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.com/

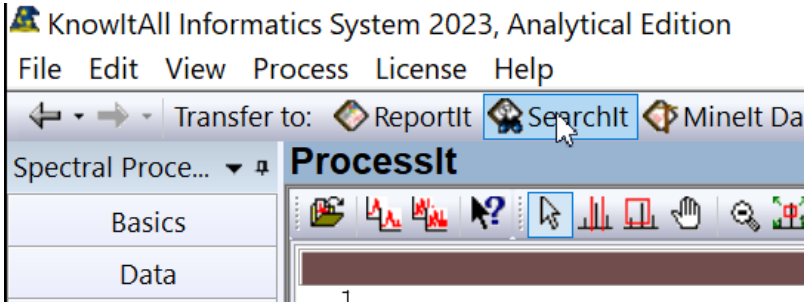
Note: Series of training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

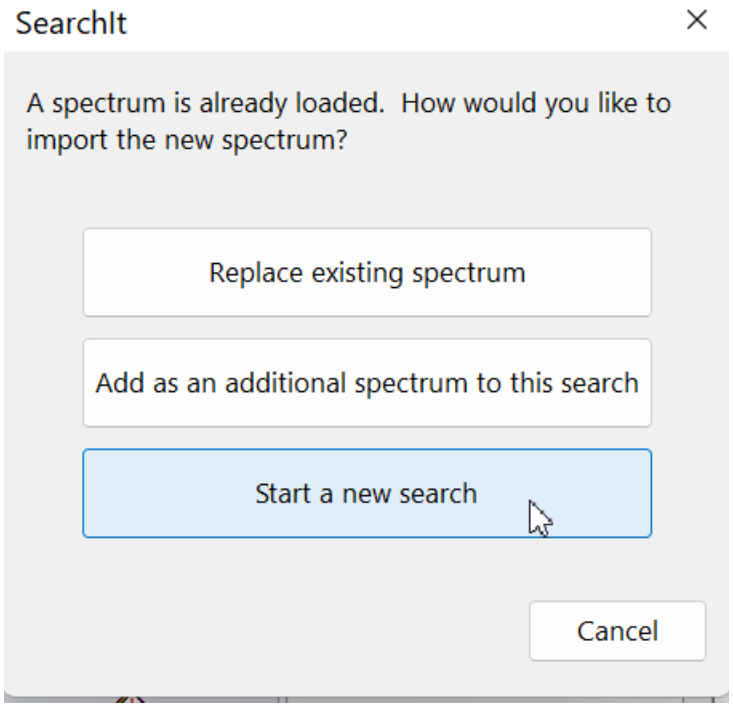
Link to Training

Sept 5, 2022

Sending a Search from ProcessIt to SearchIt

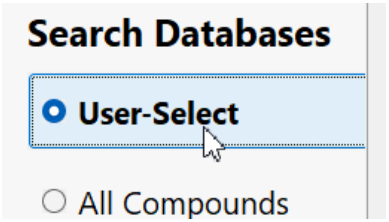
- Obtain a background subtracted spectrum from ProcessIt
- Then go to “Transfer to:” Ribbon in Menu Bar and select “SearchIt”
- In first window, select “Start a New Search”
- This will keep separate tab at bottom of page for ***each*** search performed

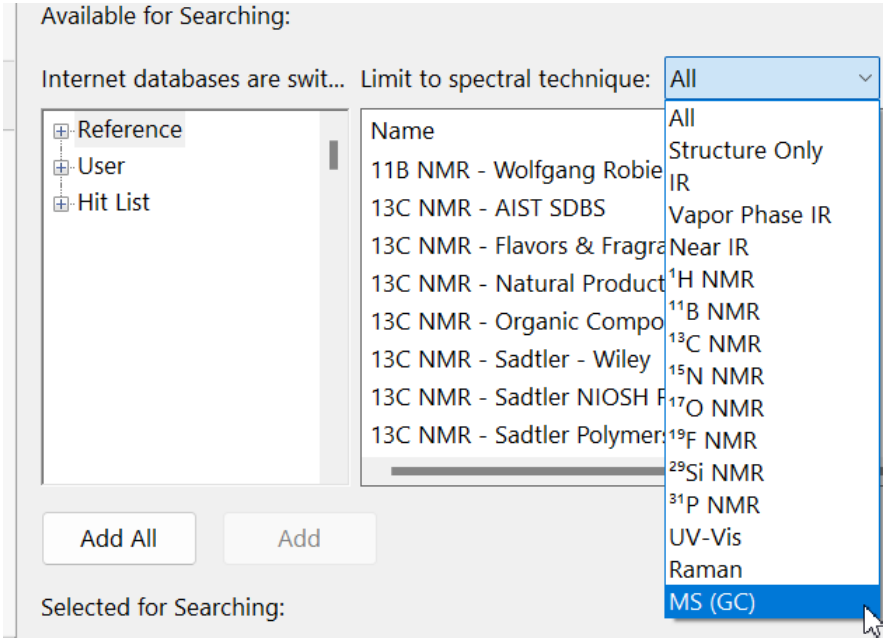


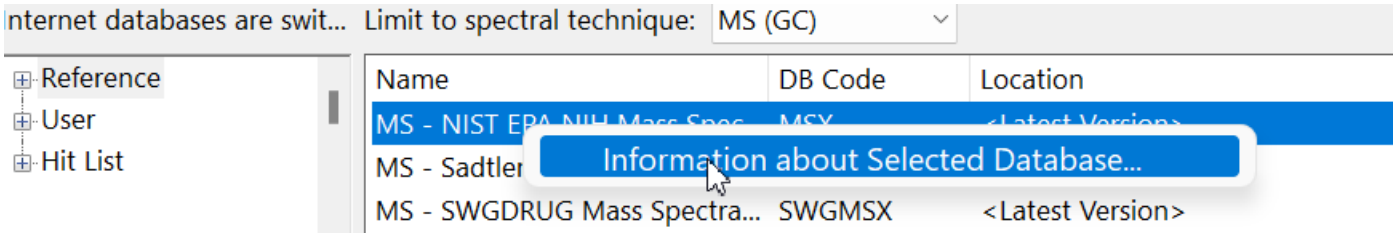


Setup of Search Functions

- 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

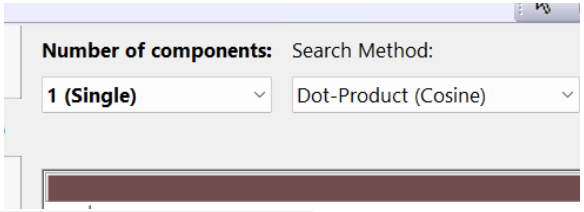


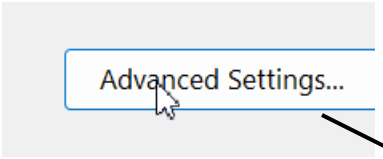


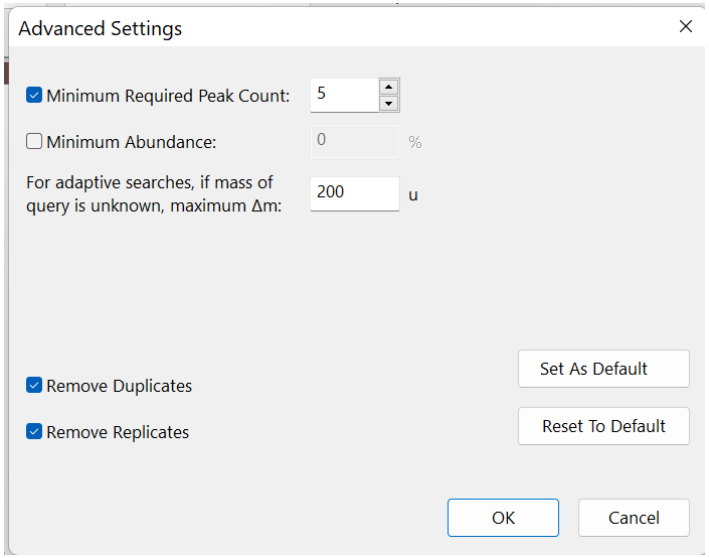


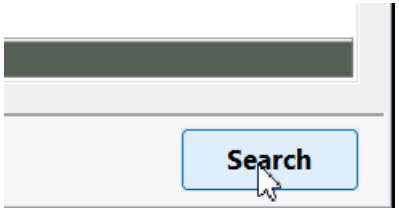
Go Back to Top Window and Setup Other Search Parameters

- 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



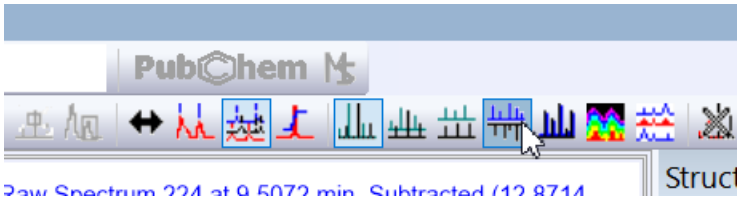


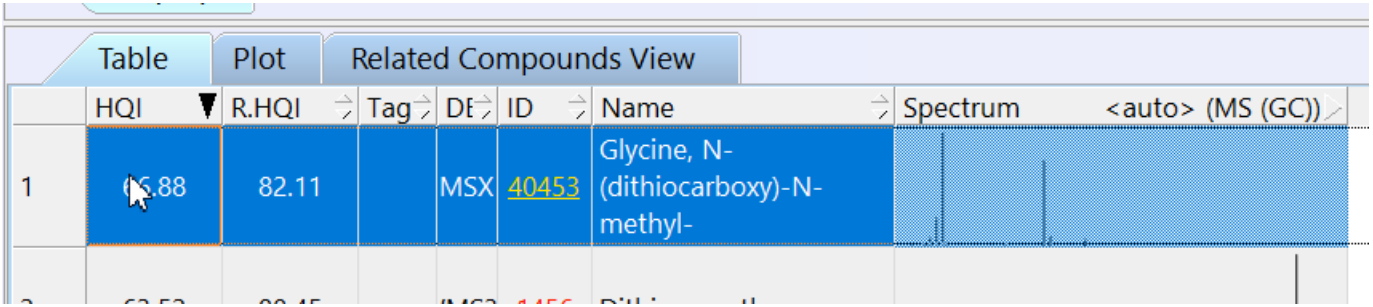




Results Displayed In MineIt

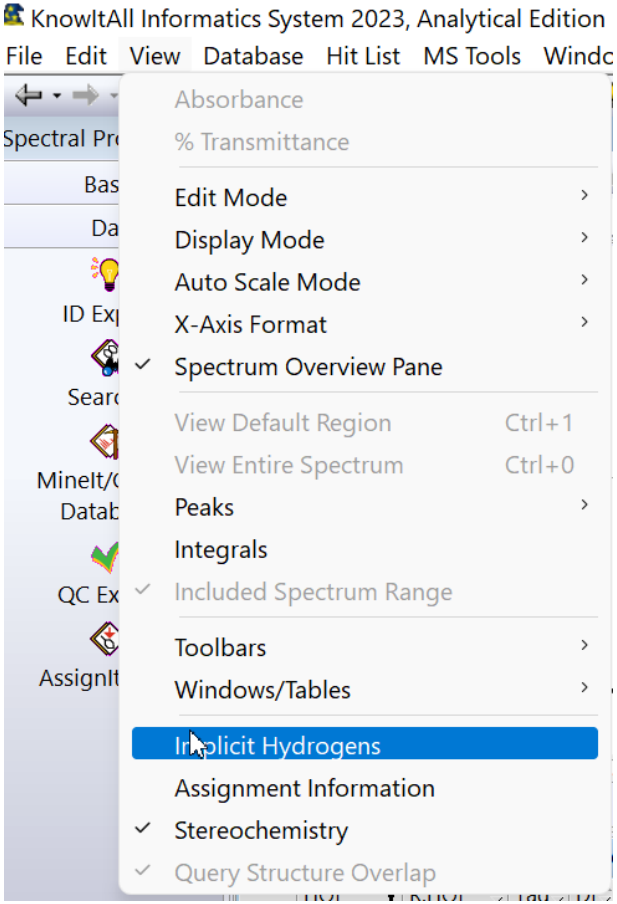
- Results of search shown in MineIt Window
- Butterfly or subtract is a good option for displaying spectrum
- Options selected from Menu Bar
- Left click on best hit in the table at bottom of page
- Use up and down arrows on keyboard to step through and compare search results



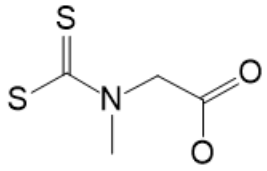


Implicit Hydrogens

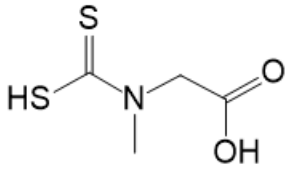
➢Best display of structures with hydrogens on N, O, S, etc. are shown by selecting implicit hydrogens



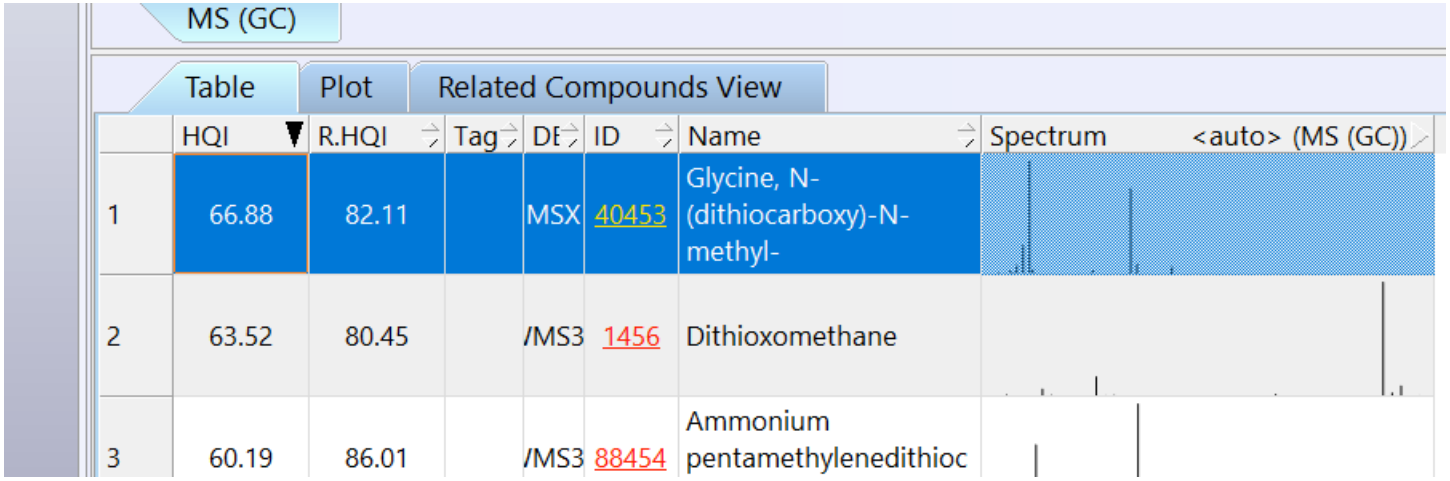
Before implicit hydrogens clicked

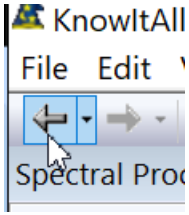
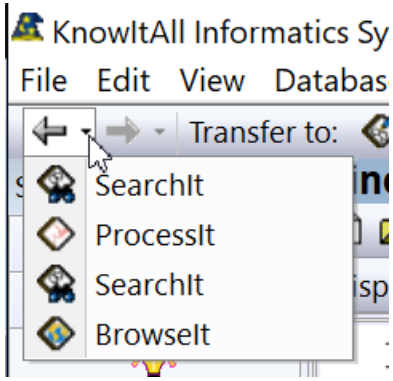
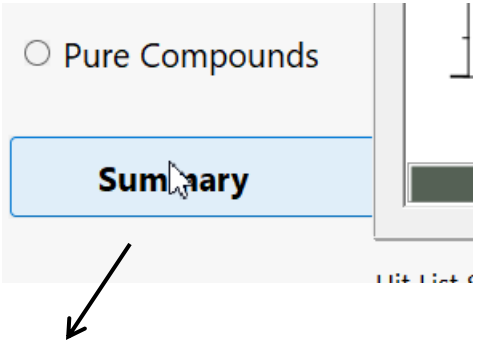
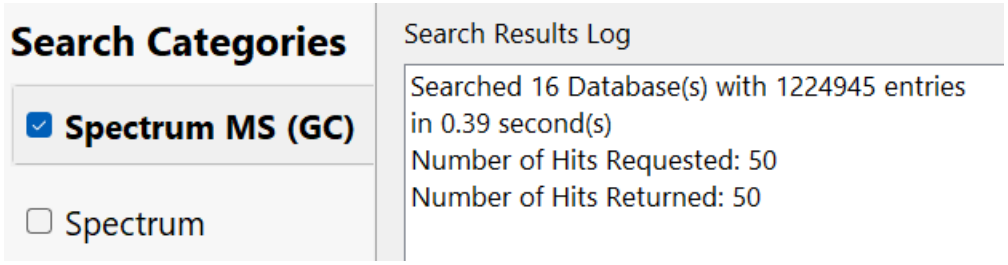


After implicit hydrogens clicked



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