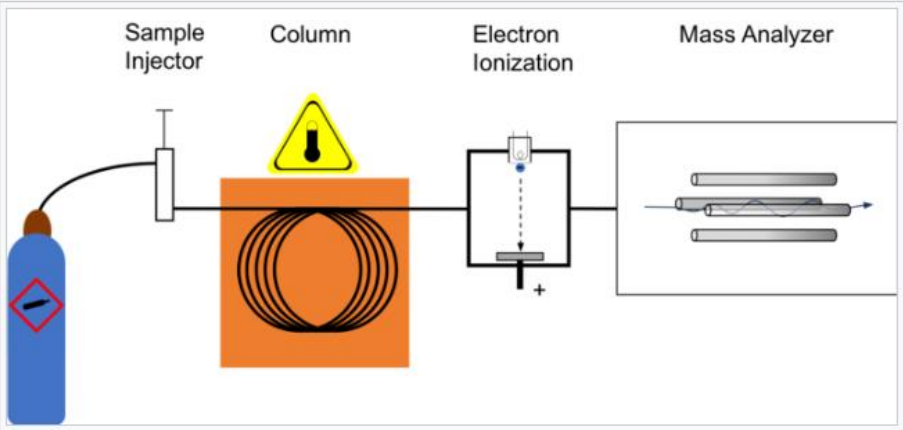
Free NIST GC-MS Software Lab for Universities:

Part 3: Library Searches



James Little

August 29, 2023

38 years Eastman Chemical Company

7 years Mass Spec Interpretation Services

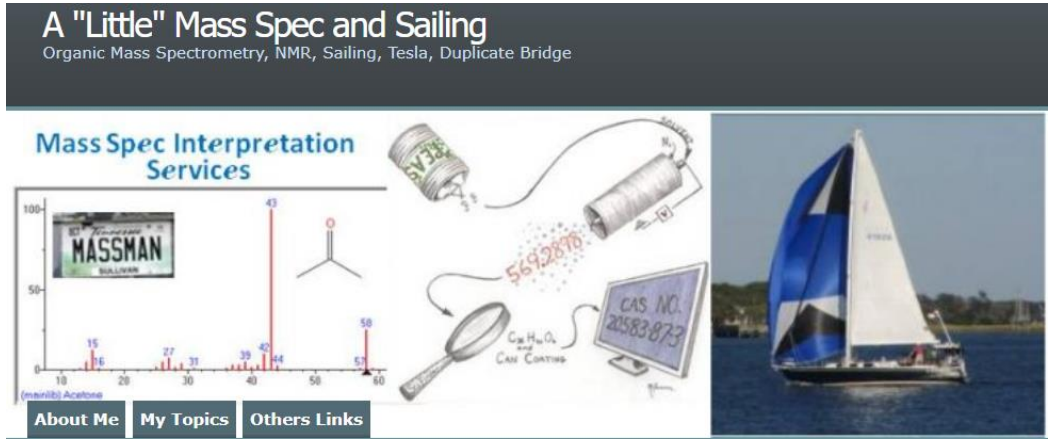
https://littlemsandsailing.wpcomstaging.com/

Link to GCMS Schematic Above

Link to University Logos

Free NIST GC-MS Software Lab for Universities

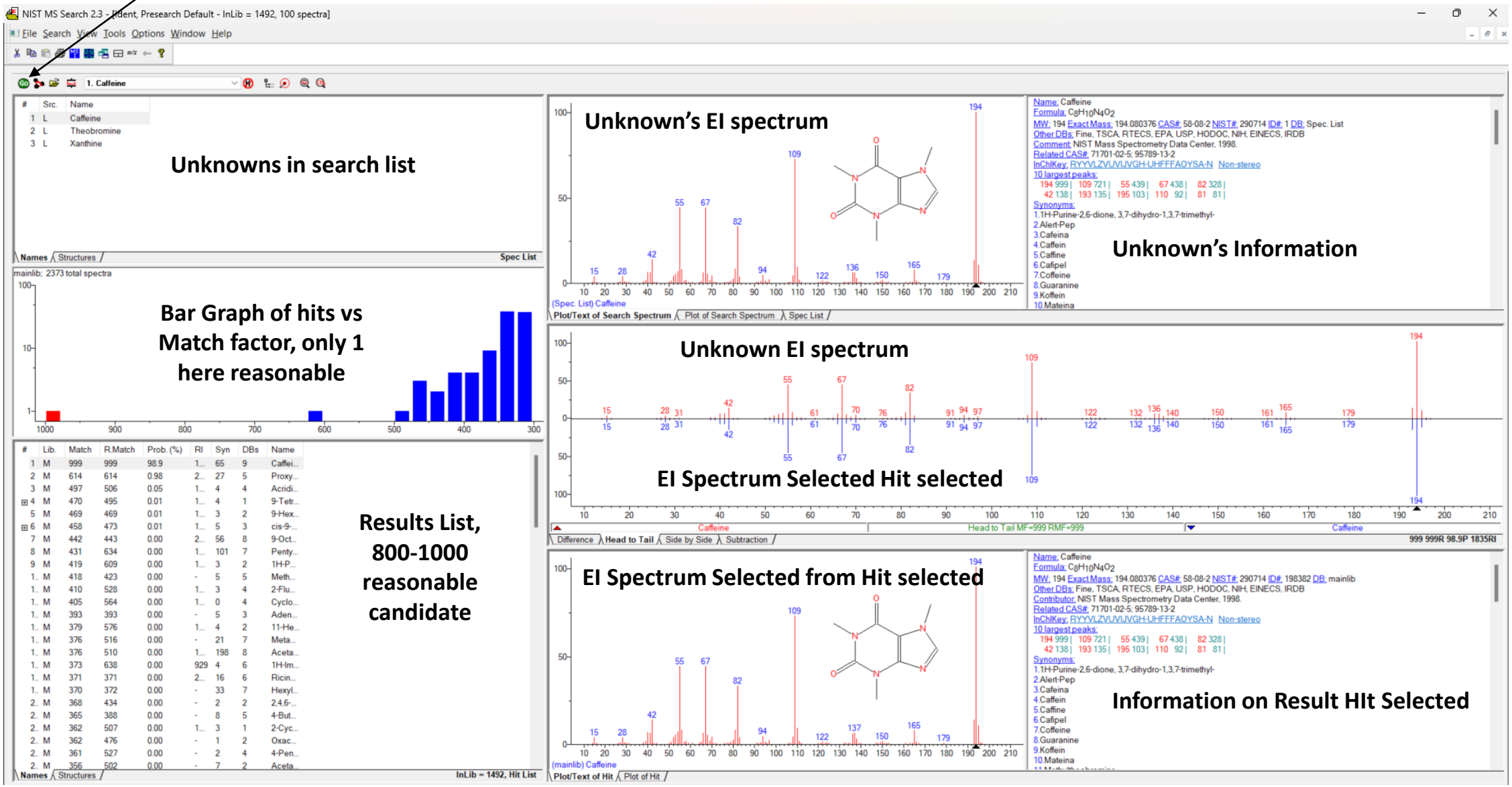
Part 1: Very Basic Theory of GCMS Analyses
Part 2: Installation of Software
Part 3: Library Searches
Part 4: Processing GCMS Data with AMDIS
Part 5: Understanding EI Fragmentation with MS Interpreter
Part 6: Structure Searches with Input from ChemSketch
Part 7: Creating a User Library
Part 8: Advanced Processing with NIST Software



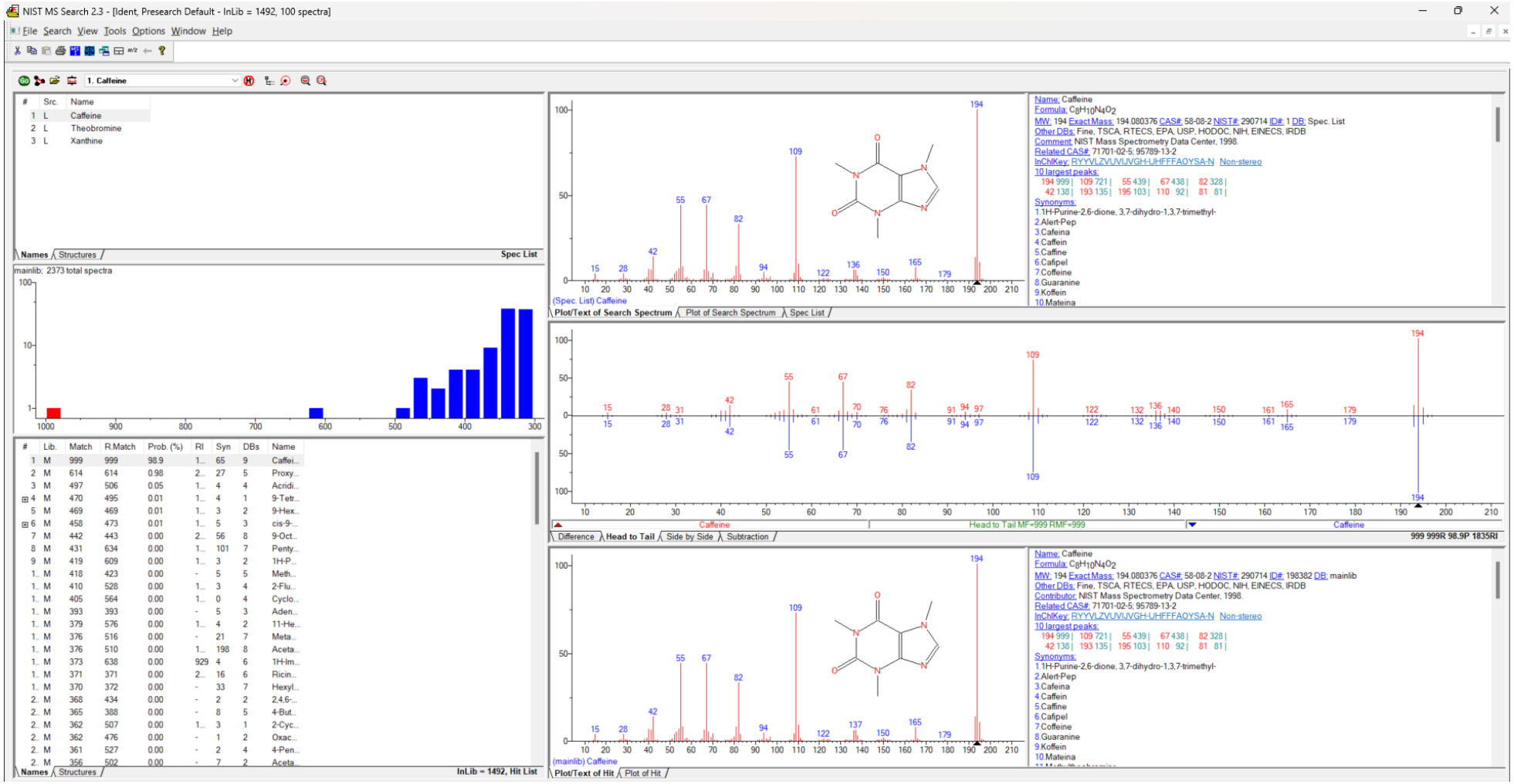
Link to Training Website

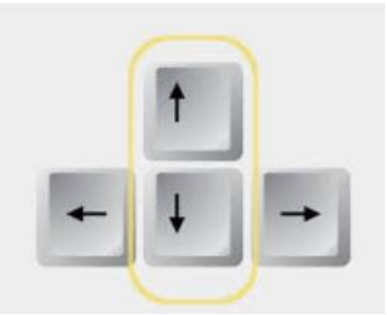
Basic Search, Just Select Spectra of Interest and Press Go Button

Select Go to search to search spectrum, or right click on entry in search list, or double left click quickly on entry search list



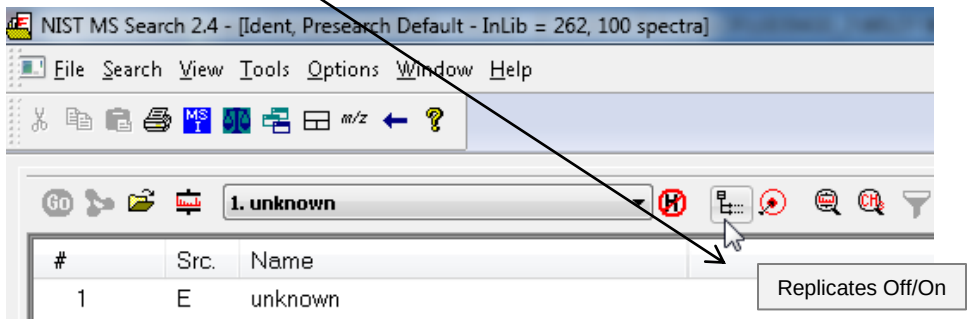
Change Between by Left Click and select, or scroll with mouse, or use up and down keys on keyboard



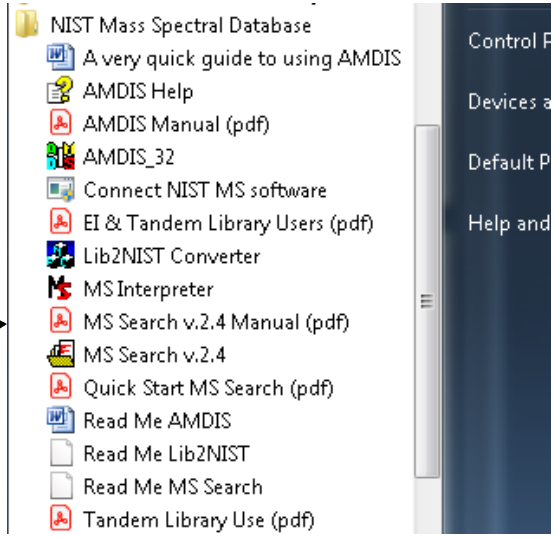


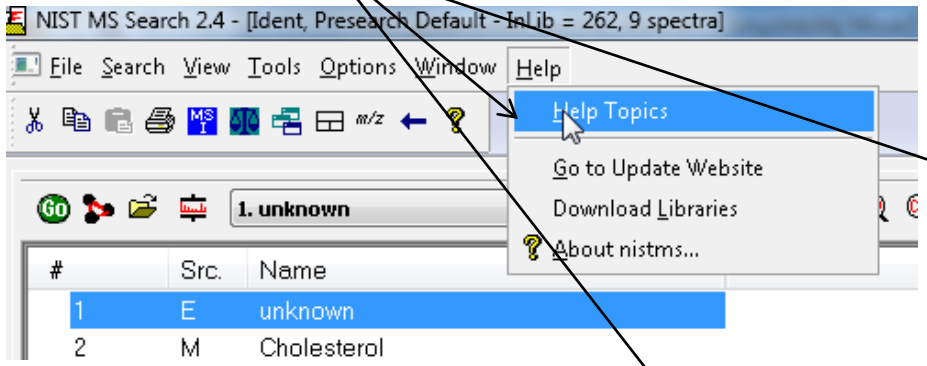
Help Files for NIST Search

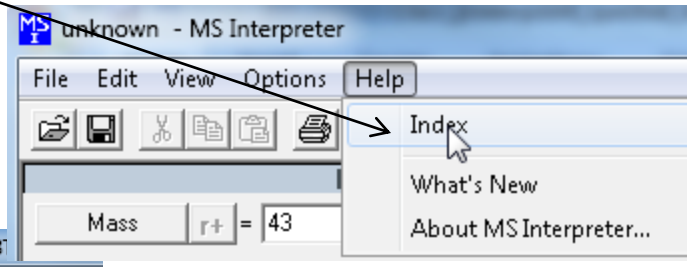
-"Hover" over Program Icon with mouse and function description displayed

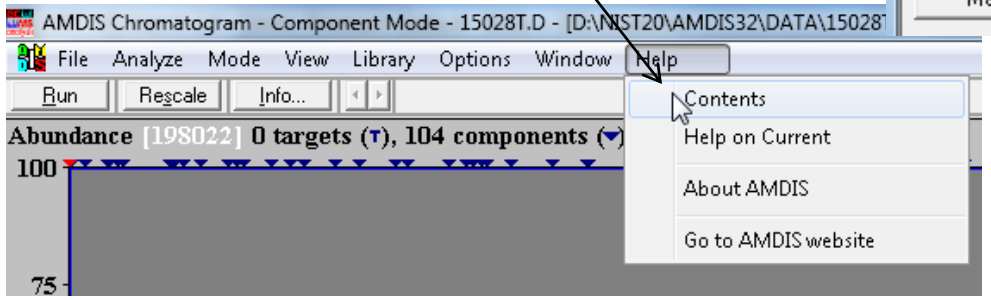


-Detailed documentation for NIST Search[2] and AMDIS[3,4,12]
-MS Interpreter included in NIST manual[2] and in posters[13-15]
-Windows Program Group
-"In program" assistance for all three programs





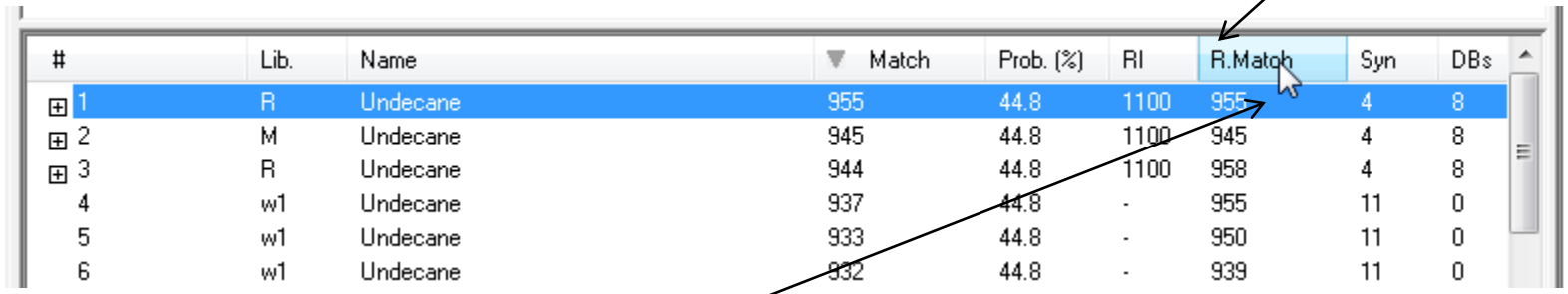




NIST Software in General is “Windows Compliant”

-***left click (LMB)*** to select an item, ***double LMB*** on that item to perform operation
-***right click (RMB)*** in area or item to see operations that can be performed or to change properties of window
-***LMB*** on first item and last item to select group ***while*** holding ***shift key***
-***LMB*** to select/deselect individual items ***while*** holding ***Ctrl button***
-use up and down arrows ***on keyboard*** to step between entries
-some NIST windows such as librarian have no delete button to delete ions, ***must*** use delete key on keyboard!
-***control a*** (select all), ***control x*** (delete selected), ***control c*** (copy); ***control v*** (paste)
-***control k*** copies entries into windows in tab-separated text format, e.g., ***paste*** into Excel
-F1 MS Search help
-F9 send spectrum to MS Interpreter
-***LMB*** and ***zoom*** mass spectral windows, ***RMB*** then ***LMB*** to ***zoom out***

Tip 3: ***LMB*** and **drag** to rearrange order of column headers



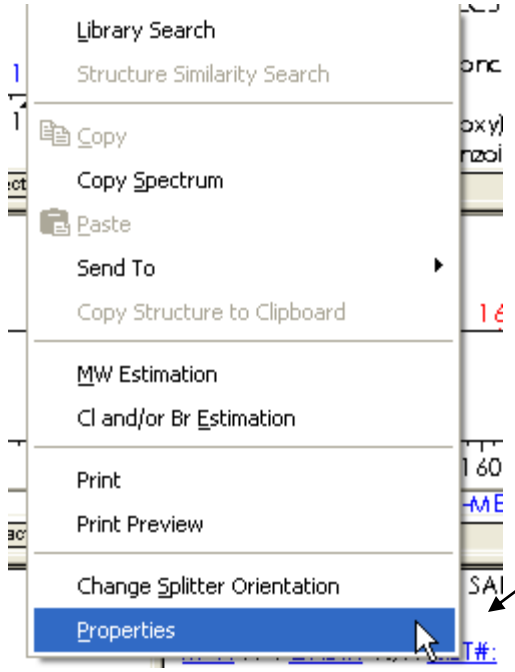
#	Lib.	Name	Match	Prob. (%)	RI	R.Match	Syn	DBs
1	R	Undecane	955	44.8	1100	955	4	8
2	M	Undecane	945	44.8	1100	945	4	8
3	R	Undecane	944	44.8	1100	958	4	8
4	w1	Undecane	937	44.8	-	955	11	0
5	w1	Undecane	933	44.8	-	950	11	0
6	w1	Undecane	932	44.8	-	939	11	0

-***LMB*** on column of interest
-Can sort in lower value first or higher
-Will show use in mixtures in example later in presentation

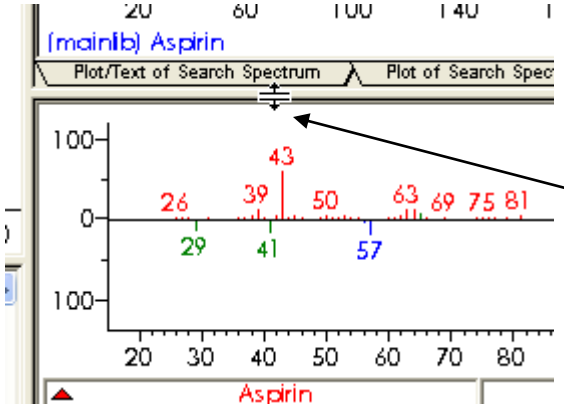
Tip 1: When reviewing search results, use up and down arrows on keyboard to quickly step through results!

Tip 2: When viewing structures in MS Interpreter, use left and right arrows on keyboard to quickly review results!

Customizing the Windows



-***RMB*** within any window of interest and select properties to change window information and/or layout



-place cursor over any bar between (***top or side***) windows and then ***LMB*** and drag to change the size of a window or make window so small it essentially disappears.

Customizing the Windows (continued)

-RMB in display windows then ***LMB*** to “Change Splitter Orientation”

Tip: ***All*** mass spectra in windows can be ***“Boxed”*** to ***expand*** by ***LMB*** and dragging to expand/enlarge; ***restore*** to original by ***RMB*** in spectrum region and selecting ***“Zoom Out”***

Tour of NIST Search Program
(Top Links)

-default to original settings with settings_EI

-Restore and Create user Configurations, named my personal one jl_default