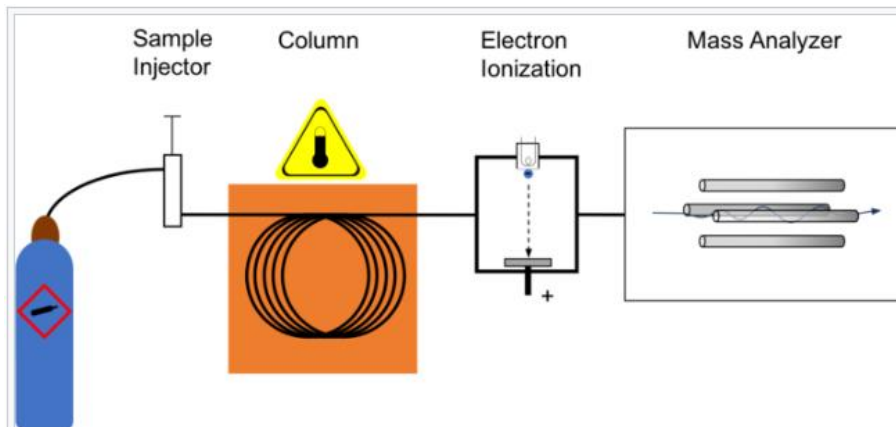


**Free NIST GC-MS Software Lab
for Universities:
Part 3: Library Searches**



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](#)

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

Unknowns in search list

#	Src.	Name
1	L	Caffeine
2	L	Theobromine
3	L	Xanthine

Bar Graph of hits vs Match factor, only 1 here reasonable

Results List, 800-1000 reasonable candidate

#	Lib.	Match	R.Match	Prob. (%)	RI	Syn	DBs	Name
1	M	999	999	98.9	1...	65	9	Caffeine
2	M	614	614	0.98	2...	27	5	Proxy...
3	M	497	506	0.05	1...	4	4	Acridi...
4	M	470	495	0.01	1...	4	1	9-Tet...
5	M	469	469	0.01	1...	3	2	9-Hex...
6	M	458	473	0.01	1...	5	3	cis-9...
7	M	442	443	0.00	2...	56	8	9-Oct...
8	M	431	634	0.00	1...	101	7	Pentyl...
9	M	419	609	0.00	1...	3	2	1H-P...
1.	M	418	423	0.00	-	5	5	Meth...
1.	M	410	528	0.00	1...	3	4	2-Flu...
1.	M	405	564	0.00	1...	0	4	Cyclo...
1.	M	393	393	0.00	-	5	3	Aden...
1.	M	379	576	0.00	1...	4	2	11-He...
1.	M	376	516	0.00	-	21	7	Meta...
1.	M	376	510	0.00	1...	198	8	Aceta...
1.	M	373	638	0.00	929	4	6	1H-Im...
1.	M	371	371	0.00	2...	16	6	Ricin...
1.	M	370	372	0.00	-	33	7	Hexyl...
2.	M	368	434	0.00	-	2	2	2,4,6...
2.	M	365	388	0.00	-	8	5	4-But...
2.	M	362	507	0.00	1...	3	1	2-Cyc...
2.	M	362	476	0.00	-	1	2	Oxac...
2.	M	361	527	0.00	-	2	4	4-Pen...
2.	M	356	502	0.00	-	7	2	Aceta...

Unknown's EI spectrum

Unknown's Information

Unknown EI spectrum

EI Spectrum Selected Hit selected

EI Spectrum Selected from Hit selected

Information on Result Hit Selected

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

NIST MS Search 2.3 - [Ident, Presearch Default - InLib = 1492, 100 spectra]

File Search View Tools Options Window Help

1. Caffeine

#	Src	Name
1	L	Caffeine
2	L	Theobromine
3	L	Xanthine

Names / Structures / Spec List

mainib: 2373 total spectra

#	Lib	Match	R.Match	Prob. (%)	RI	Syn	DBs	Name
1	M	999	999	98.9	1.	65	9	Caffe...
2	M	614	614	0.98	2.	27	5	Proxy...
3	M	497	506	0.05	1.	4	4	Acridi...
4	M	470	495	0.01	1.	4	1	9-Tetr...
5	M	469	469	0.01	1.	3	2	9-Hex...
6	M	458	473	0.01	1.	5	3	cis-9...
7	M	442	443	0.00	2.	56	8	9-Oct...
8	M	431	634	0.00	1.	101	7	Penty...
9	M	419	609	0.00	1.	3	2	1HP...
1	M	418	423	0.00	-	5	5	Meth...
1	M	410	528	0.00	1.	3	4	2-Flu...
1	M	405	564	0.00	1.	0	4	Cyclo...
1	M	393	393	0.00	-	5	3	Aden...
1	M	379	576	0.00	1.	4	2	11-Hc...
1	M	376	516	0.00	-	21	7	Meta...
1	M	376	510	0.00	1.	198	8	Aceta...
1	M	373	638	0.00	929	4	6	1H-Im...
1	M	371	371	0.00	2.	16	6	Ricin...
1	M	370	372	0.00	-	33	7	Hexy...
2	M	368	434	0.00	-	2	2	2,4,6...
2	M	365	388	0.00	-	8	5	4-But...
2	M	362	507	0.00	1.	3	1	2-Cyc...
2	M	362	476	0.00	-	1	2	Oxac...
2	M	361	527	0.00	-	2	4	4-Pen...
2	M	356	502	0.00	-	7	2	Aceta...

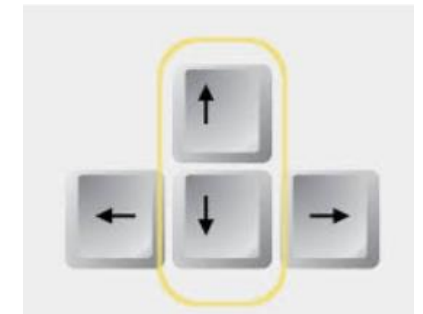
InLib = 1492, Hit List

Plot/Text of Search Spectrum / Plot of Search Spectrum / Spec List /

Name: Caffeine
Formula: C₈H₁₀N₄O₂
MW: 194 Exact Mass: 194.080376 CAS#: 58-08-2 NIST#: 290714 ID: 1 DB: Spec List
Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB
Comment: NIST Mass Spectrometry Data Center, 1998.
Related CAS#: 71701-02-5; 95789-13-2
InChIKey: RYYVLZVJVLJVGH-UHFFFAOYSA-N Non-stereo
10 largest peaks:
194 999 | 109 721 | 55 439 | 67 438 | 82 328 |
42 138 | 193 135 | 195 103 | 110 92 | 81 81 |
Synonyms:
1. 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
2. Alert-Pap
3. Caffeina
4. Caffein
5. Caffeine
6. Cafpel
7. Coffeine
8. Guaranine
9. Koffein
10. Mateina

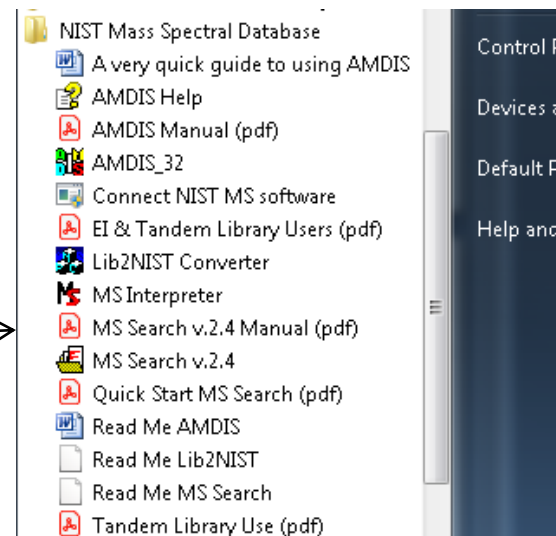
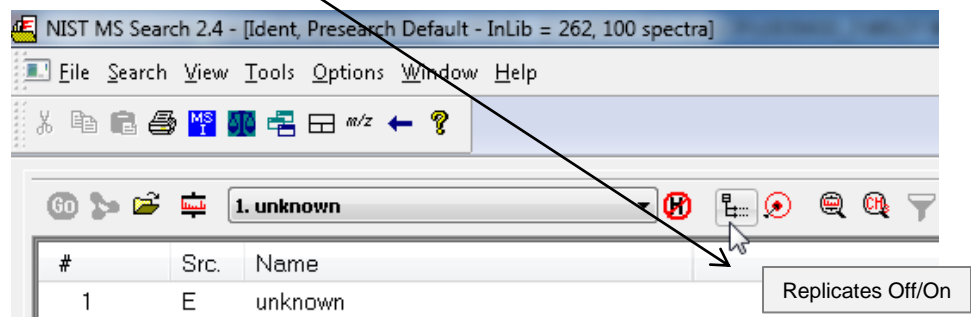
Plot/Text of Hit / Plot of Hit /

Name: Caffeine
Formula: C₈H₁₀N₄O₂
MW: 194 Exact Mass: 194.080376 CAS#: 58-08-2 NIST#: 290714 ID: 198382 DB: mainib
Contributor: NIST Mass Spectrometry Data Center, 1998.
Related CAS#: 71701-02-5; 95789-13-2
InChIKey: RYYVLZVJVLJVGH-UHFFFAOYSA-N Non-stereo
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9. Koffein
10. Mateina

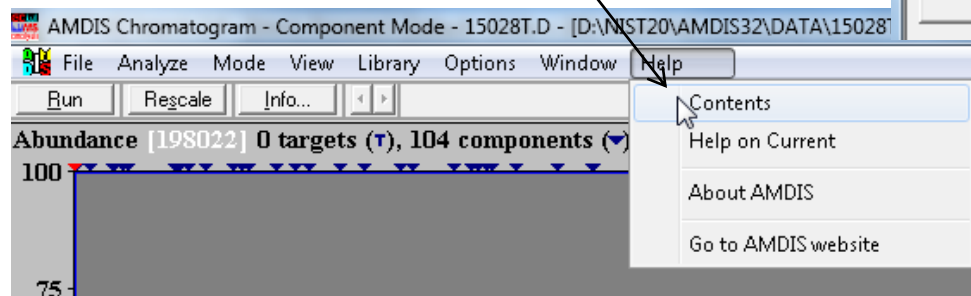
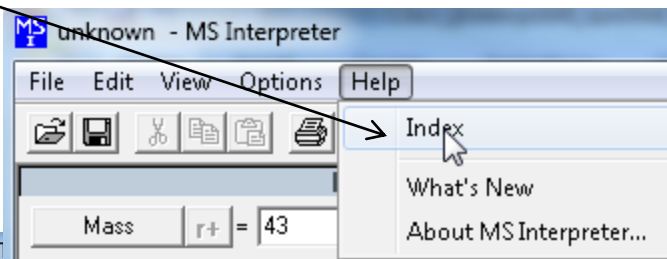
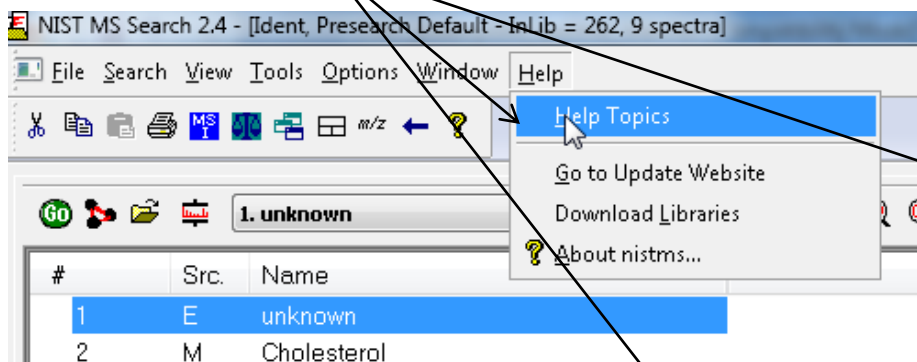


Help Files for NIST Search

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



- Detailed documentation for NIST Search² and AMDIS^{3,4,12}
- MS Interpreter included in NIST manual² and in posters¹³⁻¹⁵
- 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

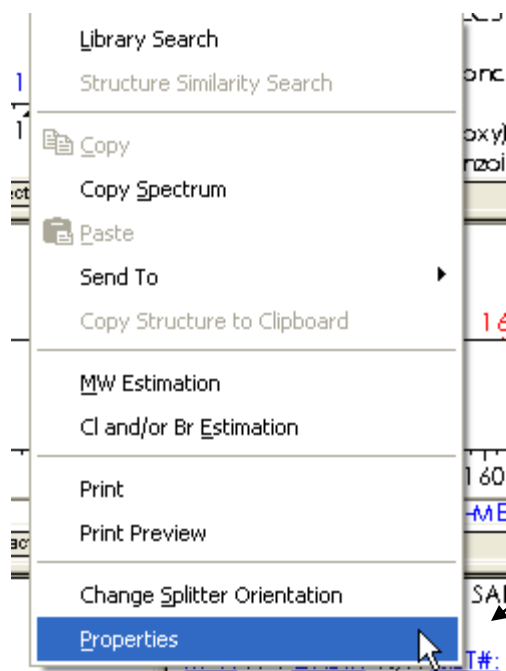
Tip 1: When reviewing search results, use up and down arrows on keyboard to quickly step through results!



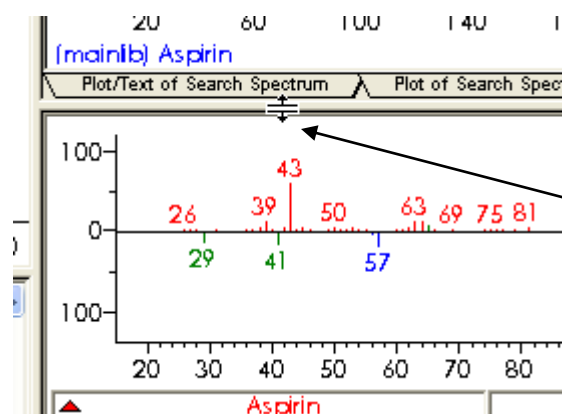
Tip 2: When viewing structures in MS Interpreter, use left and right arrows on keyboard to quickly review results!



Customizing the Windows



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

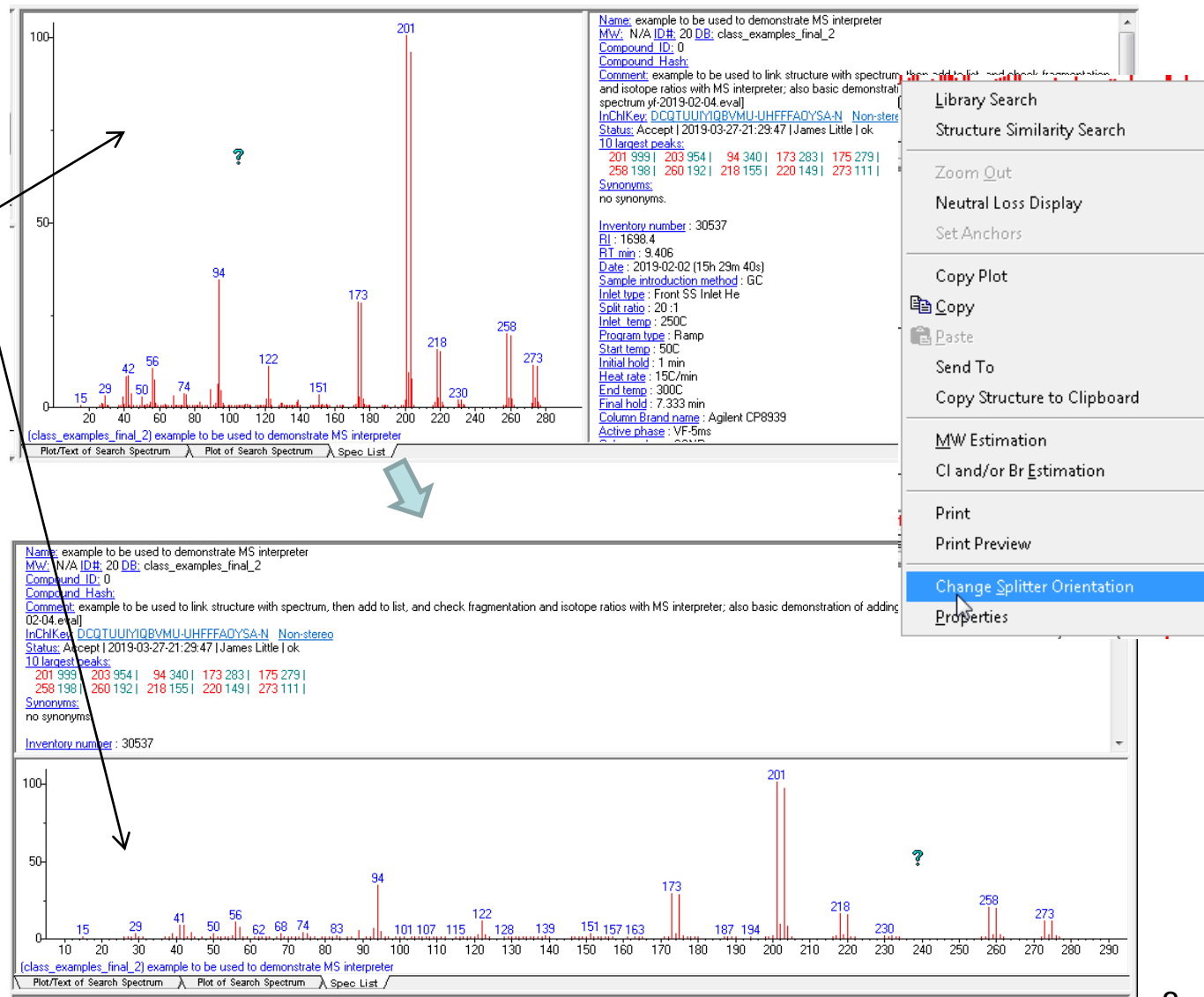


-place cursor over any bar between (**top or side**) windows and then **LMB** and drag to change the size of a window or make window so small it essentially disappears.

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

