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

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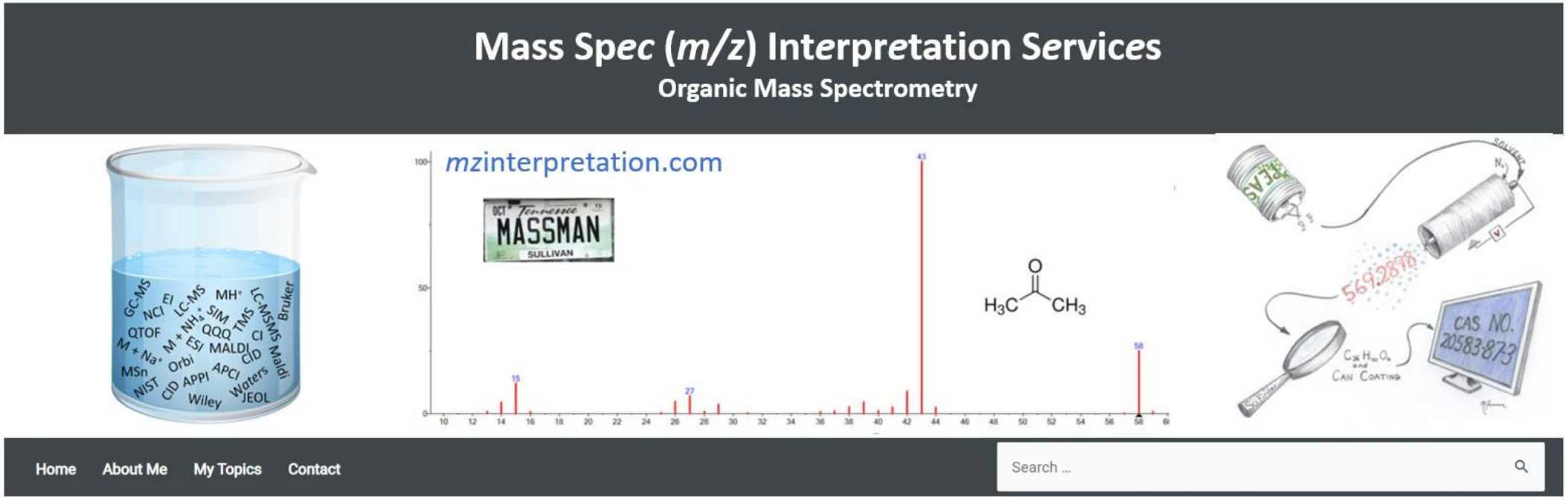
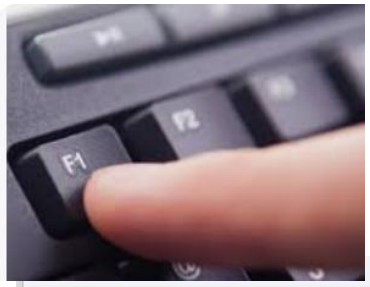
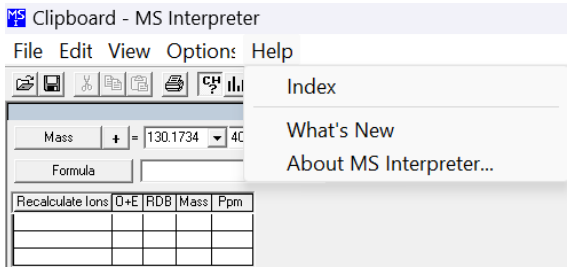
See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!

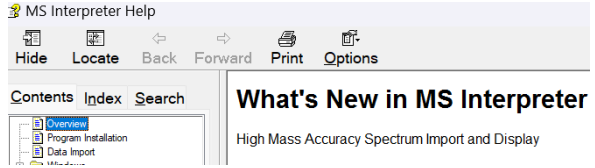


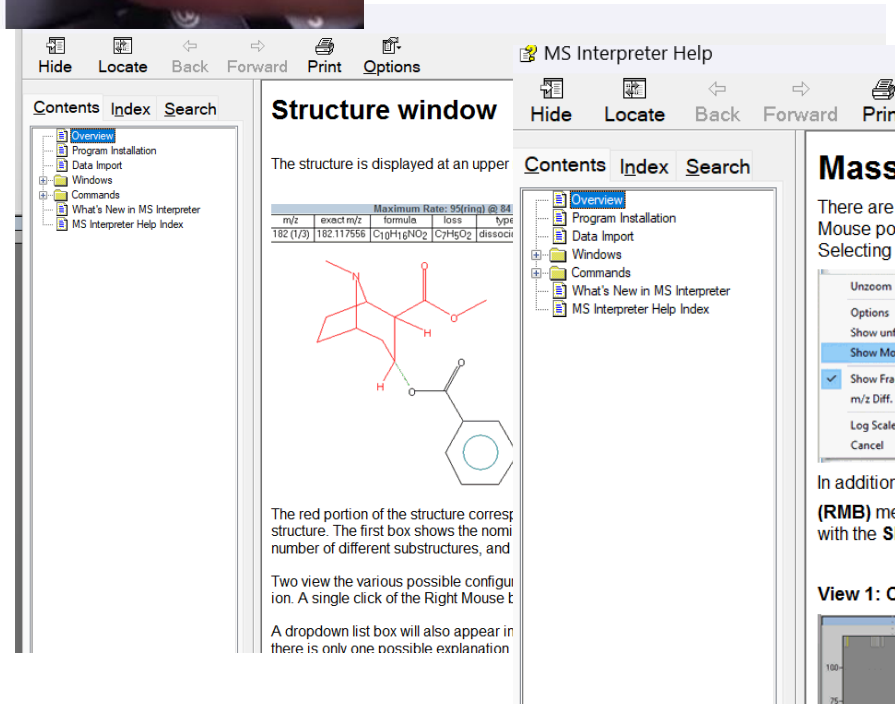
Help in Using MS Interpreter

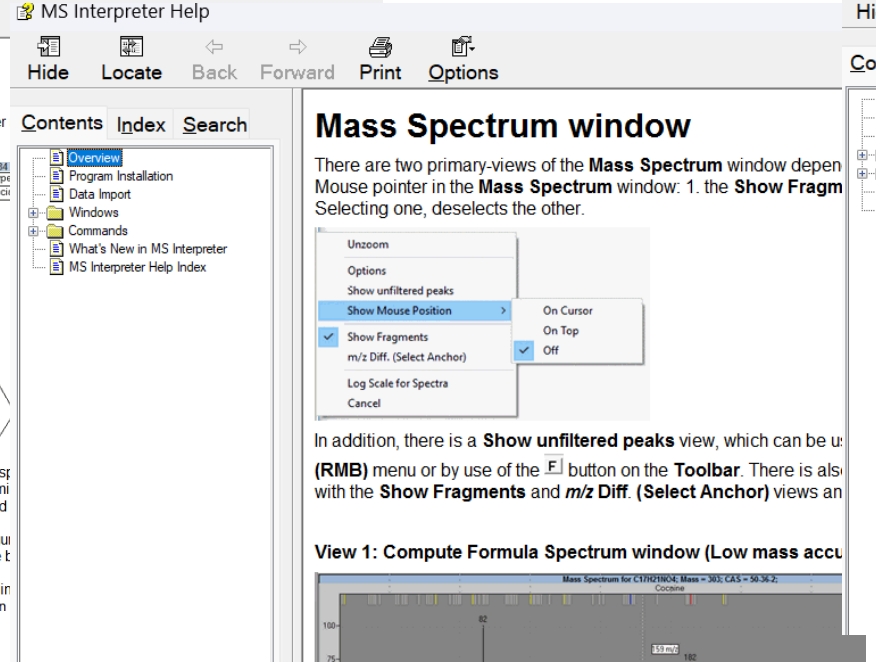
- **Use the Help on Menu Bar and see Whats New and Index**
- ***ALSO*, F1 on keyboard when *ANY* of the windows give addition information**

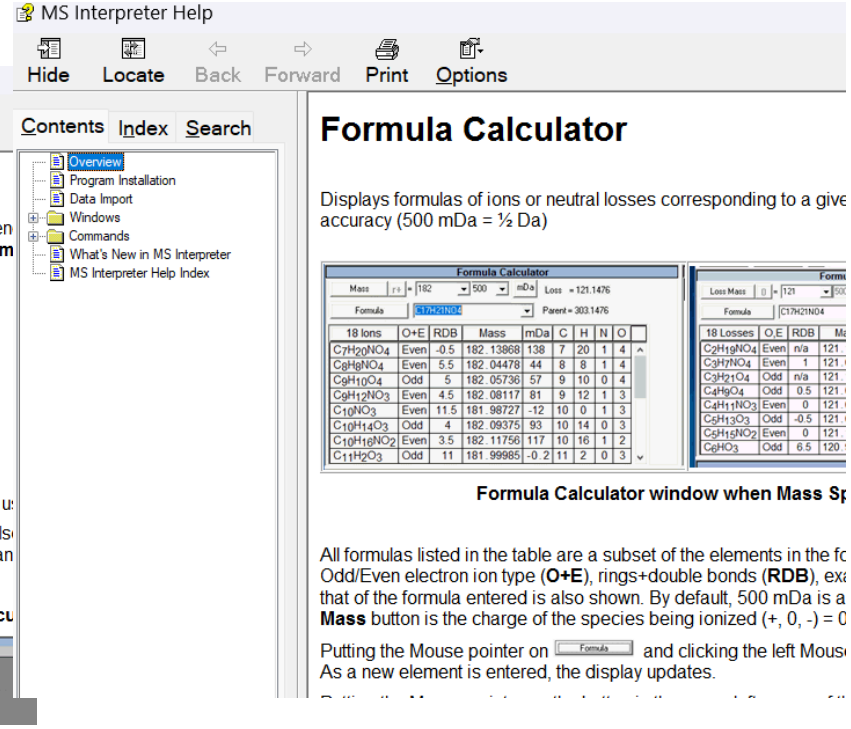








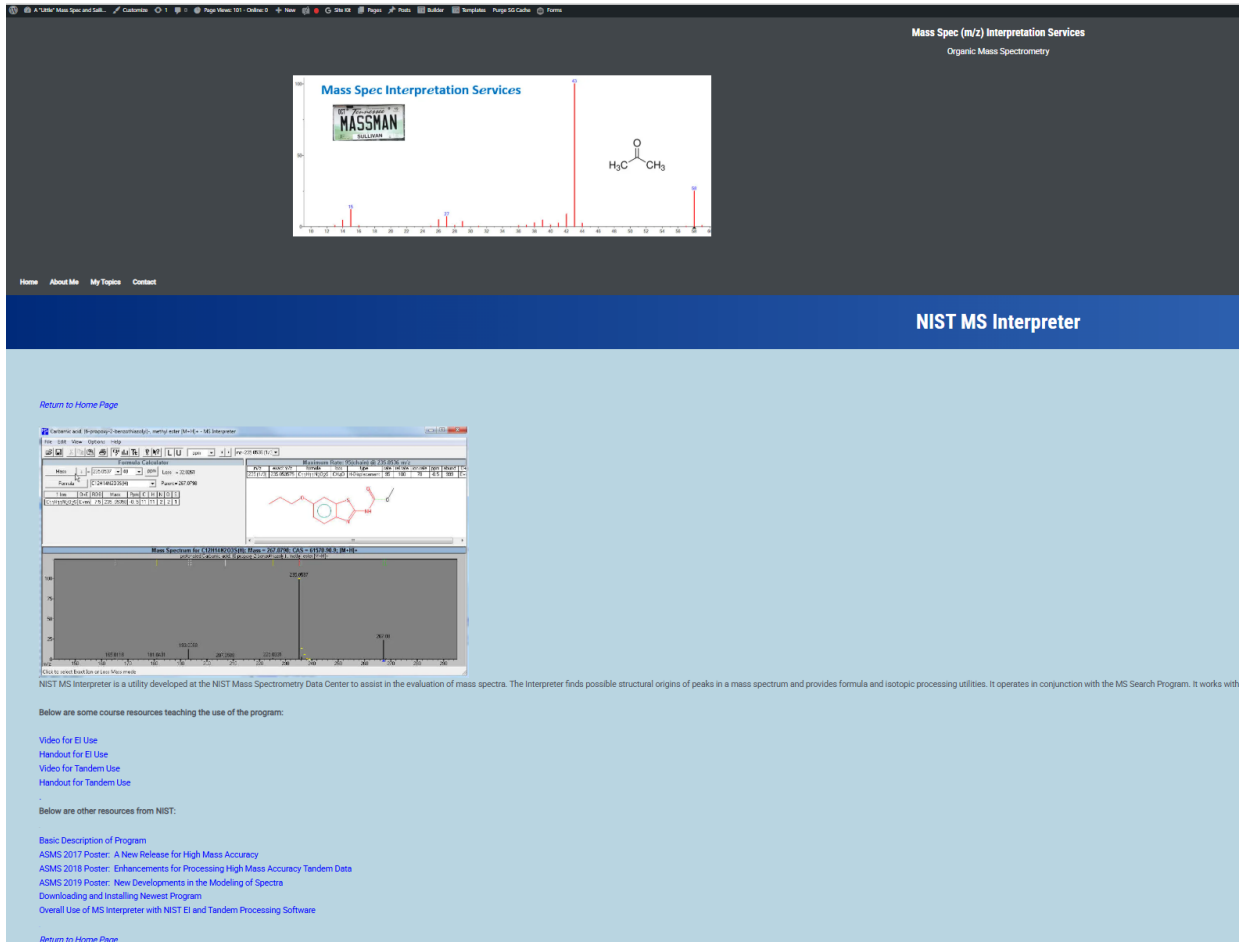




Other Training Videos and Handouts on MS Interpreter

- Many other resources from previous versions
- Very ***useful still***, especially for the ***new user!***
- ***See Links below***

See *link*



See *link*

- V4.0 (2026): start with NIST26
- V3.0 (2023): start with Part 0
- V2.4: start with Part I

Videos and Videos Zipped:

NIST26
Part 0: Changes in EI NIST23 Program (V3.0)
Part I: Spectral Searches with NIST MS Search
Part II: Structure Searches with MS Search and Using MS Interpreter
Part III: AMDIS (NIST) for Processing EI Mass Spectral Data Files
Part IV: Advanced NIST Hybrid Search of EI and MS/MS Spectra
Part V: Creating and Sharing User EI and MS/MS Libraries
Part VI: Creating and Using Retention Indices in NIST Software
Part VII: Tracking Complex Coelution with AMDIS and NIST Search

Parts 0-VI Zipped

Detailed Handouts:

Part 0: Changes in EI NIST23 Program (V3.0)
Part I: Spectral Searches with NIST MS Search
Part II: Structure Searches with NIST Search and MS Interpreter
Part III: AMDIS (NIST) for Processing EI Mass Spectral Data Files
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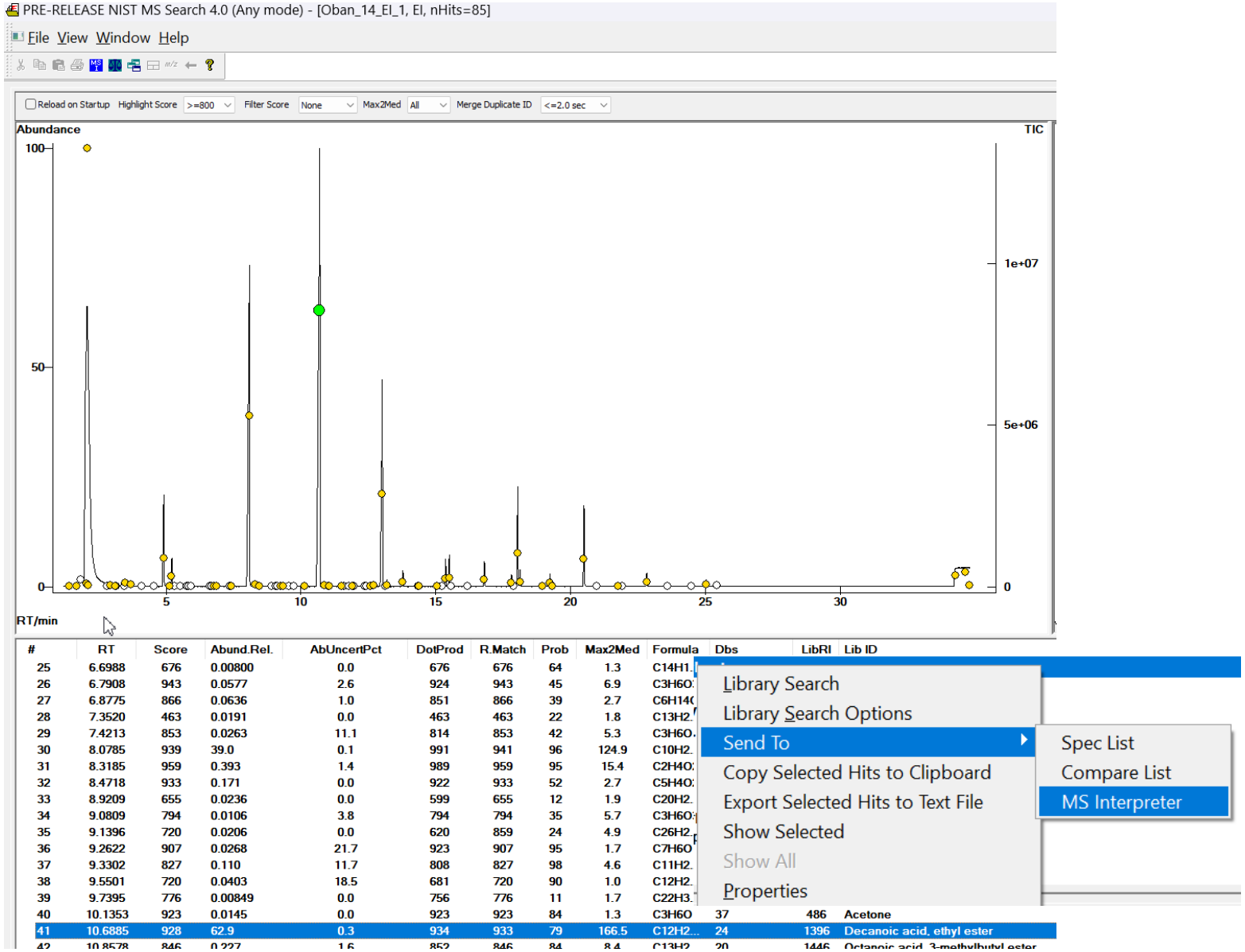
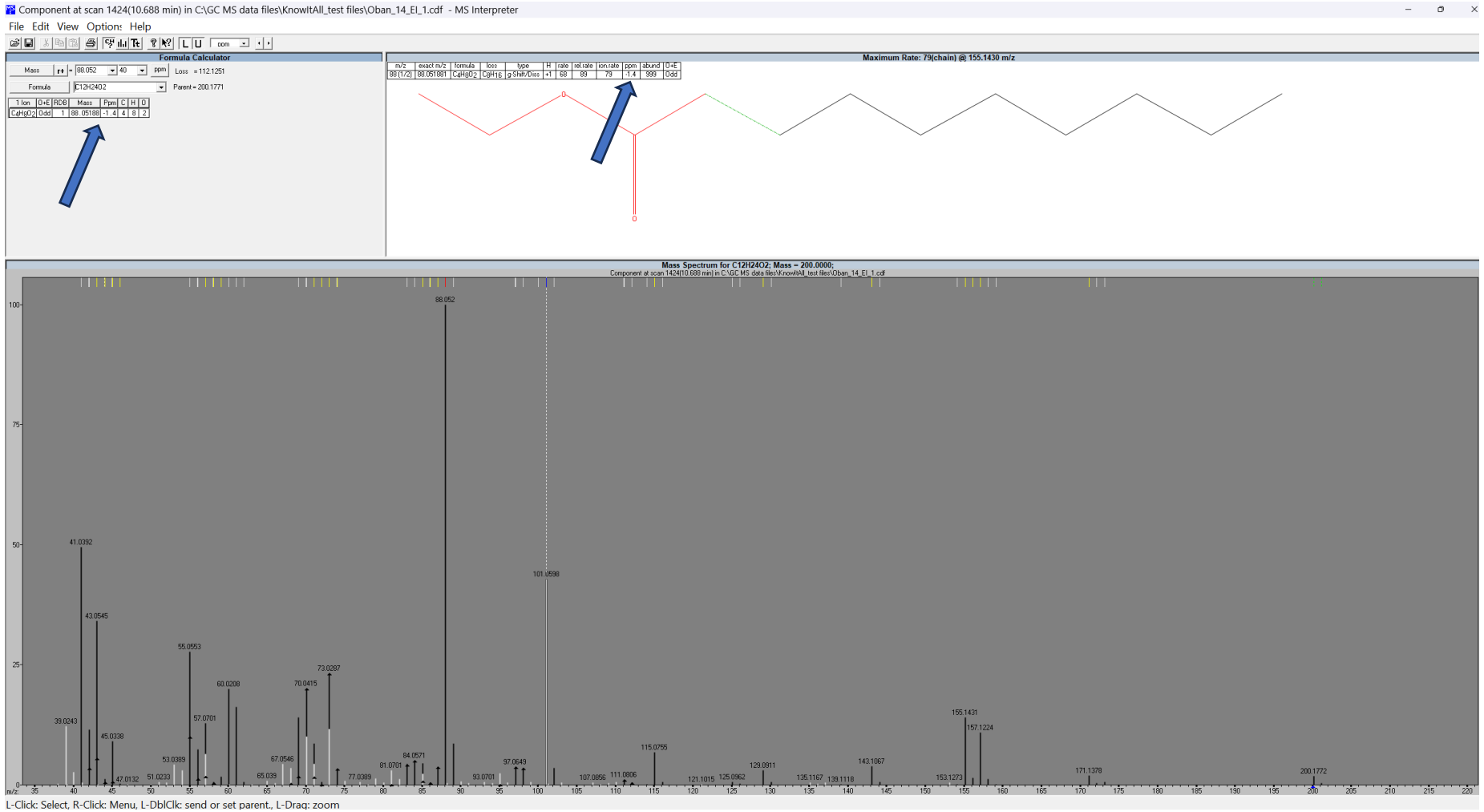
Can Send Any Result in Chromatogram List



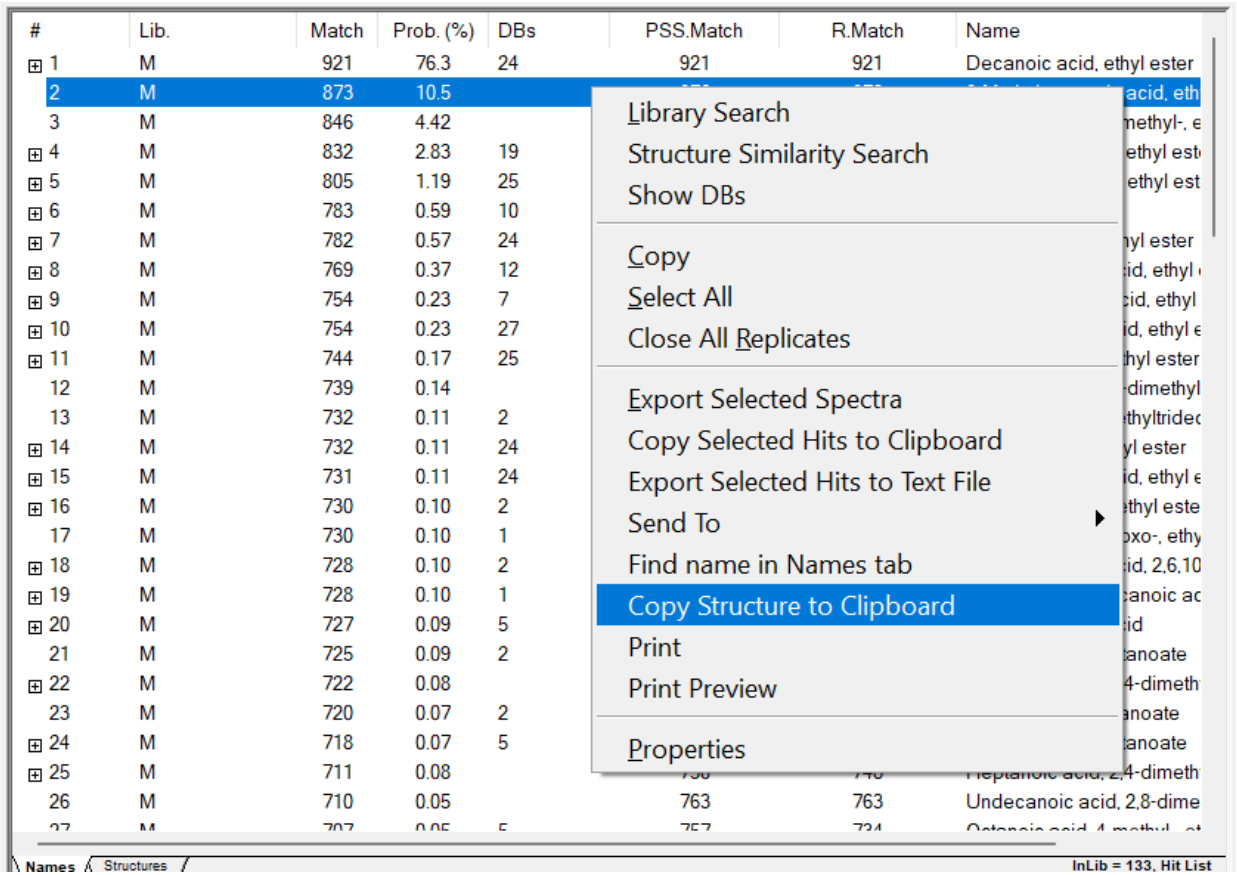
Overall Process

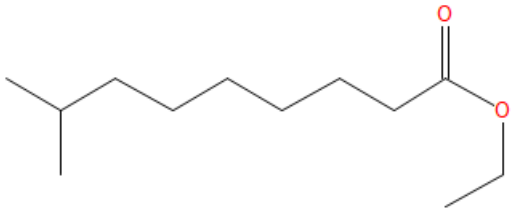
- Spectrum is sent from Chromatogram for the unknown identification from bottom list to MS Interpreter,
- Structure for known is ***paired*** with the Unknown's EI spectrum in transfer process
- User gets the accurate mass errors in ppm and the proposed substructures assigned to observed fragment ions
- Can send spectrum from text section of "Head to tail" display, but for the top one just get the accurate mass spectrum no structure
- For the bottom one, get the library spectrum and its structure



Sending Unknown Accurate Mass Spectrum to MS Interpreter and Adding Structure of Identified Component from Lib Search Window *(First Step)*

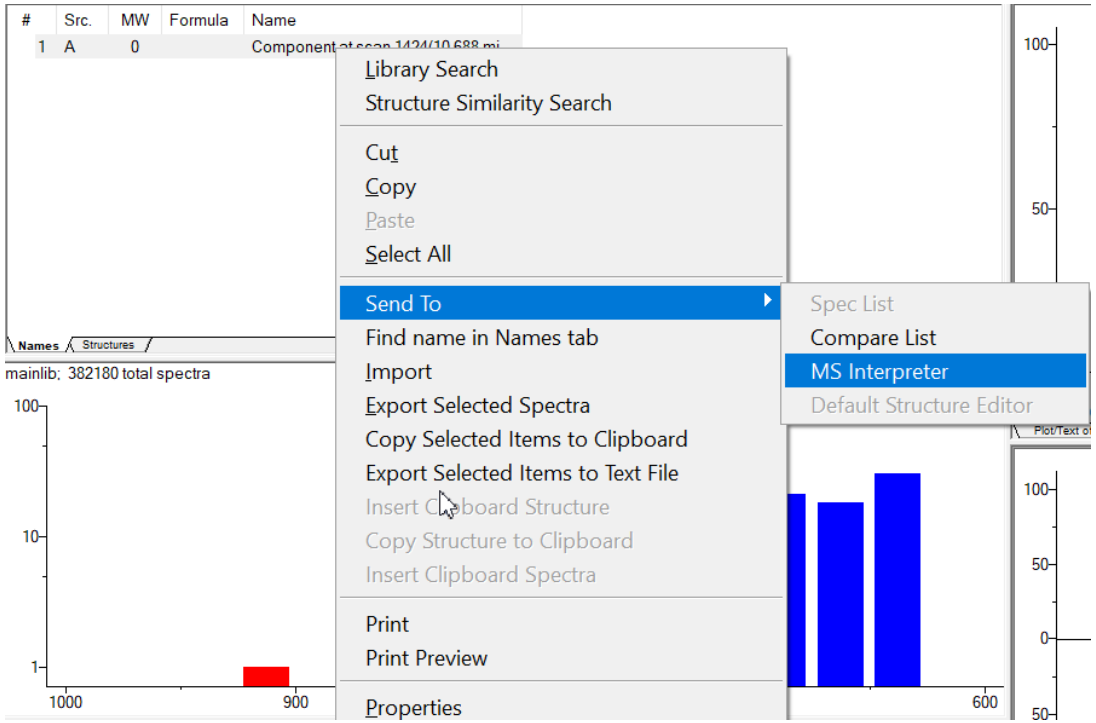
- Use this approach if the best hit in Chromatogram is ***not*** the best candidate
- Compare a hit with lower Match Factor
- Copy the structure of second-best match in Lib Search Window to clipboard



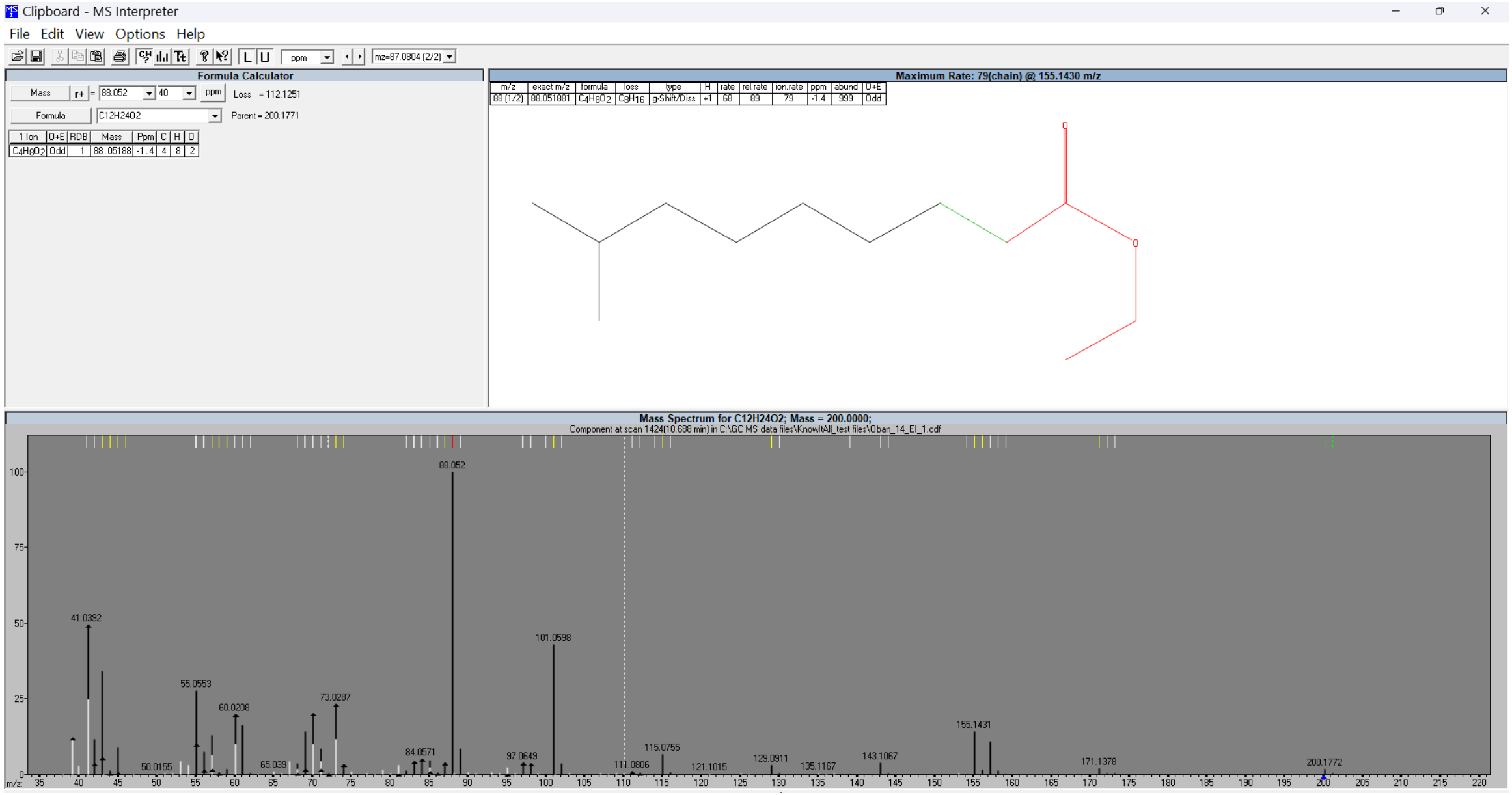


Sending Unknown Accurate Mass Spectrum to MS Interpreter and Adding Structure an Identified Component *(Second Step)*

- Send the accurate mass spectrum from top window in Lib Search to MS Interpreter



Paste Second Best Hit Into Accurate Mass Spectrum Into MS Interpreter



User Proposed Structure for Accurate Mass Spectrum

- First approach, user draws a spectrum in their preferred structural program
- Circle the structure in structural program
- Copy which puts in window clipboard
- Open accurate mass spectrum of interest in MS interpreter (send from Lib Search window)
- Edit/Paste or click on structure box in MS Interpreter then Ctrl V
- Second Approach shown below, ***Often easier,*** send structure from Lib Search to Structural program and modify it
- Much ***more efficient*** than drawing from scratch