

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

James Little Mass Spec Interpretation Services

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

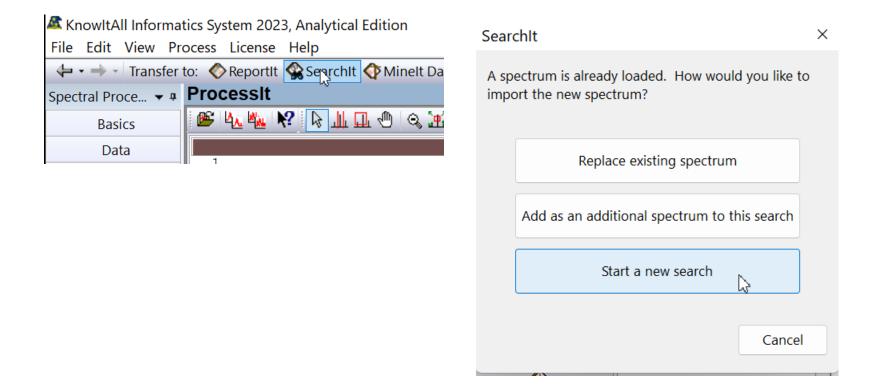
Note: Series of training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

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"

Available for Searching:

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

Search Databases • User-Select • All Compounds	Add All Add	Hit List Hit Li					
	Selected for Searching:		MS (GC)				
nternet databases are swit	Limit to spectral technique: MS (GC)	~					
Reference	Name DB Co	ode Location					
User	MS - NIST EPA NIH Mass Space MSX	el atact Varcia					
🖶 Hit List	MS - Sadtler Information about Selected Database						

MS - SWGDRUG Mass Spectra... SWGMSX

<Latest Version>

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

1		M				
Number of components:	Search Method:		<u> </u>			
1 (Single)	Dot-Product (Cosine)	~	Hit List Size Lir	nit: 50 🚖	🗌 All Hits	
· · ·	_					
Advanced Settings	Adva	anced Settings			×	
		Iinimum Required Peak Count:	5			
		1inimum Abundance:	0 %			
	For	adaptive searches, if mass of ry is unknown, maximum ∆m:	200 u			
	🗹 R	emove Duplicates		Set As Default		Search
	🜌 R	emove Replicates		Reset To Default		
				OK Cancel		

Results Displayed In Minelt

▶ Results of search shown in Minelt 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

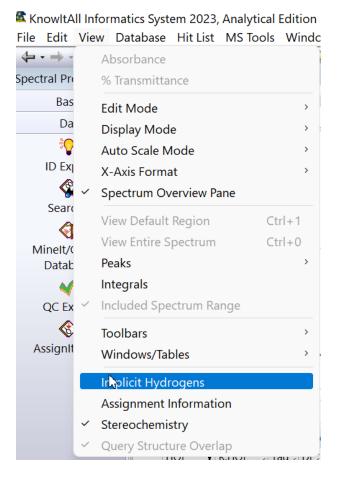
➤Use up and down arrows on keyboard to step through and compare search results



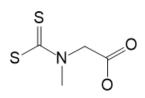
	<u> </u>					
	Table	Plot Rela	ted Compour	nds View		
	HQI 🔻	R.HQI 🗦 Tag	🗟 DE🗘 ID 🗦	Name	Spectrum	<auto> (MS (GC))></auto>
1	(§ .88	82.11	MSX <u>40453</u>	Glycine, N- (dithiocarboxy)-N- methyl-		
2	62.52	00.45		511.1 J		

Implicit Hydrogens

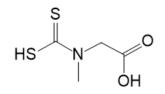
➤ Best display of structures with hydrogens on N, O, S, etc. are shown by selecting implicit hydrogens



Before implicit hydrogens clicked



After implicit hydrogens clicked



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

	MS (GC)							
	Table	Plot Related Compounds View						
	HQI 🔻	R.HQI 🗦	Tag⇒	DE⇒	ID 🗦	Name 🗦	Spectrum	<auto> (MS (GC))></auto>
1	66.88	82.11		MSX	<u>40453</u>	Glycine, N- (dithiocarboxy)-N- methyl-		
2	63.52	80.45		/MS3	<u>1456</u>	Dithioxomethane		
3	60.19	86.01		/MS3	<u>88454</u>	Ammonium pentamethylenedithioc		

To Return to Either Searchlt 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

