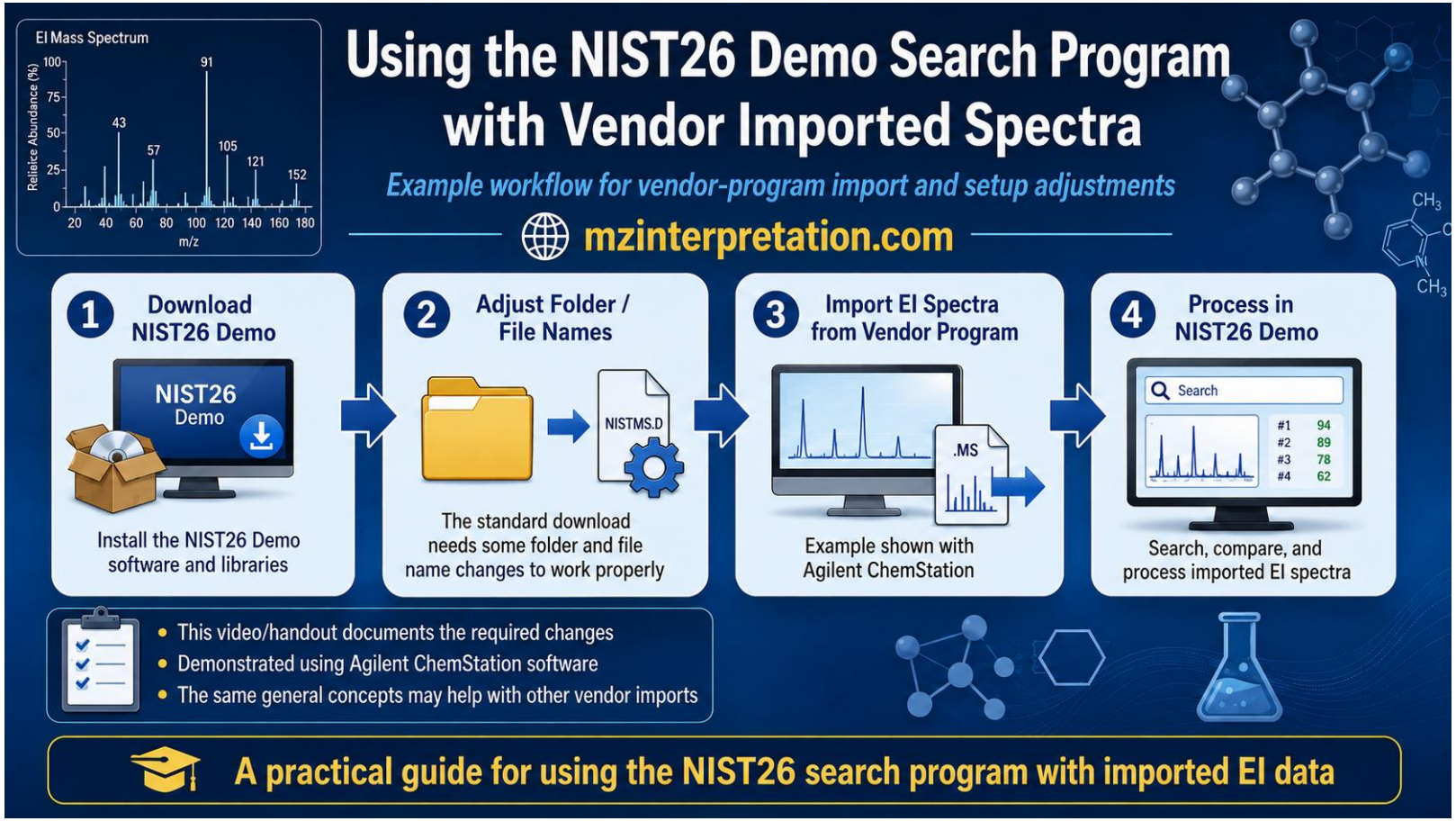
Using the NIST26 EI Demo with Spectra Imported from Vendor Software

Video and Handout (8/23/2026)

James Little
Mass Spec Interpretation Services
tvasailor@gmail.com

O. David Sparkman
Independent MS Consultant
ods@csi.com



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

link to course

Evaluating the NIST26 EI Demo as Delivered

Preferred Approach

- ***For evaluation purposes, most users will find the EI Demo as-delivered to be the preferred approach.***
- It demonstrates very efficient chromatographic processing, deconvolution, and library-searching capabilities without requiring changes to the installation.
- Vendor import of spectra is still fully supported in the purchased version of NIST26 with no significant modifications as delivered.
- ***Very useful to employ both approaches in data processing.***

Optional Configuration for Vendor-to-NIST Library Searching

Many Modifications Required

As delivered, the NIST26 EI Demo is not configured to receive spectra sent directly from vendor software. ***Vendor integration is provided as an advanced example—not as the recommended way for most users to evaluate the NIST26 EI Demo.***

The required modifications in the EI Demo include:

- Changing folder and file names
- Editing ASCII configuration files
- Updating NIST entries in the Windows win.ini file
- Providing the executable name expected by the vendor software
- Meeting vendor-specific interface requirements

This tutorial demonstrates the procedure using Agilent ChemStation. Other manufacturers may require different configurations.

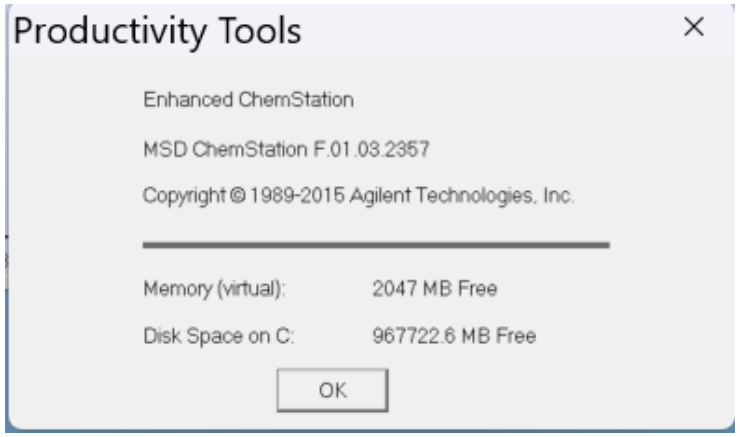
After modifications, the processing of a file will be compared in the newly developed fully integrated mode versus vendor import of spectra for library searches. ***The new approach is much more efficient in my opinion, but vendor import can still be very useful.***

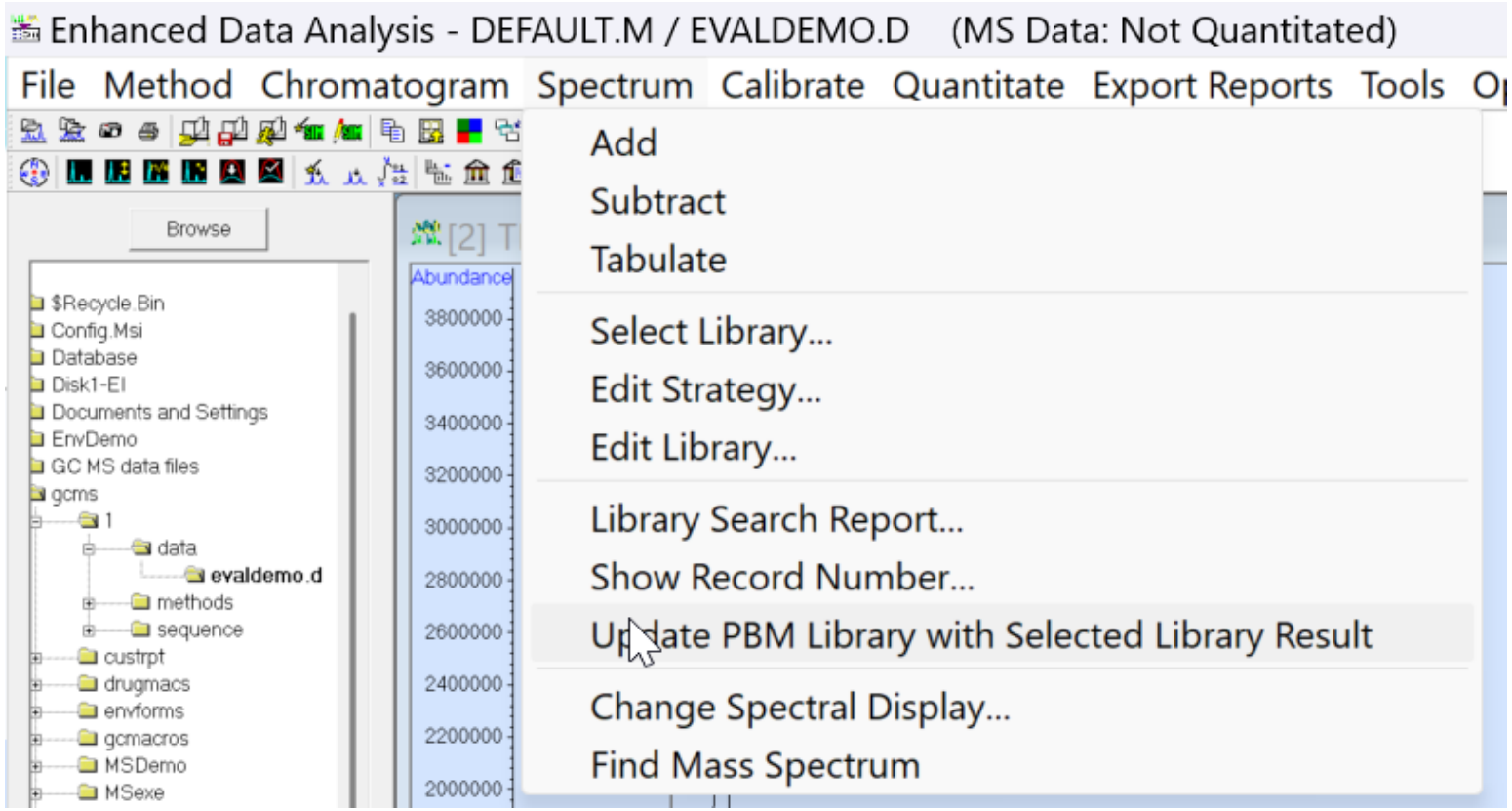
What This Handout Covers:
This handout provide a basic overview an advanced example of configuring the NIST26 EI Demo to accept spectra sent from Agilent ChemStation. Many more details in the slides on following pages.

1. **Preparing Agilent ChemStation**
    1. Download and install the required ChemStation macros
    2. Enable **Set Default Search Engine**
    3. Correct the PBMsrch.mac "Switch Failed" error
2. **Installing the NIST26 EI Demo**
    1. Download and install the Demo
    2. Accept the standard installation settings
3. **Modifying the NIST26 EI Demo Installation**
    1. Rename the installation folder to avoid path problems
    2. Provide the nistms$.exe filename expected by ChemStation
    3. Understand the roles of nistms.exe and nistms$.exe
4. **Connecting ChemStation with NIST Search**
    1. Update the NIST program path in win.ini
    2. Configure autoimp.msd for the ChemStation exported-spectrum file
    3. Create a working Windows desktop shortcut
5. **Adding Compatible EI Libraries**
    1. Add 5 free EI libraries from my website to the free mainlib supplied by NIST
    2. Any library in NIST format can be used including user-created ones
    3. Select the library directory when NIST Search first opens
6. **Configuring NIST Search**
    1. Set spectrum search and structure search libraries and other search parameters
    2. Configure the Chromatogram window
    3. Display structures on chromatographic plots
    4. Save the complete configuration for future use
7. **Examples of Data-Processing Workflow**
    1. Process the sample GROB.D data file
    2. Examine the sample in Agilent ChemStation
    3. Send spectra from ChemStation to NIST Search
    4. Use **Switch to Caller** to return to ChemStation
    5. Process and review the sample in the NIST Library Search Chromatogram window

Installation and Setup of ChemStation Software

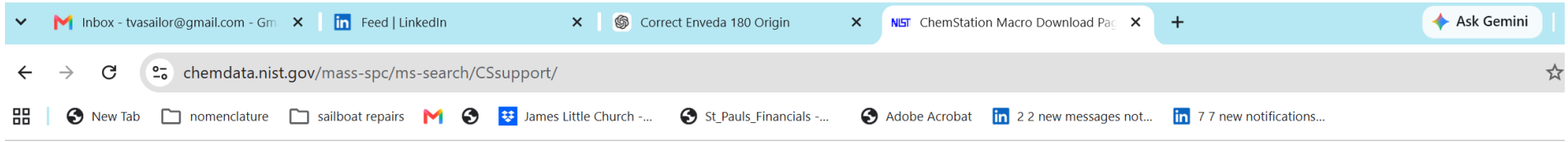
- As installed, MSD ChemStation F.01.03.2357 needs additional macro
- Ability to “Set Default Engine” as NIST Search not found in pull down menu below
- Close ChemStation program
- Download macros
- Make necessary modifications shown in next 5 slides





Download Macros for Sending Spectra to NIST Search (1 of 5)

See *Link*



Macros for ChemStation

Several macros have been created to add flexibility to the ChemStation library search and NIST Mass Spectral (MS) Search Program v.1.7. Prev ChemStation macro (NISTINT.mac) was available with the NIST MS Search Program v.1.6. This macro displays a dialog box with options to create files of spectra to be saved for use by the NIST MS Search Program, to switch to the NIST MS Search Program with automatic import of saved spe copy ChemStation user libraries to NIST User libraries. In August of 1999, James Little (Eastman Chemical Company) and O. David Sparkman (created several new macros to integrate the NIST MS Search Program with ChemStation and add flexibility to the ChemStation library search op new macros are available.

NISTSrch.mac sends the currently displayed ChemStation mass spectrum to the NIST MS Search Program to be searched against the NIST/EPA/NIH Mass Spectral Database and/or User libraries.

LS.mac performs a ChemStation PBM search using up to three different libraries with the top 20 hits returned from each library.

Switch.mac allows the user to change the default search invoked when double clicking in the ChemStation spectrum display (PBM Quick Search, NIST MS Search, or PBM Search using multiple libraries).

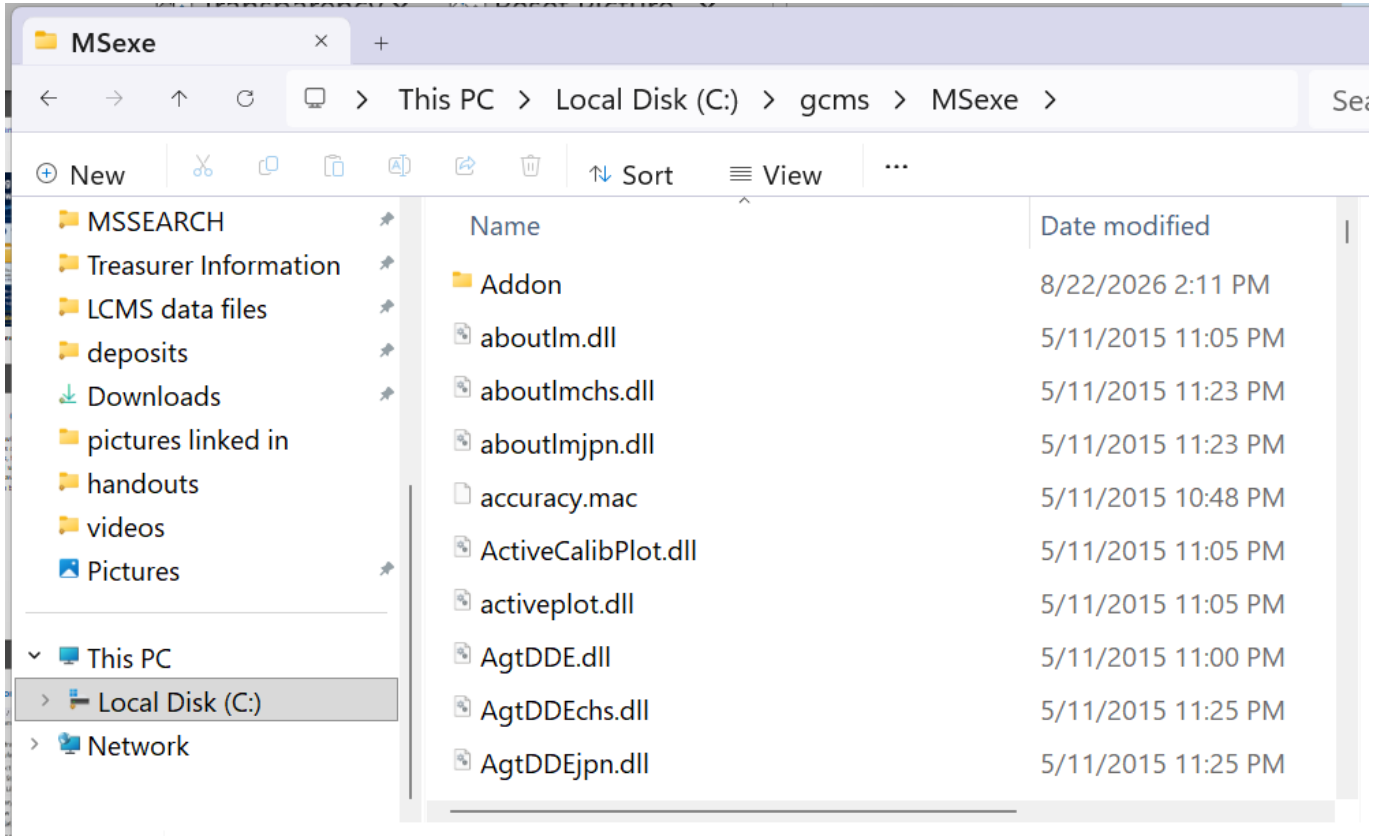
NISTINT.mac displays a dialog box with various options to save spectra for automatic importation into the NIST MS Search Program, toggles to the NIST MS Search Program, or copies HP user libraries to the NIST User library format.

AMDIS.mac loads current ChemStation data file directly into AMDIS.

PBMSrch.mac performs normal ChemStation PBM search (copy of the ChemStation system macro LIBSrch.mac).

Download Instructions

Download Macros for Sending Spectra to NIST Search (2 of 5)

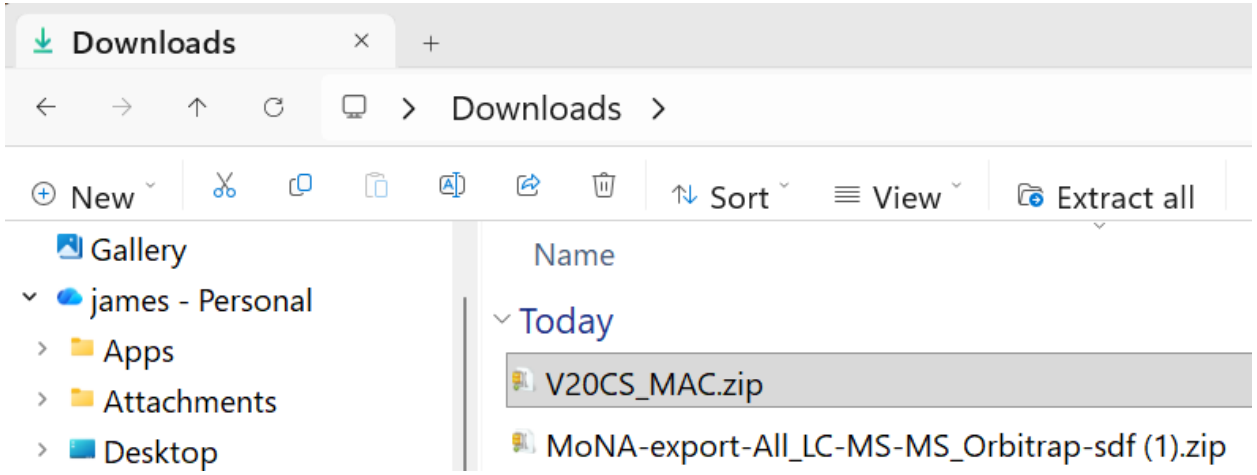


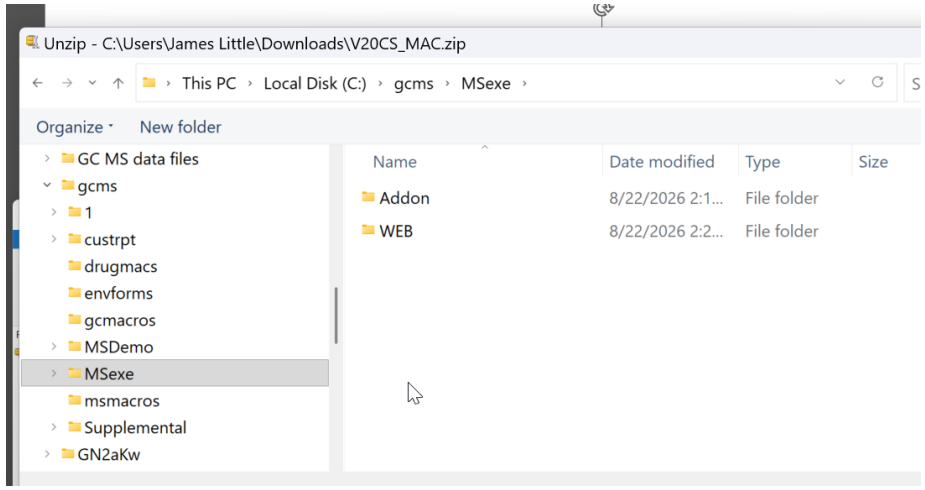
Download zip file and extract all files from the zip file into the \MSexe directory within the ChemStation directory. Further instructions are included in Menu_mod.doc in the zip file.

- ChemStation Macros for V.1.7
- ChemStation Macros for V.2

Download Macros for Sending Spectra to NIST Search (3 of 5)

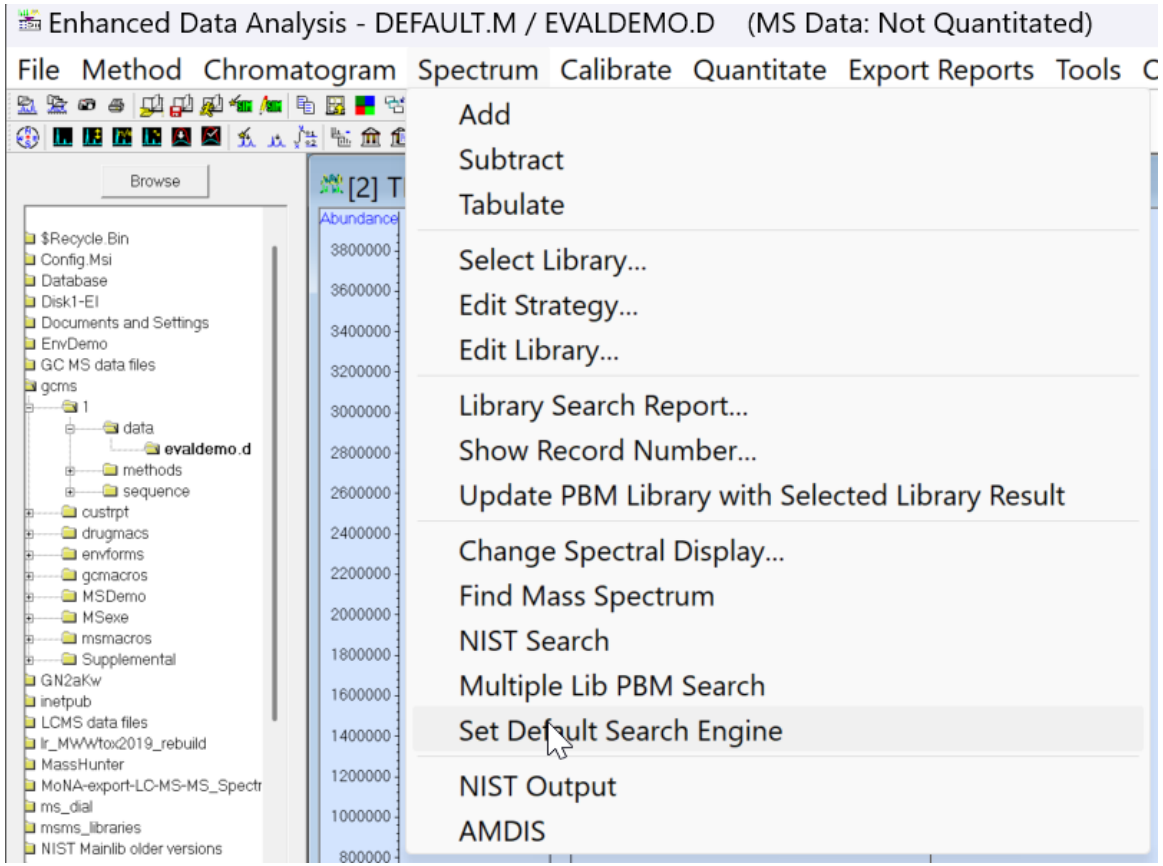
- Unzip the downloaded V20CS_MAC.zip
- Direct to Msexe folder in C:/gcms folder

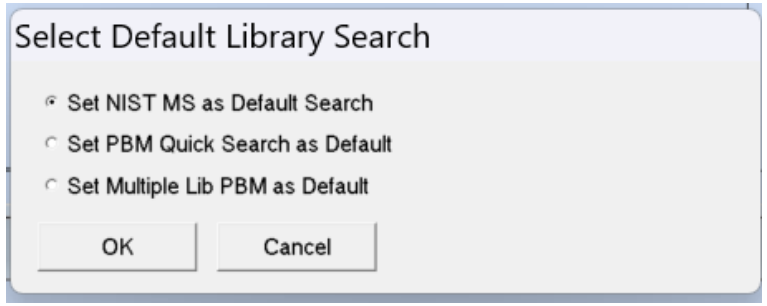




ChemStation Window Now Shows the Option “Set Default Search Engine” (4 of 5)

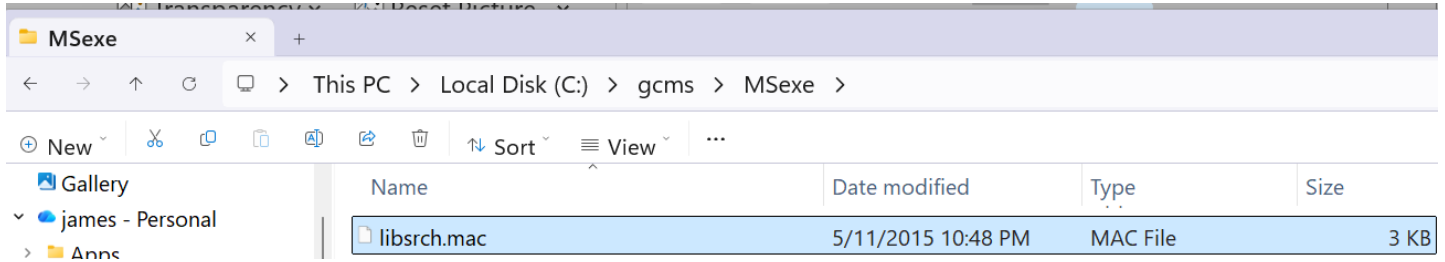
- Menu item now shown
- Attempt to use gives error at bottom of screen
- Fix noted on next slide
- After fixing, will get menu on right to select NIST Search

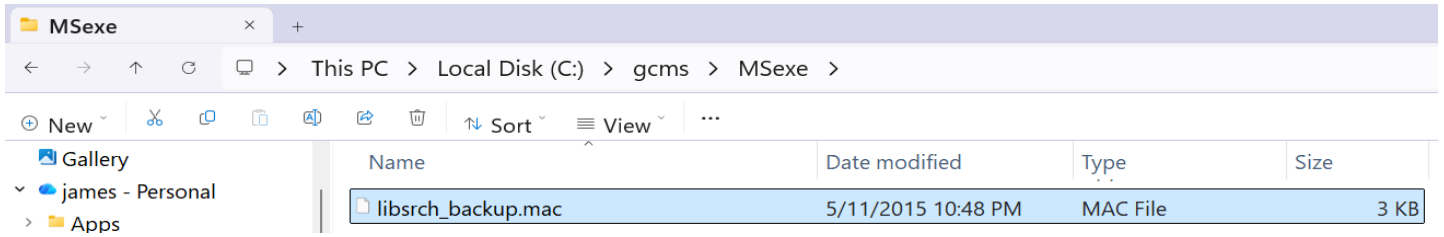


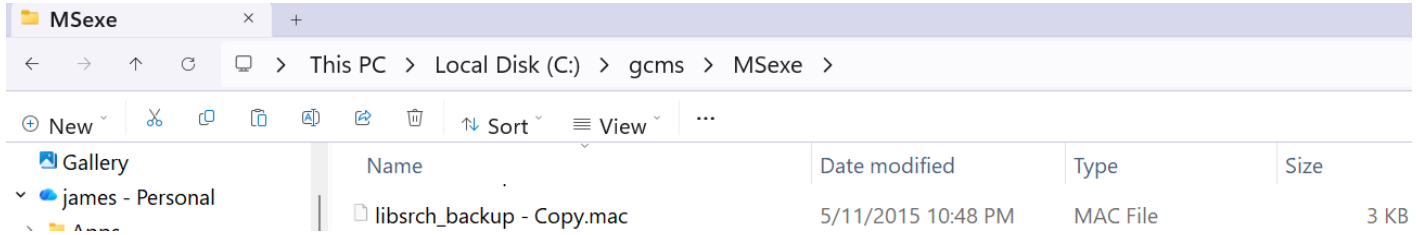


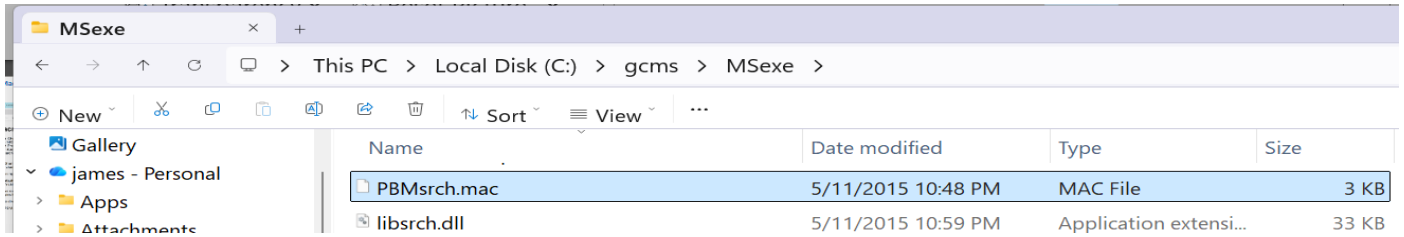
Repairing PBMsrch.mac “Switch Failed” Error (5 of 5)

- Change Name of libsrch.mac to PBMsrch.mac
- Best to make backup copy before changing
- Libsrch_backup renamed PBMsrch.mac
- See succession of menus below



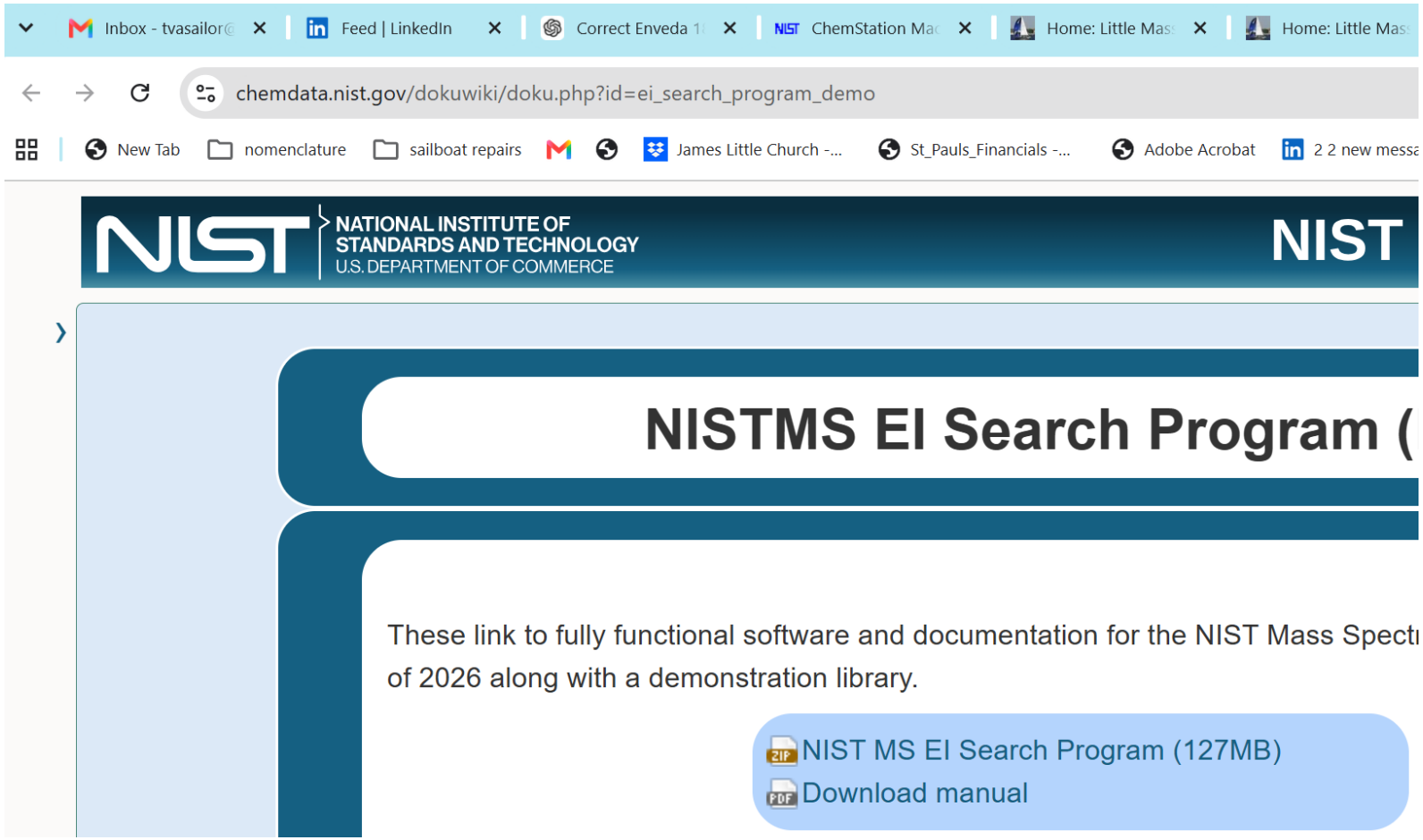






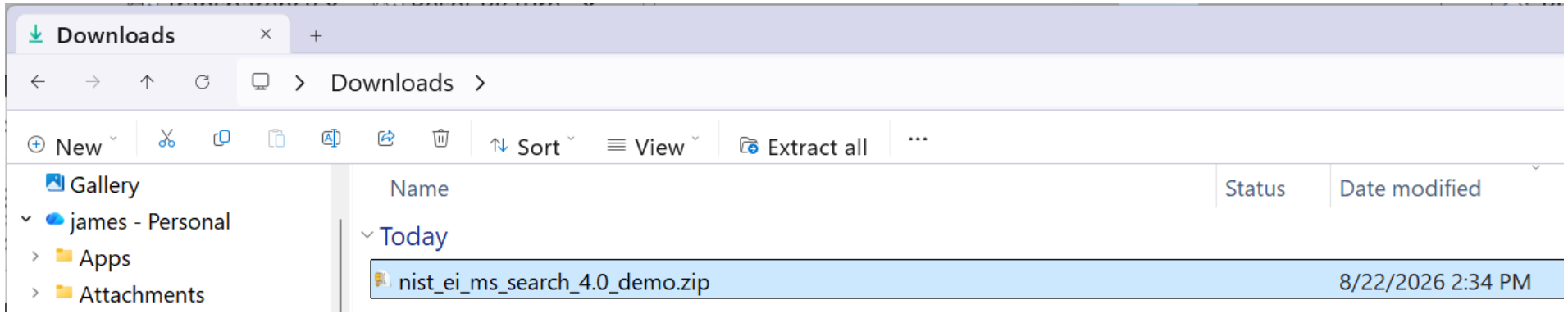
Installing NIST Demo EI Program (1 of 3)

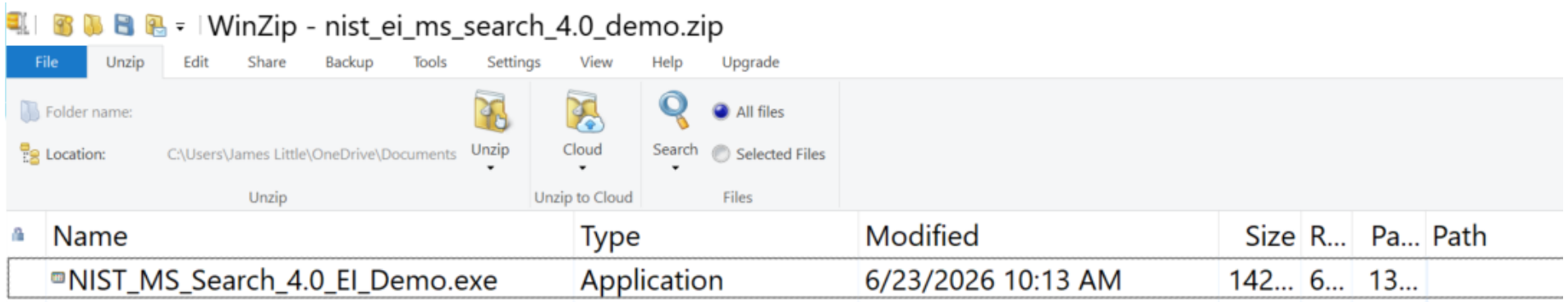
- Download the NIST Software from NIST Website (see ***Link***)



Installing NIST Demo EI Program (2 of 3)

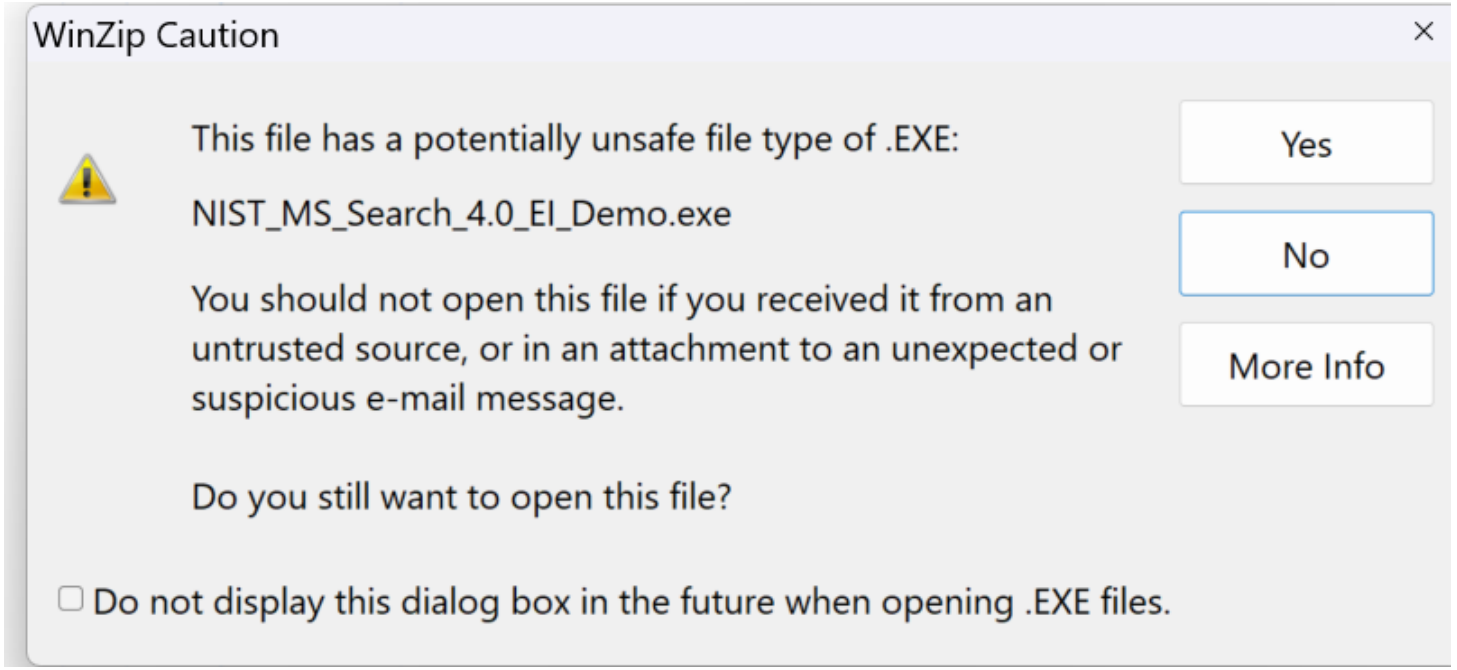
- Just double left click on the component within the Zip file to start installation





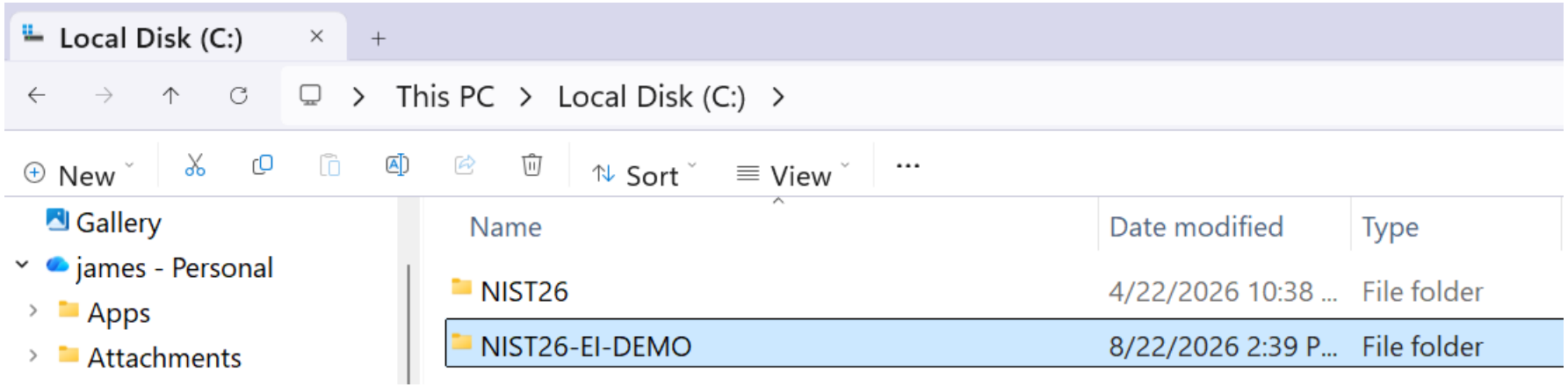
Installing NIST Demo EI Program (3 of 3)

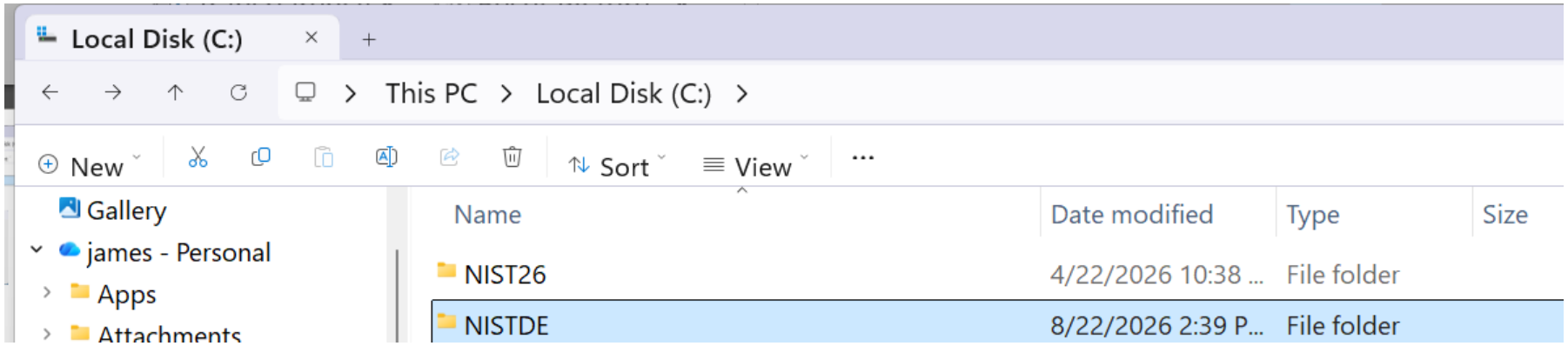
- Say yes to the WinZip caution window
- Accept all defaults in the installation process



Changing Name of Folder for NIST EI Demo Program

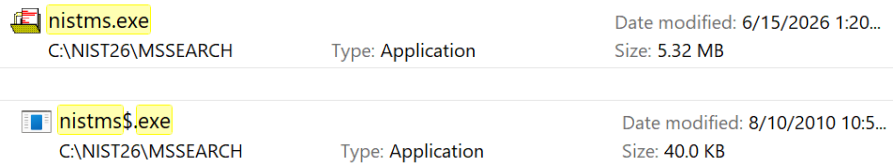
- Change the name of folder
- Some problems with hyphenated folder name in win.ini file in Windows Folder
- Picked “NISTDE” for NIST Demo EI
- Not sure the limitations for this change, but this name works
- Of course, will affect operation of any shortcuts in Program group created or other existing Window “shortcuts”

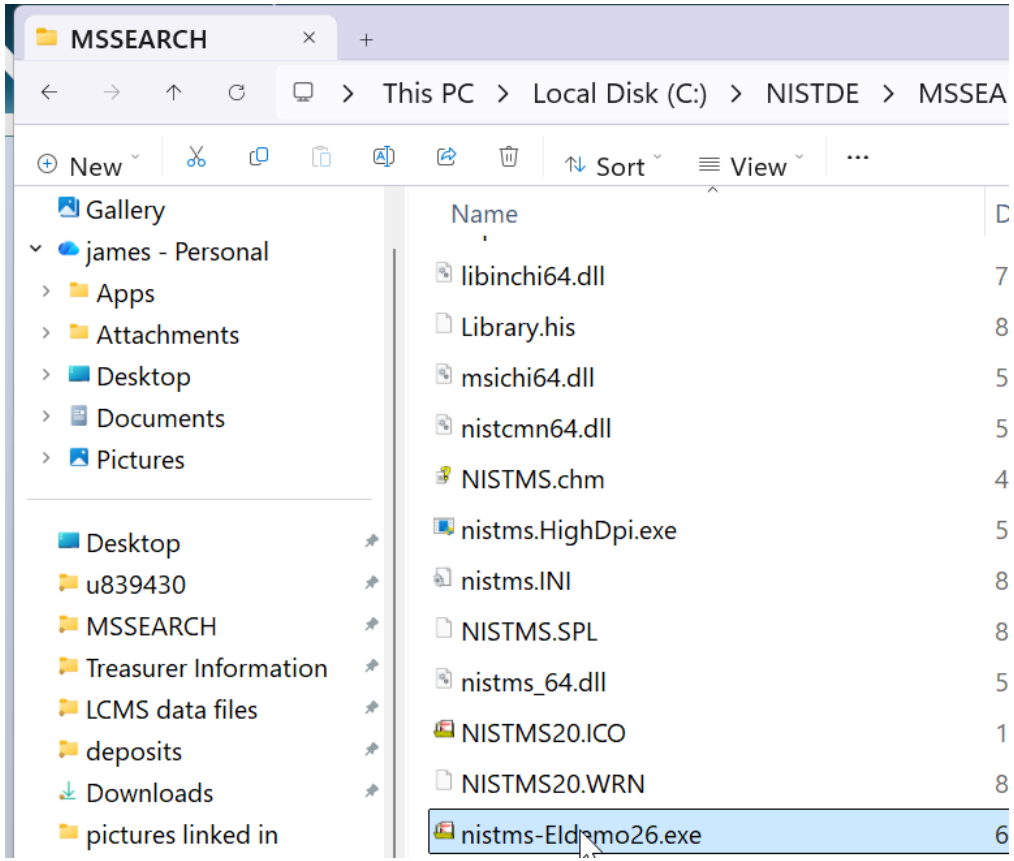


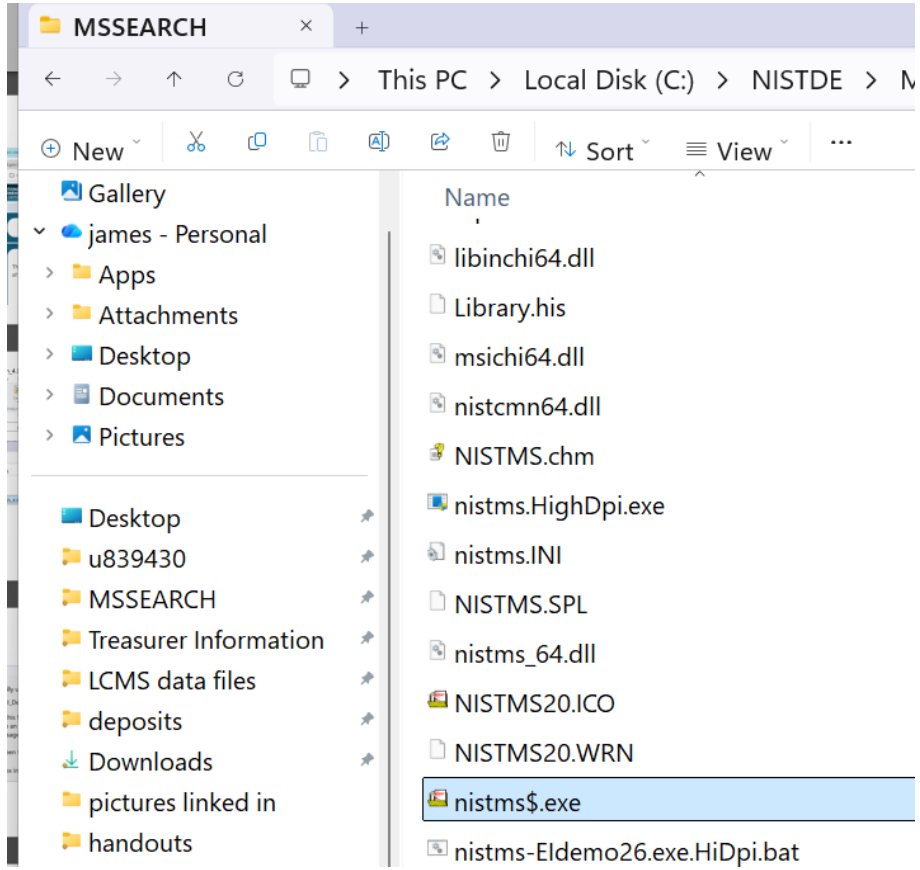


Changing Name of Program Executable for NIST EI Demo Program

- Change the name of NIST executable from default in window on left to nistms$.exe
- Executable located in C:/NISTDE/MSSEARCH
- Agilent ChemStation assumes that the executable will be nistms$.exe
- For more details on the process required of vendors, see ***Link***
- Not sure if this will work for all vendors and for all situations
- Nistms$.exe is a loader program for nistms.exe, see nest slide
- File sizes for the two programs shown to right for commercial NIST26 version







nistms.exe versus nistms$.exe (from ChatGPT)

File	Purpose
nistms.exe	The actual NIST MS Search program and user interface
nistms$.exe	A small loader that starts NIST MS Search while handling command-line options, including information passed from other software

They serve different purposes:

NIST's documentation specifically describes nistms.exe as the **main executable** and nistms$.exe as the **loader for command-line options**. Older NIST installations even created the normal Start-menu shortcut to nistms$.exe, which then loaded the main program. NIST MS Search documentation

Why some installations have only nistms.exe
Some stand-alone and demonstration packages are designed primarily to be opened directly. For example, NIST describes the current Tandem Demo as a fully functioning version based on nistms.exe v4.0. It apparently does not include every auxiliary interface file distributed with some purchased or earlier installations. NIST Tandem Search Program Demo

Why vendor software may expect nistms$.exe

Vendor programs may launch NIST with command-line instructions containing:
- The spectrum or interchange-file location
- The requested search operation
- Information telling NIST to import and search the spectrum
- Other startup parameters

That is the type of invocation for which the $ loader was historically provided.

Important caution about copying and renaming
Making a copy of nistms.exe and naming it nistms$.exe can satisfy vendor software that merely checks for that filename. This explains why your renamed copy may appear to work.
However, it does **not create the genuine NIST command-line loader**—it is still just another copy of the main executable. It may open NIST successfully but could fail to process certain vendor-supplied commands or imported spectra correctly.

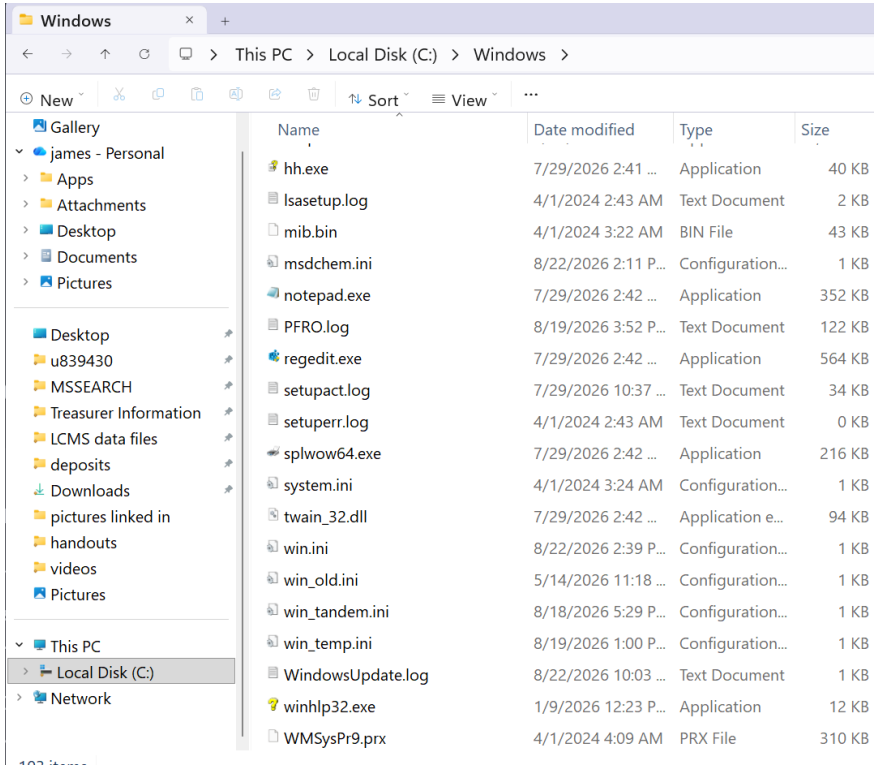
Therefore:
- For ordinary manual operation, use nistms.exe.
- For a vendor interface specifically expecting nistms$.exe, use the genuine loader when supplied.
- If the Demo lacks the loader, your renamed copy may work for a particular vendor, but it should be described as a workaround that needs testing—not as equivalent to the real nistms$.exe.

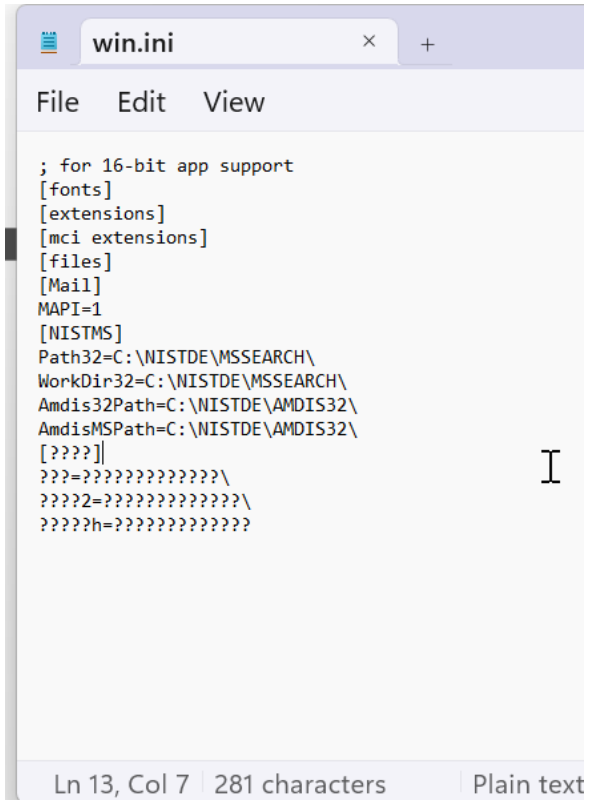
This difference is probably one reason the vendor-import configuration is substantially more complicated than evaluating the Demo through its built-in processing.

you should **not assume nistms$.exe is identical or interchangeable among NIST17, NIST20, NIST23, and NIST26**.
NIST does not publish a clear version-by-version compatibility table for the loader. However:
- NIST distributes nistms$.exe alongside the corresponding nistms.exe and supporting DLLs.
- Older NIST upgrade instructions replaced the loader along with the main program files, indicating that NIST regarded them as a matched software set.

Changing Location Vendor Program Expects to Find nistms$.exe

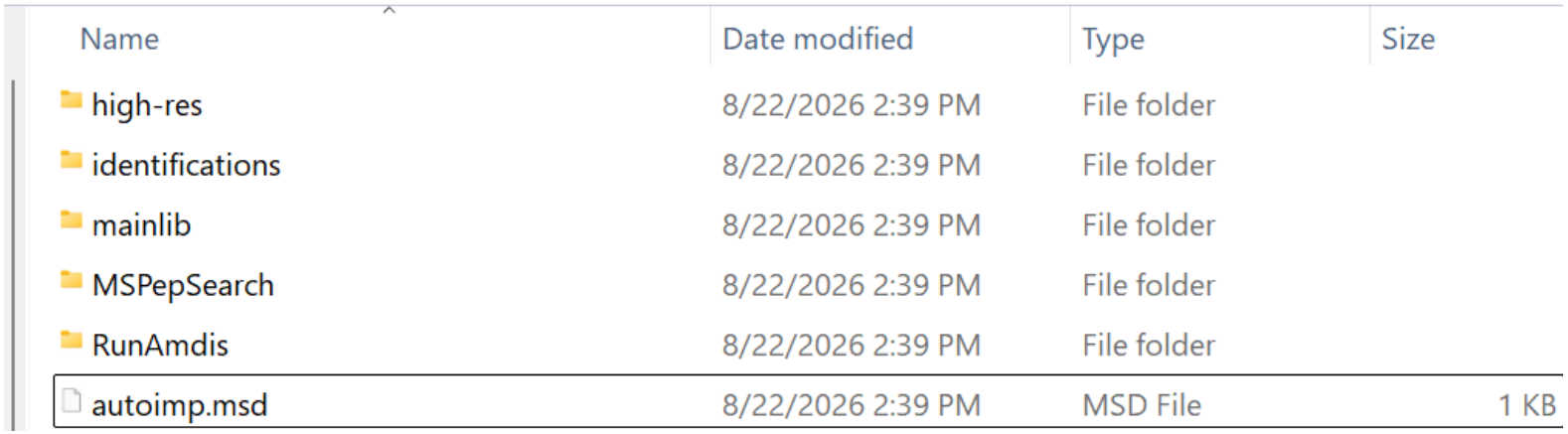
- Win.ini contains the location of nistms$.exe, the program executable
- Also, the location of AMDIS stand-alone application executable
- C:windows is a system protected folder
- Might not be able to edit directly, might need to save a copy to another folder, then modify
- Edit the file with Windows Notepad
- If so, make a copy in a another directly and make changes
- Then copy back to C:/Windows directly to overwrite
- ***Before editing*, *Best to make backup copy in the C:/Windows directory with name such as win_original.ini***
- Win.ini is a configuration file, so show file extensions to make sure it remains a configuration type

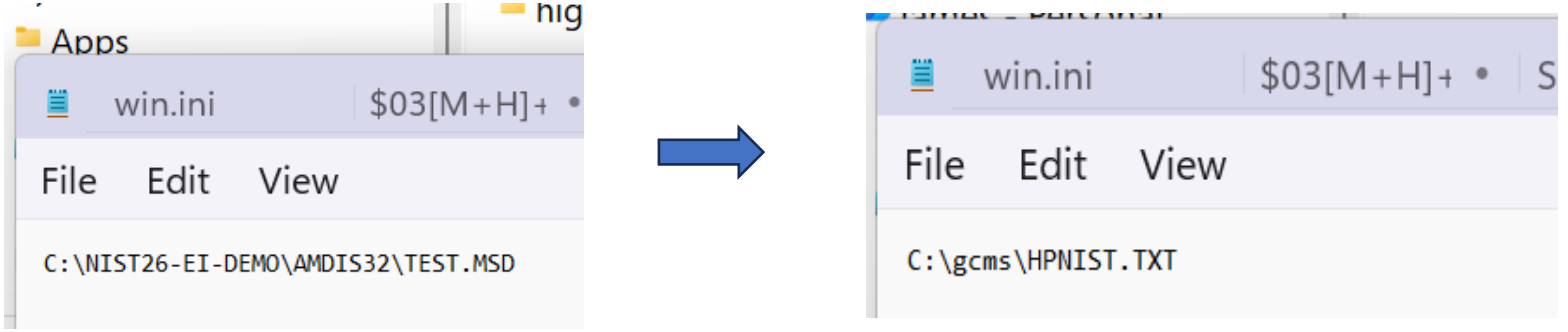




Changing Information in autoimp.msd File

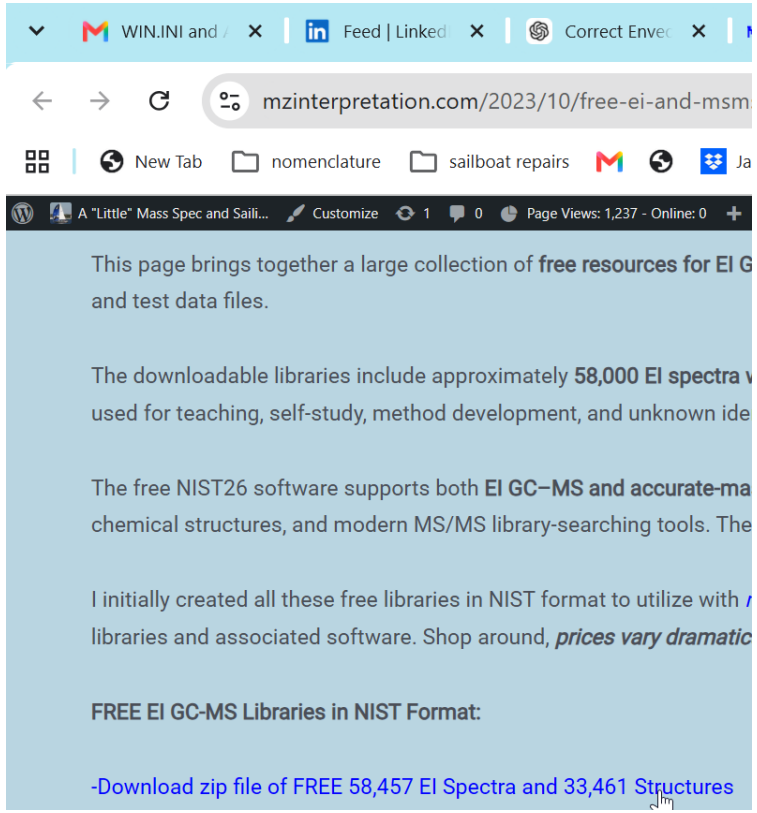
- Autoimp.msd tells the NIST program where it expects to find the temporary file with the exported spectrum in msp format
- It will be found in the C:/NISTDE/MSSEARCH folder
- Open and edit with Notepad
- Always good to keep backup copy of file before changes, so keep it *e.g.* as autoimp.msd
- Agilent assumes it should be C:/gcms/HPNIST.TXT
- For more details on process, see ***Link***



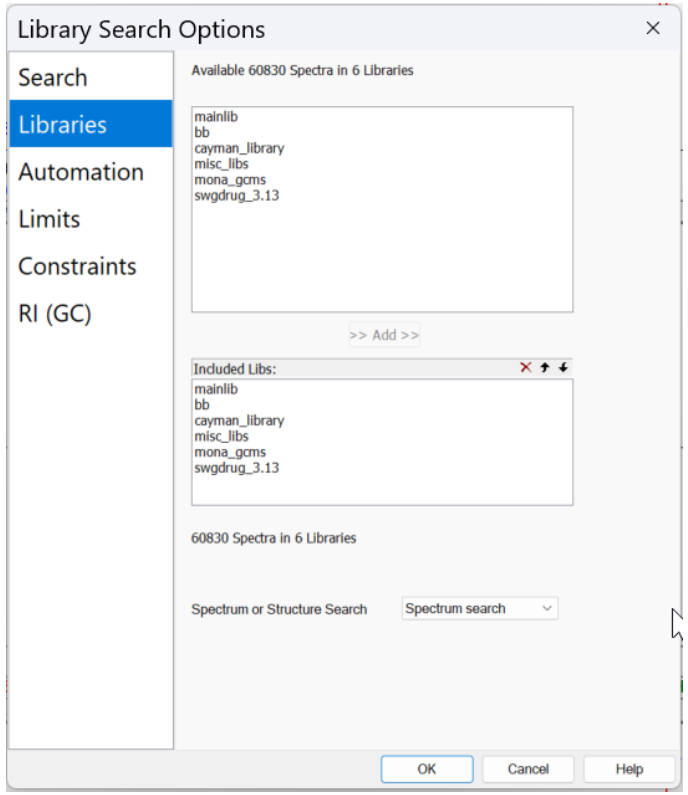


Libraries Available

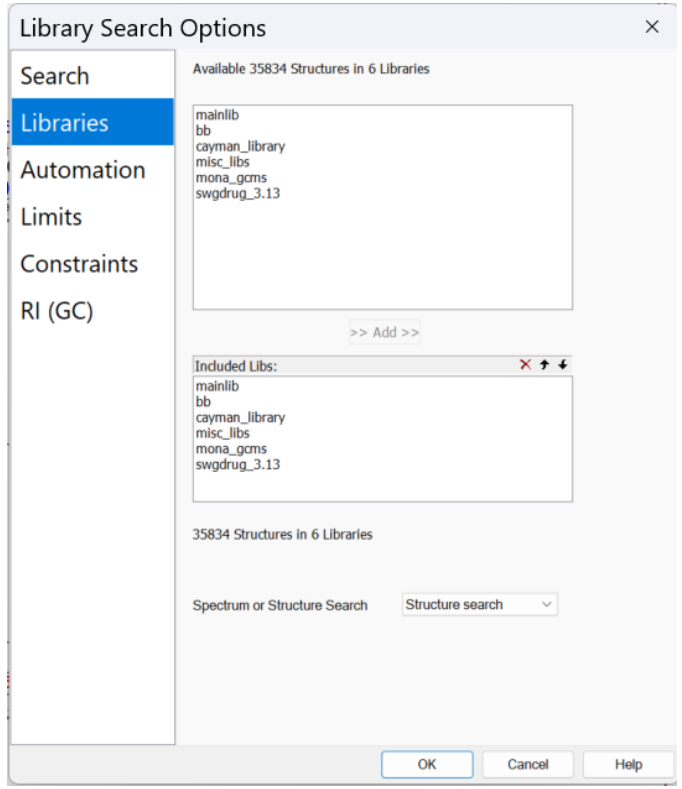
- The NIST EI Demo comes with a small mainlib library containing 2,373 EI reference spectra
- My webpage offers a group of libraries totaling 58,457 EI spectra with 33,641 structures, see ***Link***
- Downloaded as Zip
- Usually place them in C:/NISTDE/MSSEARCH directory
- Usually unzip or transfer them to C:/NISTDE/MSSEARCH directory
- Any EI library in NIST format can be searched including user-created ones
- ***Any library in NIST format can be used after the software is properly configured.***



Spectrum Search

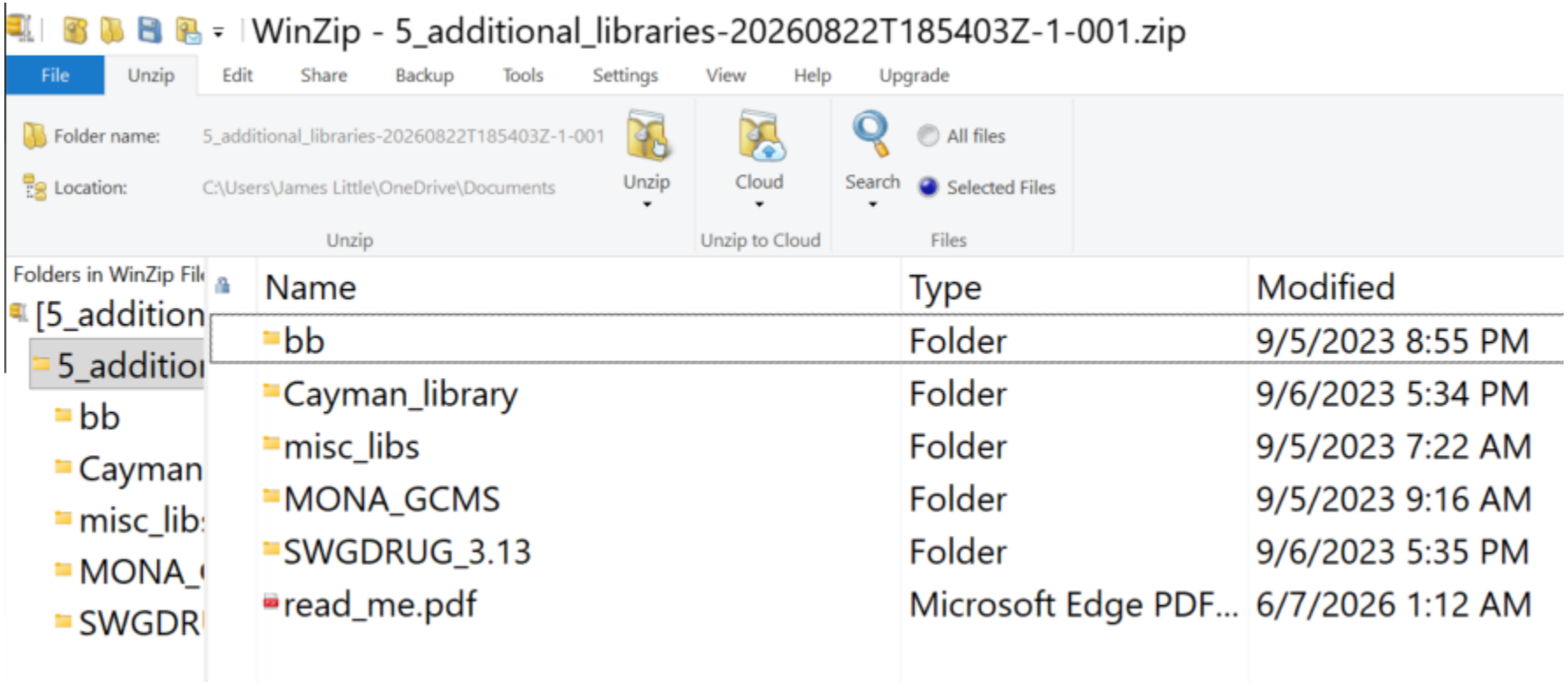


Structure Search



Libraries in Zip File from Website

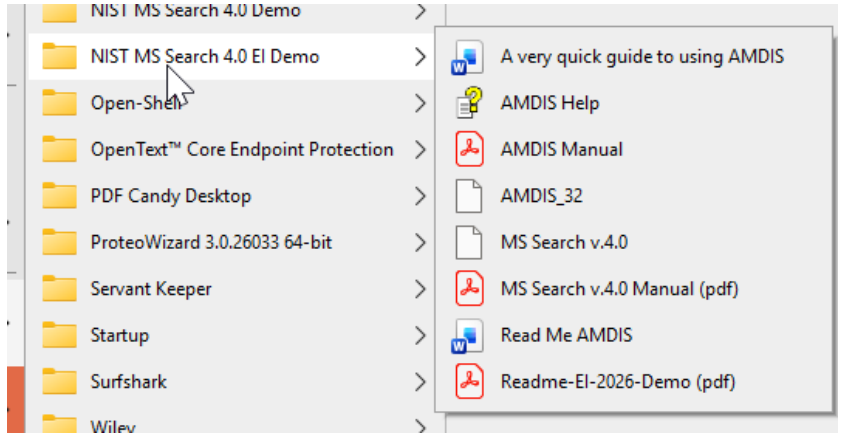
- The Zip file as seen on Google Server only shows 4 libraries on the screen
- After unzipping on your system, 5 will be noted
- “Bug” (Limitation of Google Drive)
- More information on libraries found in read_me.pdf, see ***Link***

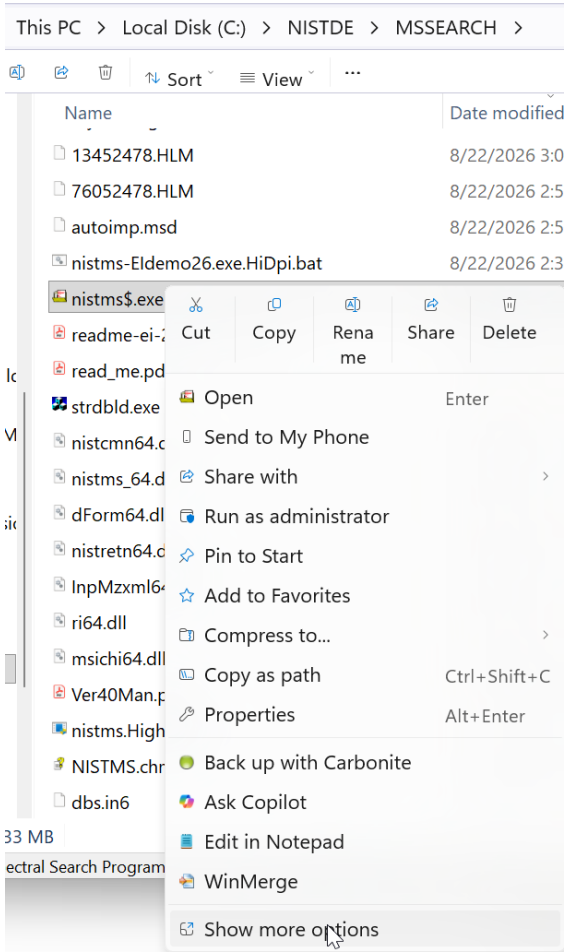


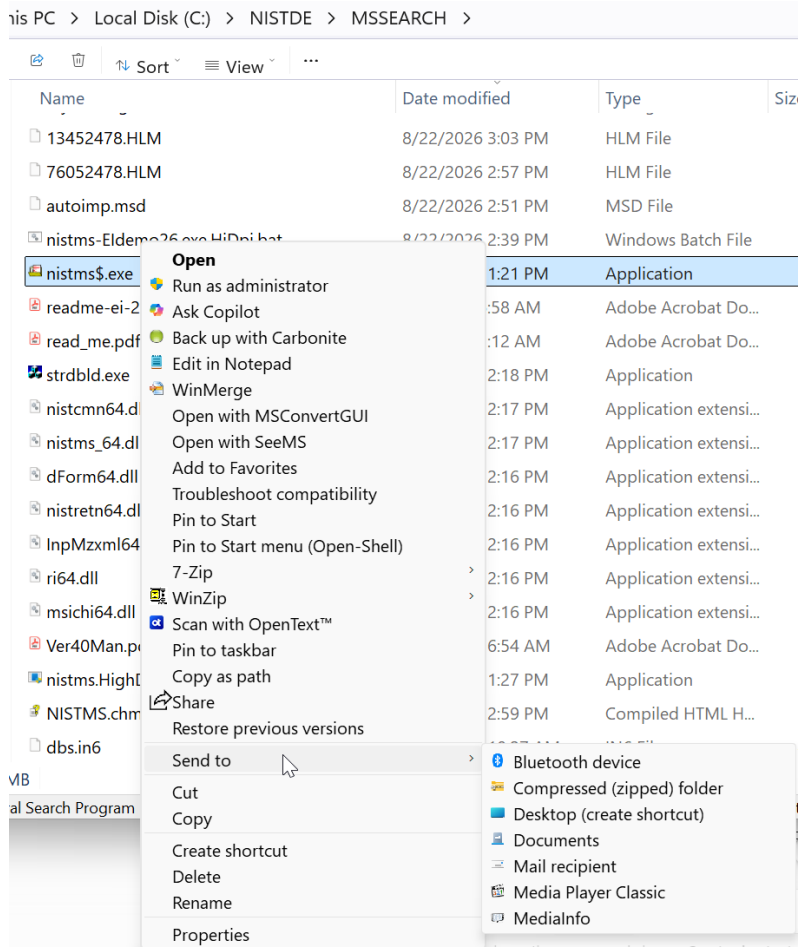
Starting NIST Search from Windows

- After changing name, NIST search will not start from program group in start menu
- Easiest for me was to send a shortcut to desktop
- Right click on nistms$.exe, then show more options, then send to Desktop (create shortcut)
- Many different ways to accomplish same task!

No Longer work to open NIST Search!

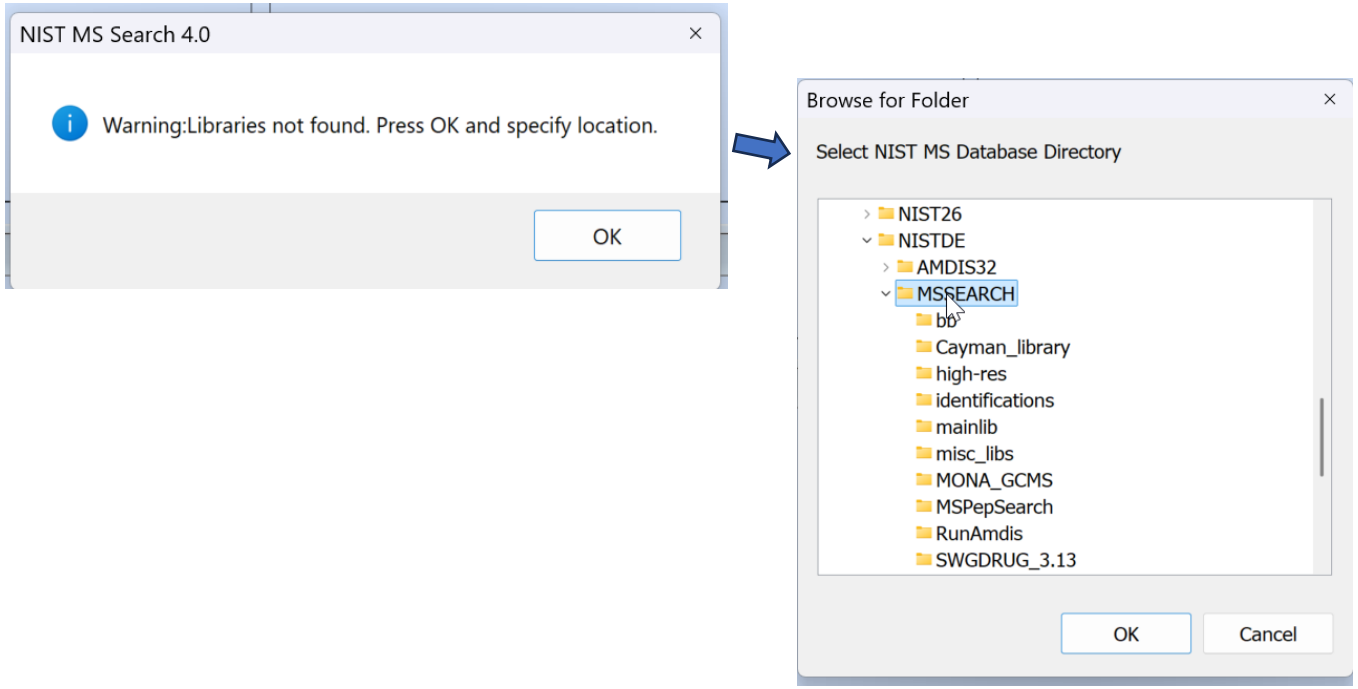


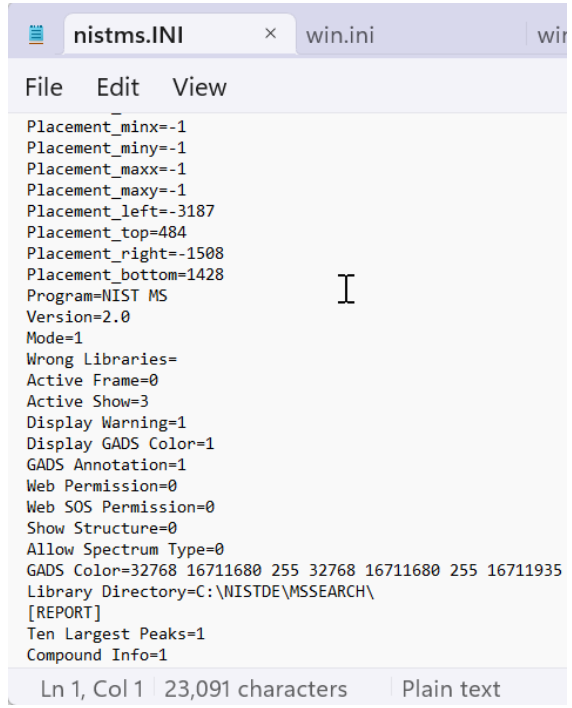




First Time Opening NIST EI Demo Program

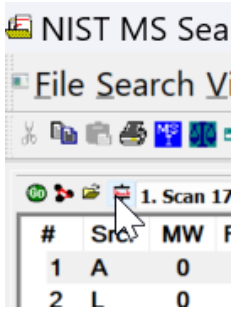
- First time opened, “Warning: Libraries not found..
- User can select the NISTDE
- Or can select another directory which contains their libraries
- Location is stored in an ASCII settings ini file,

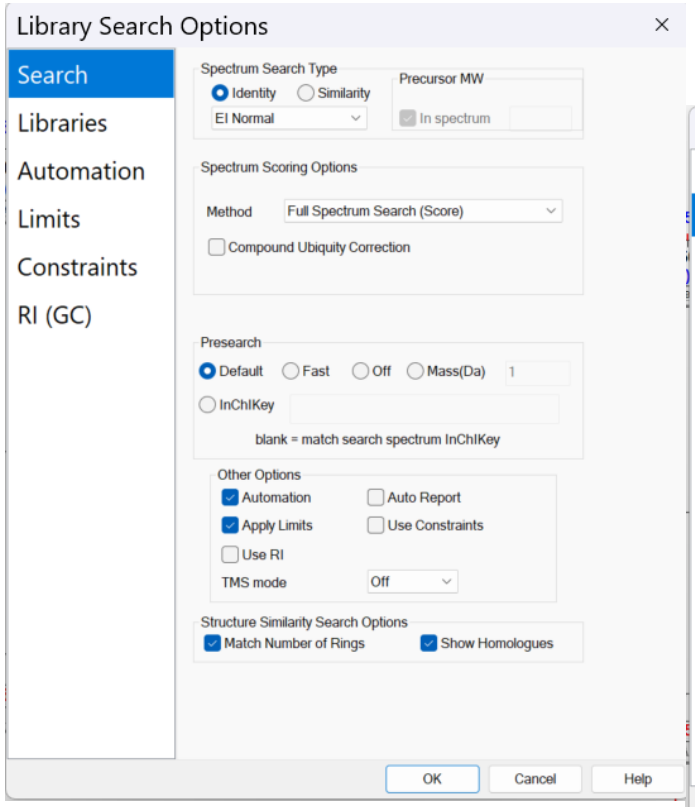


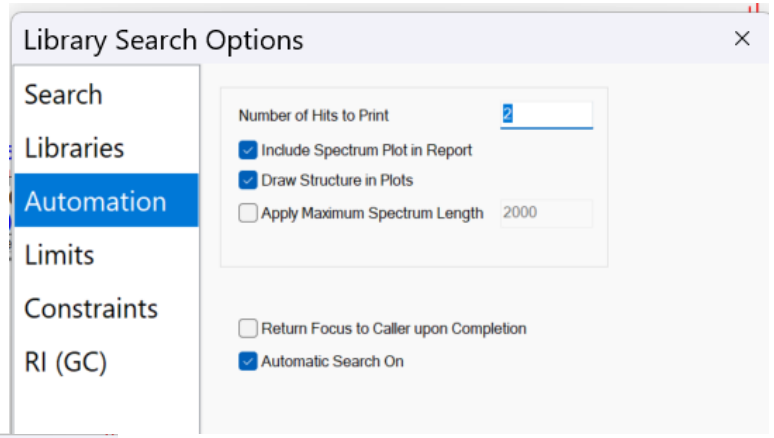


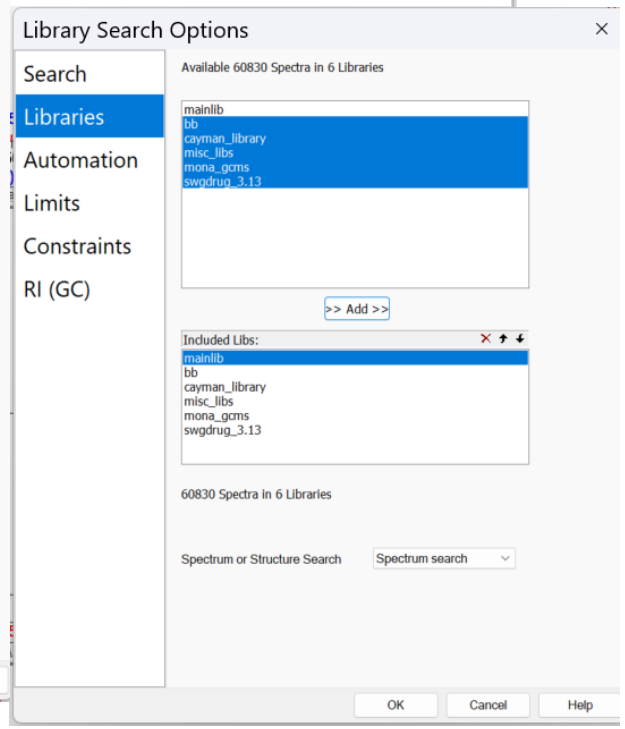
Entering Standard Search Parameters in NIST Lib Search

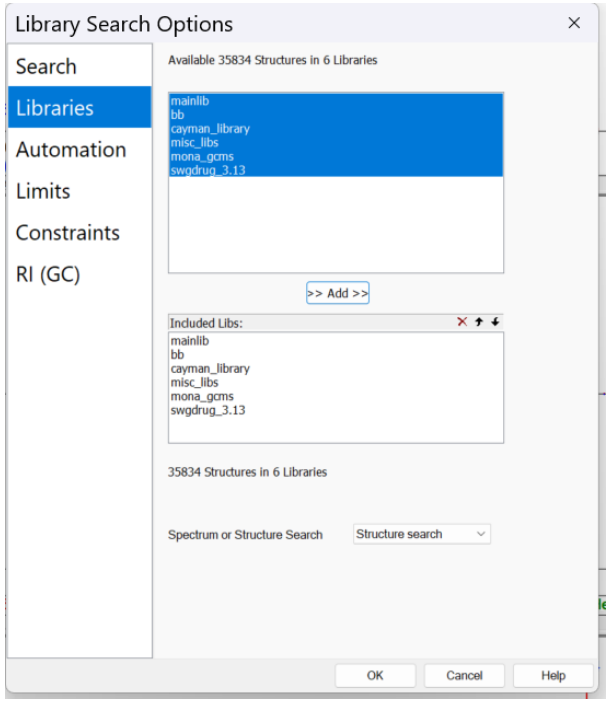
- User sets up search parameters
- Identity EI Normal, Full Spectrum search, default presearch
- Spectrum search, structure search
- Automation On



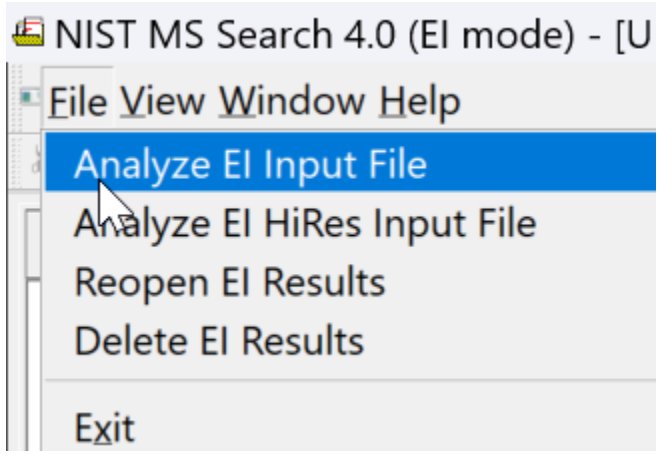


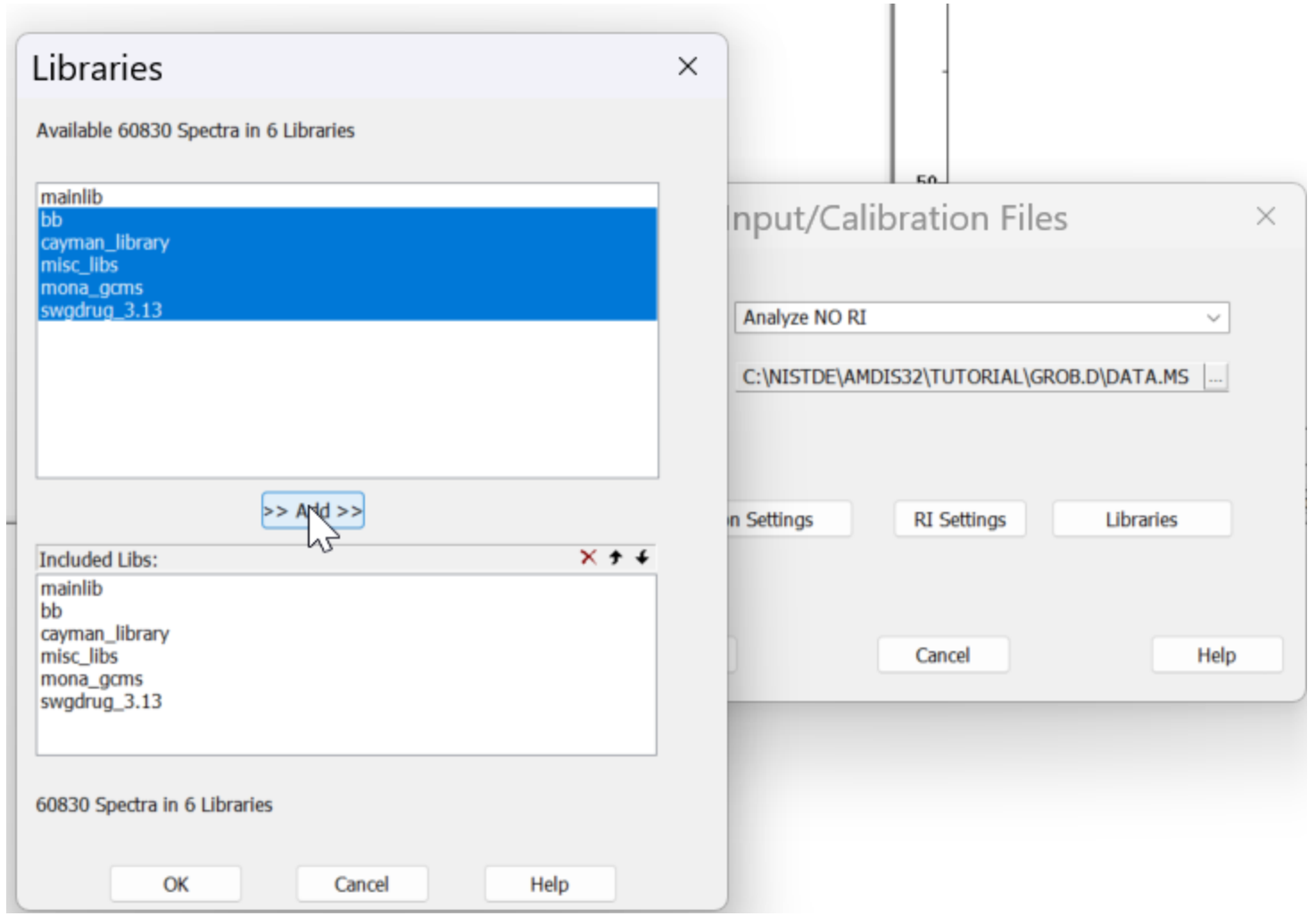




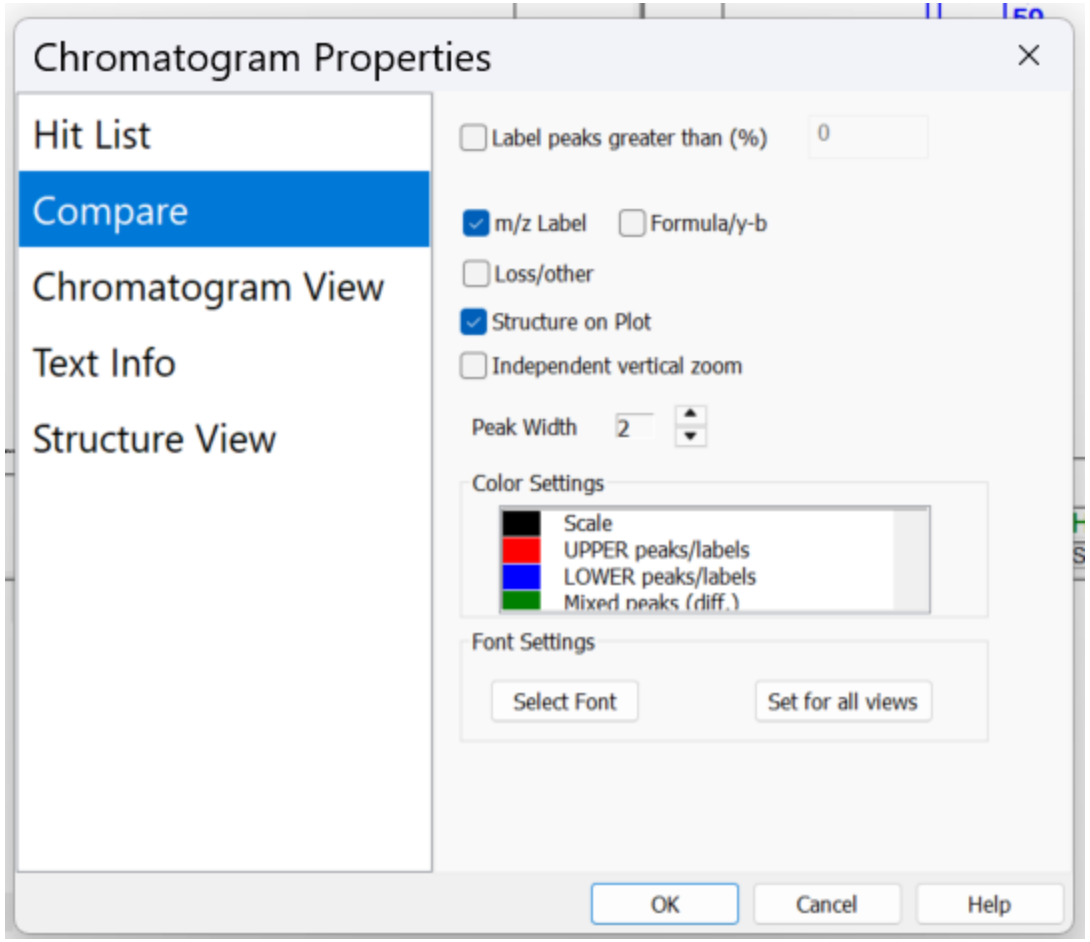


Entering Standard Search Parameters in NIST Lib Search Chromatogram Window

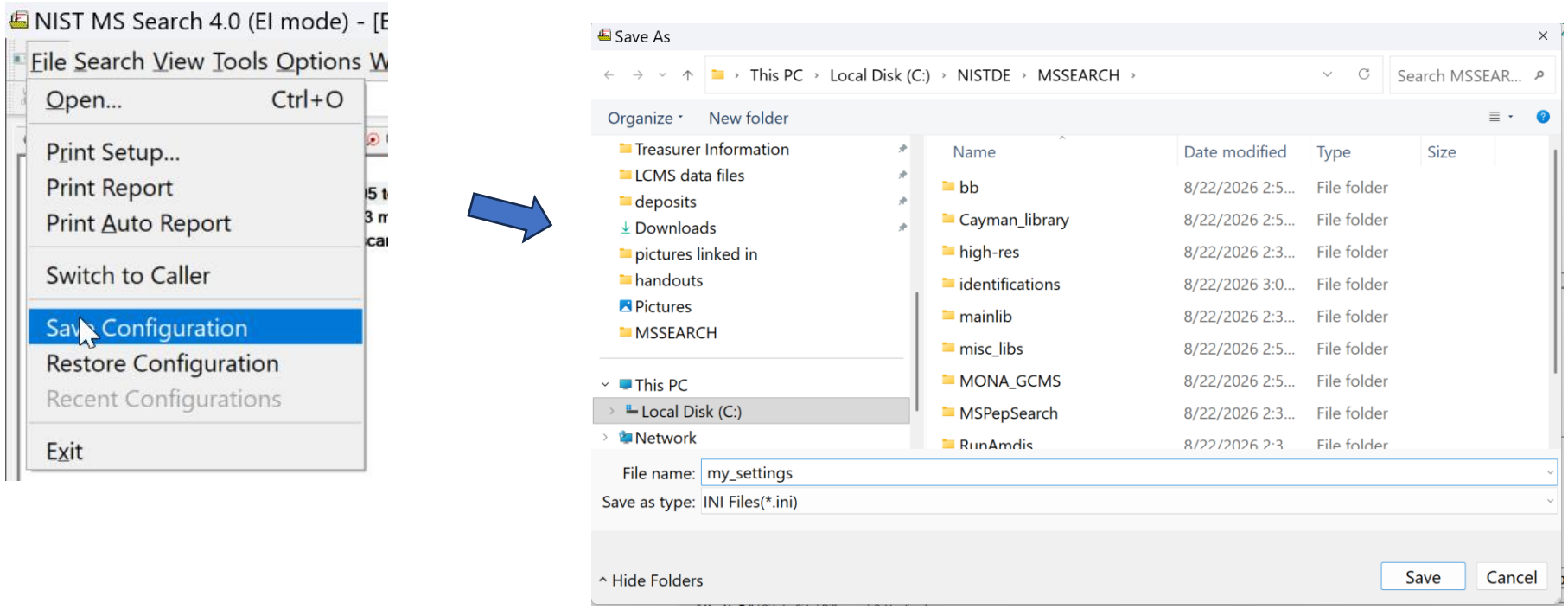




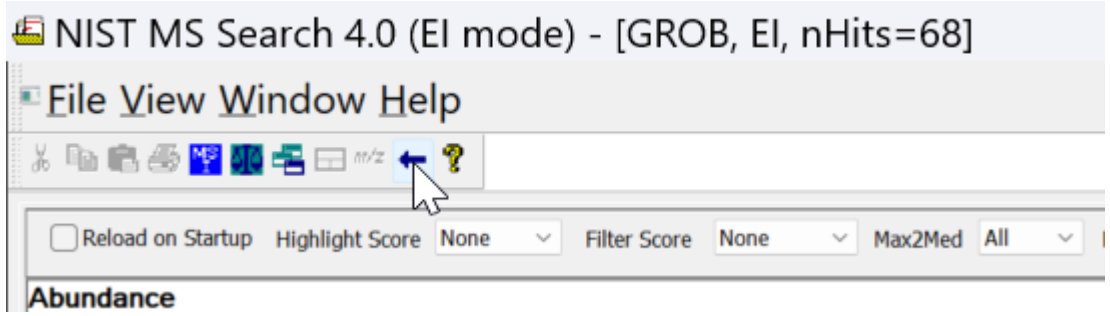
Setup “Structure on Plot” in Chromatogram Window



Save Configuration Keeps all the Setting in All the NIST Search Program Windows



Switch to Caller Brings the ChemStation Window Back into Focus



Examples of Data-Processing Workflow

- Demonstrate file processing on GROB.D
- Shown in Agilent ChemStation
- Shown in NIST Library Search Chromatogram Window

