# Using NIST MS Search with Agilent OpenLab Software for Unknown Identifications

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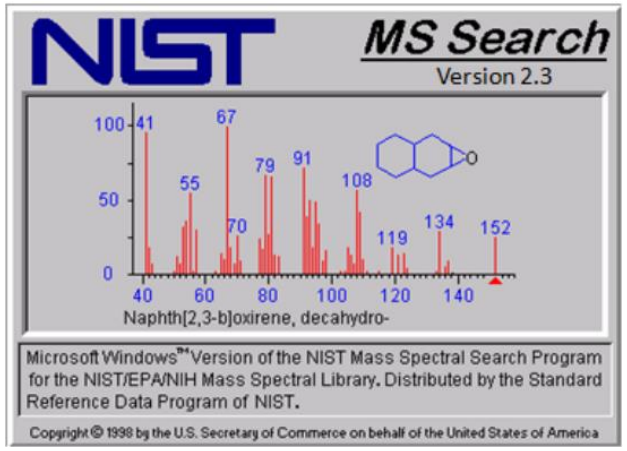
https://littlemsandsailing.com/

- Some tips on using NIST MS Search for unknown identifications
- Search with Agilent GC MSD/OpenLab CDS transferred to NIST MS Search
- Information supplied from Agilent (Emily Adams, Product Support Engineer)
- *YouTube Video*

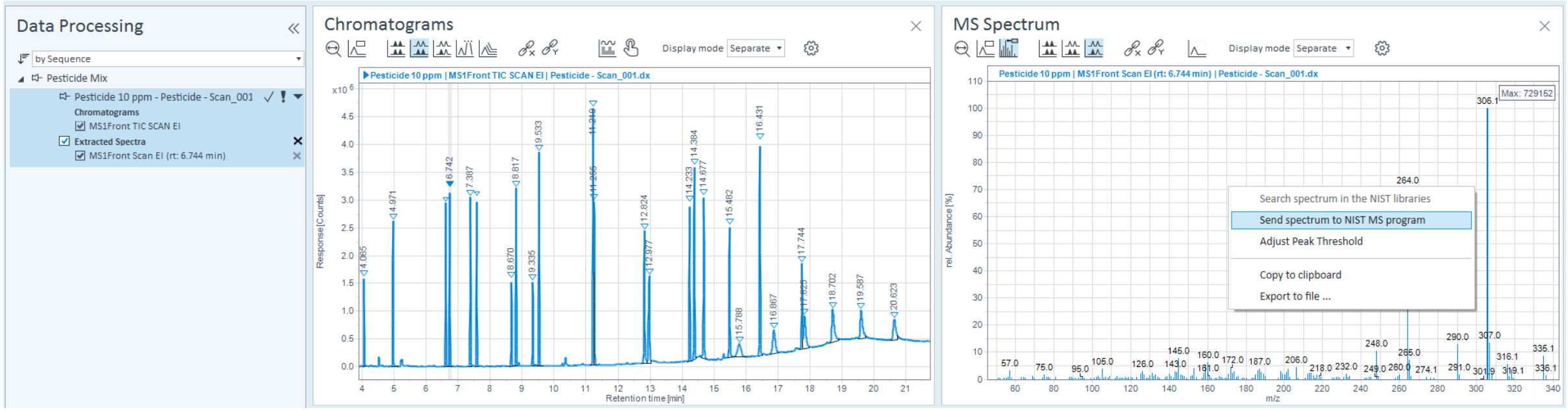



## Topics Discussed

1. Sending spectra for search from OpenLab to external NIST MS Search Program
2. Processing OpenLab Files in Agilent MassHunter
3. Export files in netCDF (AIA) format for processing with AMDIS, Wiley KnowItAll, *etc.*
4. Data file locations in OpenLab file directories
5. Searching using NIST *dll* with results returned for internal display in OpenLab
6. Library format supported by OpenLab and interconversion of library formats with NIST Lib2NIST utility program
7. Adding an entry to existing user library or creating first entry in a new user library
8. Initial Settings for NIST Search V3.0 in EI and MSMS (tandem) modes
9. Extensive user help found on “Agilent OpenLab Help & Learning” website

*1) Can you send spectra to NIST's MS Search program?*

Yes! The simplest way is to right-click on the spectrum in OpenLab CDS and select Send spectrum to NIST MS Search program. (Note that this option is greyed out until NIST's MS Search package is installed on the same PC as OpenLab CDS.)

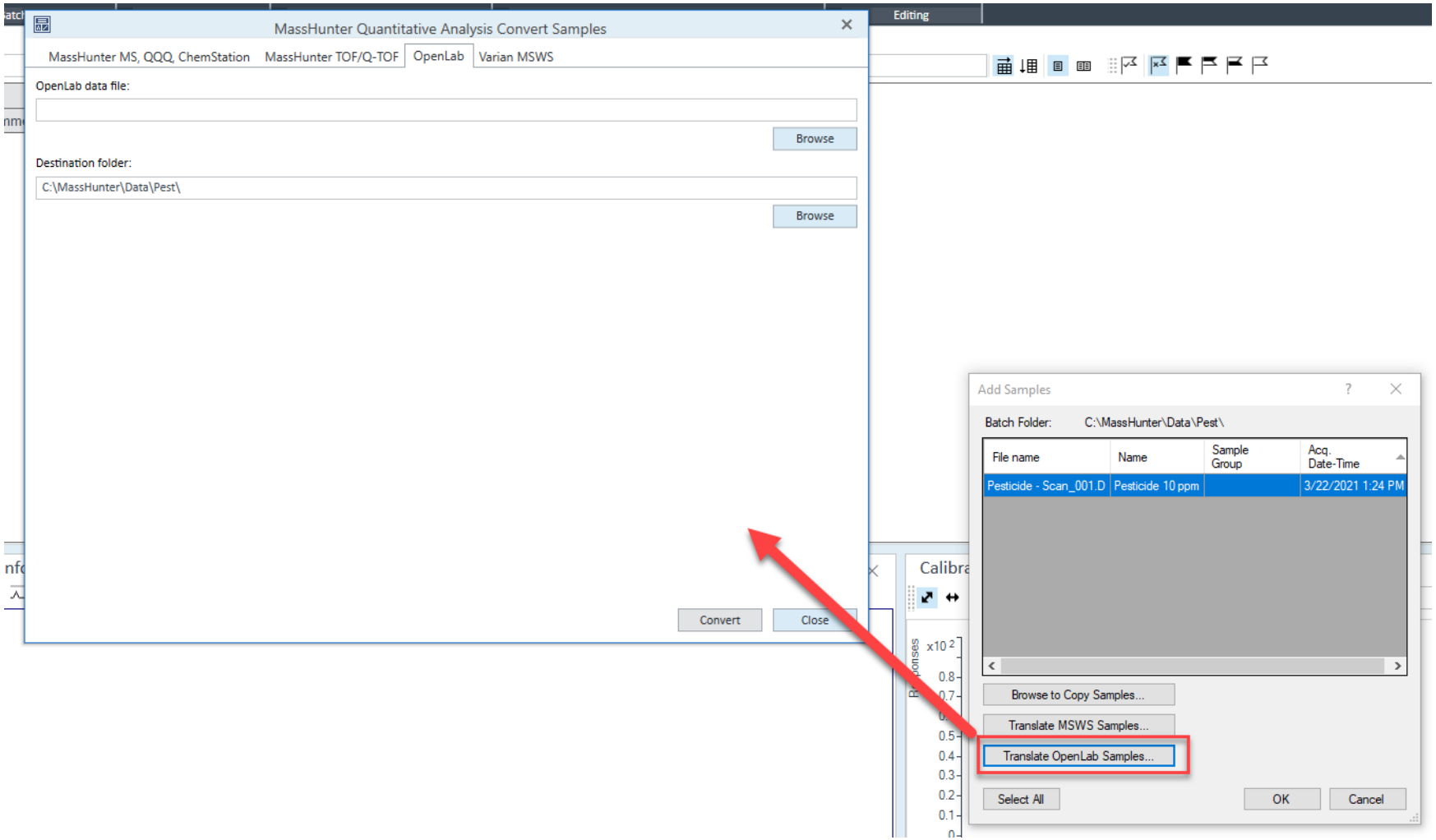


1) This will open NIST MS Search and load the spectrum you sent.

***Note:*** When you click “Send spectrum to NIST MS program”. The MSP text file is generated and saved to a temporary folder (C:\Usrs\<CurrentUser>\AppData\Local\Temp\SPECTRA.MSP), should you need to access it

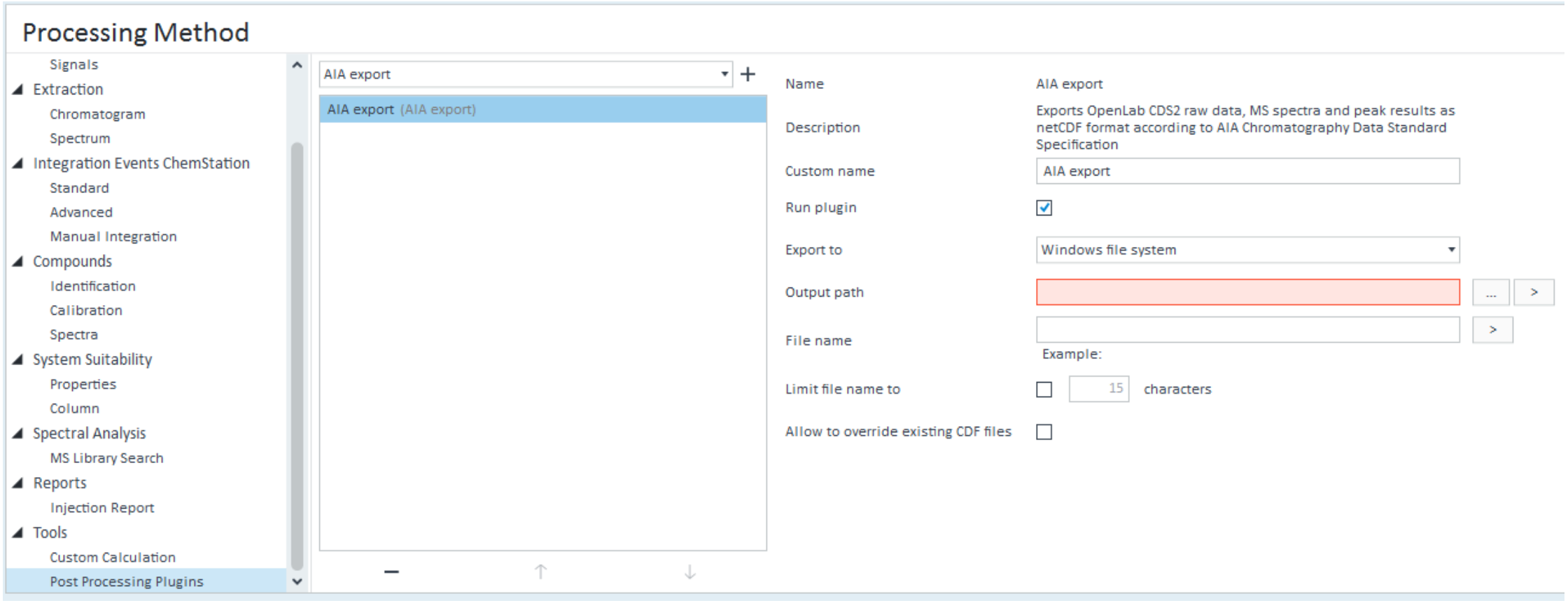
*2) Can you process the OpenLab mass spec file in MassHunter?*

Yes, you can convert OpenLab CDS data to MassHunter format. You can then analyze the converted data in MassHunter Quant, Qual, and Unknowns Analysis. You ***cannot*** open it in MSD ChemStation Data Analysis. There is a conversion tool you can access starting in MassHunter Quant 11.1.



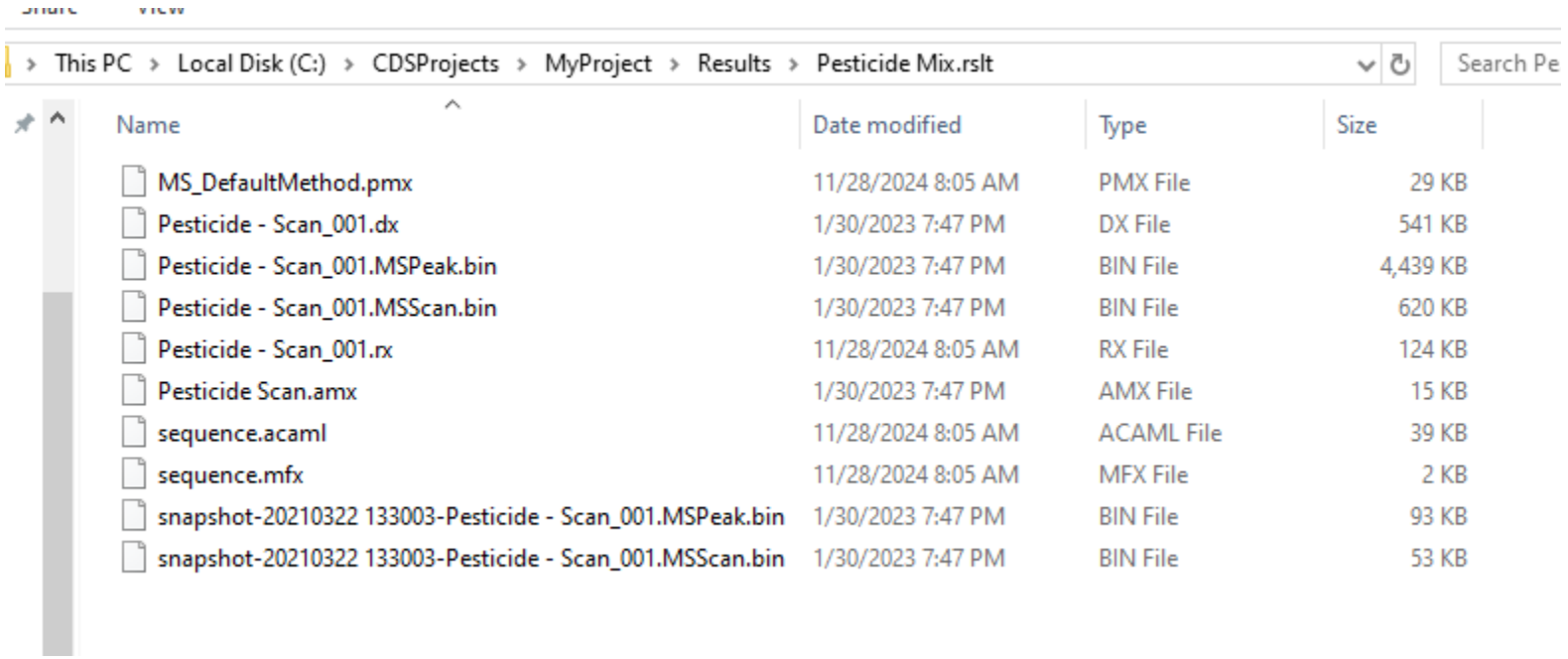
*3) Can you convert OpenLab to netCDF (AIA) files?*

Yes. The AIA export functionality in Post Processing Plugins allows the export in NetCDF format. For example, if you wanted to use NIST's AMDIS program or Wiley KnowItAll, this is how you can export your data.



# 4) Data File Locations in OpenLab

- CDS is organized in result sets – files are grouped together based on the sequence they are run with into folders called <MyResultName>.rslt (or <MyResultName>.sirslt for single injections). This *.rslt or *.sirslt folder contains all the data and processing information needed to reconstruct the analysis (acquisition method, processing method, raw data, results, etc.)
- Raw data is stored in *.dx files. Results are stored in *.rx files. Each injection will have one *.dx and one *.rx file.
- The MS data is stored in the same format that MassHunter uses – namely for GCMS single quads there are two binary files which contain the raw data - *.MSPeak.bin and *.MSScan.bin.



*5) Can library searches be performed with NIST dll and then returned to OpenLab for Display?*

Yes, see page 29 in the following *link* to Agilent documentation

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## Use MS Libraries Within OpenLab CDS

3 Under **MS Library Search > Properties**, select the desired library from the drop-down list and click the + icon to add it. For details, search for "Use the MS library search" in OpenLab Help and Learning.

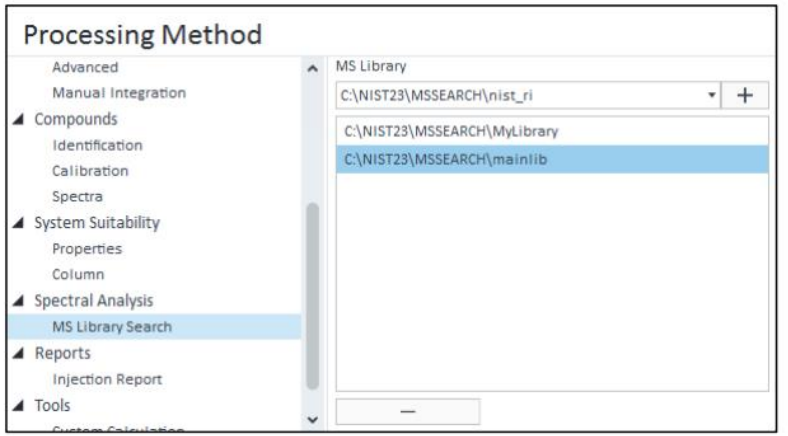



**Figure 22** MS library properties

4 Save the processing method.

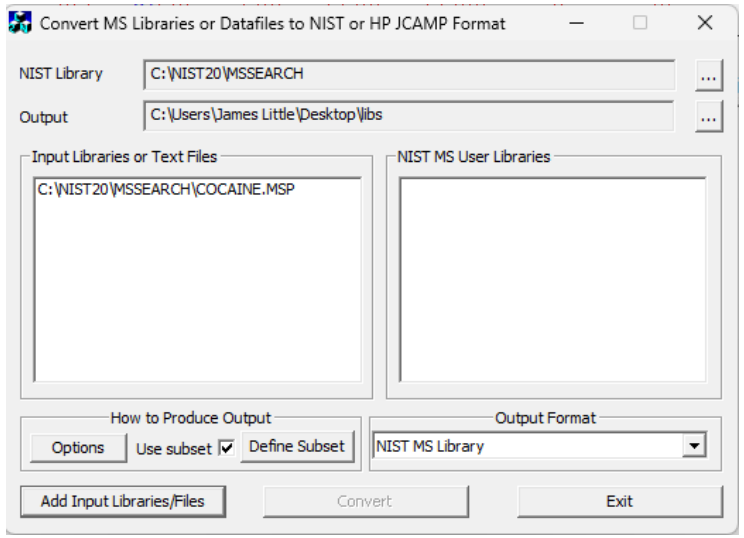
5 Load MS data and link it to the prepared processing method.

6 For details on performing an MS Library search, refer to OpenLab Help and Learning.

## 6) What library formats are used with OpenLab?

OpenLab CDS can only use libraries in NIST format – so for users with existing .L (PBM) libraries, we direct them to convert using NIST's Lib2NIST utility. mslibrary.xml libraries can also be converted, if you first send them to JCAMP format, then use Lib2NIST.

Information can also be found in section 5 of the following manual, *here is the link*




Agilent

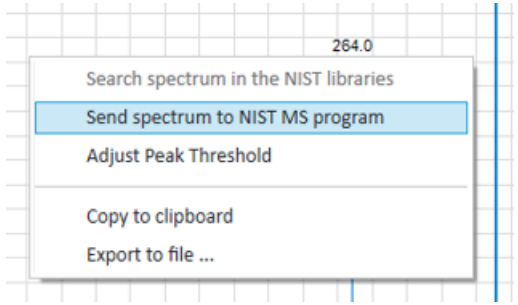
OpenLab CDS

**Setup and Configuration of MS Library Search**

# 7) How do I add to or create a user library?

1. All libraries used in OpenLab are in NIST format
2. Thus, to add a library entry or to create the first entry in a new user library, first send the spectrum to NIST MS Search from OpenLab by using the “Send spectrum to NIST MS program”
3. Then the Librarian Tab is selected at bottom of the NIST MS Search Program
4. The remaining details are found in my videos with associated handouts on my web page
5. EI MS libraries, https://littlemsandsailing.com/2020/08/ms-master-class/, Part V
6. MSMS libraries, https://littlemsandsailing.com/2020/12/lcms-unknown-identification-with-nist-search-using-msms-libraries/, Part VII

1

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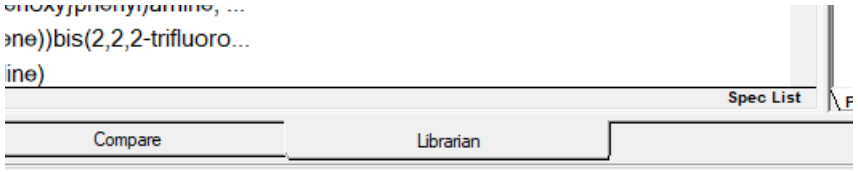

## 8) Initial Settings for NIST Search V3.0 in EI and MSMS (tandem) Modes

- There are many settings to setup when first using NIST MS Search
- After setup, user saves as a configuration which makes easy to restore if changed during processing
- ***EI*** Quick Start Guide for Settings *Link*
- ***MSMS (tandem)*** Quick Start Guide for Settings *Link*

# 9) Agilent OpenLab Help & Learning

- Great resource for a large group of topics
- https://openlab.help.agilent.com/
- After choosing language, *e.g., one* can find information on library search
- https://openlab.help.agilent.com/en/index.htm#t=mergedProjects%2FDataAnalysis%2FUseMSlibrarysearch.htm
- Easily search for useful topics, *e.g.,* look for information on AIA netCDF file export as shown below on right side of screen