

KnowItAll Mass Spectrometry Training

*Vendor Neutral Data Processing
Solution for Spectral Analyses*

WILEY



KnowItAll™

“Automatic GC-MS Data Processing Using MS Expert”

James Little

Mass Spec Interpretation Services

Handouts for Videos:

Website: Little Mass Spec and Sailing

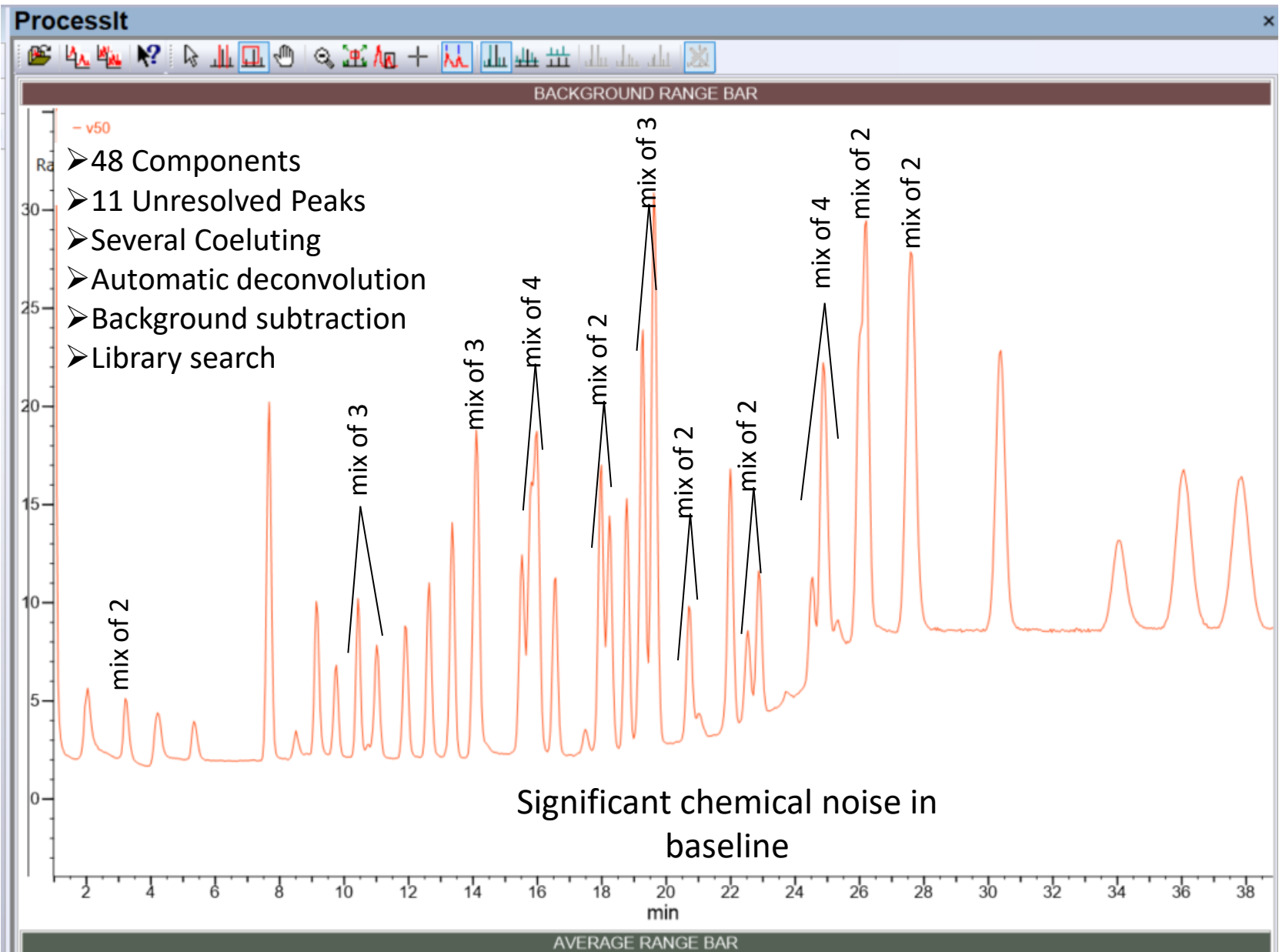
<https://littlemsandsailing.wordpress.com>

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

MS Expert Capabilities for Automatic Data Processing

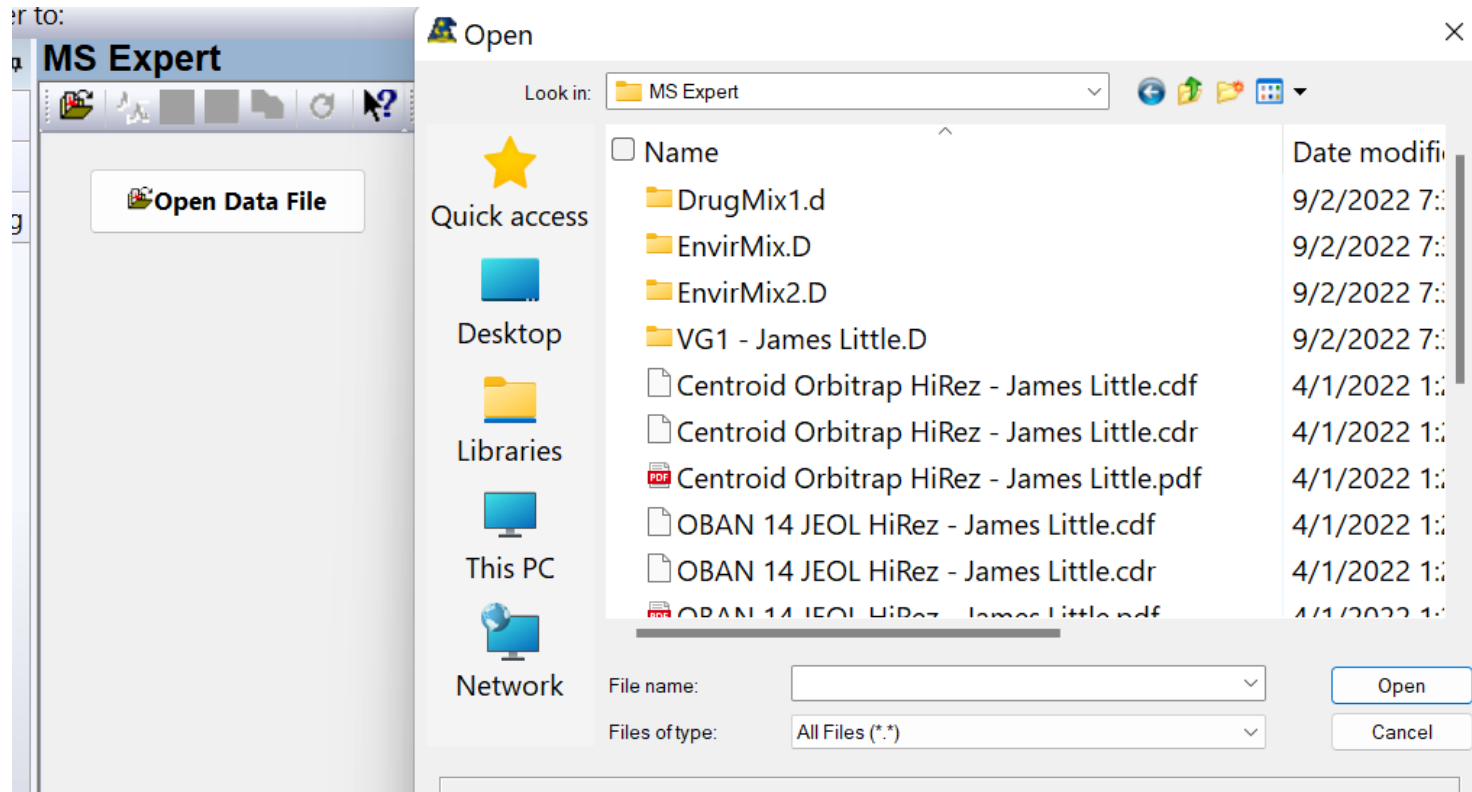
- Deconvolution of unresolved peaks in EI GC-MS files
- Processes both nominal and accurate mass data
- Automatic background subtraction from spectra of detected components
- *Extremely* fast library searches
- Efficient capabilities for reviewing data
- Easy export of results in Excel for reporting

Demo of MS Expert with V50.cdf File Supplied with KnowItAll



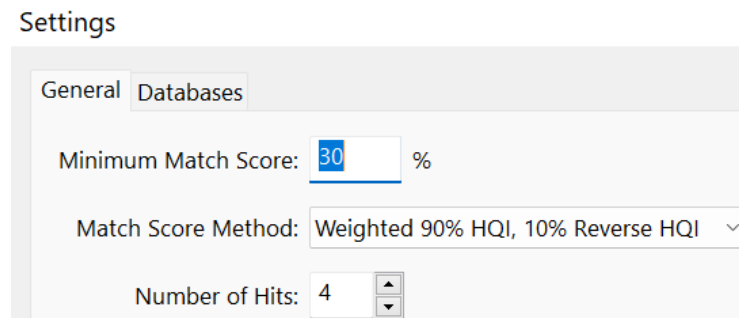
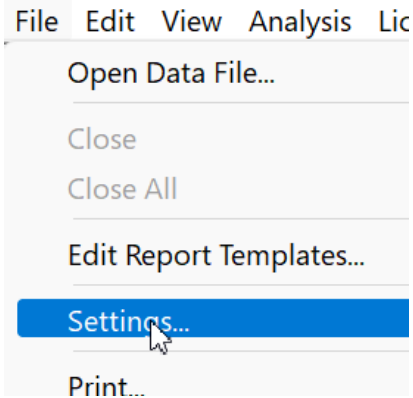
Location of Demo File Supplied with KnowItAll

- Left click on “Open Data File”
- Locate the test files to be used

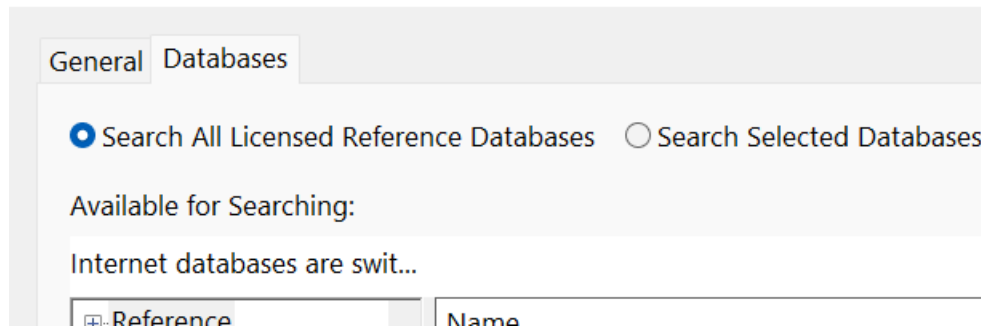


Setup Default Settings

- Go to settings before opening data file
- General tab has number of hits, 4-10 reasonable
- General tab setting for minimum match, 30% reasonable
- Wiley suggests a “Weighted score of 90 % HQI, 10% Reverse HQI”
- HQI should also be a good “Minimum Score Method”
- HQI for match score method would
- Can select “All Licensed Reference Databases” or “Select Search Selected Databases”



Settings



Reviewing of Results

- Select the first entry in list by left clicking in Components window
- Then use the up and down arrows on your keyboard to step through them
- When you are on a result in the components window, “open” the list to show other suggested hits using left and right keys on your keyboard or click on the “+” in the components window
- Manually process any components with low scores using ProcessIt with manual library searches
- Good results should have scores 80

Components		
Components		
RT [m...	#	Match
0.7241	1	Argon
0.9833	1	Carbamic acid, monoammonium salt
2.0297	1	Chloromethane
3.1198	1	Methane, oxybis-



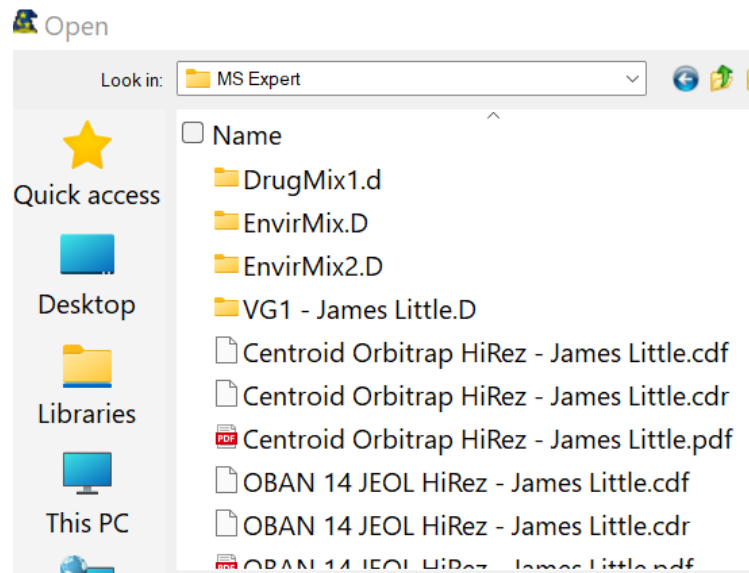
Other Hits reviewed by expanding list



0.9833	1	Carbamic acid, monoammonium salt
2.0297	1	Chloromethane
	2	METHANE, CHLORO-
	3	CHLOROACETIC ACID
	4	Acetic acid, chloro-

Accurate Mass Test Files to Analyze

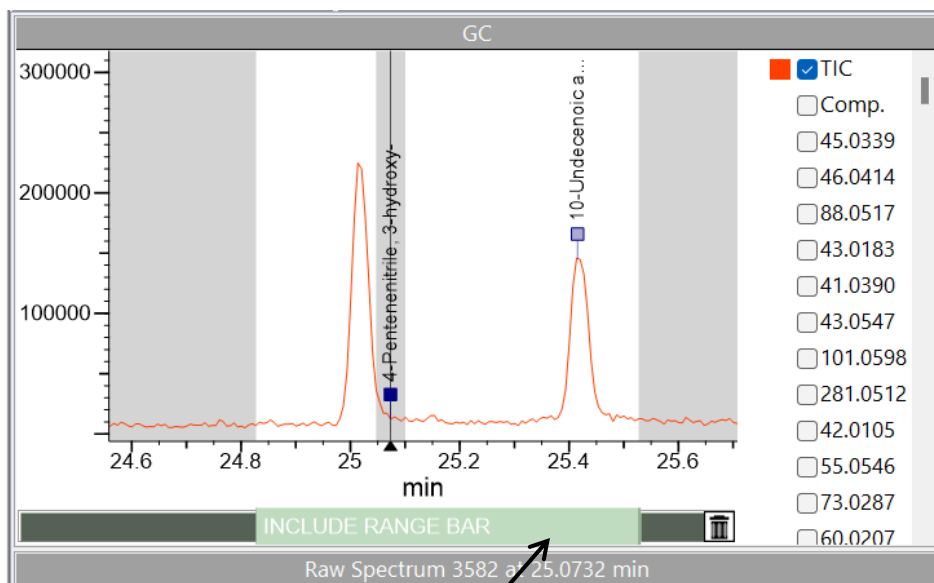
- MS Expert will process both nominal molecular weight and accurate mass files
- The JEOL time of flight file best to try, OBSN 14 JEOL HiRez-James Little.cdf
- Also Thermo file, Centroid Orbitrap HiRez-James Little.cdf, useful because shows capability to resolve an overlapping peak
- However, orbi files tend to give lower hit quality index, HQI, results compared to EI quadruple or time of flight instruments
- Click the following [link](#) for discussion of orbitrap EI spectra
- The results for both the HiRez files can be found as PDF files in the same folder as the cdf files



NOTE: PDF files for expected results of searches in same folder as data files!

Fine Tuning Deconvolution Parameters in MS Expert Analyses

- Can use include range bar to narrow the part of the data file deconvoluted
- Very useful when trying to optimize signal, removing solvent peaks in report, etc.
- First right click and use “Box Zoom Mode” to get narrow part of spectrum
- Then hover over the “Include Range Bar” to left click and select narrow range
- Deselect “Automatic” in bottom “Deconvolution” window
- Try different settings on the parameters, but “Sensitivity” is usually the most critical
- Using narrow range greatly ***speeds the process*** of optimizing these parameters!
- After satisfied, throw narrow range in trash can on bar, and whole file deconvoluted



Deselect Automatic



Left click and select range while in “Include Range Bar”

Conclusions

- MS Expert very quick and effective process for identifying components in a GC-MS file
- Processes both nominal and accurate mass data
- Still useful to employ manual processing and library searches when low scores noted
- See the other videos in this series:

[ProcessIt: manual spectral processing](#)

[SearchIt/MinIt: similarity library search](#)

[SearchIt/MinIt; novel new adaptive library search](#)

[SearchIt/MinIt: unresolved peak analyses and library search](#)

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NOTE: See other mass spec KnowItAll training videos on my personal website