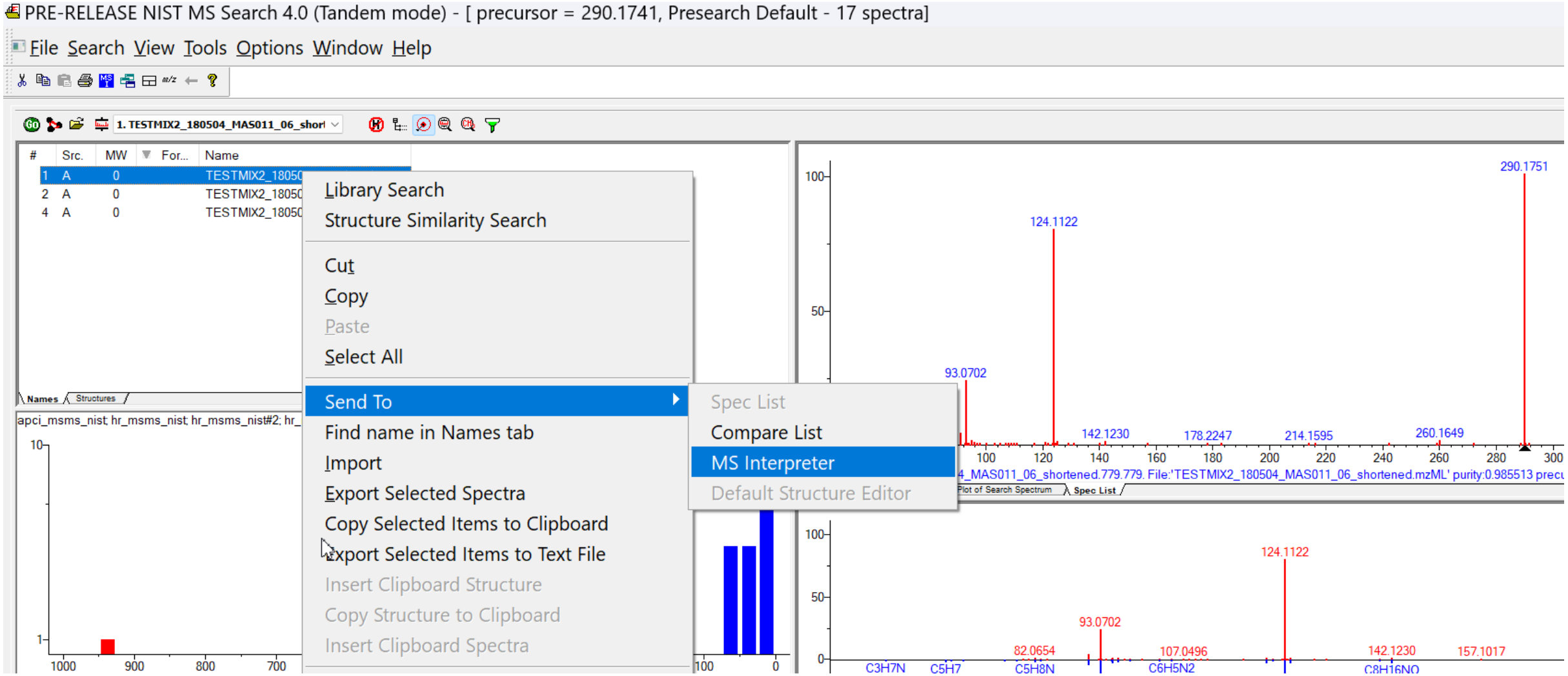
Note Protonated Selected Automatically in MS Interpreter Options



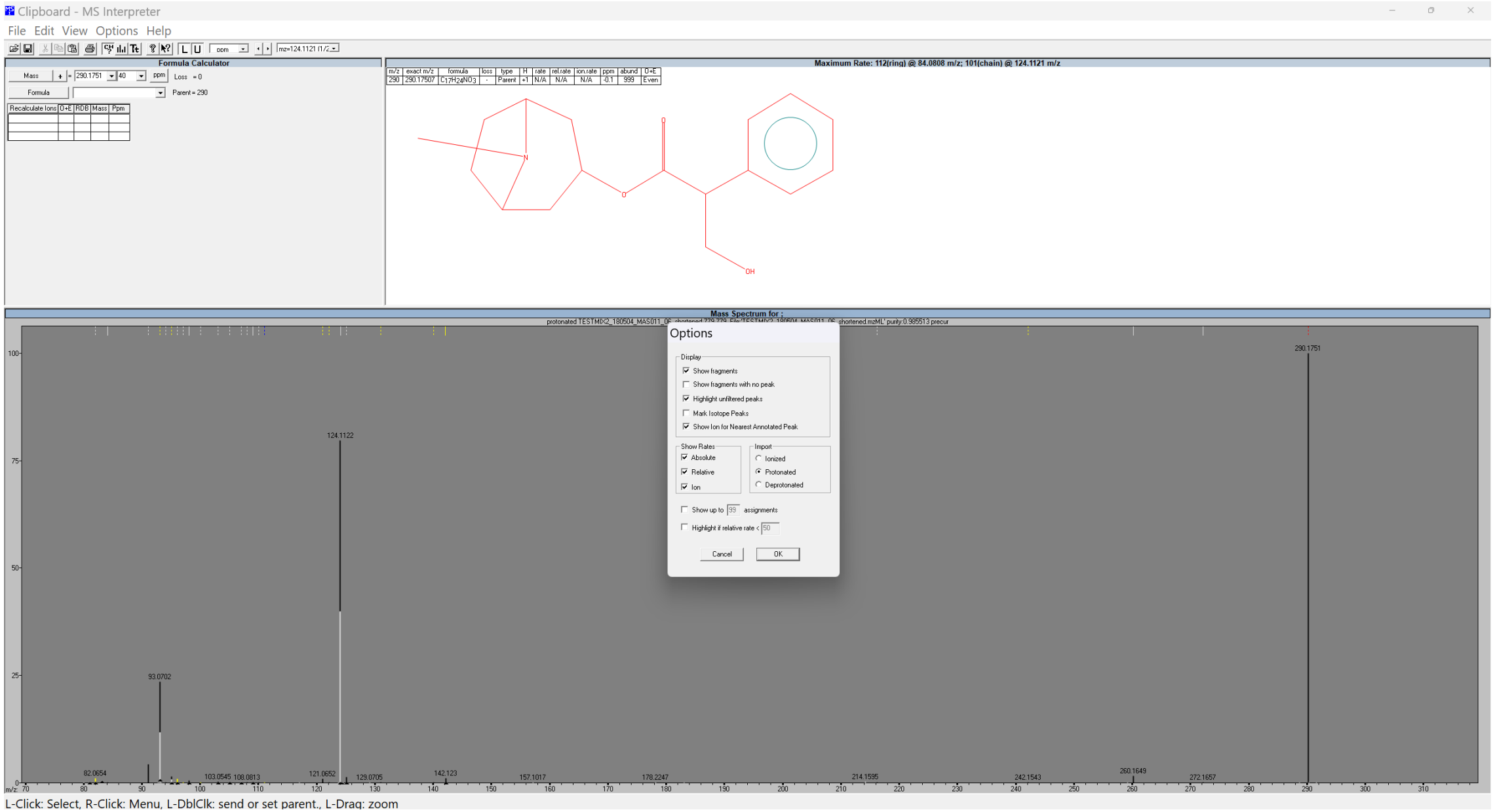
You can add your own spectrum in MS Interpreter, Get a Structure from Results List or Drawing Program



Then Send the Spectrum of Your Unknown from Spec List Window

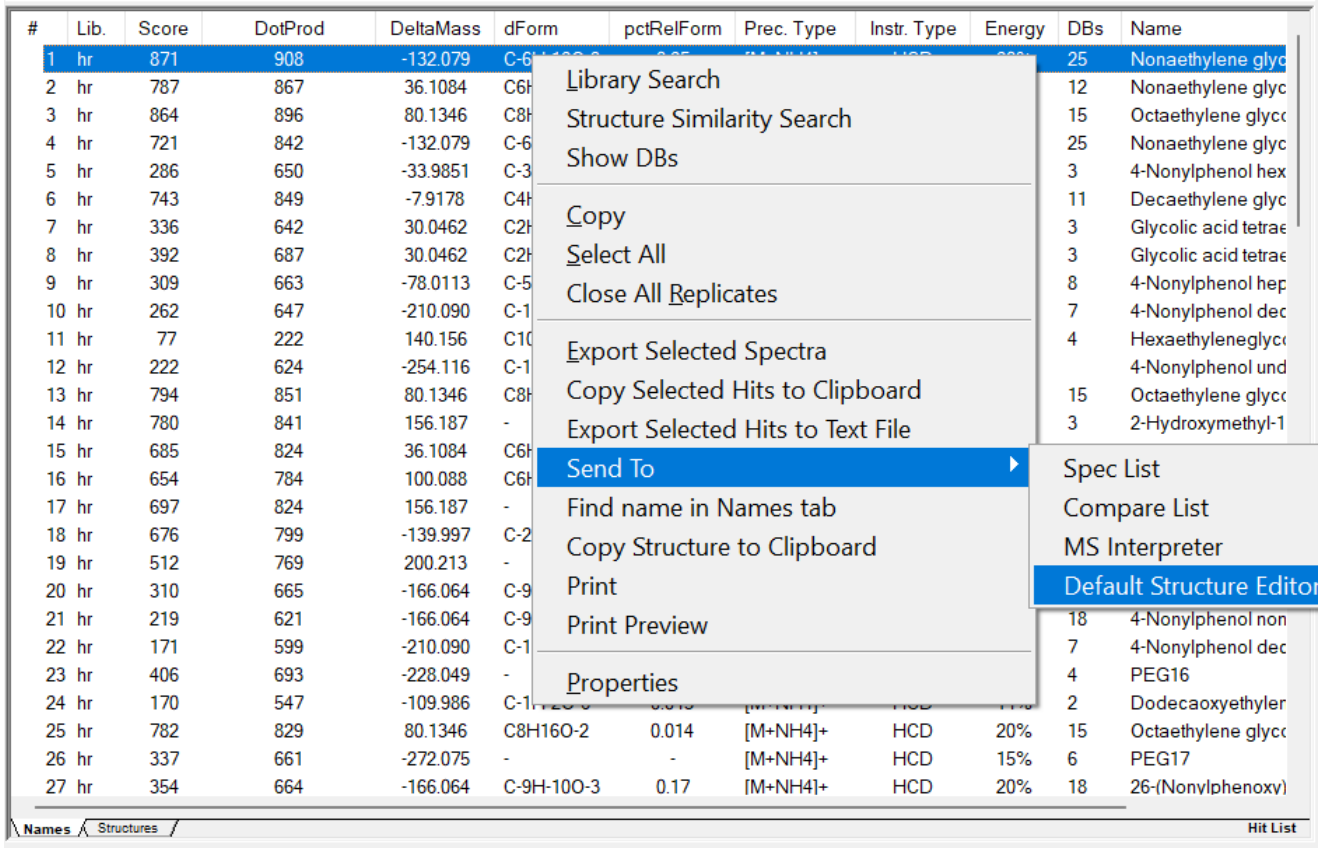


Can Either Edit/Paste or Ctrl V (keyboard sequence) to add structure to MS Interpreter Window

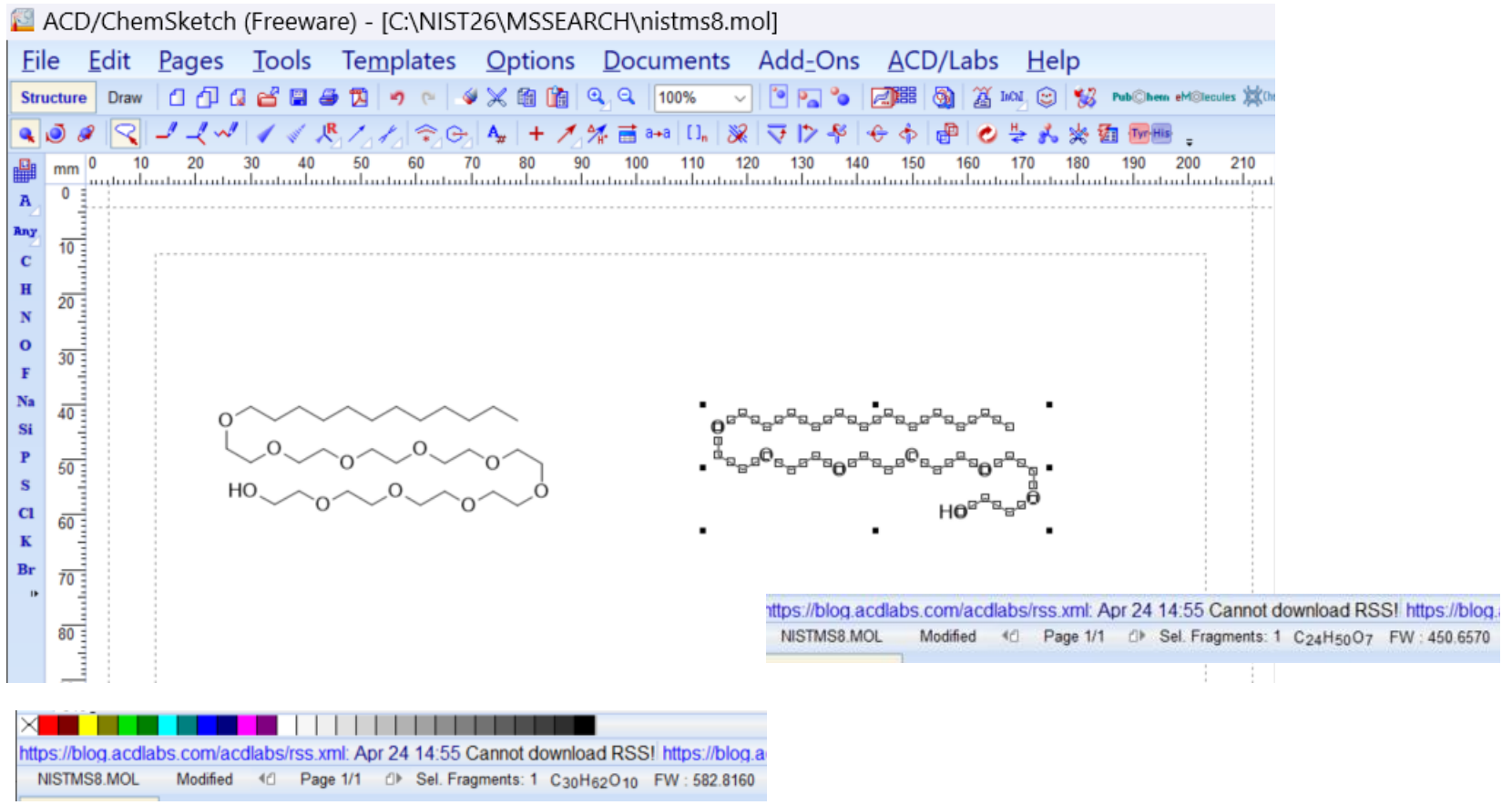


Adding Your Own Structure from Drawing Program and Pairing with Unknown Spectrum
Example with Hybrid Search Result in Lib Search Window

- **Take Advantage of Modifying Structures with NIST Windows**
- ***Much faster*** **than drawing from scratch!**
- ***e.g.,*** **I had a proposed structure that differed by 3 ethylene oxide groups**
- **Took best match and sent to structure editor**



- **Erased 3 of the Ethylene Oxide Groups**
- **Highlighted new structure and copied to clipboard**
- **Then pasted it into MS Interpreter to evaluate**



Evaluation of Proposed Structure in MS Interpreter After Editing Similar Structure in Structure Drawing Program

Note: Change from Ionized as Default to Protonated