OpenLab CDS

Setup and Configuration of MS Library Search

Notices

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Software Revision

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Contents

In This Book

This document describes the installation and configuration of the NIST library framework within different OpenLab CDS topologies, including Workstation, Workstation Plus, client/server, and Citrix/Terminal Server. It also discusses the use and management of other commercial and user-created libraries, and the MS library search within OpenLab CDS.

Table 1 Terms and abbreviations used in this document

Terms	Description
AIC	Agilent's Analytical Instrument Controller

1 Introduction

The NIST installation package includes NIST libraries, the NIST MS Search program, the Lib2NIST Library Converter, and other NIST software components:

- The NIST MS Search program must be installed locally on each Workstation, Workstation Plus, client, or AIC that performs the library search within OpenLab CDS.
- NIST libraries can be installed locally or on shared network drives.
- With the Lib2NIST Library Converter, NIST provides a tool to convert existing libraries into NIST format. This enables the use of other commercial and user-created libraries together with the NIST libraries.

NOTE

This document is written for NIST23. The instructions apply also for prior versions of NIST. For these versions, substitute **NIST23** for your version, for example NIST17.

2 Licensing

NIST's commercial libraries (and some other commercial libraries as well) require a license for their use:

- For one-user-at-a-time computers (any Workstation or Workstation Plus computers which are searching locally stored NIST libraries), a license is needed for each computer where the NIST libraries are installed.
- For NIST libraries in a shared environment, a license is needed for each possible simultaneous user of the NIST libraries.
  Shared environments are:
  - Workstation or Workstation Plus computers searching NIST libraries on a shared location
  - Clients[1]
  - AICs[1]
  - Clients within a multi-user (Citrix/Terminal Server) environment[1]

Upgrades (for both scenarios) require an upgrade license – for example, to move from NIST17 to NIST23 would require an upgrade to each license described above (each license that will access the upgraded NIST library would need an upgrade license). For more information, reference the EULA (End User License Agreement) shipped with the NIST library.

You do not need a license for the NIST MS Search program and the Lib2NIST Library Converter. You can download NIST MS Search and the Lib2NIST Library Converter only, without the NIST commercial libraries. This allows you to create and use custom libraries without the purchase of the NIST commercial libraries.

Please refer to Open Source Licenses for OpenLab.

[1] regardless of whether the NIST library is local to the client, AIC, or Citrix/Terminal Server, or on a share

3 Library Topologies

These are the possible topologies to set up the NIST libraries to work with OpenLab CDS.

- Local
  - Libraries are installed, stored, and used locally.
  - Sharing user-created libraries requires copying them between PCs.
  - One NIST license is needed for each system.
  - This is the default configuration for Workstation and Workstation Plus.
- Shared
  - Libraries are installed on a network share.
  - One NIST license is needed for each possible simultaneous user of the shared NIST library (including AICs).
  - AICs need to have access to this library for unattended processing including a library search (that is, using a processing method during acquisition that contains a library search).
- Mixed
  - You can use a combination of local and shared libraries.
  - To decrease search time and network traffic, it is recommended to install the large NIST commercial libraries locally, while keeping user-modified libraries on a share.
  - This is a typical configuration on an OpenLab CDS client or AIC.

NOTE

For commercial libraries that users can't modify we recommend storing them locally, as they impact performance otherwise.

It is recommended that libraries and MS Search should be the same version on all AICs, clients, Workstations, and Workstation Plus systems to ensure that search results are consistent regardless of where the search is run. Check the *OpenLab CDS Requirements and Supported Instruments Guide* delivered with your version of OpenLab CDS for a list of compatible NIST libraries.

4 Installation

When the NIST installer runs, it adds information to the local computer's win.ini file, which OpenLab CDS and NIST MS Search both reference to determine the location of the libraries.

```
[NISTMS]
Amdis32Path=C:\NIST23\AMDIS32\
AmdisMSPath=C:\NIST23\AMDIS32\
Path32=C:\NIST23\MSSEARCH\
WorkDir32=C:\NIST23\MSSEARCH\
```

Figure 1 Directories

- It is recommended to update win.ini only via the NIST installer. Do not change win.ini manually.
- Libraries must be located in the directory referenced in win.ini to be available for use in OpenLab CDS and in NIST MS Search.

  For non-local libraries on shared drives, the path in win.ini should still point to the local machine as in the screen shot above. Within that directory will be folders containing shortcuts to the libraries on the network share. See "Prepare mapping to libraries on a shared network drive" on page 16.

Install NIST With Local Libraries

1 Launch the NIST installer using an account with local administrator privileges.

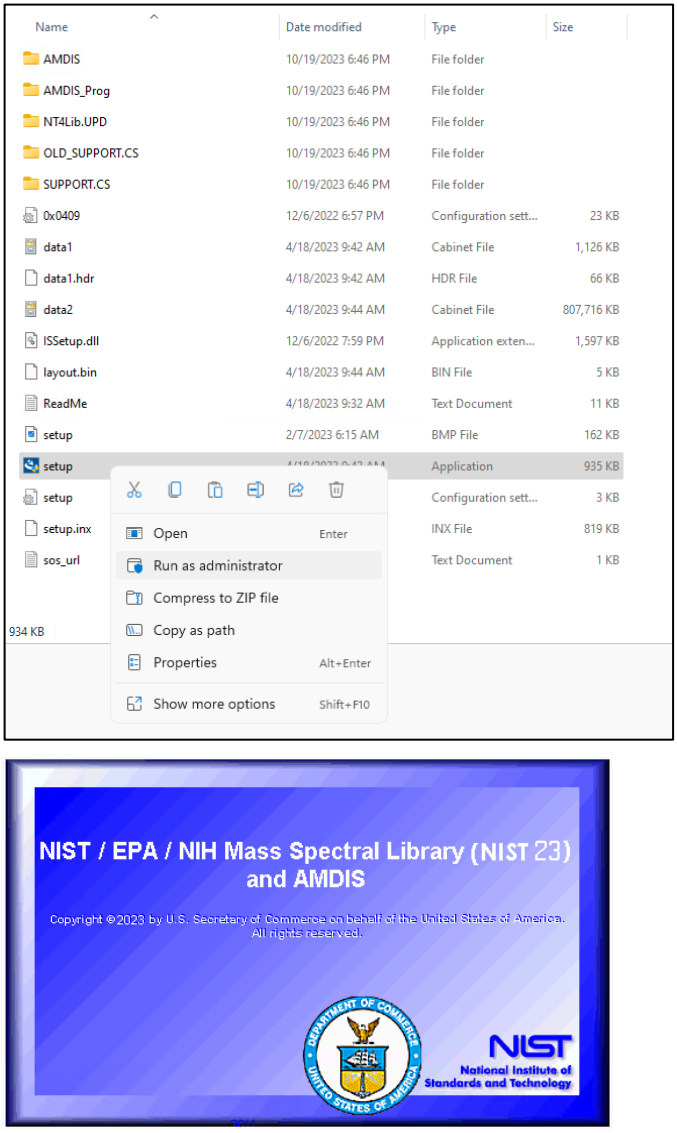


Figure 2 Setup file

2 Follow the installation wizard until you reach the **Setup Type** screen.

3 From here, you can select the **Typical** setup for ease of installation, or **Custom** to control which components are installed.

If you select **Custom**, ensure that you install the following:

- NIST MS Library components
- NIST MS Search Program

It is not recommended to change the path the libraries are saved in. If you want to change the location, choose a local drive (not on a network share or removable drive).

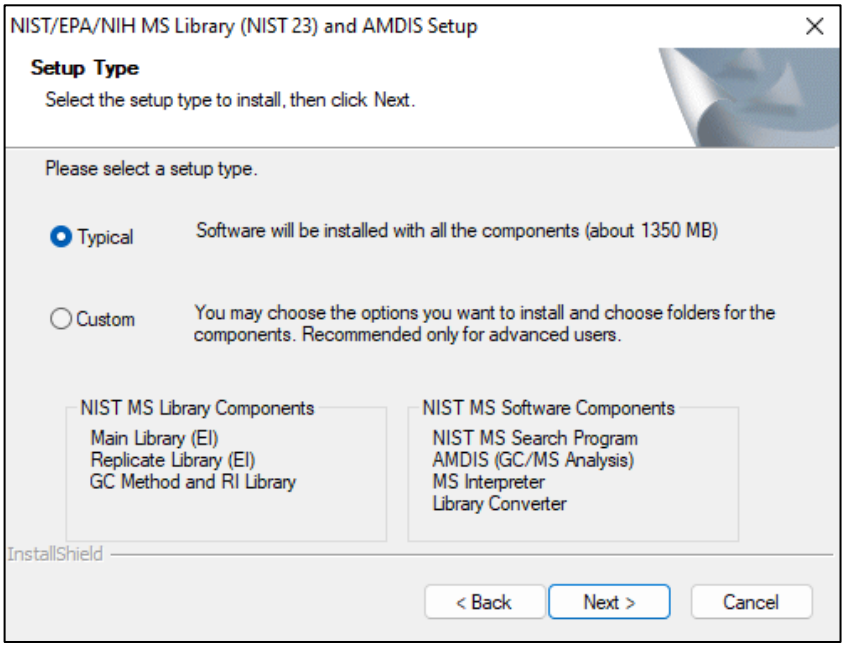


Figure 3 Setup type – **Typical**

4 If other commercial or user-created libraries in NIST format already exist, copy them into the NIST MS Search folder using the installer. If the installer does not automatically locate existing libraries, click **Search for User Libraries**.

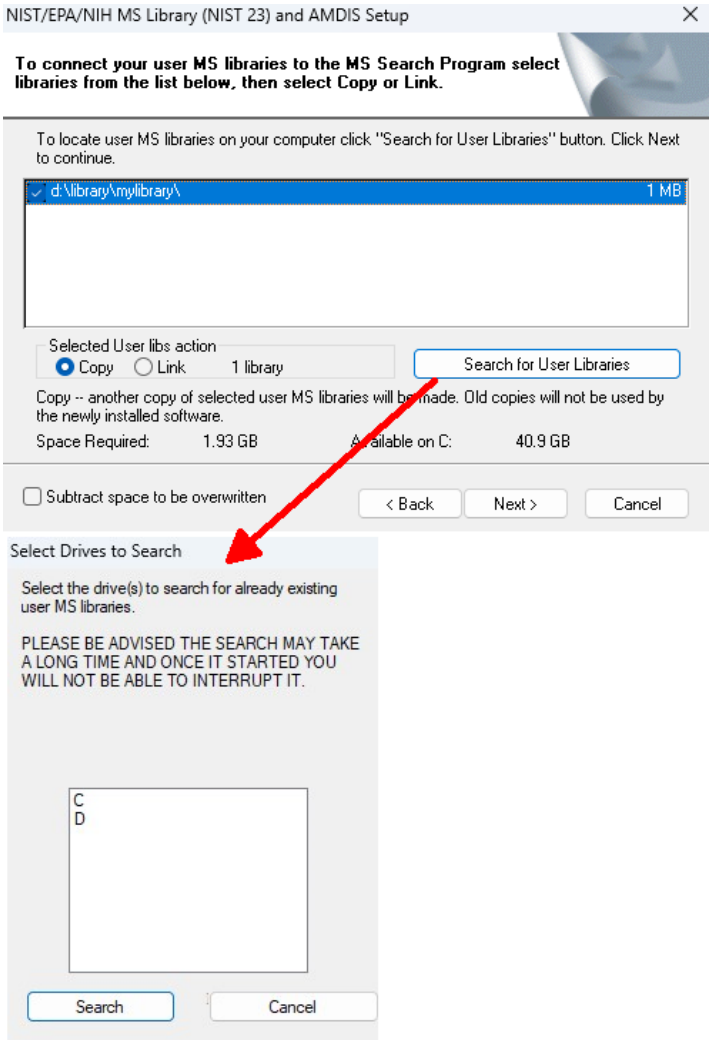


Figure 4 User libraries selection

Typical setup should show all components being installed; **Custom** setup may have less, but all installation locations must be local.

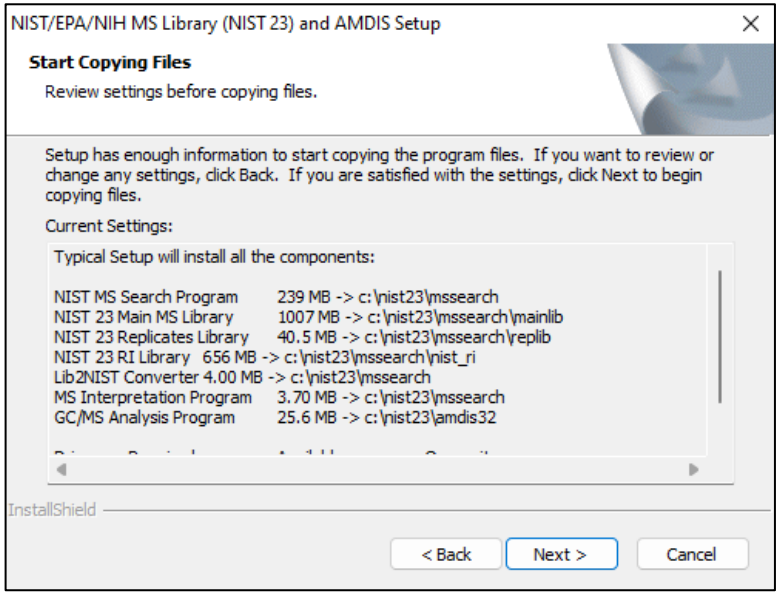


Figure 5 Program files – **Typical** setup

5 Complete the installation.

NIST MS Search is now installed. Installed libraries are now visible in MS methods in Data Analysis, see "Use MS Libraries Within OpenLab CDS" on page 28.

6 If you want to add libraries after installation, see "Add Libraries After Installation" on page 22.

Prepare Usage of Shared Libraries

To decrease search time and network traffic, it is recommended to install the large NIST commercial libraries locally, while keeping user-modified libraries on a share.

Set up a shared network drive

1. Create and configure a shared network drive that will contain the libraries. For example. \\MyServer\MSSEARCH
2. Share the folder with **Everyone** (**Full Control**).

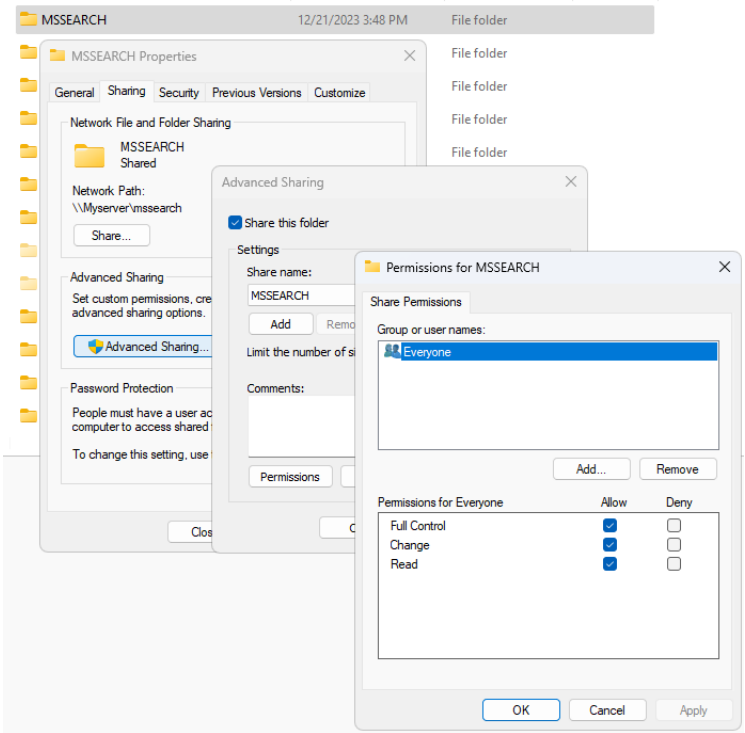


Figure 6 Sharing and permission options

3 If it is necessary to limit write access to specific users or user groups, do so at the file level using the **Security** tab, not via the permissions on the **Sharing** tab. These **Security** settings can be inherited to every library within the shared folder, or they can be applied to individual libraries.

NOTE Commercial NIST libraries cannot be user edited.

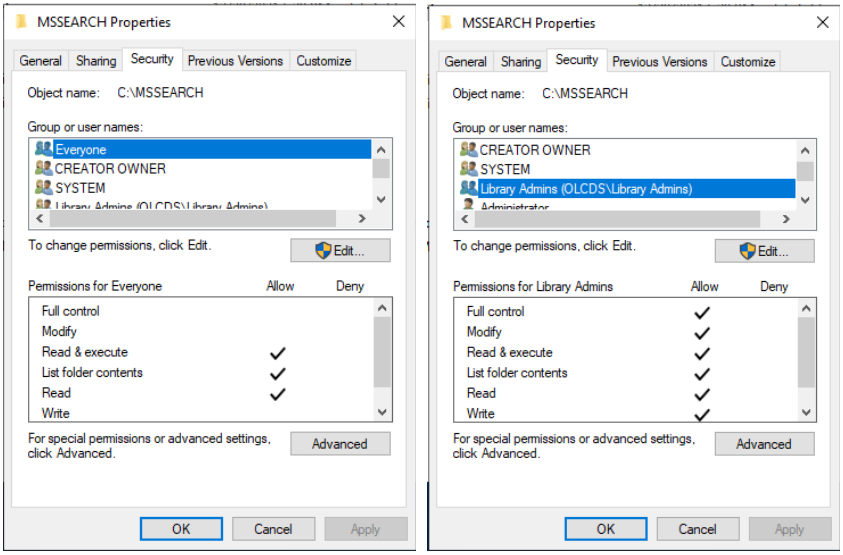


Figure 7 **Security** tab

4 In this example, a domain group was created called Library Admins. Any user in the Library Admins group has permissions to modify the libraries in the shared MSSEARCH folder. Any other user not in the Library Admins group can search (view) the libraries but cannot modify them.

See "Library Maintenance" on page 23 for more information.

NOTE MS Search does not need to be installed on the server hosting the share. If you want to allow local use of the libraries on the server, you can install the NIST MS Search Program using a custom setup (see "Install NIST With Local Libraries" on page 9).

Configure Log On user for instrument service

Carry out the following steps if you want to search shared libraries during unattended processing (that is, using a processing method during acquisition that contains a library search).

To ensure that your AIC, Workstation, or Workstation Plus can access the shared library, the Agilent OpenLab Instrument Service must be run under a specific account. This Log On account must have the following properties/privileges:

- Domain user
- Part of the local administrators group
- Can access the library network share
- Can log on as a service

Set up the Log On account for the **Agilent OpenLab Instrument Service** through the Windows Services application:

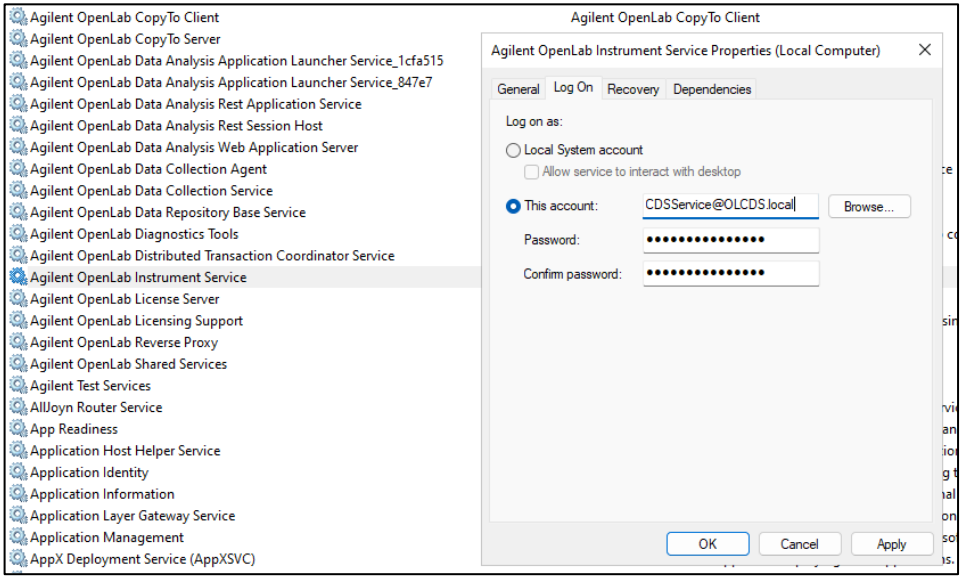


Figure 8 Instrument service properties

Prepare mapping to libraries on a shared network drive

NOTE

For this procedure, file extensions need to be visible. To show file extensions, open the File Explorer, go to **View > Show**, and select the **File name extensions** check box.

1. In a location that is available to everyone (for example, \\MyServer\MSSEARCH\maps), create one new folder for each library you plan to share. For example: \\MyServer\MSSEARCH\maps\MyLibrary
2. Inside each of these folders, create a new ALIAS.TXT file.
3. Inside each ALIAS.TXT text document, type the network location of the respective library, for example: `\\MyServer\MSSEARCH\MyLibrary`
4. Rename the ALIAS.TXT files to ALIAS.MSD.

Copy user-modified libraries to the share

Copy your user-modified libraries from a local installation (for example, C:\NIST23\MSSEARCH\MyLibrary) to the network share (for example: \\MyServer\MSSEARCH\MyLibrary).

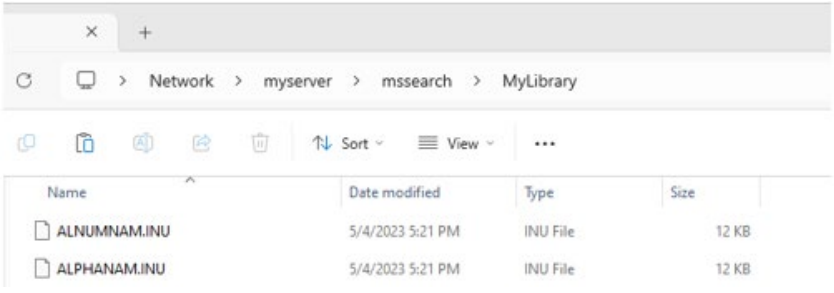


Figure 9 User-modified library on the server

Install NIST With Shared Libraries

Preparation

- See “Prepare Usage of Shared Libraries” on page 13

1. Install NIST, see “Install NIST With Local Libraries” on page 9.
2. Navigate to the location where you prepared the mapping to the shared libraries (for example, \\MyServer\MSSEARCH\maps).
3. Copy the subfolders into the local **C:\NIST23\MSSEARCH** folder.

   The copied folders contain the ALIAS.MSD files, which point to the network location of each library.

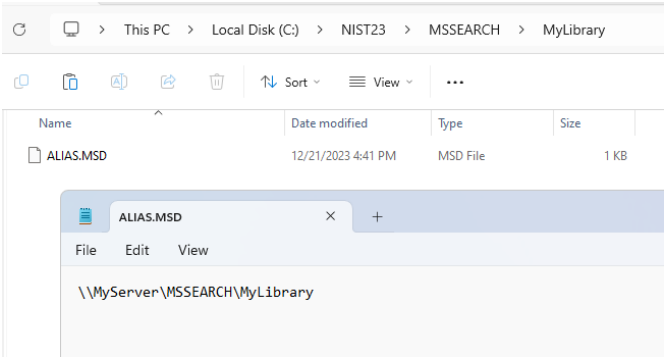


Figure 10 ALIAS.MSD file

All libraries, shared and local, are now visible in MS methods in Data Analysis, see “Use MS Libraries Within OpenLab CDS” on page 28.

Installation on Citrix/Terminal server

Preparation

- See “Prepare Usage of Shared Libraries” on page 13

1 Perform the installation for a Citrix/Terminal:

a Mount the ISO image using a tool such as Daemon.

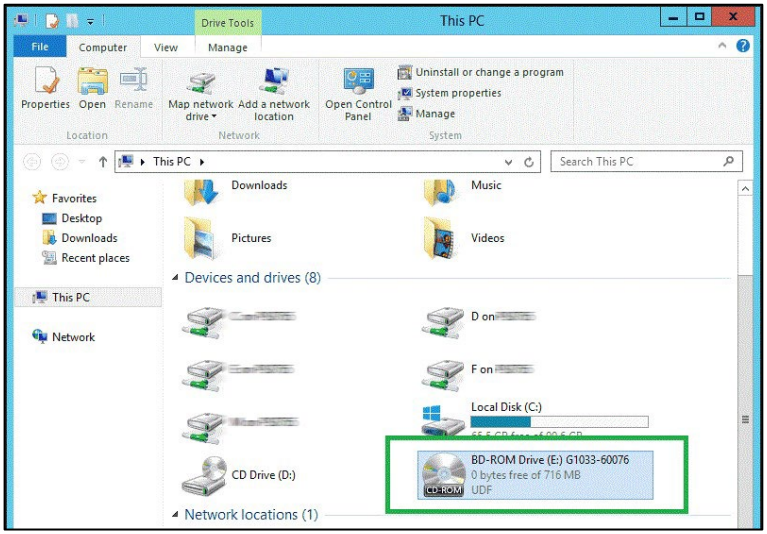


Figure 11 Example: ISO image mounted as drive E:

b Start the installation via **Install Application on Remote Desktop**.

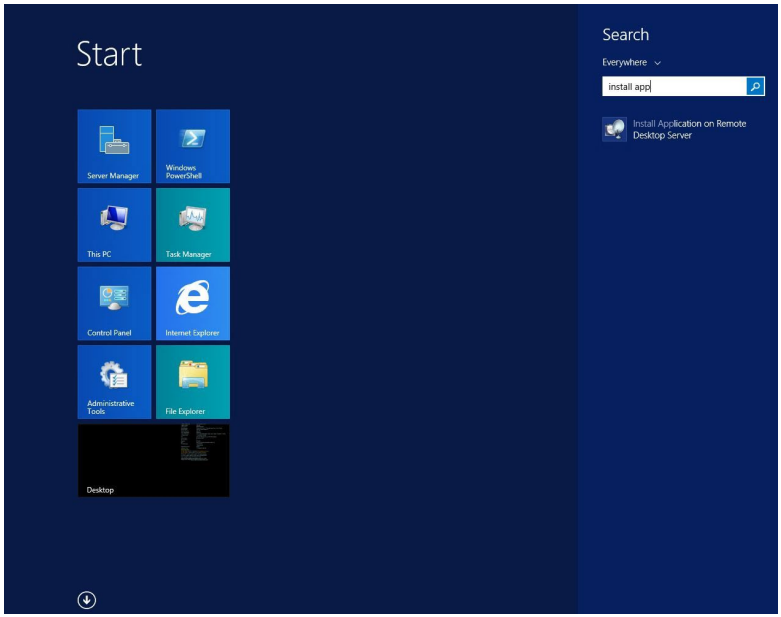


Figure 12 Start screen

c Run the installation program from the mounted ISO image.

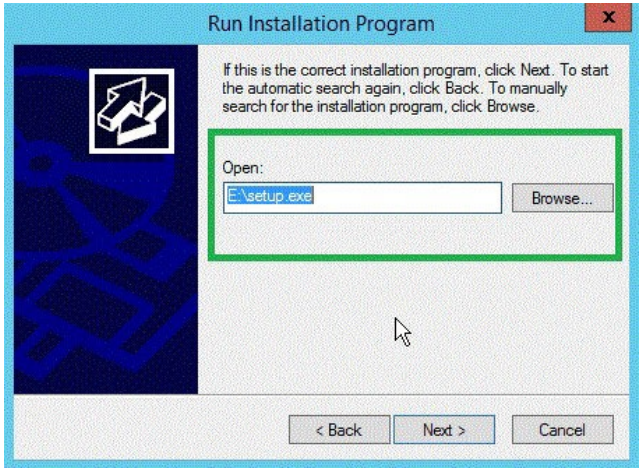


Figure 13 Installation program

The NIST installation wizard opens.

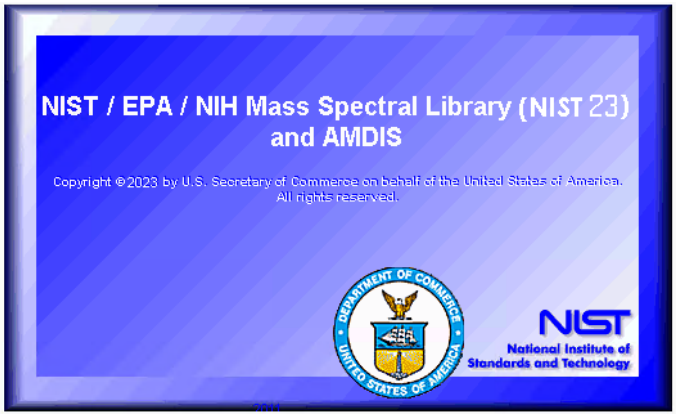


Figure 14 Installation wizard

d Carry out the installation as described in "Install NIST With Local Libraries" on page 9, starting from step 2.

2 If you want to use shared libraries:

a Navigate to the location where you prepared the mapping to the shared libraries (for example, \\MyServer\MSSEARCH\maps).

b Copy the subfolders into the local **C:\NIST23\MSSEARCH** folder.
The copied folders contain the ALIAS.MSD files, which point to the network location of each library.

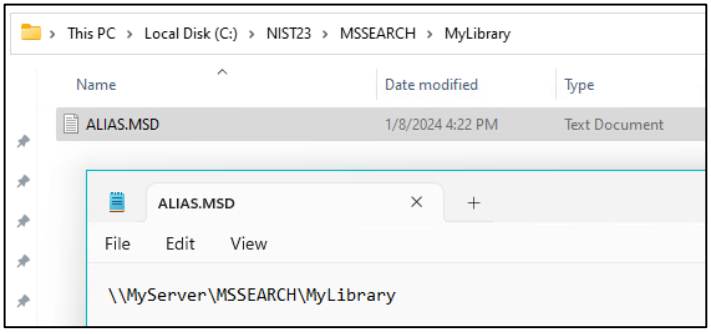


Figure 15 ALIAS.MSD

Ensure permissions for the additional library on the network share are set as in "Set up a shared network drive" on page 13.

3 Publish the application from Citrix/Terminal Server setup.

4 From a thin client, access the Citrix/Terminal Server published link.

5 If you want to add more libraries after installation, see “Add Libraries After Installation” on page 22.

Add Libraries After Installation

To use additional user-created or commercial libraries, they must be in NIST library format and available in the local NIST library location (by default, **C:\NIST23\MSSEARCH**).

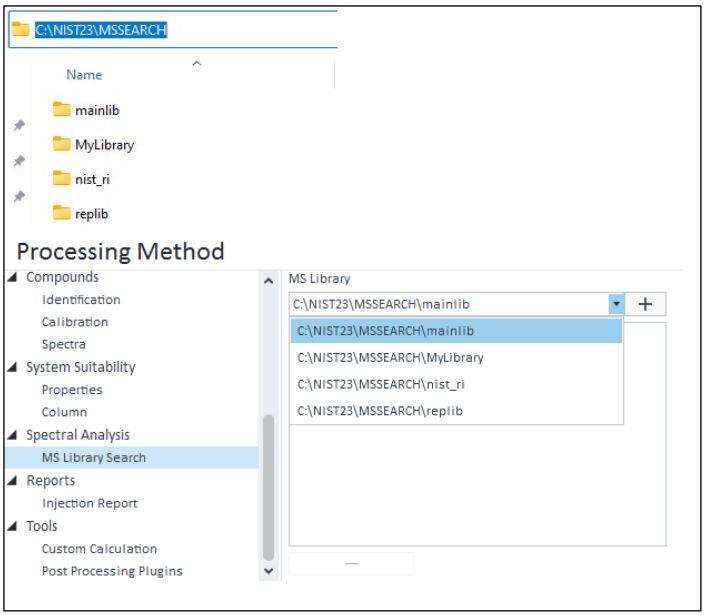


Figure 16 User-created or commercial libraries

1. Convert any libraries to NIST format using the Lib2NIST tool. This tool is installed by default when running the NIST installer. See "Library Maintenance" on page 23 for details.
2. For libraries that you want to store and use locally in addition to the shared libraries, copy them into the local library folder designated at installation (by default, **C:\NIST23\MSSEARCH**) on each Workstation, Workstation Plus, AIC, or client which should have access to them.
3. For libraries which are to be utilized on a network share, copy the library to the network share location. On each client, AIC, Workstation, Workstation Plus, or Citrix/Terminal server which should have access to the library, make a copy of one of the library linking folders which contains the ALIAS.MSD file pointing to the network location of a library.

5 Library Maintenance

Modify or Create a Library

- Use NIST's MS Search program. Libraries cannot be created or modified from within OpenLab CDS.
- Instructions for MS Search can be found in the MS Search Manual and Quick Start Guides and in the help file in MS Search. The Manual and Quick Start Guide can be launched from the start menu on a system with NIST MS Search installed.

Modify a Library in a Shared Configuration

- The NIST commercial libraries are not user editable.
- The network share on which the library resides must be set to full control for everyone.

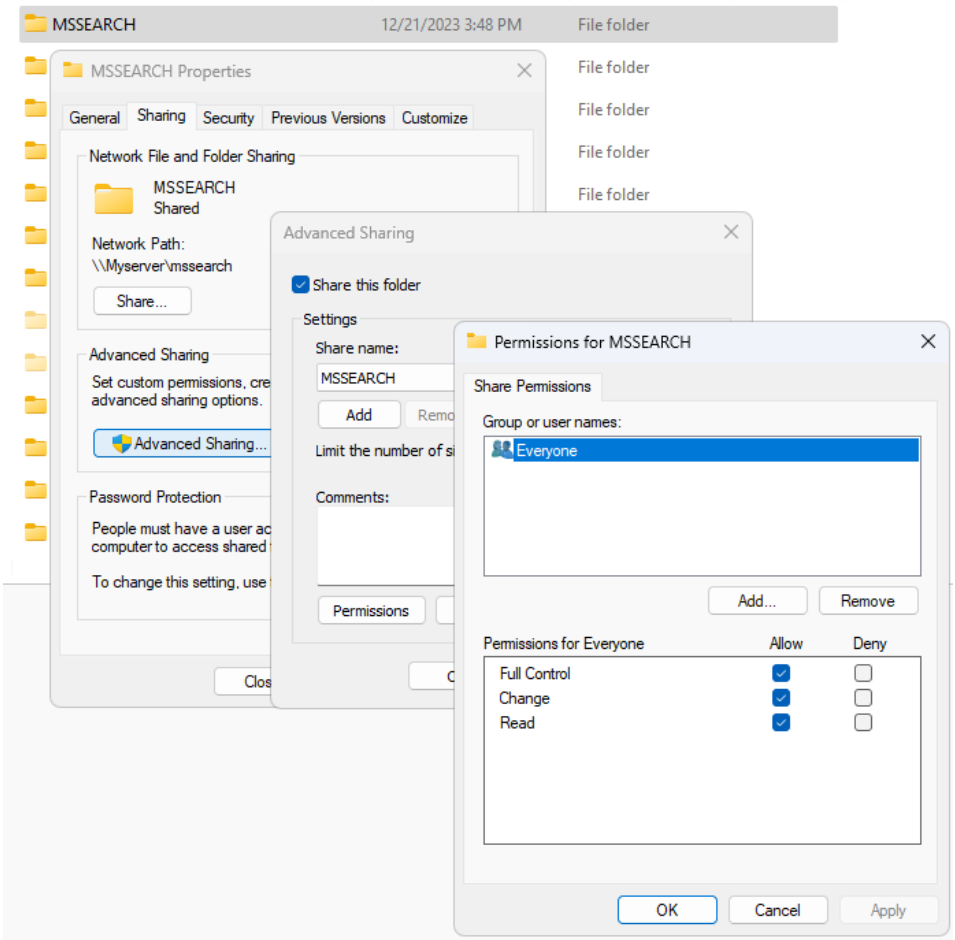


Figure 17 Permission settings

- The currently logged in user must have permissions to modify and write under **Security** tab for each library to be edited. This may be inherited from the share folder, or it may be set for each individual library. In the example below, only members of the Library Admins group can modify the libraries.

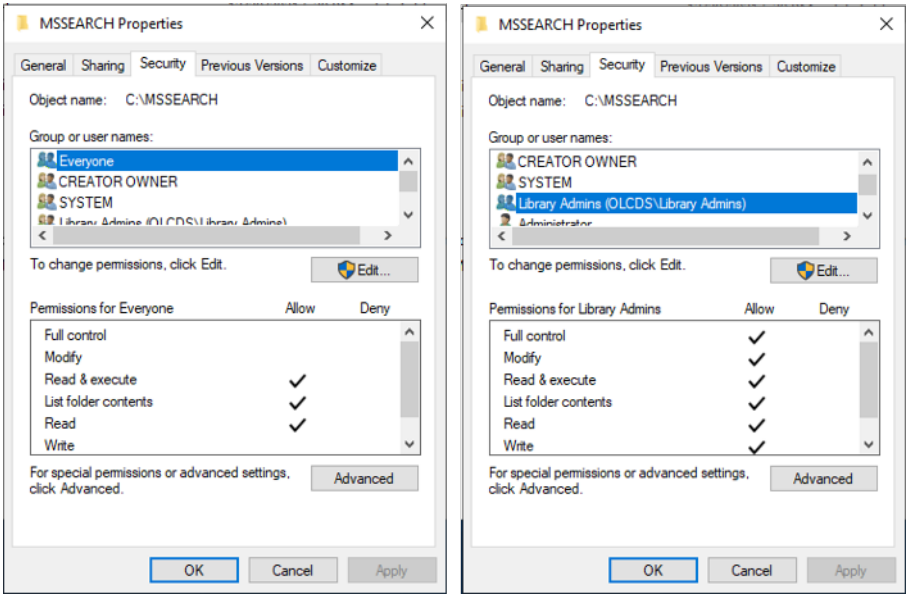


Figure 18 Security tab

- No one else can be connected to the library:
  - All instances of CDS Data Analysis which have been used to perform a search of that library must be closed.
  - All copies of MS Search which are connected to the library will either need to be closed, or they must be used to add an entry to a different library to "disconnect" them from the library which is to be edited.
  - All running and queued sequences which use processing methods which perform library searches must be completed.
  - It is recommended to schedule a Library Maintenance timeframe when all users disconnect from the library for updates to be performed.

Create a New Shared Library

1. Create the new library locally on a Workstation, Workstation Plus, or client from within MS Search.
2. Copy the library folder to the network share (see "Copy user-modified libraries to the share" on page 16) and set the permissions as above (shared with full control for **Everyone**; limit who has access to modify the library using the **Security** tab).
3. Create the link folder containing ALIAS.MSD, modify ALIAS.MSD to point to the new library, and copy the link folder to each client, Workstation, Workstation Plus, or AIC that should have access.

Convert an Existing Library to NIST Format

The Lib2NIST tool may be used. It is installed automatically when the NIST commercial libraries are installed. Alternatively, it may be downloaded from the NIST website.

1. Launch the Lib2NIST tool.

   If you use NIST23:

   a. Run a command prompt,

   b. Navigate to the Lib2NIST installation folder (by default, C:\NIST23\MSSEARCH).

   c. Execute the command:
   ```
   Lib2NIST.exe /AccuratePeakMZ
   ```

   If you use NIST20 or lower, launch Lib2NIST Converter from the Start menu.
2. Navigate to and select the library to be converted.

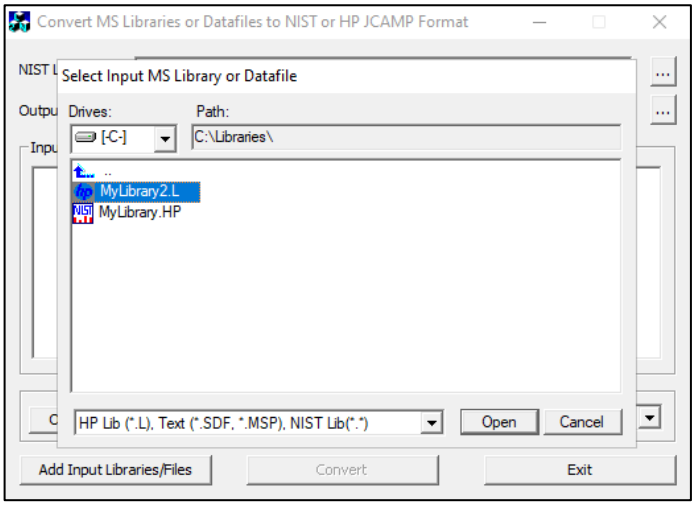


Figure 19 Library selection

3 Select the NIST output format and the output folder.

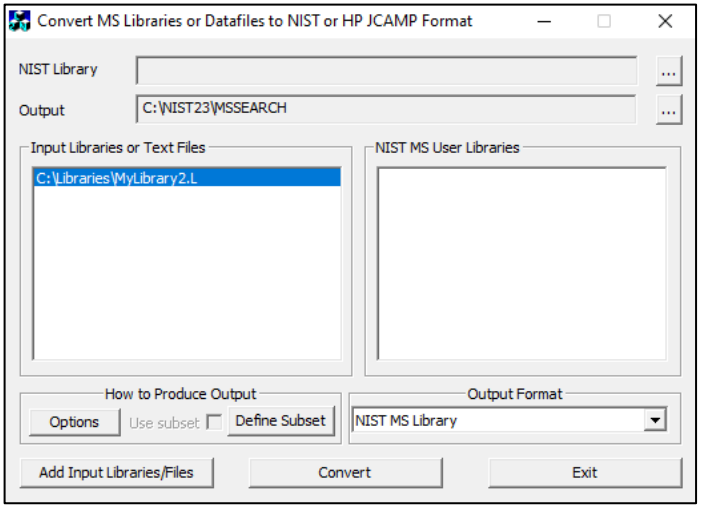


Figure 20 Output format and folder

4 The program will convert the libraries and copy them to the specified output location; be sure this is the same location where the NIST libraries were installed so that CDS and MS Search find the newly converted libraries.

6 Use MS Libraries Within OpenLab CDS

To use MS libraries, you must reference these libraries in a processing method.

1 Log in to OpenLab CDS and start Data Analysis.

2 Create a new MS processing method.

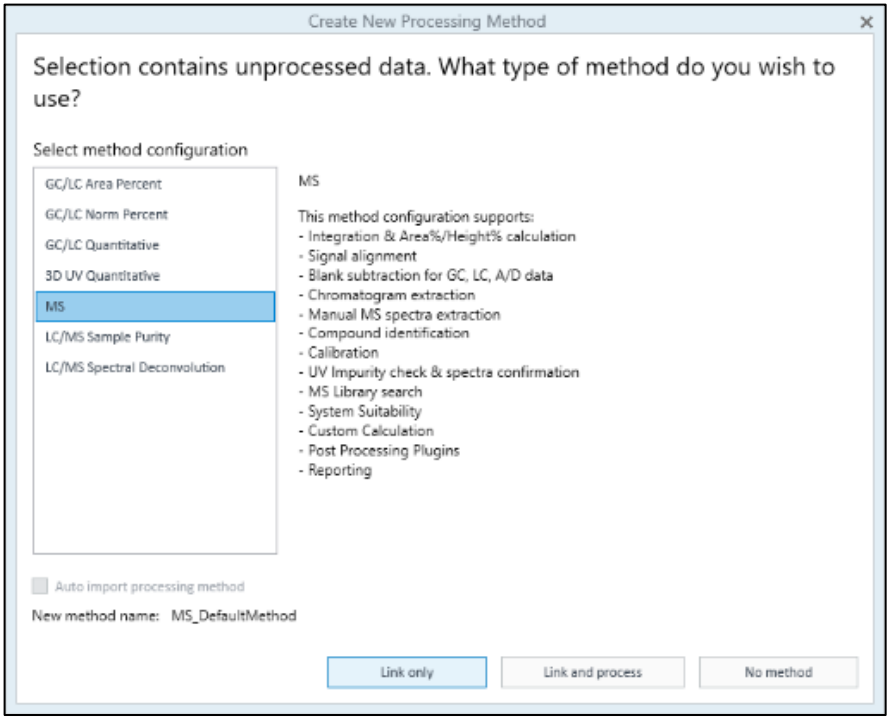


Figure 21 Processing method creation screen

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.

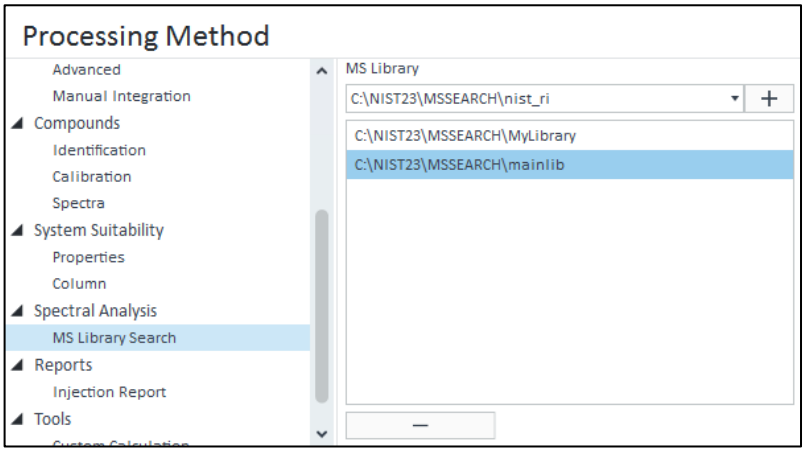


Figure 22 MS library properties

4 Save the processing method.

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

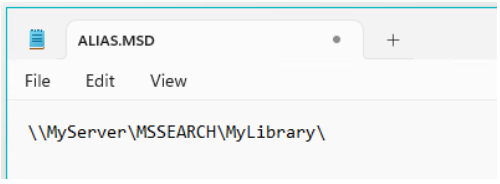
6 For details on performing an MS Library search, refer to OpenLab Help and Learning.

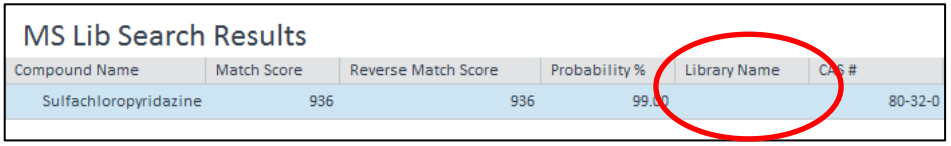
7 Troubleshooting

When searching the libraries, if the library name is not shown in the library search window or in the generated reports, open the ALIAS.MSD file within that library's folder and delete the "\" at the end of the network path.

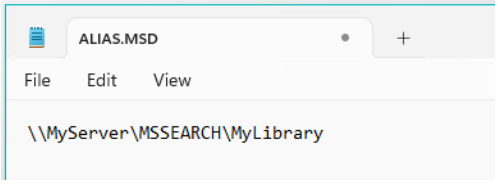
This "\" prevents OpenLab CDS from reading the name of the library correctly.

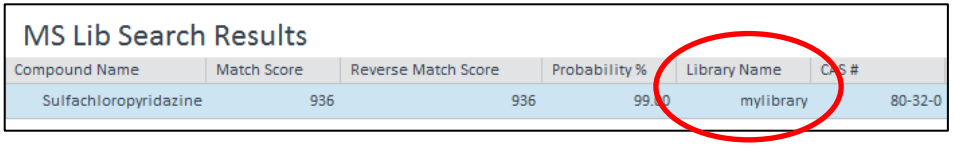
For example, if the file ALIAS.MSD reads **\\MyServer\MSSEARCH\MyLibrary\:**





ALIAS.MSD reads **\\MyServer\MSSEARCH\MyLibrary**:





To solve the issue:

1. Update and save all ALIAS.MSD files to remove the final "****".
2. Place copies of all the linking folders containing ALIAS.MSD in a location which can be accessed during all future NIST library installations.

In This Book

This manual describes the installation and configuration of the NIST library framework within standalone, client/server, and Citrix/Terminal Server OpenLab CDS setups. It also discusses the use and management of other commercial and user-created libraries with OpenLab CDS MS library search.

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