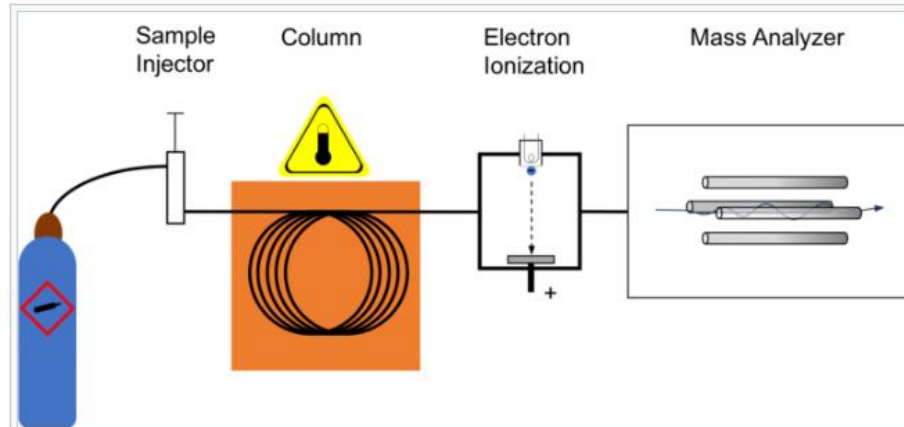


**Free NIST GC-MS Software Lab for
Universities:
Part 9: 58,456 Additional Reference
Spectra for NIST Demo Search**



Resource Link to 5 Additional Libraries in Combined in One Zipped File

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](#)

Topics Discussed Concerning Libraries in Presentation (Video/Handout)

- Overview of libraries
- Brief description of origin of the 5 libraries
- Lib2NIST for MONA conversion
- Relative Quality and Displaying Source in Search
- Installing the libraries in Demo Search
- Updating index files
- Setting up libraries to search

Summary of *All* Free Libraries in the Laboratory Course

- Additional libraries needed to use Demo software to solve “Real-World” problems
- Included 5 additional libraries, 58,456 additional EI reference spectra and 34,933 associated structures
- There can be errors in *any* library
- The NIST main library with software the highest quality
- Others vary widely in quality and actual quality unknown
- Remember, library searches give *proposed* structures, there are an aid to identification
- Always consider sample history and organic chemistry
- *Be skeptical* and make sure library spectrum looks reasonable (i.e. check in MS Interpreter)

Library Name	No. EI Spectra	No. of Structures	Quality	Comment
mainlib	2,373	2,373	Very good	Library from NIST supplied with Demo
SWGDrug_3.13	3,598	3,593	good	Library downloaded from internet, drug related
Cayman	2,262	506	good	Library downloaded from internet, drug related
Misc_lib	20,049	10,547	Unknown/ Good	From internet and Kodak library; 10,501 are Kodak ~95% good quality, remaining unknown, wide variety of compound types
MONA	18,914	18,815	good	Crowd sourced, wide variety of compound types
BB	13,633	1,472	good	Six peak index from ASTM and Eastman Chem. Co., wide variety of compound types, useful for low MW compounds and when no full spectrum available
Total	60,829	37,306		

My Opinion on Order of Quality

MAINLIB >>> BB* > SWGDrug or Cayman > Misc_lib > MONA

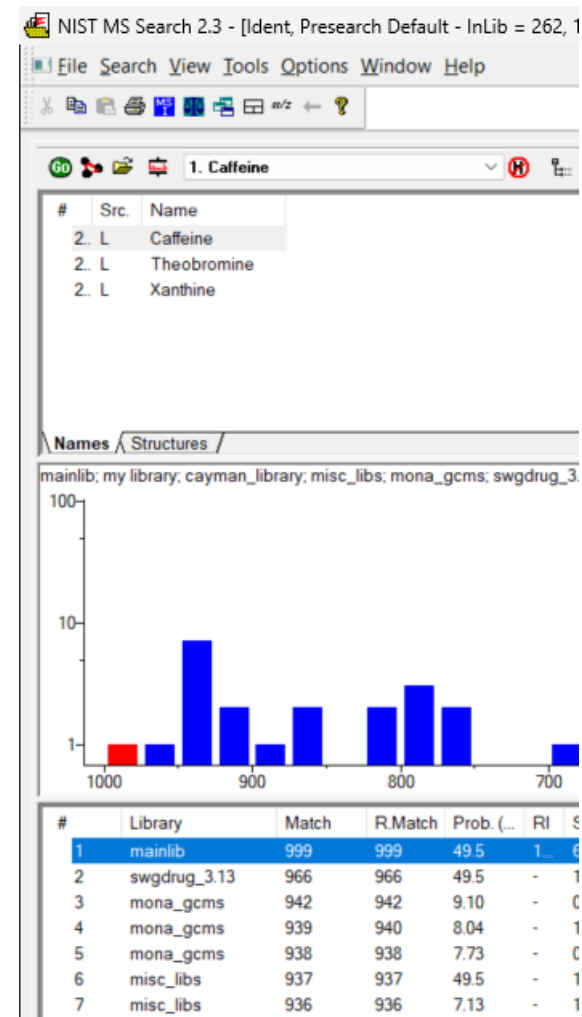
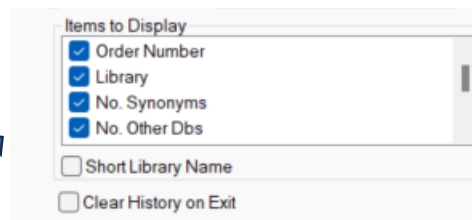
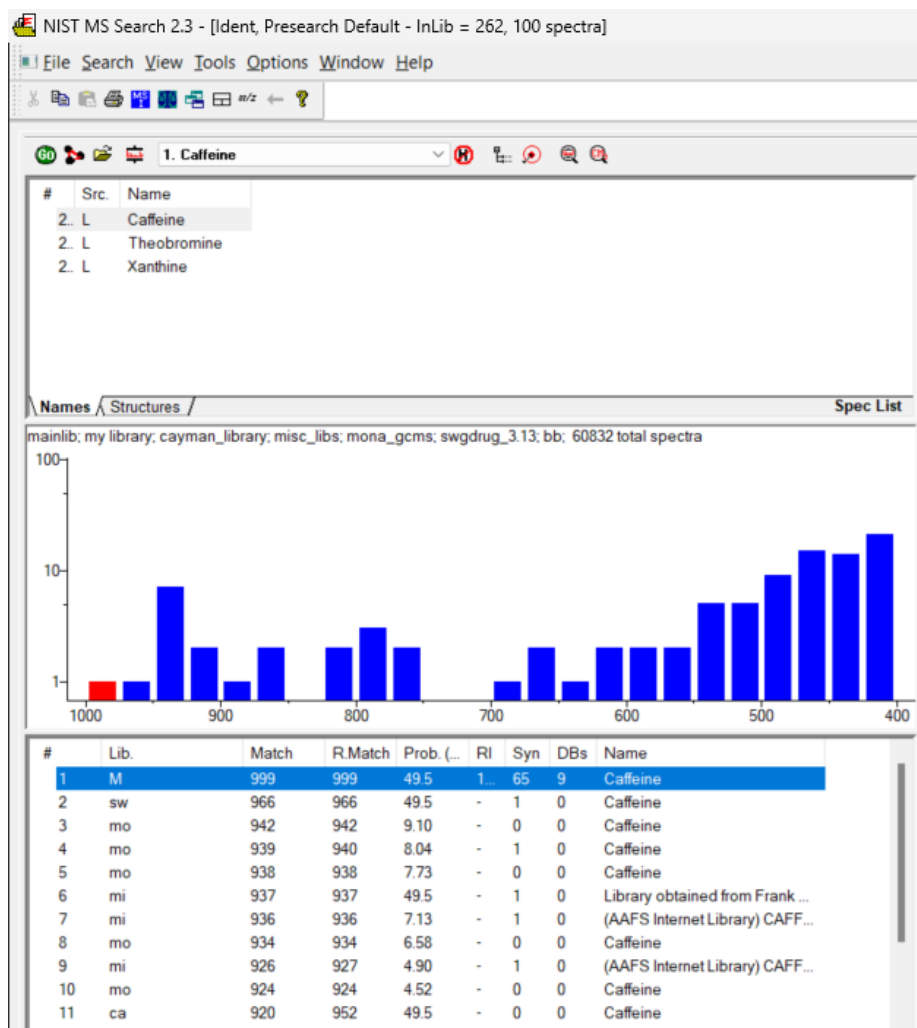
Higher Quality

Lower Quality

*Lower relative match due to only 6 largest peaks

Library Name Shown with Search Results

- Useful to know the origin of hit
- Change to full name, right click on bottom window, “un-select” Short Library Name



Miscellaneous Library (Misc_lib)

- Various free libraries that I have had over the years
- 10,501 are from Kodak collection, the rest are from internet sources such as Agilent VOCS, Finnigan Xcalibur demo library, Frank Antolasic in Wsearch demo, TIAFT, Agilent PCB, AAFS, *etc.*
- Kodak spectra were evaluated by NIST before entries were added to their library
- Some removed, but no editing of the ones in this copy were performed
- However, ~95% are good quality
- Quality of the remaining 9,548 spectra are unknown

Cayman Library

- Library curated by Cayman's forensic team
- Contains newly synthesized novel psychoactive substances (NPS's)
- Downloaded file on 9/4/2023
- Contains 2,262 EI spectra
- Download future versions at link below

[Link to Cayman Library Download](#)

SWGDrug Library

- Variety of drug related and other chemicals
- Scientific Working Group for the Analysis of Seized Drugs
- Library continuously being updated
- Downloaded copy on 9/4/2023
- Contains 3,598 EI entries
- Download future versions at link below

[SWGDrug Library Download link](#)

Black Book (BB) Library

- Library is a six peak index of EI spectra
- Majority from ASTM collection
- Some entered by Eastman Chemical and contain structures
- Useful when a compound's spectrum is not present in the other libraries
- If more complete spectra present, will definitely have a *lower* relative match
- 13,634 spectra with 1,472 structures
- Library searched manually using a group of "Black Books" in the mid 1970's

MONA Library Additional Information

- Copy of the MONA EI GC-MS library on my website in 2021, 18,886 entries
- Version in zip file more current, 18,914 entries (9/4/2023)
- Used the SDF version of MONA from their website
- Lib2NIST program converts from SDF format to NIST format with structures
- Not sure which is the newest version of Lib2NIST?
- Some problems with derivatives in MONA library, see ***next 2 slides***

[Link My Old Version MONA EI library in NIST format](#)

[Link to MONA Website for file in NIST SDF format](#)

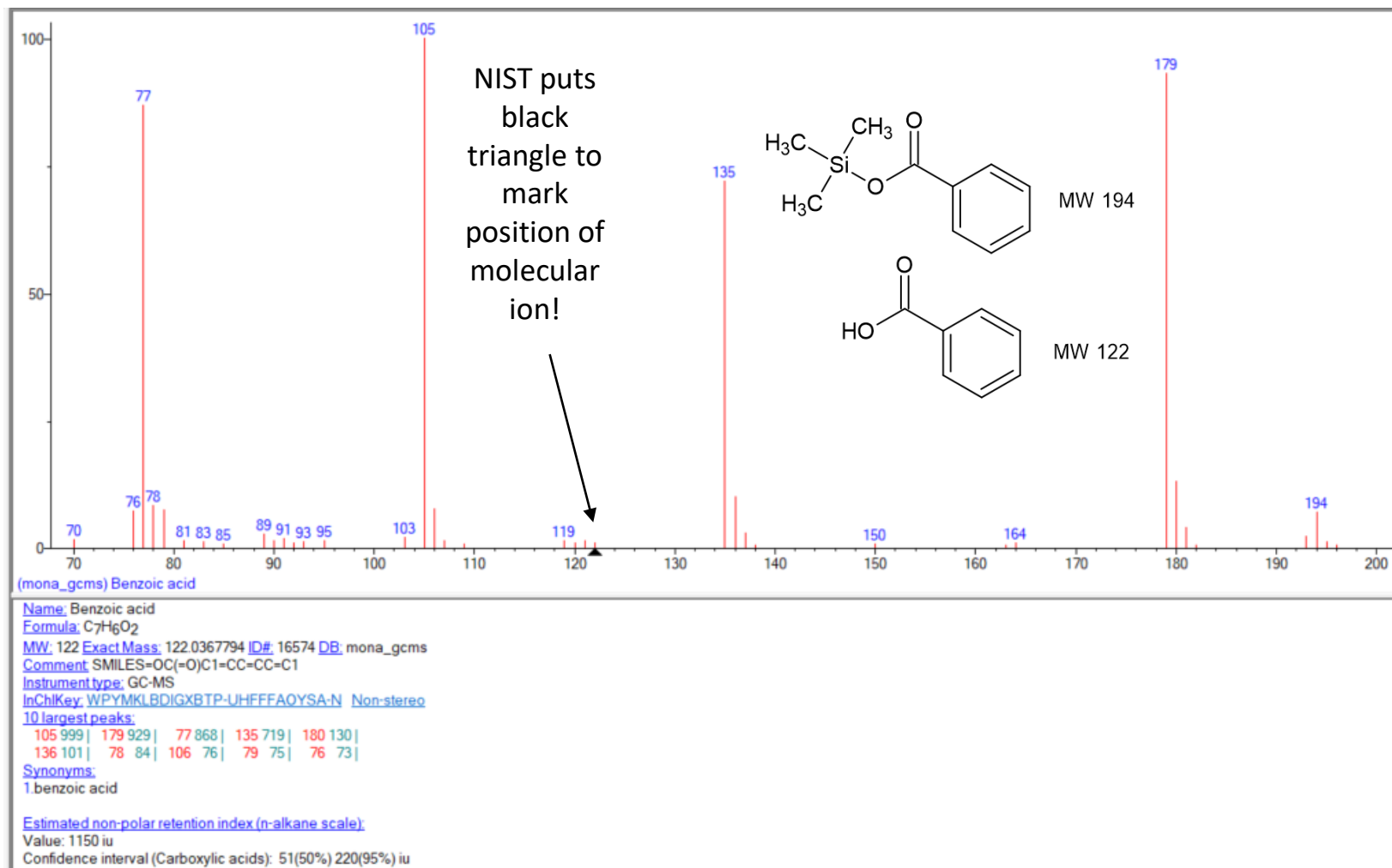
[Link to Lib2NIST program download on my website](#)

[Documentation on Lib2NIST](#)

[Link to Lib2NIST program on NIST website](#)

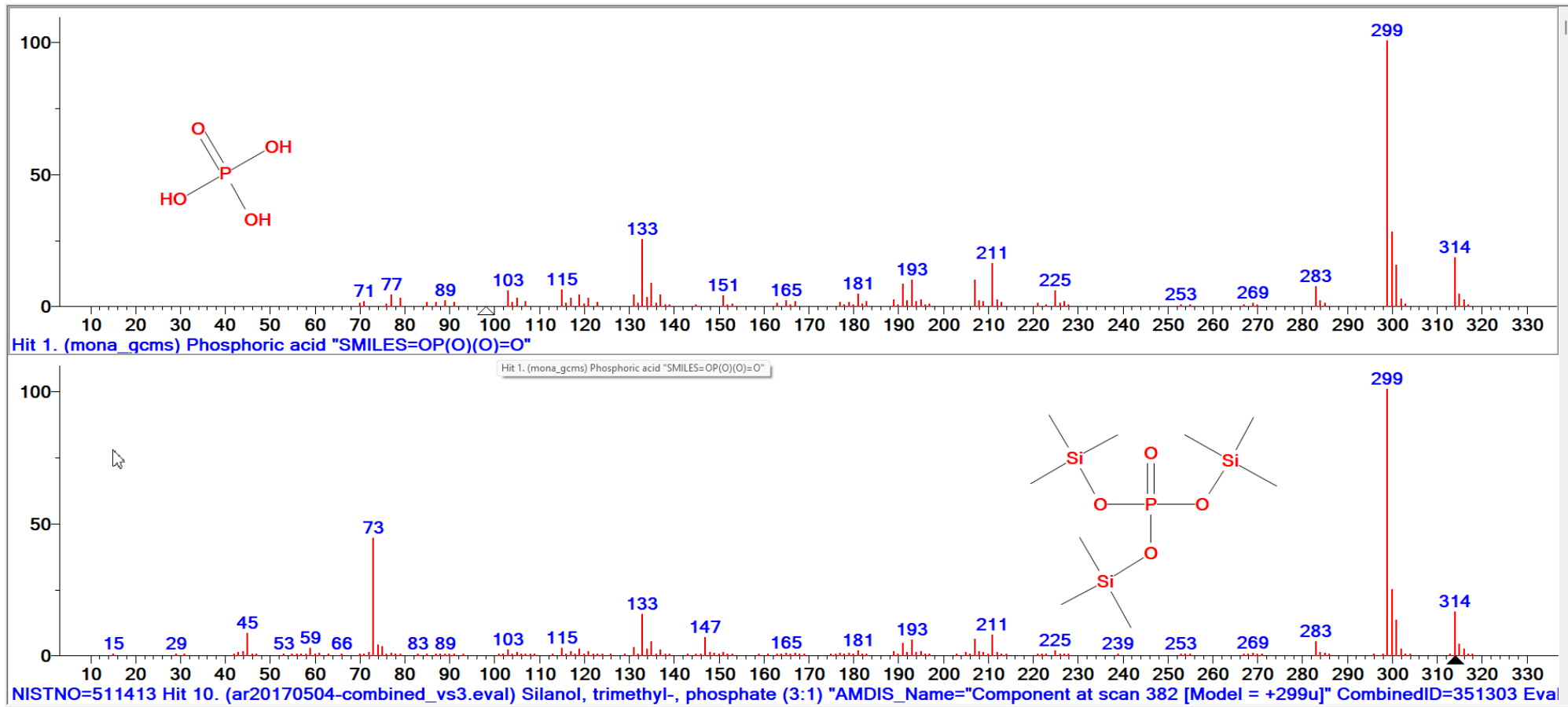
MONA TMS Library Derivative Problems

- The spectrum below is the TMS derivative, **NOT** the free acid
- Will not cause searching problem, but user might not notice
- It will affect the structure search, will not find the TMS derivative by structure!
- Not, NIST always put a little black triangle to mark the molecular ion!



MONA TMS Library Derivative Problems

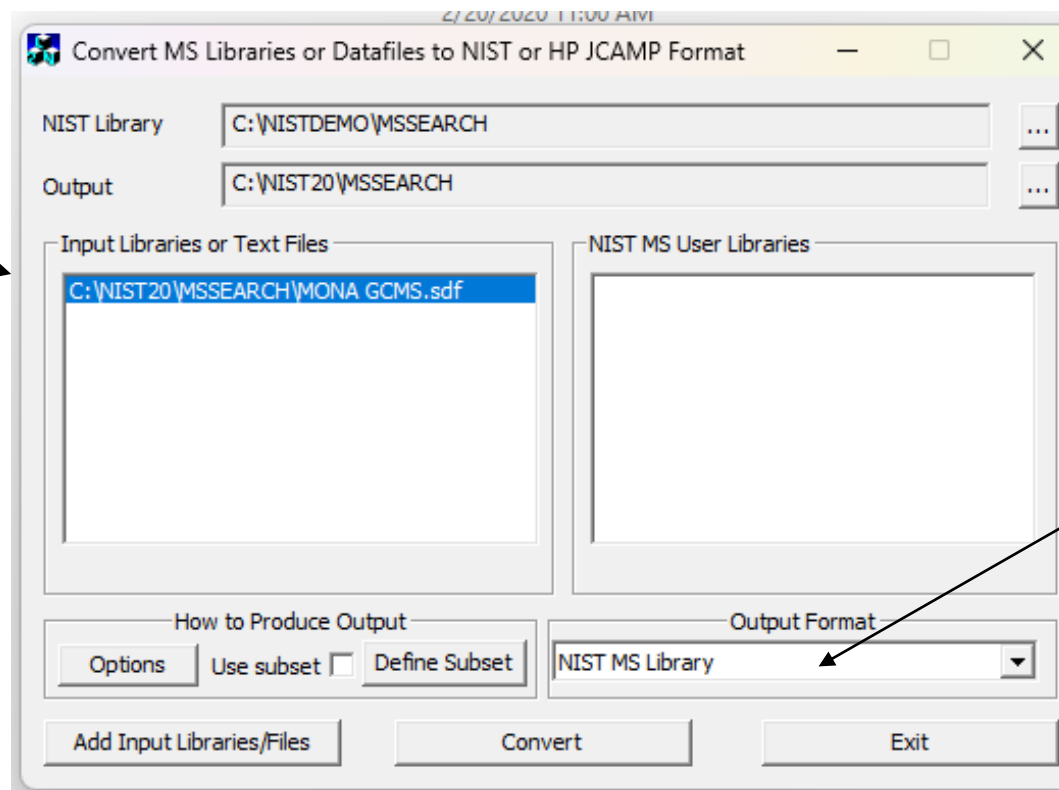
- For phosphoric acid, again shown as the structure of free acid **NOT** tris-trimethylsilyl derivative
- Also, for **SOME** trimethylsilyl derivatives, they leave out their ubiquitous mass fragments at m/z 73, 74, 75, 147, 148, and 149
- Compare the NIST library spectrum to the MONA spectrum below
- Similar approach taken for the free GOLM Metabolome Library, [see link](#)



Screenshot of Lib2NIST: Converting Mona.sdf to NIST-Formatted EI Library

- Used to convert and combine libraries
- NIST utility, usually delivered with full version NIST
- Not too difficult to use
- Download MONA in sdf format
- Select in Lib2NIST then convert, then click convert button with Output format NIST MS Library

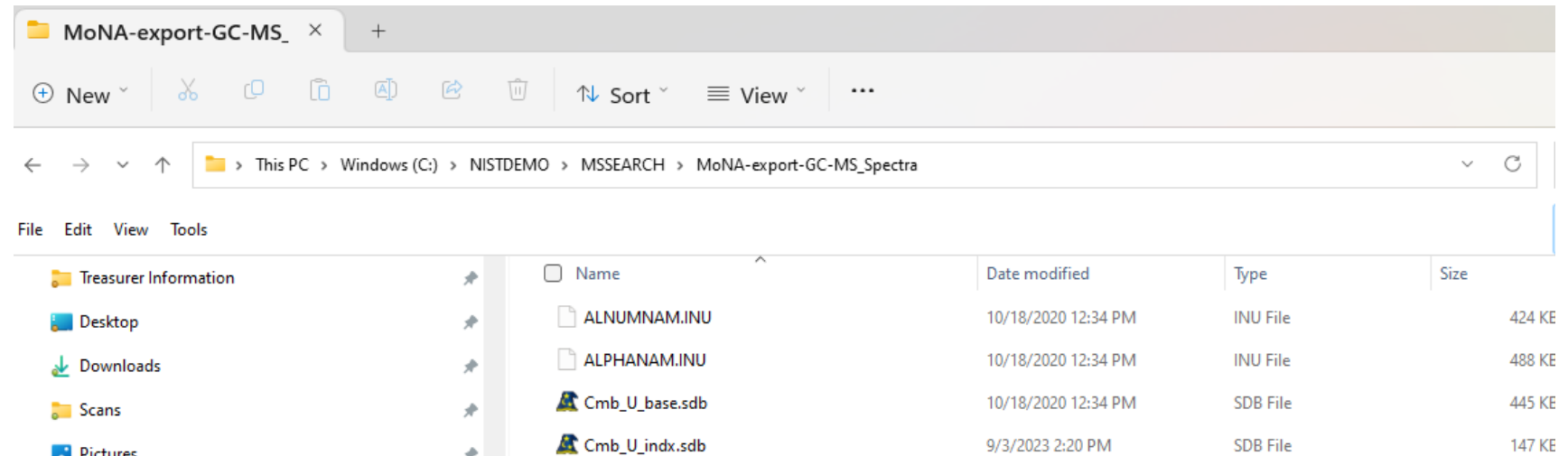
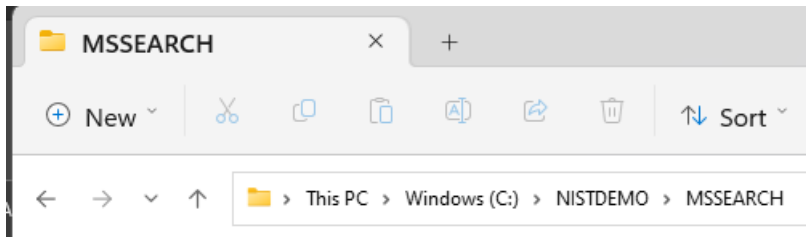
After download,
find on computer
and select



Then convert with
output forma and
NIST MS Library

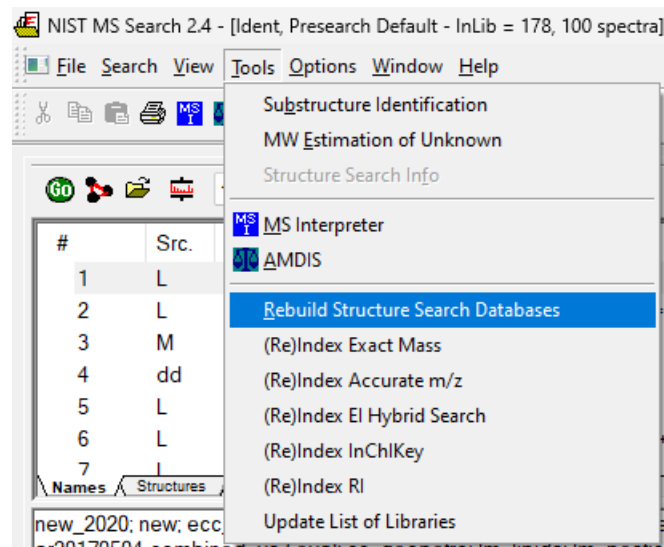
Installing Libraries in NIST Demo Program

- Find the NIST Demo Folder on C drive, see my location below
- Put the three libraries in the MSSEARCH Folder
- Make Sure when you open each library in this folder that the next level down contains the indices
- E.g. See the view for MONA library below
- Should see around 34 files
- If they are obtained further down the file tree in another folder, you will not see them when you open the NIST program!



Making Sure Index Files for All Added and User Libraries are Updated

- Make sure structural indices current for all these 5 libraries
- In addition, if any new spectra added to your personal library, it needs to be updated after every new addition plus the hybrid searches index
- If not updated, the structure searches will not work
- If you want to do hybrid type searches, also update those indices also
- If not updated, the hybrid searches will not work
- Also update in InChIKey
- See how these options accessed below:



Selecting Libraries to Search

- Select the icon shown below in NIST Search Program
- Go to Libraries Tab and select all 5 including main library plus your personal library if it exists
- Add them to the list
- Make sure to add to **both** the Spectrum search and Structure search windows
- Exit my selecting OK

Click Library
Search
Options

The screenshot shows the NIST MS Search 2.4 application window. The title bar reads "NIST MS Search 2.4 - [Ident, Presearch Default - InLib = 178, 100 spectra]". The menu bar includes File, Search, View, Tools, Options, Window, and Help. The toolbar contains icons for file operations and search parameters. The main window displays a table with columns for "#", "Src.", and "Name". The "Library Search Options" dialog box is open, showing tabs for Search, MS/MS, Libraries, Automation, Limits, Constraints, and RI (GC). The "Spectrum Search Type" section has "Identity" selected. The "Spectrum Search Options" section has "Reverse Search" and "Penalize rare compounds" unchecked.

#	Src.	Name
1	L	Clipbo
2	L	Compo
3	M	(S)-(+)-3
4	dd	4-Fluor
5	L	Clipbo
6	L	Compo
7	L	p-fluoro

This screenshot shows the "Library Search Options" dialog box with the "Libraries" tab selected. It displays "Available 26899 Spectra in 5 Libraries" with a list of library names: mainlib, caymanspectrallibrary-june_23.hp, mona-export-gc-ms_spectra, my library, and swgdrug3.9. Below this is an "Add >>" button. The "Included Libs:" section shows the same five libraries, with a red "X" icon and up/down arrows. At the bottom, it states "26899 Spectra in 5 Libraries".

This screenshot shows the "Library Search Options" dialog box with the "Libraries" tab selected. It displays "Available 26899 Spectra in 5 Libraries" with a list of library names: mainlib, caymanspectrallibrary-june_23.hp, mona-export-gc-ms_spectra, my library, and swgdrug3.9. Below this is an "Add >>" button. The "Included Libs:" section shows the same five libraries, with a red "X" icon and up/down arrows. At the bottom, there is a dropdown menu for "Spectrum search" with "Spectrum search" and "Structure search" options. At the very bottom are "OK", "Cancel", and "Help" buttons.