Searching Normal NIST Search with Chromatogram Results

Video/Handout

James Little
Mass Spec Interpretation Services
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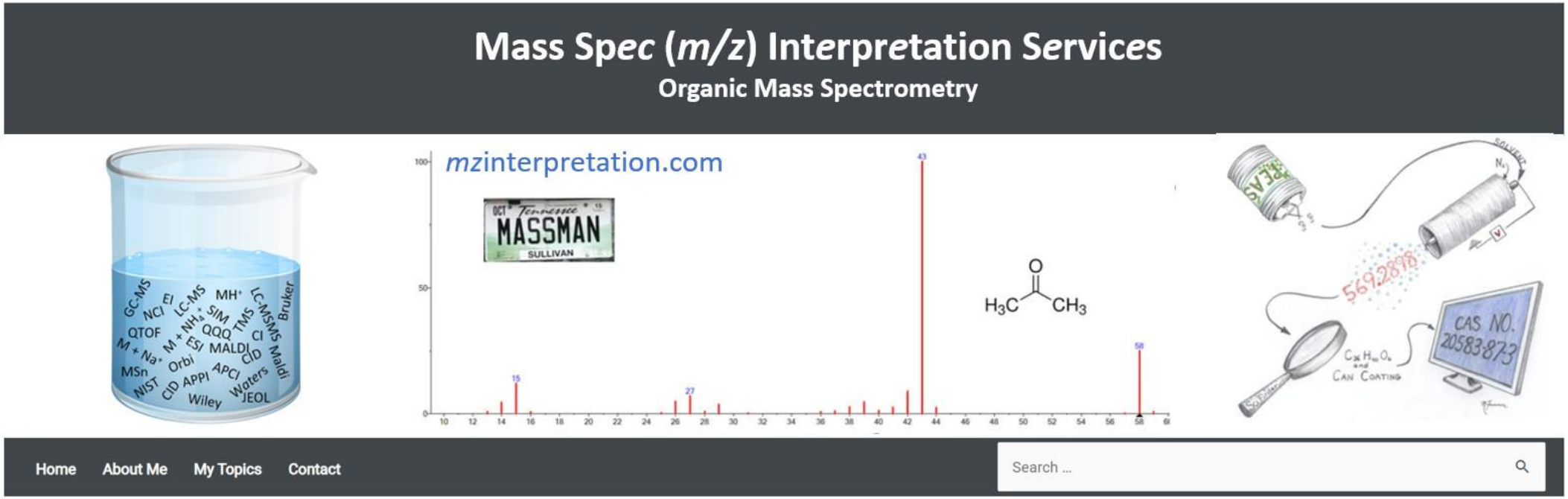
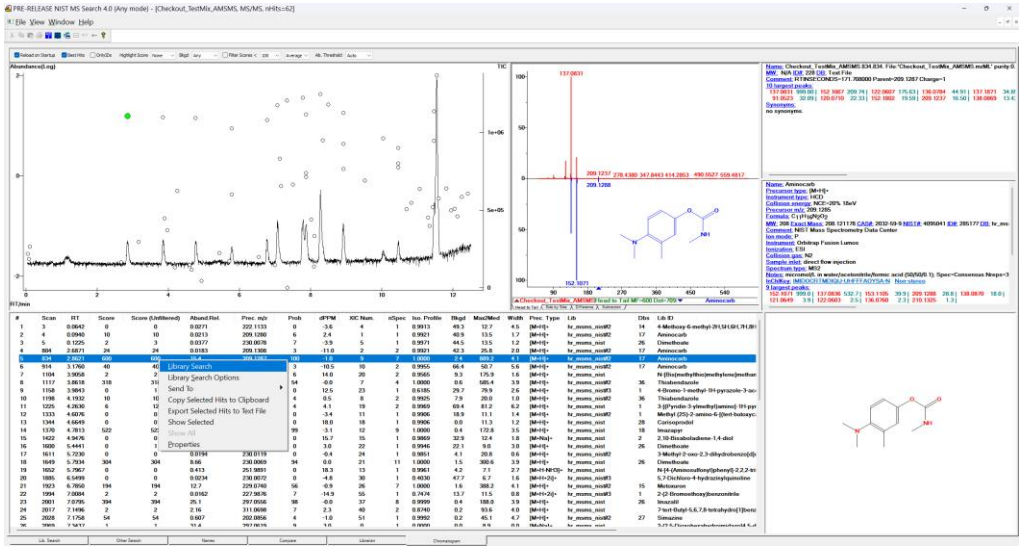
mzinterpretation.com

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

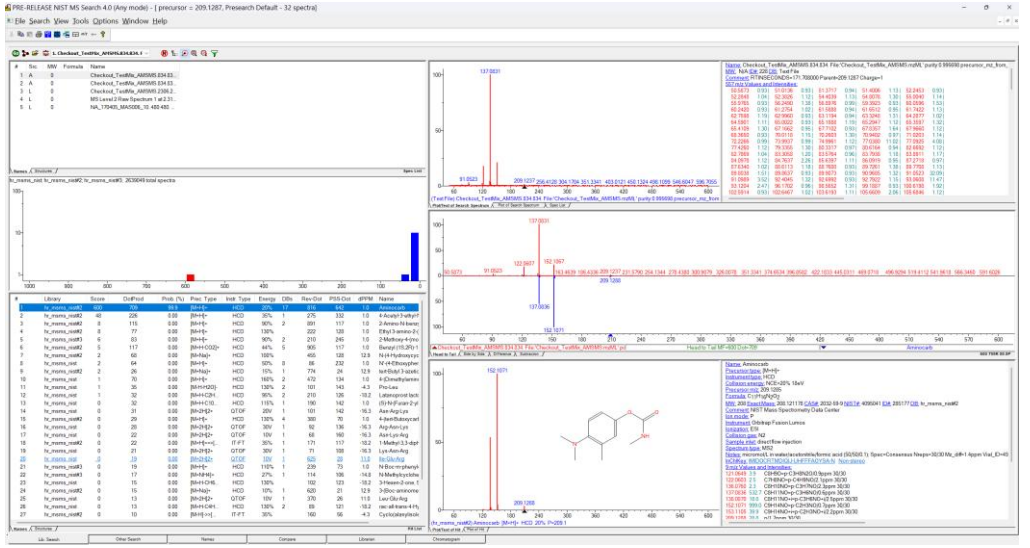


Reasons for Sending Results from Chromatogram to Normal Lib Search Window

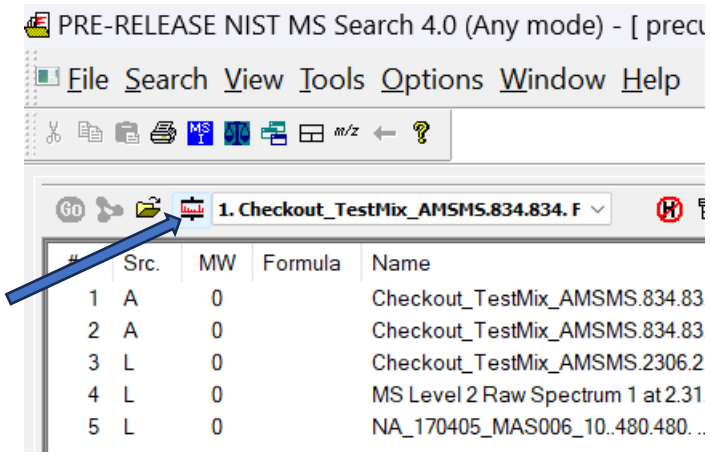
- The search results in Chromatogram only show the best result, Lib Search shows alternate candidates
- Chromatogram ***only capable*** of performing MS/MS and hybrid search with precursor automatically specified
- Identity MS/MS and Similarity Hybrid allows user to select Precursor
- Lib Search has an additional Identity MS/MS HiRes No Precursor searching for substructural information
- Lib Search offers Full Spectrum, Impurity Tolerant (Rev. Dot), or Partial Spectrum Search (PSS-Dot)
- Hybrid Similarity discussed in separate video
- Sent to Lib Search by right clicking on component of interest then selecting “Library Search”



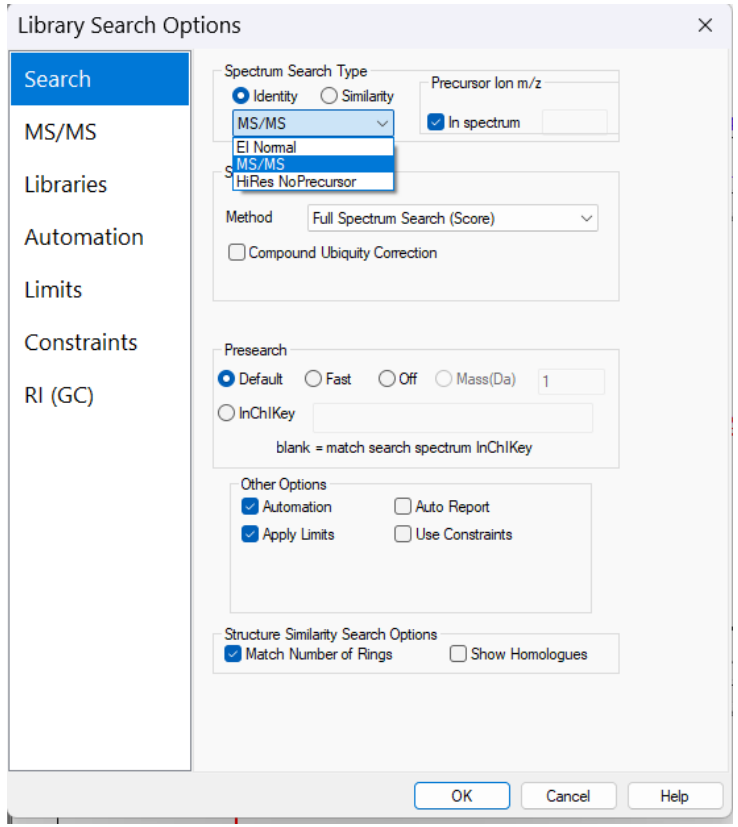
Chromatogram Result List to Lib Search



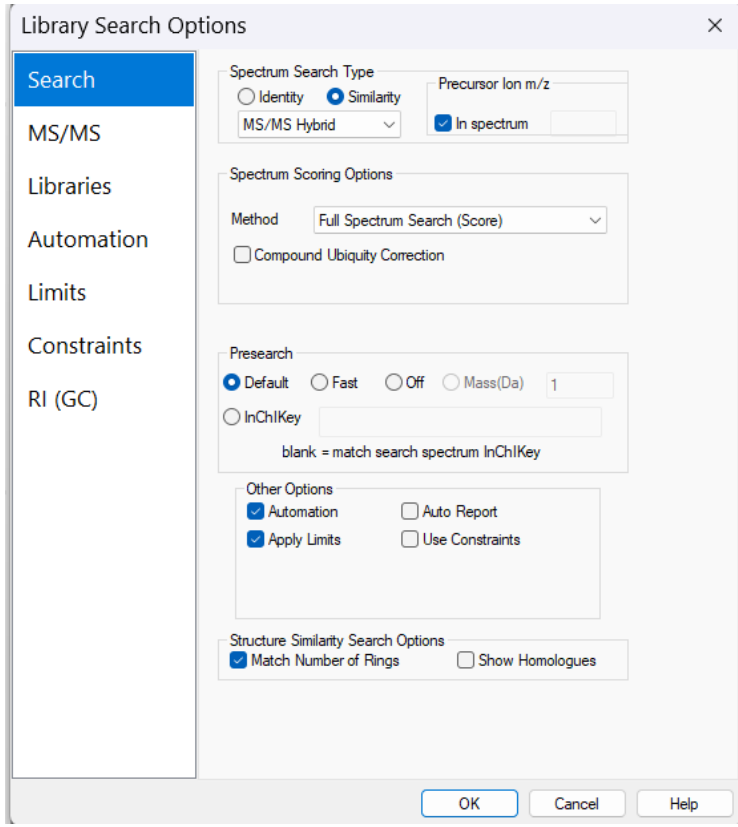
Open Settings

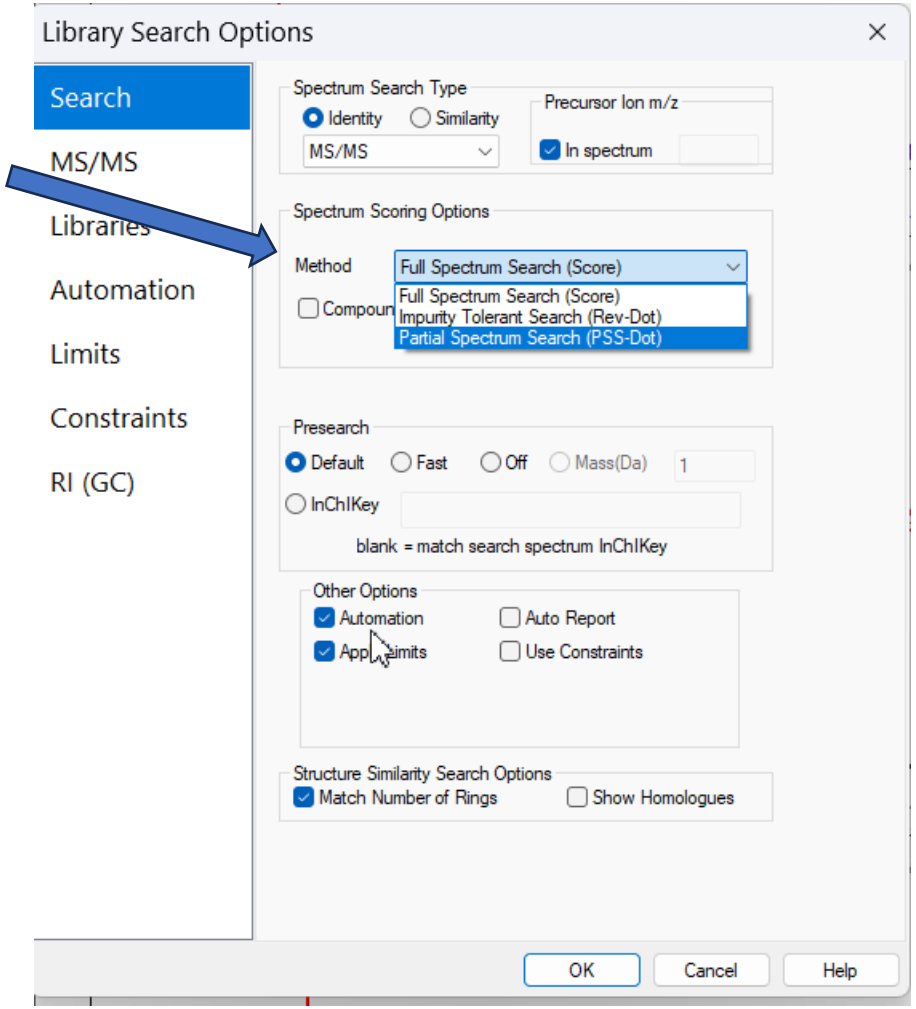


- Identity Radio Button selected
- MS/MS is the same search done in Chromatogram
- In spectrum checked, will use the precursor sent from chromatogram, can uncheck and add your own
- HiRes No Precursor just compares the spectra but does not limit by precursor specified or imported



- Similarity Radio Button selected
- Hybrid Search
- Discussed in separate video/handout
- In spectrum checked, will use the precursor sent from chromatogram, can uncheck and add your own

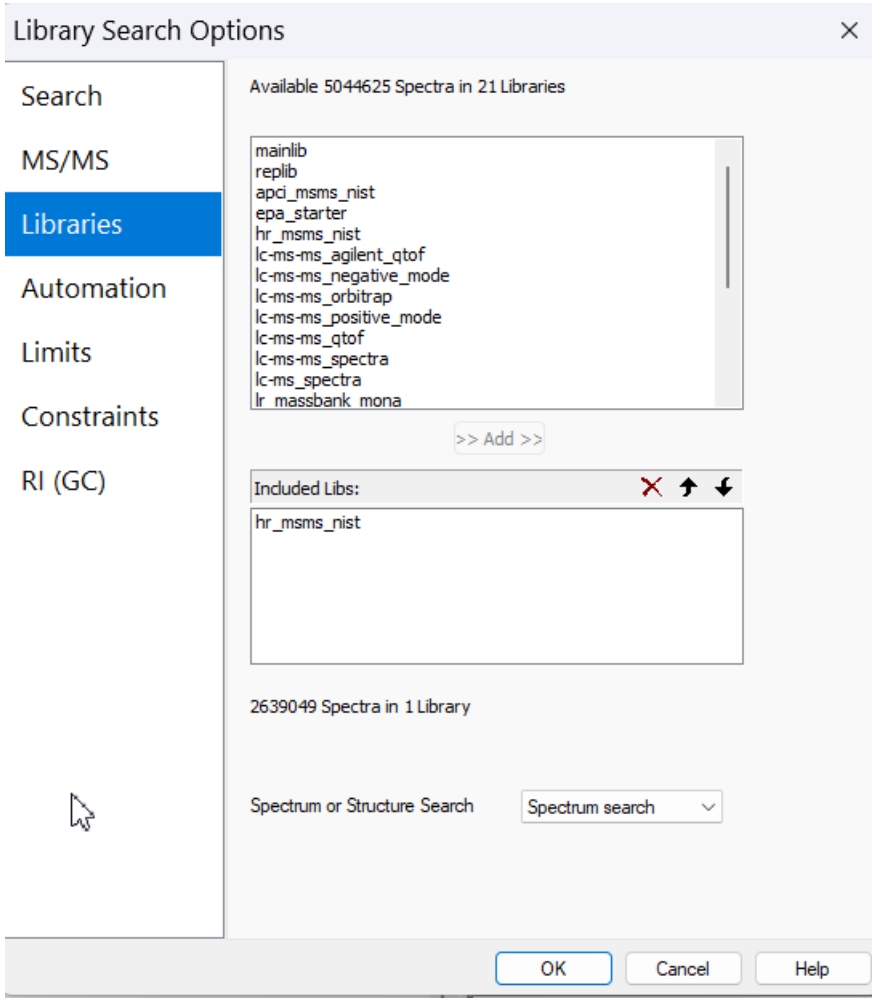


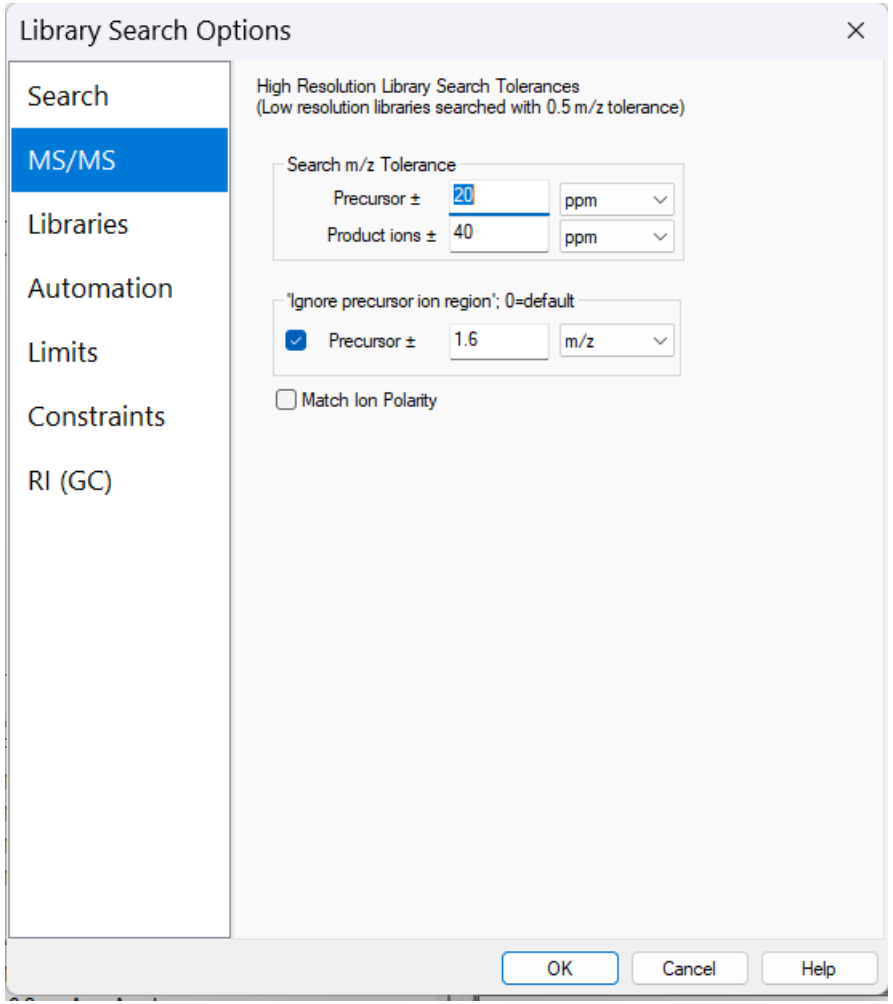


Method Selected:

- 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. Partial search matching is designed for incomplete spectra, such as MS/MS or filtered data, where only a subset of fragment ions is observed
- Reverse-Dot search does not penalize for extra peaks in spectrum that are not present in library spectrum
- Partial spectrum does not penalize for peaks absent in spectrum that are found in library spectrum
- Can see all these values 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 search to get candidate spectra that are more processed in more detail

Select Libraries and Tolerances





Similar to Our Discussion of the Chromatogram Window:

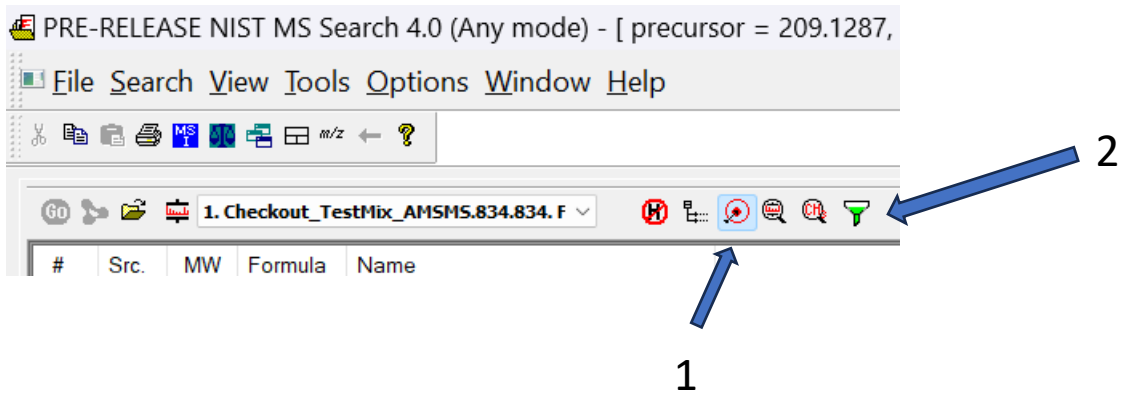
- Windows can be resized by left clicking on bar and dragging
- ***Hovering*** over item on menu bar shows information
- Properties can be added by right clicking and selecting properties
- Order of Properties can be left clicked and dragged to change order and resized
- Left click to sort by the property, normally initially sorted by score
- Use keyboard up and down arrows to step through results

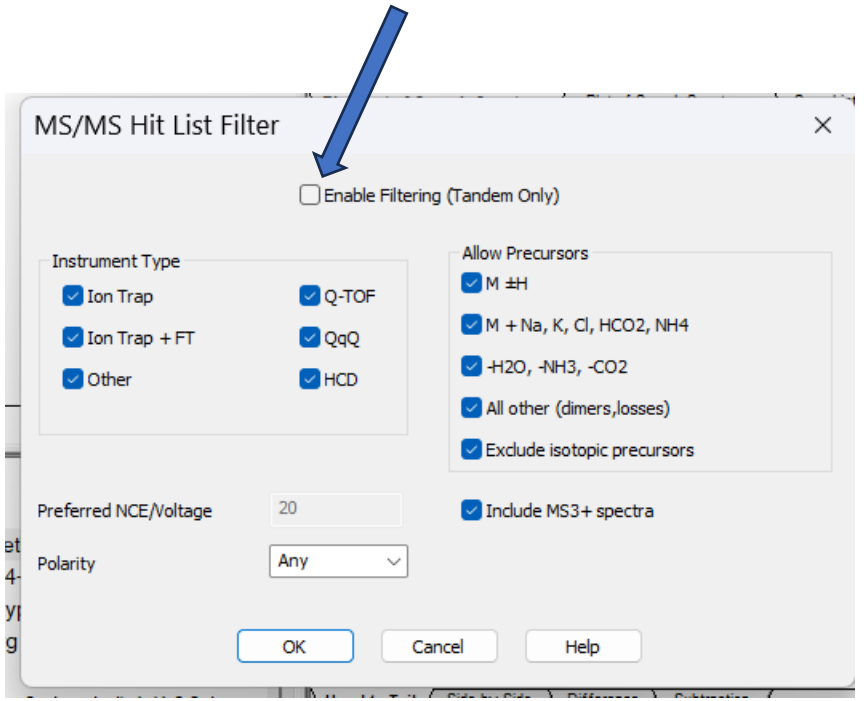
#	Library	Score	DotProd	Prob. (%)	Prec. Type	Instr. Type	Energy	DBs	PSS...	Rev-Dot	dPPM	Name
1	hr_msms_nist#2	600	709	99.9	[M+H]+	HCD	20%	17	642	816	1.0	Aminocarb
2	hr_msms_nist#2	48	226	0.00	[M+H]+	HCD	35%	1	332	275	1.0	4-Acetyl-3-ethyl-N,5-dimethyl-1H-py...
3	hr_msms_nist#3	6	83	0.00	[M+H]+	HCD	90%	2	245	210	1.0	2-Methoxy-4-(morpholin-4-yl)aniline
4	hr_msms_nist	2	64	0.00	[M+H]+	HCD	50%	8	232	86	1.0	N'-(4-Ethoxyphenyl)-N,N-dimethylur...
5	hr_msms_nist	0	22	0.00	[M+2H]2+	QTOF	10V	1	160	68	-16.3	Asn-Lys-Arg
6	hr_msms_nist	1	35	0.00	[M-H-H2O]-	HCD	130%	2	143	101	-4.3	Pro-Leu
7	hr_msms_nist	0	32	0.00	[M+H-C10...	HCD	115%	1	142	190	1.0	(S)-N-(Furan-2-ylmethyl)-1-(1,2,3,4-t...

- The dot product measures the raw similarity between two spectra based on shared peaks and intensities. The NIST score builds on this by applying weighting and scaling so that meaningful matches can still be found even when spectra are incomplete, such as in MS/MS or filtered data
- Normally the ***score is the best way*** to sort before reviewing the results
- Can sort by ***Rev-Dot and Partial Spectrum (PSS)***, but remember some important ***results can be loss*** during the standard Presearch when standard Full Spectrum (Score) method employed

Other Useful Filters:

- Best matching Only (1)
- MS/MS Hit Filter List Options (2)
- These filters applied ***after*** Presearch, and can be ***easily reversed***





- When Best Matching Only Selected, it removes most duplicates
- Makes reviewing data more efficient
- Toggle on and off by depressing button

I usually keep these off initially
Select as needed by Enable Filtering ***(tandem only)***