Lib Search: Normal EI Search for Spectra Sent from Chromatogram Window

Video/Handout

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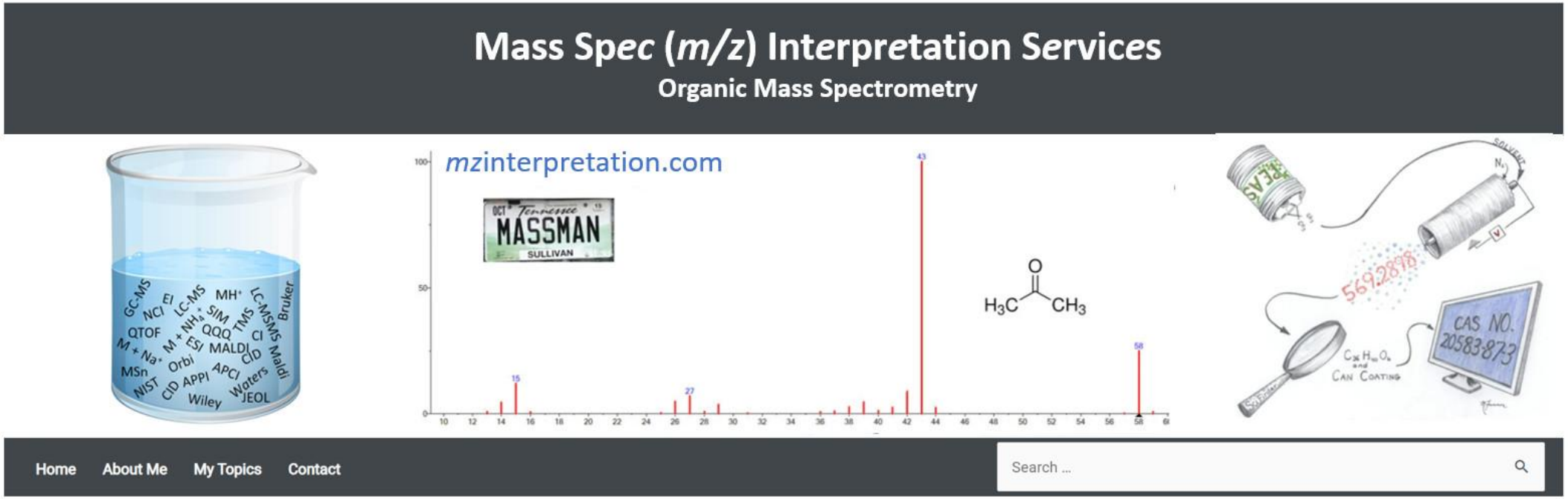
See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!



Lots of Previous Information on Lib Search and Other NIST Software on My Website

NIST Search of EI Mass Spectral Databases in Unknown Identifications

- ***Extensive*** Resources on Lib Search and Other Programs within NIST Search
- See *Link*
- This video ***only*** discuses program ***basics***
- No information on Chromatogram Window

Videos and Videos Zipped:

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

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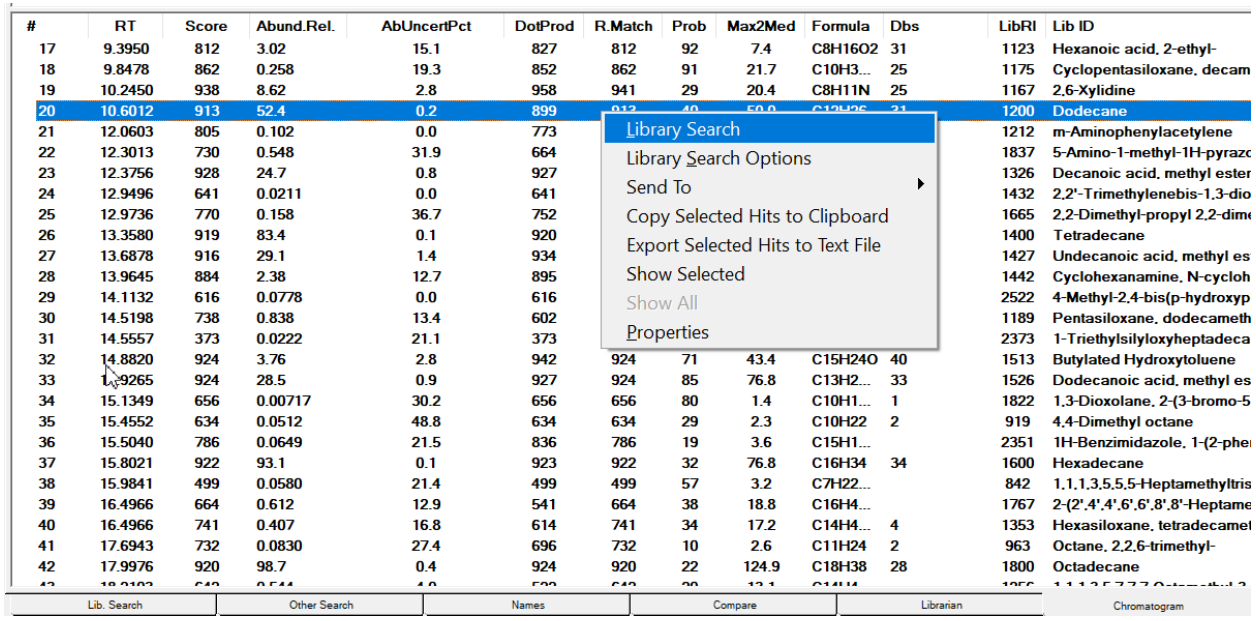
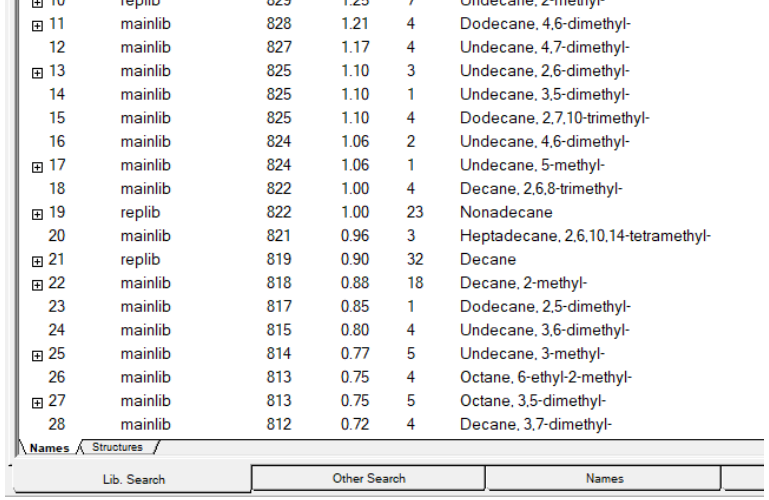
Other Webinar Resources:

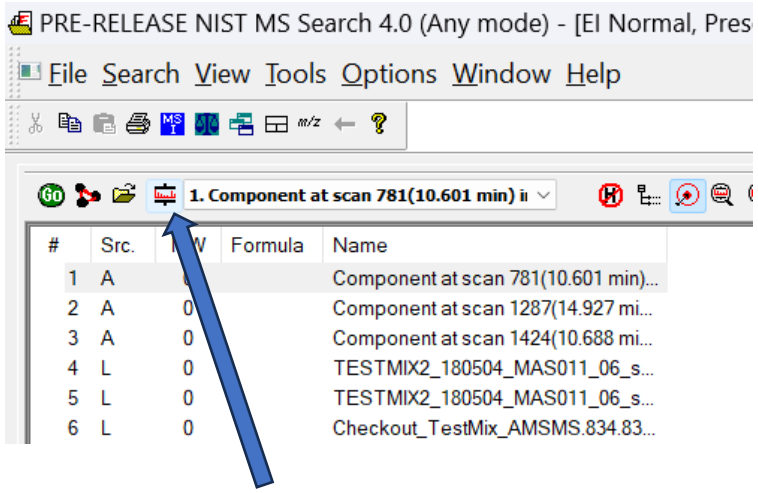
Main Reasons for Sending Results from Chromatogram to Lib Search Window

- The EI Normal Identity search results in Chromatogram ***only*** show the ***best*** result, *i.e.*, only one hit per unknown
- The same search in Lib Search Shows Large List of candidates
- Send to Lib Search by right clicking on component of interest then selecting “Library Search”

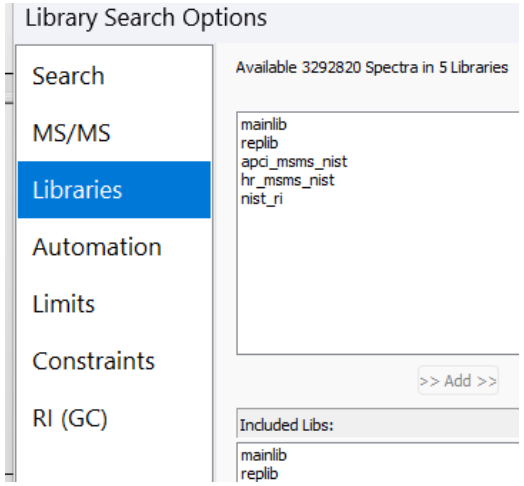




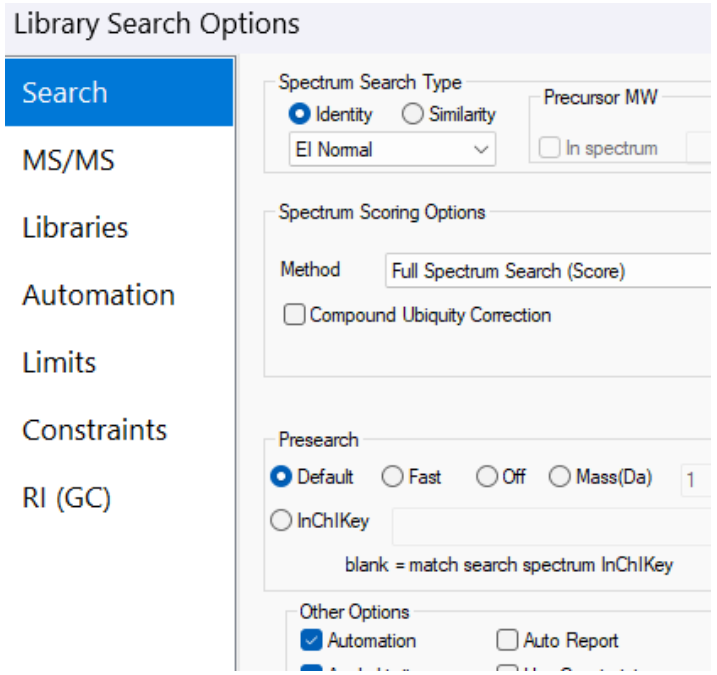
Open Settings



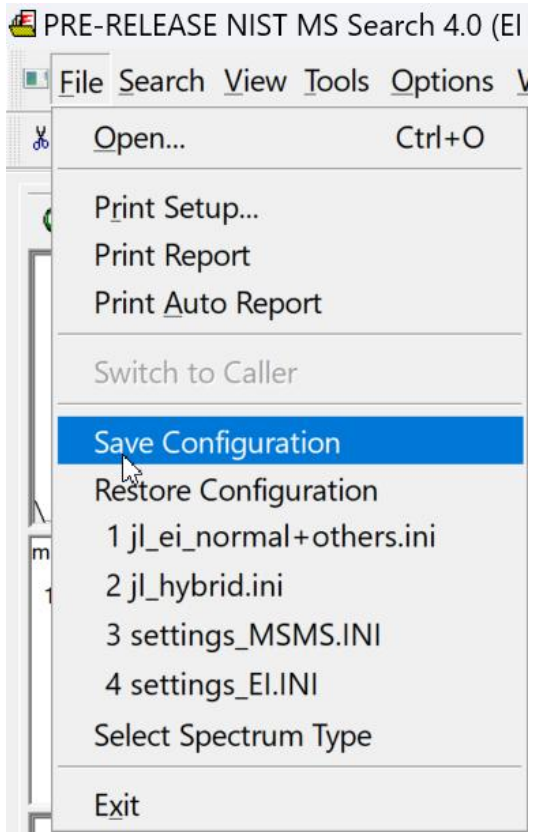
- Select Libraries
- Commercial Libraries *e.g*. Wiley
- User Libraries, *etc.*
- Results combined



- Identity Radio Button selected
- EI Normal is the same search performed in Chromatogram Window
- Full Spectrum Search



- Save configuration
- Settings, Font and window sizes, etc.

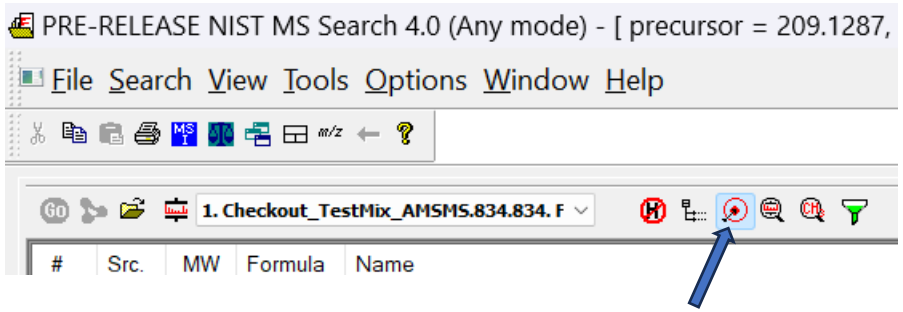


EI Normal Identity Search

- Note no, of spectra top bar
- Note Type of Search, bottom right bar
- Type of information displayed bottom right bar

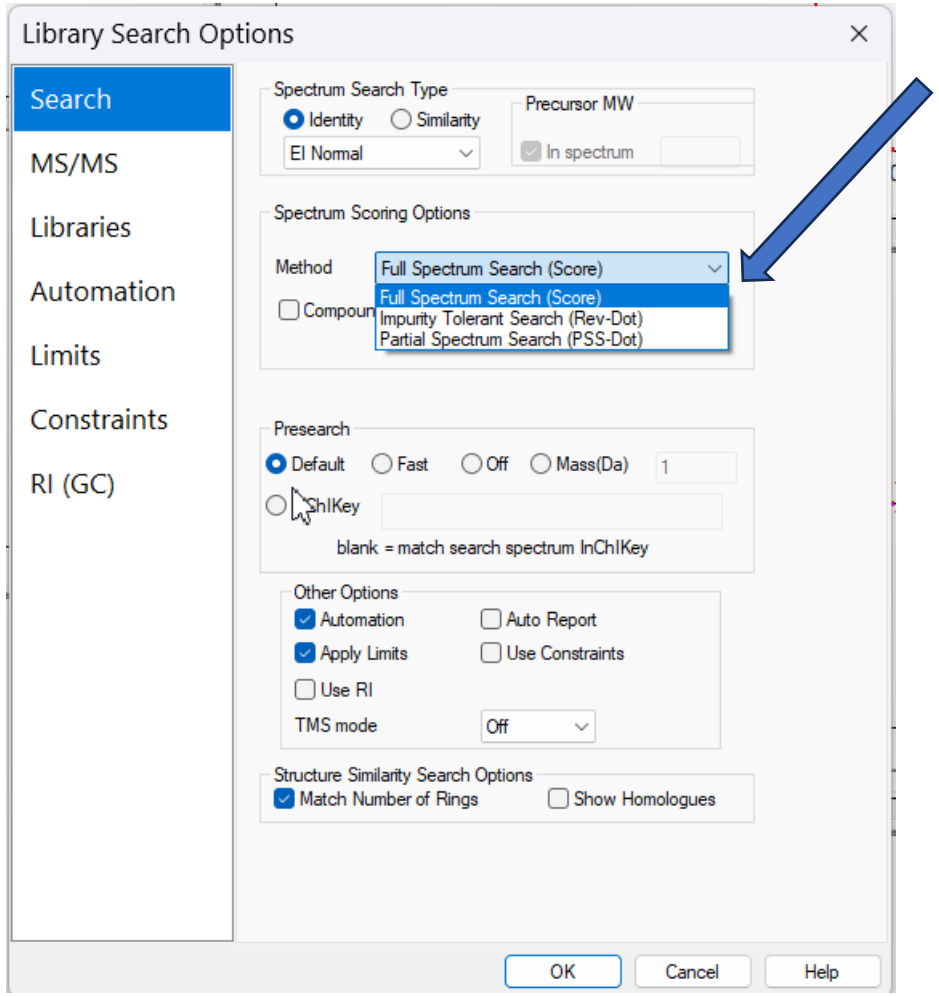
Useful Filter Best Matching Only

- Best matching Only
- When selected, it removes most duplicate search results
- Makes reviewing data easier
- Toggle on and off by depressing button
- Done after the Presearch, thus reversable
- These filters applied ***after*** Presearch, and can be ***easily reversed***



Best Matching Only

Other Options Besides Standard Full Spectrum Search (Score)



Method Selected:

- Full spectrum matching compares entire spectra and works best for clean data. Reverse matching focuses on whether key library peaks are present, making it robust to chemical noise.
- In other words, Reverse-Dot search does not penalize for extra peaks in spectrum that are not present in library spectrum
- The Wiley Library contains many partial spectra from the literature
- Thus, the Reverse Search (Impurity Tolerant Search, Rev-Dot) gives better search results against an unknown pure spectrum for these partial library reference spectra
- Can sort by left clicking on R.Match in results for full spectrum search, but entries that are filtered out in Presearch ***will not be found*** in results
- Thus, might need to ***specify the method before*** Presearch
- ***Presearch*** employed to ***greatly increases speed*** of final search
- Partial Spectrum search (PSS-Dot) more useful in tandem applications

Manipulating Search Results in Lib Search Results

#	Lib.	Match	Prob. (%)	DBs	R.Match	Name
⊞ 1	M	923	39.5	31	923	Dodecane
⊞ 2	M	877	5.78	31	889	Tridecane
⊞ 3	M	867	4.20	30	884	Undecane
⊞ 4	M	860	3.36	33	861	Tetradecane
⊞ 5	M	859	3.25	33	860	Pentadecane

- Additional column above added for R. Match
- Normally Match is best value to sort the results
- Can sort after the Full Spectrum search by left click on R.Match, but some values for R. Match might not be present after presearch
- Thus, for best R.Match results, do a “Impurity Tolerant Search (Rev-Dot)
- Then review results

Impurity Tolerant Search (Reverse, Rev-dot) with Results Sorted by R. Match

- No. of hits shown on top bar
- The type of search noted and the type displayed on right bottom bar
- Note, Rev for Reverse, Impurity Tolerant Search, on bottom right corner
- Results are sorted by R Match
- Can reset for standard results by left clicking on Match