

Lib Search: Cleaning Up Workspace and Temporary HLM Files in NIST26

James Little

Mass Spec Interpretation Services

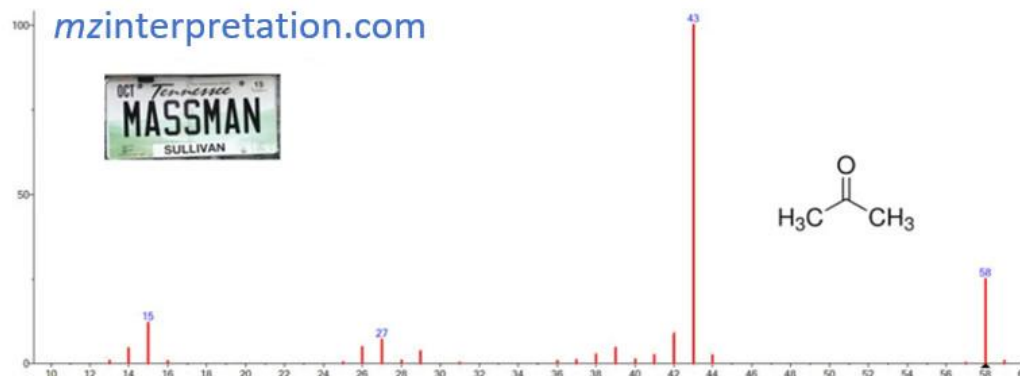
June 28, 2026

mzinterpretation.com

See **Full Course** on NIST26 with new **Integrated** Deconvolution/Library Searching for **EI GC-MS** and **LC-MS/MS**!

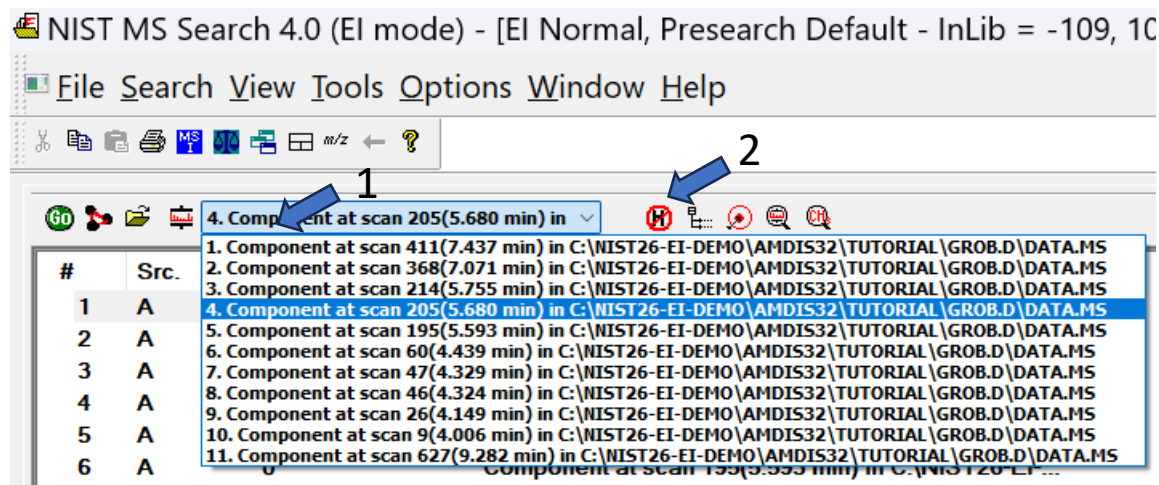
Mass Spec (m/z) Interpretation Services

Organic Mass Spectrometry



Manually Cleaning Up Lib Search Window of Search History, HLM Files

- Every time a search is performed, the results are change in an HLM file and can be recalled from a pull-down menu, 1
- Searches are so quick, I just usually search again instead of recalling
- These results are stored in a named HLM file and stored in MSSEARCH folder
- Click on Clear History icon, 2, to delete them and save disk space and “folder clutter”
- These files are created in either EI or MS/MS Searches



Automatically Cleaning Up Lib Search Window of Search History, HLM Files

- Right click on Spec List Window
- Open Properties
- Select Hit List
- Check “Clear History on Exit” box

NIST MS Search 4.0 (EI mode) - [EI Normal, Presearch Default - InLib = -181, 100 spectra]

File Search View Tools Options Window Help

1. Component at scan 5332(13.891 min)

#	Src.	MW	Formula	Name
1	L	0		Component at scan 5332(13.891 min) in C:\NIST26-E...
2	L	146	C6H4Cl2	Clipboard #3
3	L	0		Component at scan 2090(6.268 min) in C:\NIST26-EI...

Names / Structures /

mainlib; bb; cayman_library; misc_libs; mona_gcms; swgdr...

100
10
1

1000 900 800

Lib. Match Prob. (%) LibRI DBs

1	bb	845	74.0	
2	bb	807	14.0	
3	bb	755	2.66	
4	bb	739	1.59	
5	bb	728	1.12	
6	bb	724	0.98	
7	bb	723	0.95	
8	mo	710	0.63	
9	mo	710	0.63	
10	bb	707	0.57	
11	bb	703	0.40	

Library Search
Structure Similarity Search

Cut
Copy
Paste
Select All

Send To
Find name in Names tab
Import
Export Selected Spectra
Copy Selected Items to Clipboard
Export Selected Items to Text File
Insert Clipboard Structure
Copy Structure to Clipboard
Insert Clipboard Spectra

Print
Print Preview

Properties

Library Search Properties

Hit List

Spec List

Plot of Hit

Unknown Plot

Spec List Plot

Hit Text Info

Unknown Text Info

Spec List Text Info

Structure View Options
Structure Size in %: 50 ☐ Structures Only

EI no RI Search
Items to Display
☒ Order Number
☒ Library
☒ Prob.(%)
☒ LibRI
☒ Other DBs
Default

☒ Short Library Name ☒ Clear History on Exit

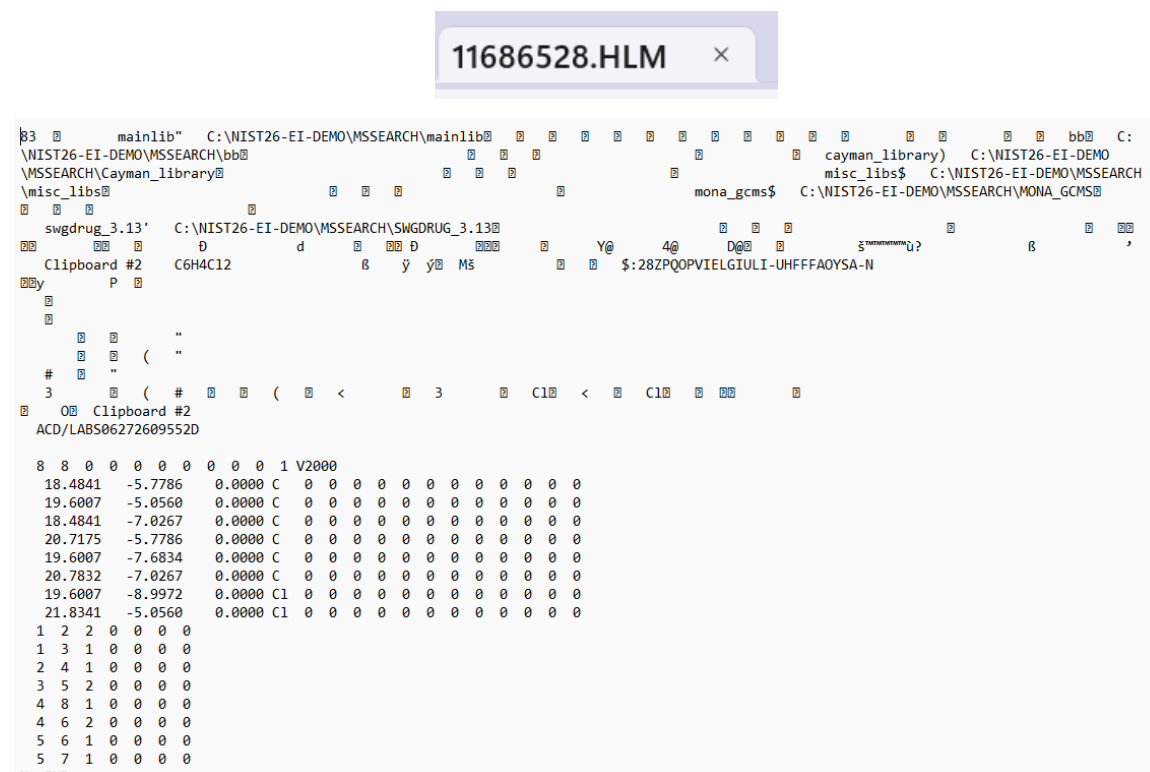
Color Settings
☒ Bonds and Rings
☒ Atomic Symbols
☒ Compound Name

Font Settings
Select Font Set for all views

OK Cancel Help

Screenshot of Typical HLM Files Found in MSSearch Folder

01786528.HLM	6/27/2026 9:58 ...	HLM File	3 KB
03017528.HLM	6/27/2026 10:37 ...	HLM File	51 KB
08886528.HLM	6/27/2026 10:01 ...	HLM File	3 KB
11686528.HLM	6/27/2026 9:56 ...	HLM File	51 KB
13786528.HLM	6/27/2026 9:58 ...	HLM File	51 KB
15151528.HLM	6/26/2026 7:05 P...	HLM File	14 KB
17786528.HLM	6/27/2026 9:59 ...	HLM File	51 KB
19151528.HLM	6/26/2026 7:06 P...	HLM File	4 KB
22296528.HLM	6/27/2026 10:07 ...	HLM File	15 KB
25065528.HLM	6/27/2026 6:27 ...	HLM File	15 KB
25786528.HLM	6/27/2026 9:59 ...	HLM File	51 KB
26907528.HLM	6/27/2026 10:36 ...	HLM File	51 KB
28686528.HLM	6/27/2026 9:58 ...	HLM File	51 KB
29196528.HLM	6/27/2026 10:06 ...	HLM File	15 KB
29417528.HLM	6/27/2026 10:44 ...	HLM File	4 KB
33066528.HLM	6/27/2026 9:13 ...	HLM File	51 KB
38686528.HLM	6/27/2026 9:58 ...	HLM File	51 KB



Cleaning Up Lib Search Spec List Window

- Every search performed creates an entry in the Spec List Window
- To remove them, right click, "Select All," then right click "Cut"

NIST MS Search 4.0 (EI mode) - [EI Normal, Presearch Default - InLib = 124, 100 spectra]

File Search View Tools Options Window Help

1. Component at scan 411(7.437 min) in

#	Src.	MW	Formula	Name
1	A	0		Component at scan 9/4 006 min) in C:\NIST26-ELDE
2	A	0		Compo
3	A	0		Compo
4	A	0		Compo
5	A	0		Compo
6	A	0		Compo
7	A	0		Compo
8	A	0		Compo
9	A	0		Compo
10	A	0		Compo

Names Structures

mainlib: bb; cayman_library: misc_libs; mona_g

100-
10-
1-

1000 900 800

Lib. Match Prob. (%)
1 mo 857 97.2
2 bb 755 2.38
3 mi 726 2.38

Library Search
Structure Similarity Search
Cut
Copy
Paste
Select All
Send To
Find name in Names tab
Import
Export Selected Spectra
Copy Selected Items to Clipboard
Export Selected Items to Text File
Insert Clipboard Structure
Copy Structure to Clipboard
Insert Clipboard Spectra
Print
Print Preview
Properties



NIST MS Search 4.0 (EI mode) - [EI Normal, Presearch Default - InLib = 124, 100 spectra]

File Search View Tools Options Window Help

1. Component at scan 411(7.437 min) in

#	Src.	MW	Formula	Name
---	------	----	---------	------

Names Structures

mainlib: bb; cayman_library: misc_libs; mona_g

Spec List

mainlib: bb; cayman_library: misc_libs; mona_g; acms: swadrui 3.13: 60830 total spectra