KnowItAll
Mass Spectrometry
Training

*Vendor Neutral Data Processing
Solution for Spectral Analyses*

WILEY

KnowItAll™

"Identity Search of GC-MS Data with SearchIt/MineIT"

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Handouts for Videos:
Website: Little Mass Spec and Sailing
https://littlemsandsailing.wordpress.com

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

Sending a Search from ProcessIt to SearchIt

➢Obtain a background subtracted spectrum from ProcessIt
➢Then go to "Transfer to:" Ribbon in Menu Bar and select "SearchIt"
➢In first window, select "Start a New Search"
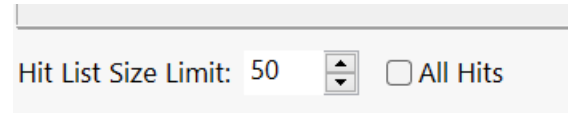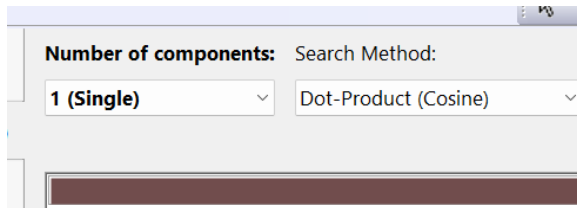➢This will keep separate tab at bottom of page for *each* search performed
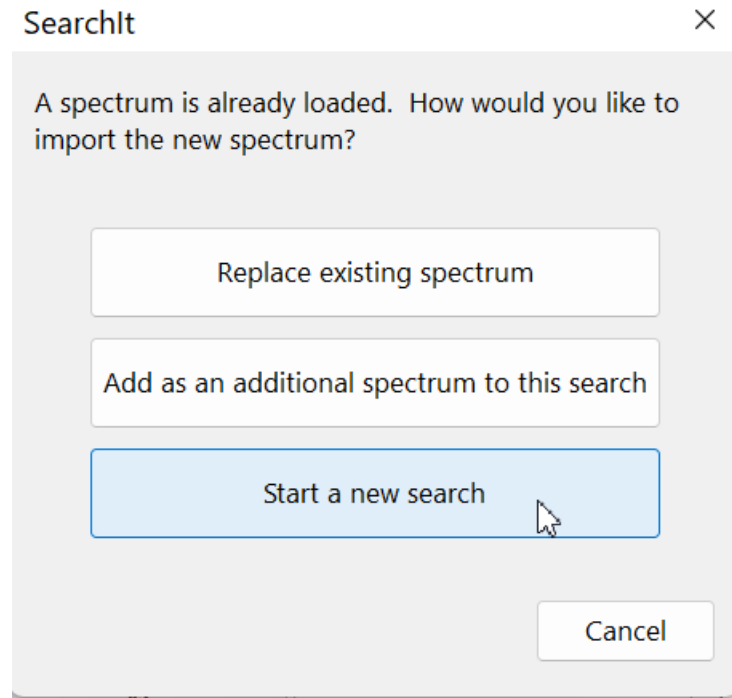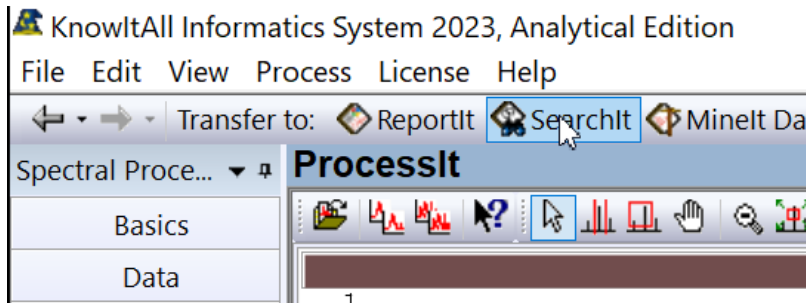
Setup of Search Functions

➤Left click on "User Select" radio button to select libraries to use for search
➤ Use pull down menua and select "MS(GC)" and "Add All"
➤Approximately 1.2 million would be selected if all licensed ones are available
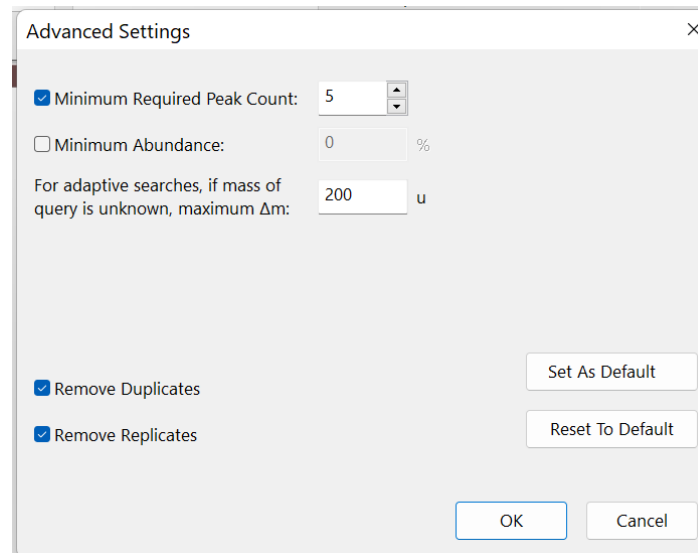➤Can right click on a library in the top window then left click to see information on number of entries
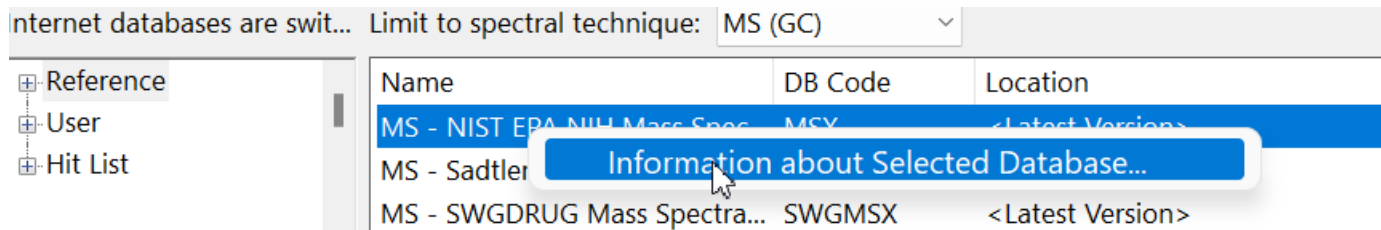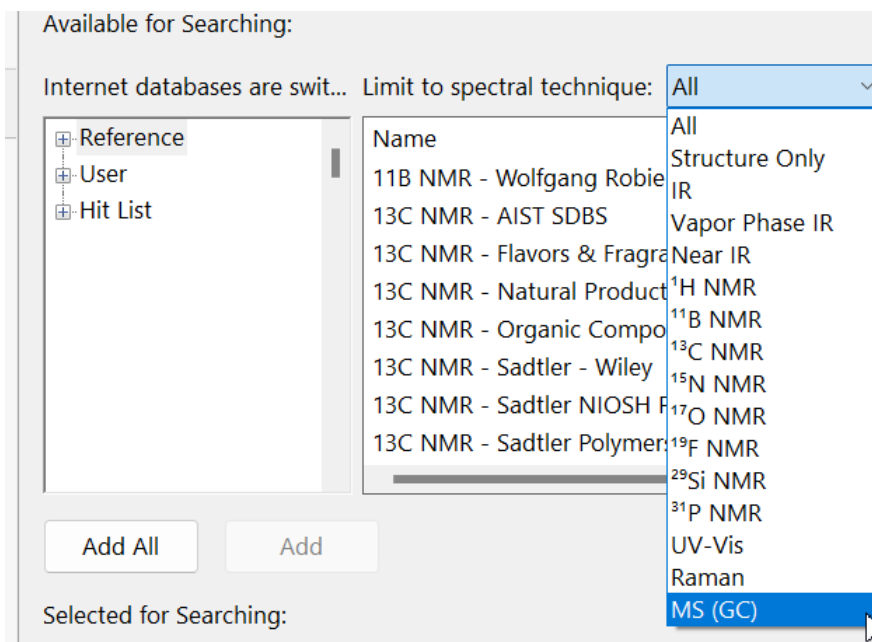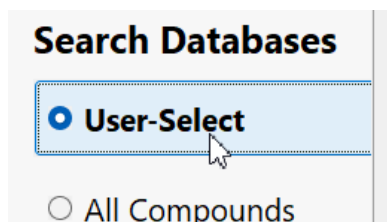
Go Back to Top Window and Setup Other Search Parameters

➤MUST Left mouse click on the Spectrum MS (GC) to get back to top level window

➤Chose a 1 (Single) Dot Product (Cosine Search), the basic similarity or identity search normally employed

➤Can select at bottom of page the number of hits, 50 is reasonable

➤Left click on "Advanced Settings…" button and see suggested default settings

➤If searching a spectrum with only a few peaks in its spectrum, the Min. Required Peak Count might need to be changed

➤Left click on "Search" Button at bottom of page to start search

Results Displayed In MineIt

➢Results of search shown in MineIt Window

➢Butterfly or subtract is a good option for displaying spectrum

➢Options selected from Menu Bar

➢Left click on best hit in the table at bottom of page

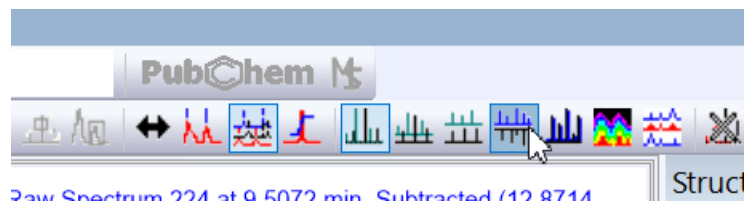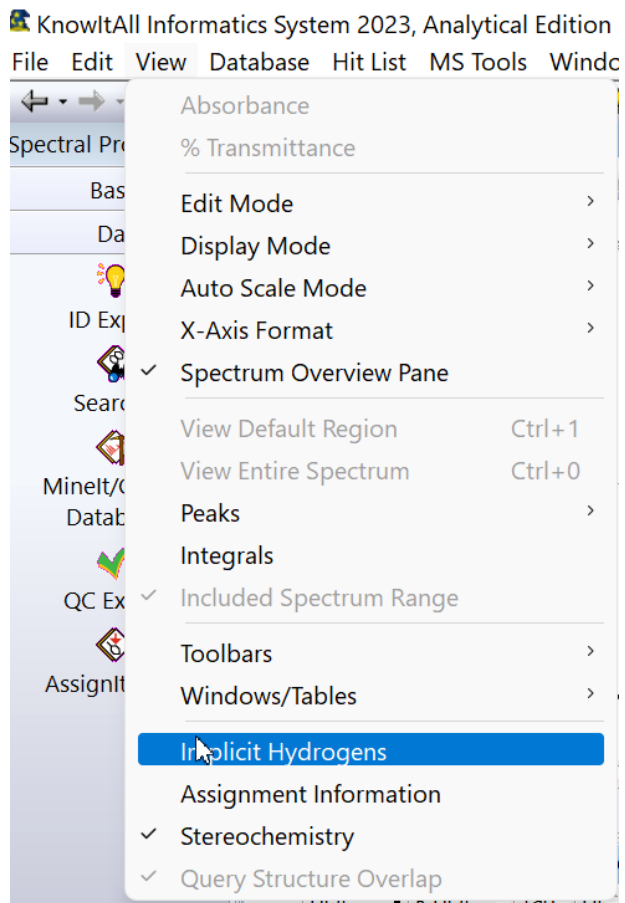➢Use up and down arrows on keyboard to step through and compare search results

Raw Spectrum 224 at 9.5072 min. Subtracted (12.8714

Struct

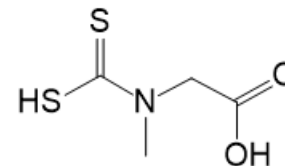|	HQI	▼ R.HQI	Tag	DE	ID	Name	Spectrum <auto> (MS (GC))
1	6.88	82.11		MSX	40453	Glycine, N-(dithiocarboxy)-N-methyl-	

Implicit Hydrogens

➢Best display of structures with hydrogens on N, O, S, etc. are shown by selecting implicit hydrogens

Before implicit hydrogens clicked
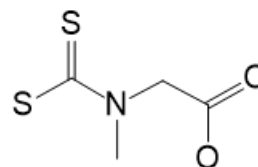
After implicit hydrogens clicked

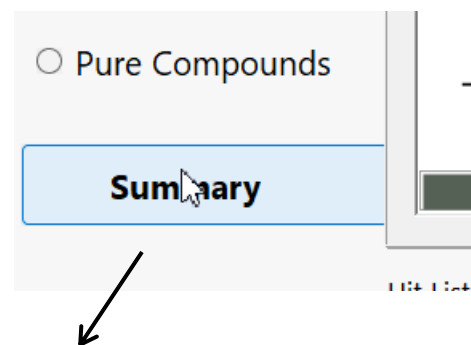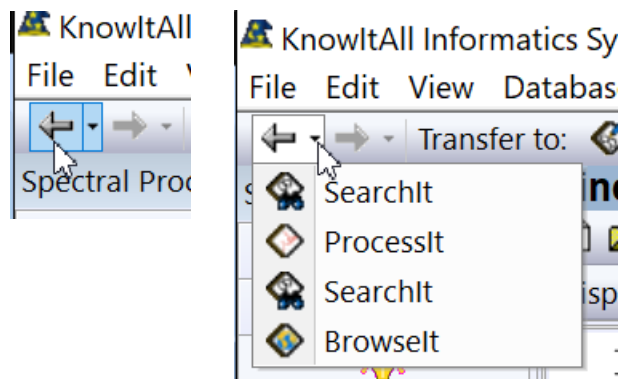# The Search Results in MineIt are Stored in Separate Tabs at Bottom of Page for Later Review

To Return to Either SearchIt or ProcessIt

➢Can return to either SearchIt to change parameters and create another search

➢Or can return to ProcessIt to obtain another spectrum for searching

➢Two Options, use the back arrow at top left of menu bar

➢Or the arrow to pull down all the windows to open

➢Two clicks of the back arrow would return the user to ProccessIt, one left click to return to SearchIt

➢If you return to SearchIt, the Summary of the search can be seen