



OpenLab CDS

## Setup and Configuration of MS Library Search

# Notices

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# 1

## Introduction

This document 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.

### NOTE

In order to use MS library searching within CDS, the NIST MS Search program must be installed locally on the Workstation, Workstation Plus, Client, or AIC which is to perform the library search. This enables the use of the NIST libraries, as well as other commercial and user-created libraries, provided they are in NIST library format. NIST provides a tool to convert existing libraries into NIST format.

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## 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 required for each computer where the NIST libraries are to be installed. For NIST libraries in a shared environment<sup>1</sup>, a license is required for each possible simultaneous user of the NIST libraries. Upgrades (for both scenarios) require an upgrade license – for example, to move from NIST17 to NIST20 would require an upgrade to each license described above (each license that will access the upgraded NIST library would need an upgrade license). For additional information, reference the EULA that shipped with the NIST library.

If the NIST commercial libraries are not needed or purchased, the NIST MS Search tool and the Lib2NIST library conversion tool (without the NIST commercial libraries) may be downloaded from NIST. This allows for creation and use of custom libraries without the purchase of the NIST commercial libraries. This download does not include the NIST libraries, only the searching and conversion tools. Using NIST MS Search only to create and manage user-created libraries or using Lib2NIST to convert only existing user-created libraries does not require a NIST license.

---

<sup>1</sup> Workstation or Workstation Plus computers searching NIST libraries on a shared location; also, Clients, AICs, and Clients within a multi-user (Citrix/Terminal Server) environment, regardless of whether the NIST library is local to the Client, AIC, or Citrix/Terminal Server, or on a share

# 3

## Topologies

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

### Standalone Workstation

- NIST MS Search and libraries are installed, stored, and used locally on each Workstation, Workstation Plus, Client, or AIC.
- Sharing user-created libraries requires copying them between PCs.
- One NIST license is needed for each Workstation or Workstation Plus.
- One NIST license is needed for each possible simultaneous user when working in a distributed environment (Clients or AICs).
- AICs need to have locally installed MS Search and libraries for any processing method containing a library search to be run during acquisition.
- This is the default configuration for Workstation and Workstation Plus.

### On a Network Share

- NIST MS Search is installed locally on every Workstation, Workstation Plus, Client, or AIC.
- Libraries are installed on a network share.
- Can use a mix of local and network share libraries – it is highly recommended to install the large NIST commercial libraries locally to decrease search time and network traffic, while keeping user-modified libraries on the share.
- One NIST license needed for each possible simultaneous user of the NIST library on a share (including AICs).
- AICs need to have access to this library for any processing method which contains a library search to be run during acquisition.

### On a Citrix/Terminal Server

- Installed the same way as the Standalone approach (NIST MS Search and libraries installed locally on the server).
- One NIST license is needed for each possible simultaneous user (including AICs).
- AICs need to have access to this library for any processing method which contains a library search to be run during acquisition.

### On a Network Share With Multiple Citrix/Terminal Servers

- Each Citrix/Terminal Server has NIST MS Search installed locally.
- Libraries are installed on a network share.
- Can use a mix of local and network share libraries – it is highly recommended to install the large NIST commercial libraries locally to decrease search time and network traffic, while keeping user-modified libraries on the share.
- One NIST license is needed for each possible simultaneous user (including AICs).
- AICs need to have access to this library for any processing method which contains a library search to be run during acquisition.

## 4 Installation

### NOTE

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

```
[NISTMS]
Amdis32Path=C:\NIST20\AMDIS32\
AmdisMSPath=C:\NIST20\AMDIS32\
Path32=C:\NIST20\MSSEARCH\
WorkDir32=C:\NIST20\MSSEARCH\
```

**Figure 1** Directories

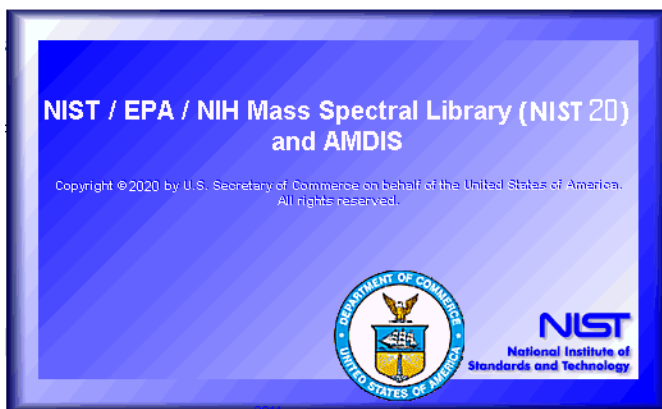
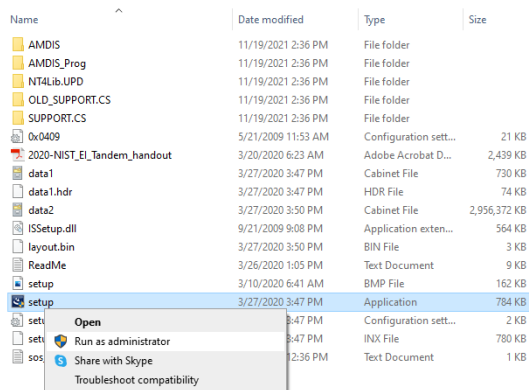
- It is recommended only to use the NIST installer to update win.ini. Do not modify win.ini manually.
- For libraries to be available for use in CDS and in NIST MS Search, they must be located in the directory referenced in win.ini.

For non-local libraries on shared drives (for sharing between multiple Citrix/Terminal Servers), 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 [“On a Network Shared Drive”](#) on page 14 for more information.



# Standalone Workstation

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



**Figure 2** Setup file

- 2 Follow the prompts until reaching the **Setup Type** screen.

From here, the **Typical** setup may be selected for ease of installation, or **Custom** may be chosen in order to save disk space by skipping libraries which are not needed (for example, the MS/MS libraries).

It is not recommended to change the path the libraries are saved in – but if a different location is desired, it must be local (not on a network share or removable drive). Updating library modification privileges and network share installations are discussed in “[On a Network Shared Drive](#)” on page 14.

## Installation

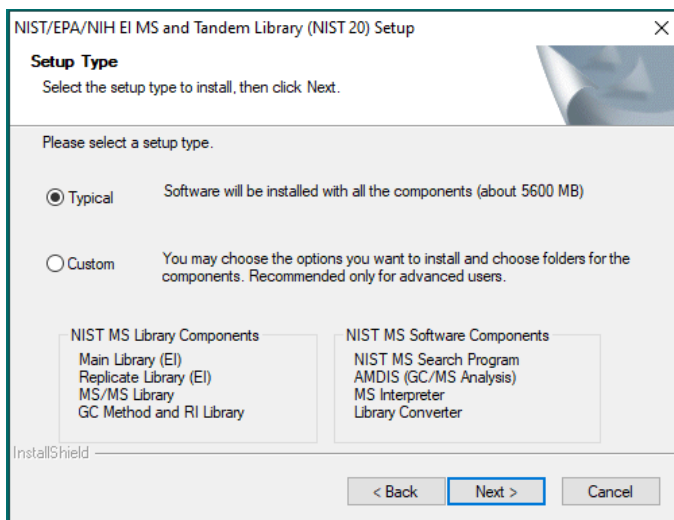


Figure 3 Setup type – Typical

Or

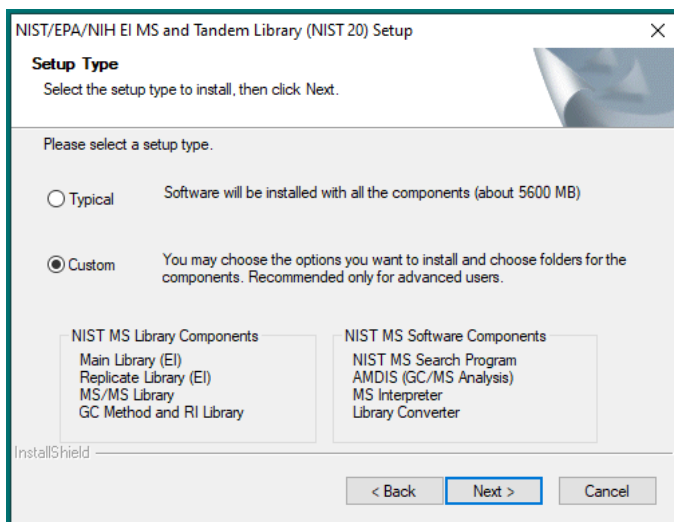


Figure 4 Setup type – Custom

## Installation

- 3 If other commercial and/or user-created libraries already exist in NIST format, they may be copied into the NIST MS Search folder by the installer if desired. Otherwise, this may be done after the installation is complete. If the installer does not automatically locate existing libraries, the **Search for User Libraries** button may be used.

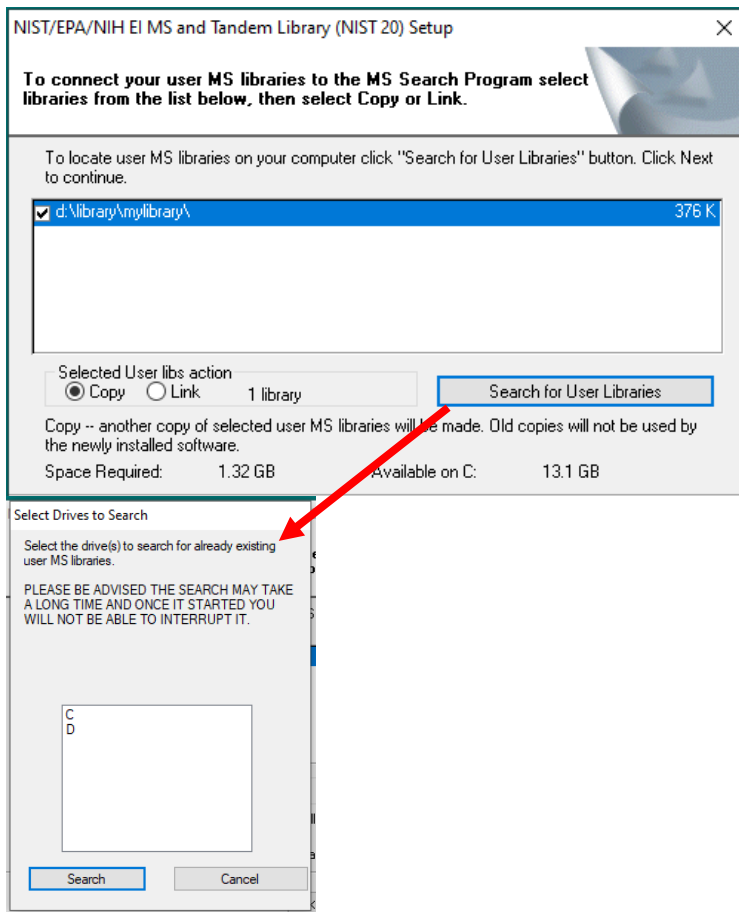


Figure 5 User libraries selection

## Installation

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

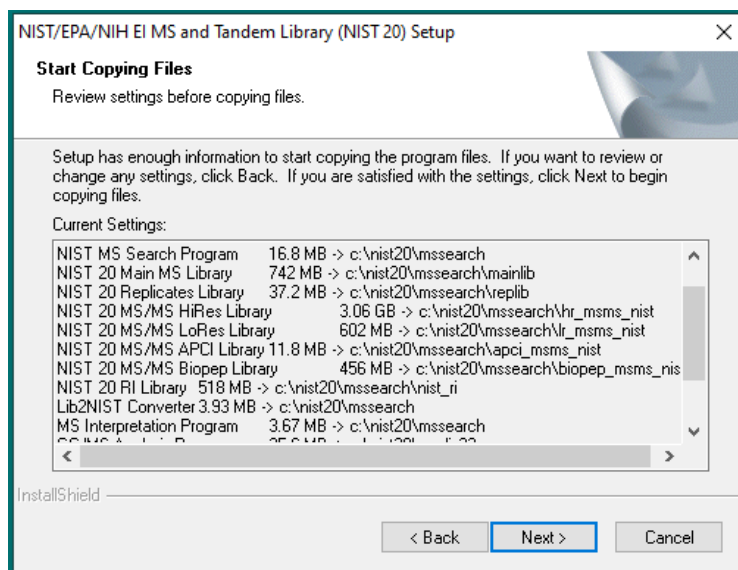


Figure 6 Program files – Typical setup

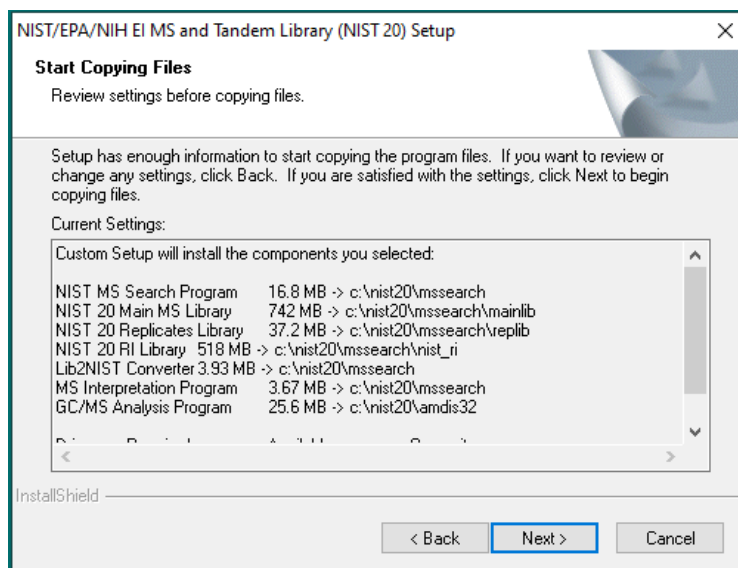


Figure 7 Program files – Custom setup

## Installation

- 4 Complete the installation.

NIST MS Search is now installed. Upon relaunch of CDS Data Analysis, the installed libraries should now be visible from any MS method.

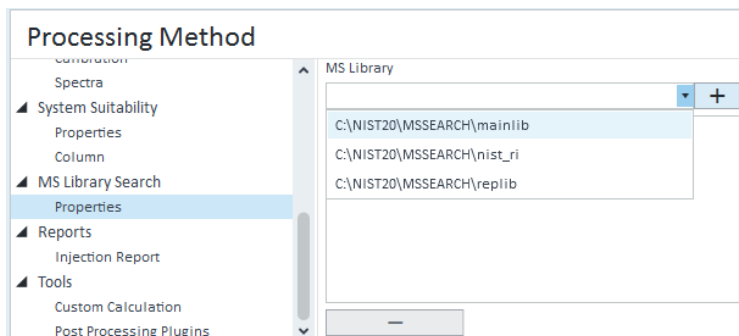


Figure 8 Processing Method window

- 5 To use additional user-created or commercial libraries, they must be in NIST library format, and available in the local NIST library location (C:\NIST20\MSSEARCH by default).

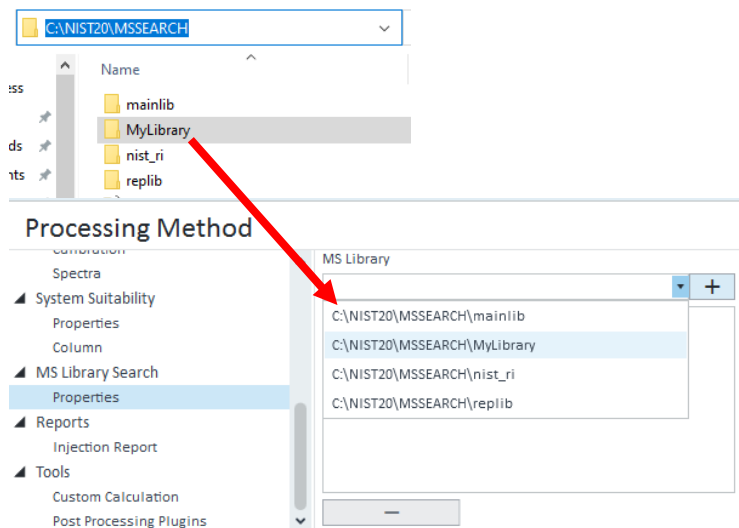


Figure 9 User-created or commercial libraries

- 6 Libraries may be converted to NIST format using the Lib2NIST tool which is installed by default when the NIST installer is run. See "Library Maintenance" on page 56 for details.

## On a Network Shared Drive

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.

- 1 First, create and configure the network shared drive.
  - a Share the folder containing the libraries with **Everyone (Full Control)**.

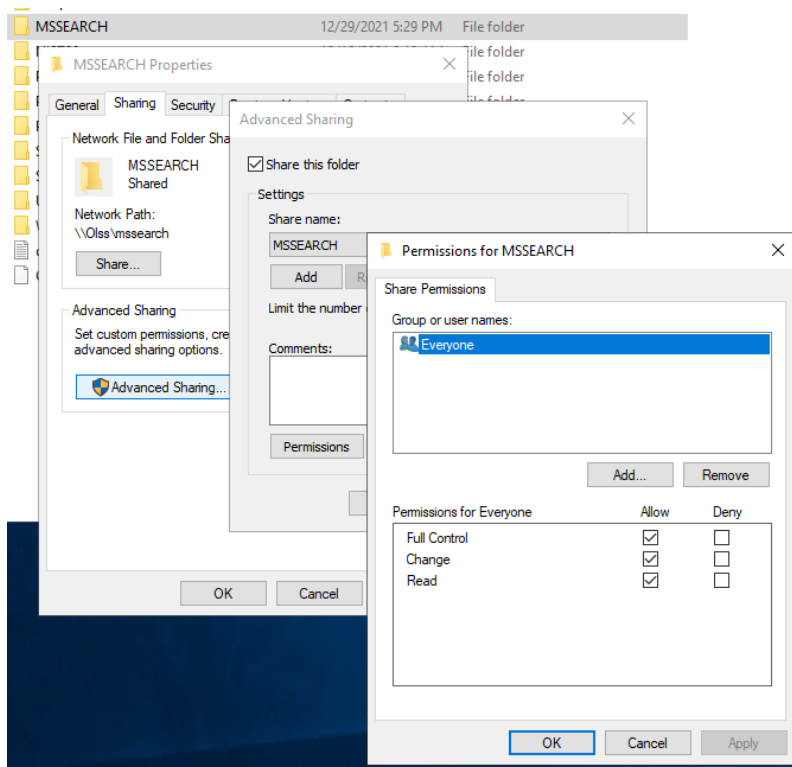


Figure 10 Sharing and permission options

## Installation

- b** If it is necessary to limit the ability to modify the libraries to specific users or user groups, this should be done 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, as needed.

### NOTE

Commercial NIST libraries cannot be user edited.

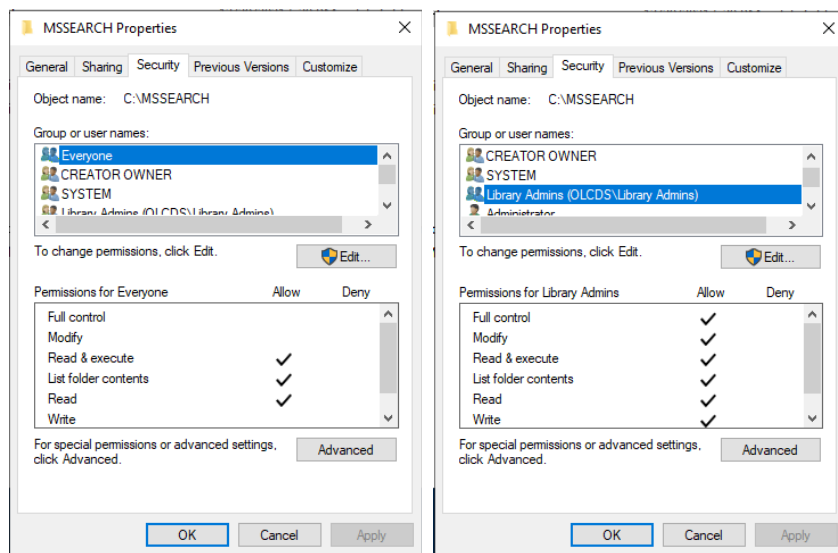


Figure 11 Security tab

- c** 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 56 for more information.
- 2 Copy any existing user-created libraries in NIST format (use the Lib2NIST conversion tool if needed) to the share – see “[Library Maintenance](#)” on page 56 for details. If libraries exist which need to be converted, but the Lib2NIST tool has not yet been installed, they can be added later.
  - 3 NIST’s MS Search program (installed as part of the NIST commercial library installation) must be installed on every Workstation, Workstation Plus, Client, and AIC which will perform library searching. MS Search does not need to be installed on the server hosting the share, although it can be to allow local use of the libraries on the server if needed.

## Installation

### On each Workstation, Workstation Plus, Client, or AIC:

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

Name	Date modified	Type	Size
AMDIS	11/19/2021 2:36 PM	File folder	
AMDIS_Prog	11/19/2021 2:36 PM	File folder	
NT4Lib.UPD	11/19/2021 2:36 PM	File folder	
OLD_SUPPORT.CS	11/19/2021 2:36 PM	File folder	
SUPPORT.CS	11/19/2021 2:36 PM	File folder	
0x0409	5/21/2009 11:53 AM	Configuration sett...	21 KB
2020-NIST_EI_Tandem_handout	3/20/2020 6:23 AM	Adobe Acrobat D...	2,439 KB
data1	3/27/2020 3:47 PM	Cabinet File	730 KB
data1.hdr	3/27/2020 3:47 PM	HDR File	74 KB
data2	3/27/2020 3:50 PM	Cabinet File	2,956,372 KB
ISSetup.dll	9/21/2009 9:08 PM	Application exten...	564 KB
layout.bin	3/27/2020 3:50 PM	BIN File	3 KB
ReadMe	3/26/2020 1:05 PM	Text Document	9 KB
setup	3/10/2020 6:41 AM	BMP File	162 KB
setup	3/27/2020 3:47 PM	Application	784 KB
seti	3:47 PM	Configuration sett...	2 KB
seti	3:47 PM	INX File	780 KB
sos	12:36 PM	Text Document	1 KB

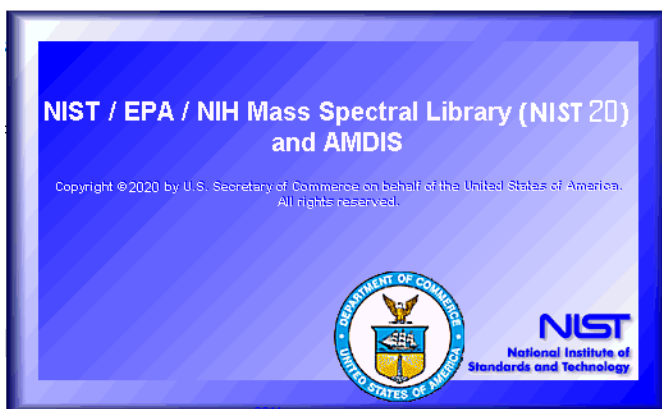


Figure 12 Setup file



## Installation

- Follow the prompts until reaching the **Setup Type** screen. Select the **Custom** installation.

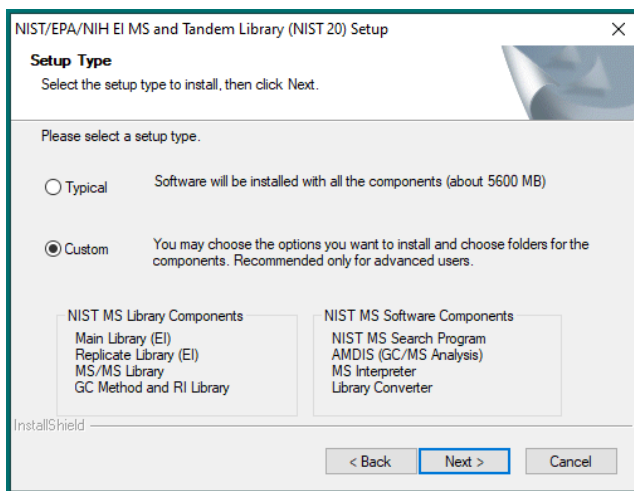


Figure 13 Setup type – Custom

- For the first installation of the NIST libraries only. Continue with step 4 for subsequent installations.

Browse to or type the location of the network share as the installation path of the NIST 20 Main Library and all other NIST libraries which are to be installed.

- The NIST MS/MS libraries may be deselected in order to save disk space, if desired.

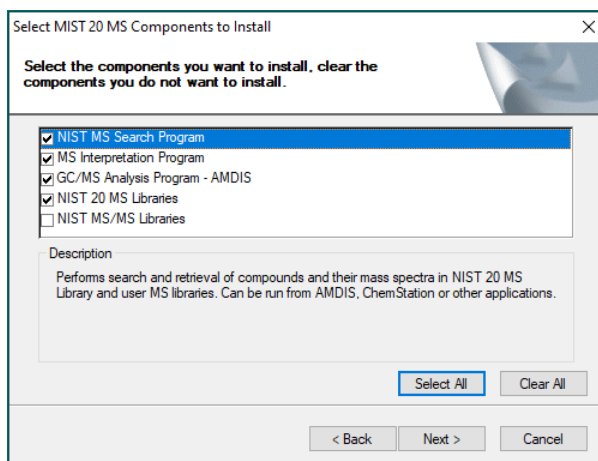
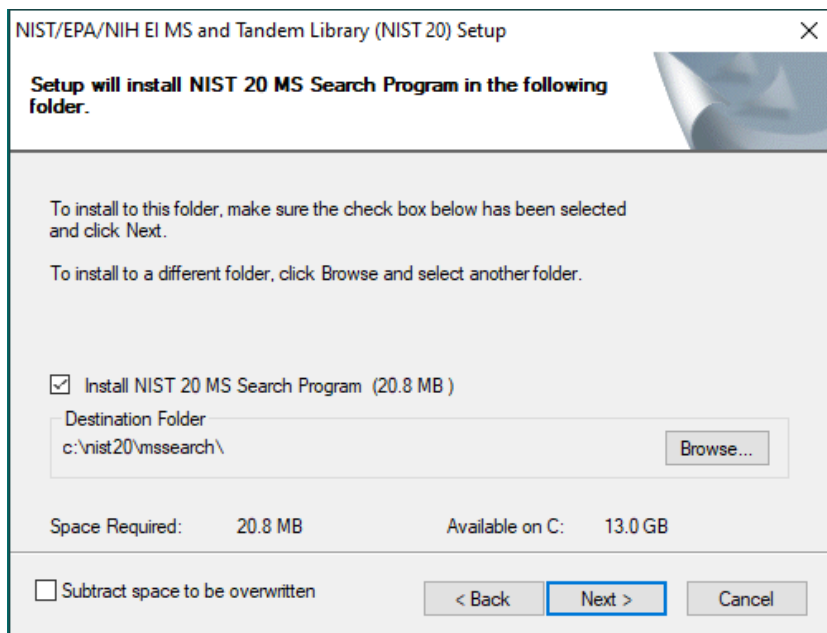


Figure 14 Component selection

## Installation

- b** Do not change the installation path of the NIST 20 MS Search program – MS Search must be installed locally.



**Figure 15** MS search program

## Installation

- c Browse to or type the location of the network share as the installation path of the NIST 20 Main Library and all other NIST libraries which are to be installed.

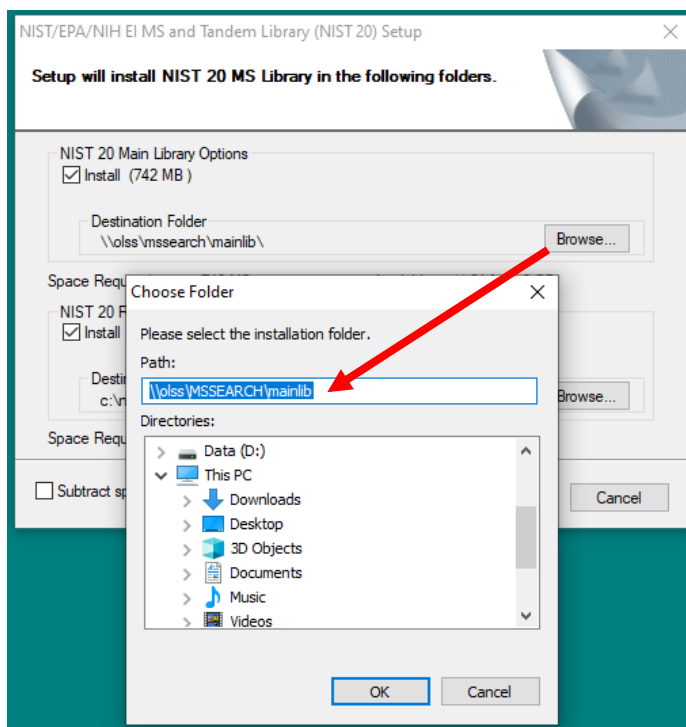


Figure 16 Installation path

- d If the installer locates the other libraries on the network share, you may link (not copy) to them –if they are not found, this can be done later.

## Installation

- e The MS Interpretation Program and AMDIS may be installed if desired; they should be installed locally (not on the network share).

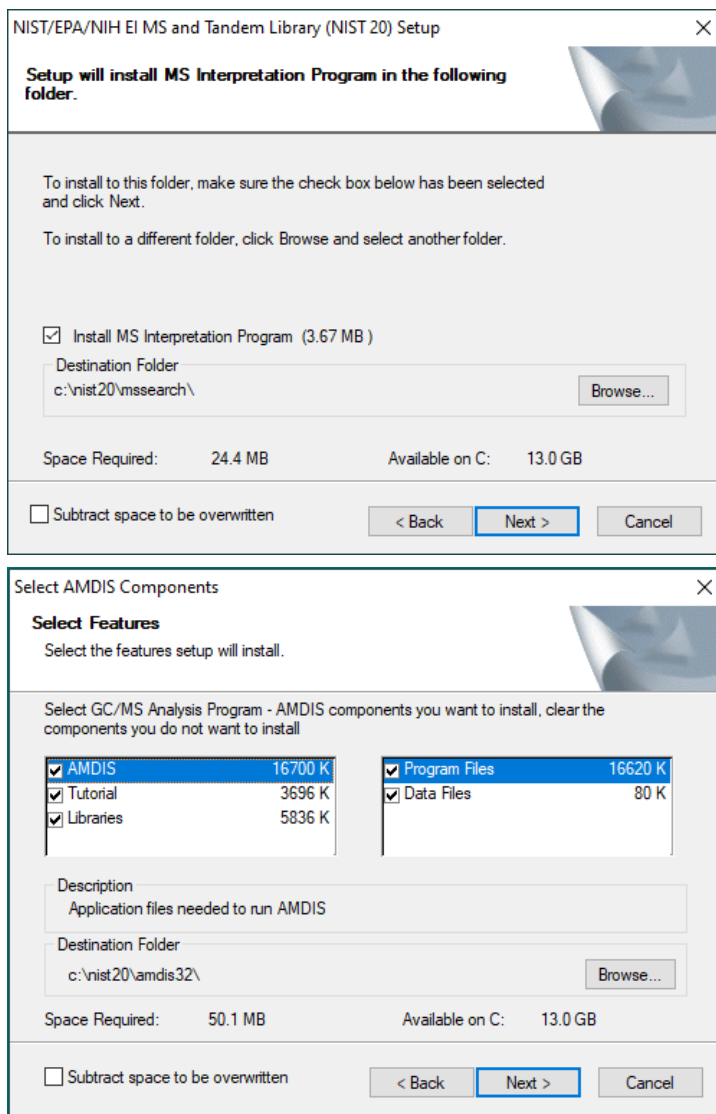


Figure 17 MS Interpretation program and AMDIS

## Installation

- f Select a program folder for program icons.

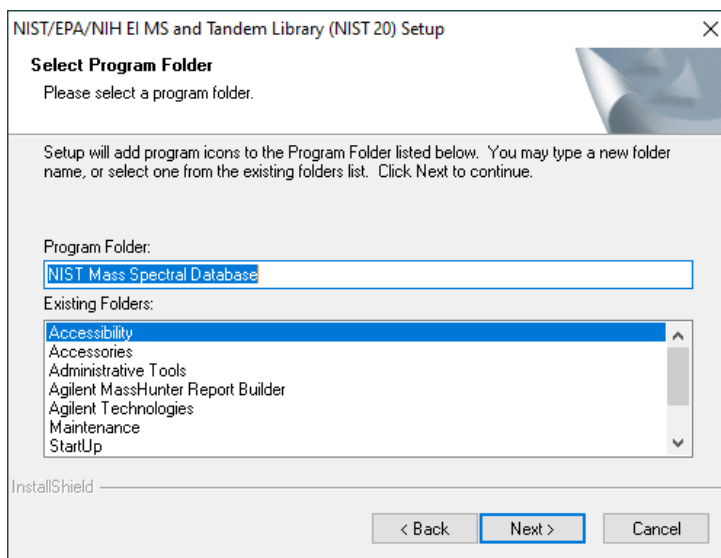


Figure 18 Program folder window

- g The installation settings should be as follows:

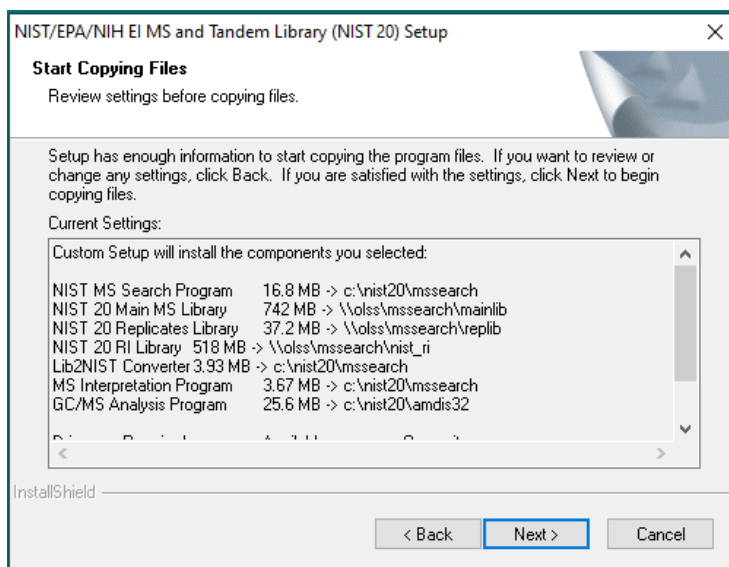
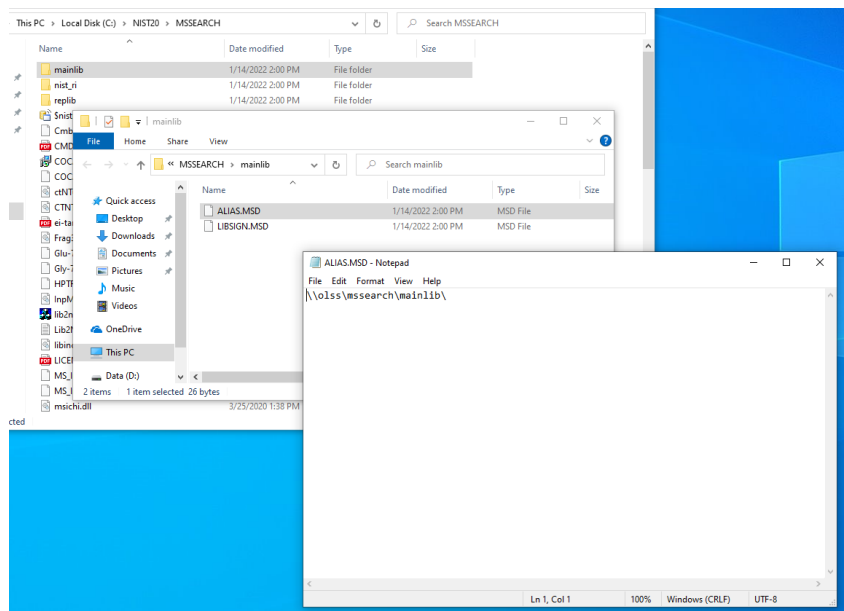


Figure 19 Installation settings

## Installation

- h Complete the installer.

NIST MS Search is now installed. The NIST libraries selected have installed on the network share drive. They have also installed links to the shared libraries on the local machine:



**Figure 20** MSSearch

This link, via the ALIAS.MSD file is how both CDS and MS Search find the libraries on the network share. It may be edited from a text editor like Notepad.

## Installation

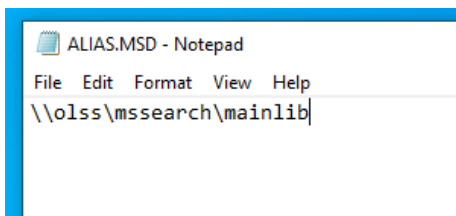
### NOTE

On the first installation, when the link files are created, the installer will create the network path with a final '\ ' at the end. This '\ ' must be removed for CDS to read the name of the library correctly. In the above example, the file will need to be edited so the path reads: **\\olss\mssearch\mainlib**. If this is not done, the library name will be empty in CDS data analysis and on generated reports:

#### MS Lib Search Results

Compound Name	Match Score	Reverse Match Score	Probability %	Library Name	AS #	NIST #
Naphthalene-D8	890	892	91.8		1146-65-2	

ALIAS.MSD reads **\\olss\mssearch\mainlib\**



#### MS Lib Search Results

Compound Name	Match Score	Reverse Match Score	Probability %	Library Name	AS #	NIST #
Naphthalene-D8	890	892	91.8	mainlib	1146-65-2	

ALIAS.MSD reads **\\olss\mssearch\mainlib**

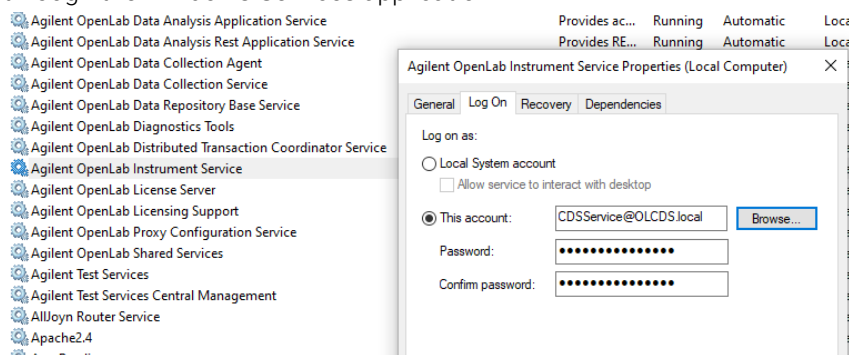
- i All **ALIAS.MSD** files generated by the installer should be updated to remove the final '\ ' and saved. Copies of all linking folders – containing **ALIAS.MSD** and **LIBSIGN.MSD** – should also be placed in a location which can be accessed during all future NIST library installations.

## Installation

### NOTE

For all AIC, Workstation, and Workstation Plus systems:

For library searching of a network shared library which is run during data acquisition (library searches run in a processing method attached to a sequence or single sample run), the Agilent OpenLab Instrument Service on each acquisition PC (AIC, Workstation, and Workstation Plus) must be run under an account which is 1) a domain user and 2) part of the local administrators group. This can be accessed through the Windows Services application:





## Installation

### 4 For all subsequent installations:

Once the first connection to the shared libraries has been created, all additional systems should be installed as follows.

- a Run the NIST installer as described in step 1 and 2. Choose the **Custom** installation.

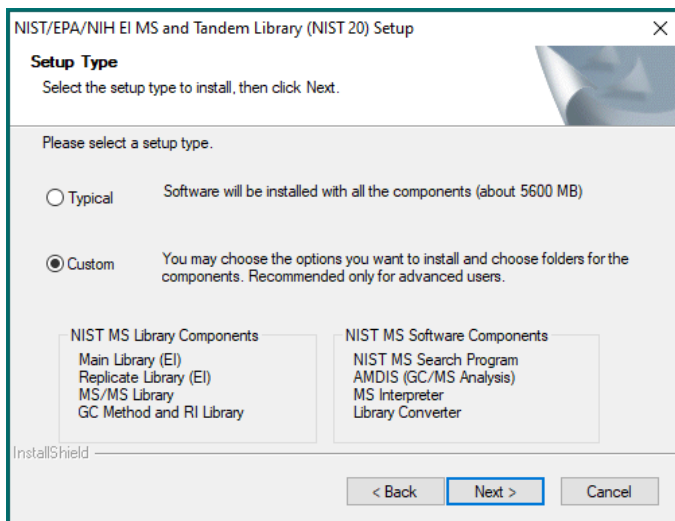


Figure 21 Setup type – Custom

- b Deselect the NIST libraries so they are not installed.

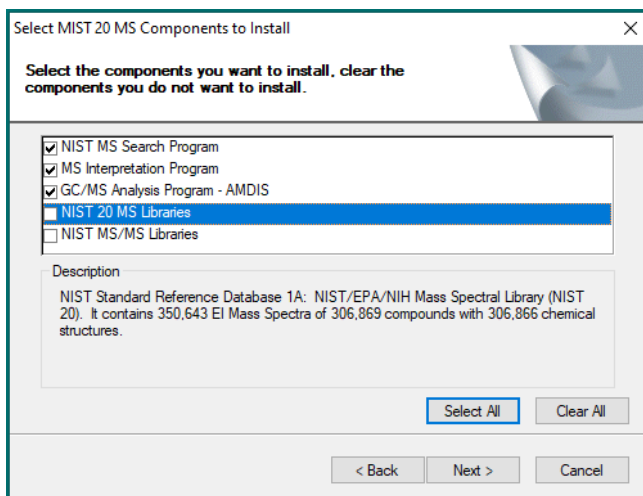


Figure 22 Component selection

## Installation

- c Install the NIST MS Search program locally in the default directory.
- d The installer will pop up a warning about not finding the main and replicates libraries – select **Yes** to continue without them.

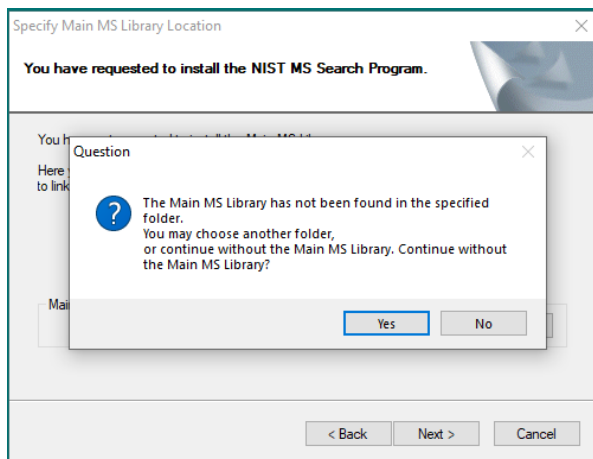


Figure 23 Installer pop-up

- e Unless local libraries are intended to be used along with network shared libraries, do not select any libraries to link or copy on the next installer screen. If local libraries are to be used, they may be linked now, or they may be manually linked later.

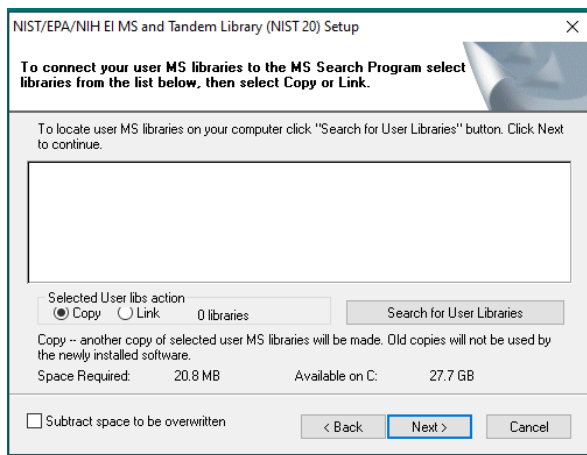
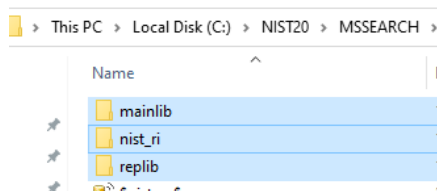


Figure 24 Local libraries

- f Click through the rest of the prompts and complete the installer.

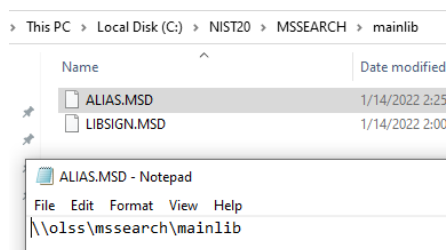
## Installation

- g** Navigate to the location where the copies of the library link folders are saved (see step 3h). Copy these folders into the **C:\NIST20\MSSEARCH** folder.



**Figure 25** Library link folders

- h** These folders contain the **ALIAS.MSD** file, which points to the network location of the library.



**Figure 26** ALIAS.MSD file

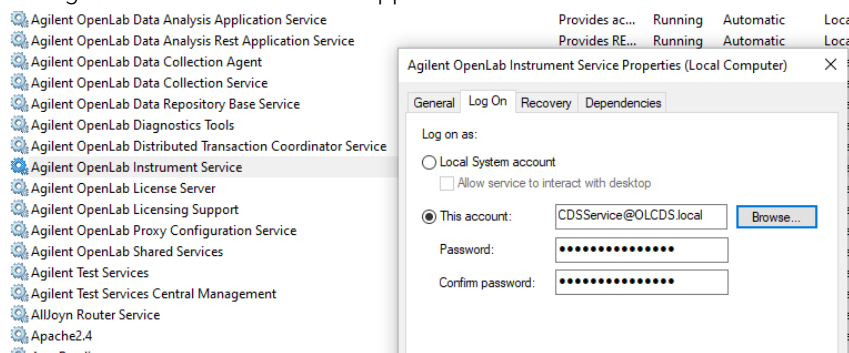
- i** Repeat for each additional system which should have access to the NIST commercial libraries on the network share.

## Installation

### NOTE

For all AIC, Workstation, and Workstation Plus systems:

For library searching of a network shared library which is run during data acquisition (library searches run in a processing method attached to a sequence or single sample run), the Agilent OpenLab Instrument Service on each acquisition PC (AIC, Workstation, and Workstation Plus) must be run under an account which is 1) a domain user and 2) part of the local administrators group. This can be accessed through the Windows Services application:



- 5 To use additional existing user-created or commercial libraries, they must be in NIST library format. Many commercial libraries are provided in NIST library format; any libraries created using NIST MS Search will also be in NIST format.
- 6 Existing libraries not in NIST library format may be converted using the Lib2NIST tool which is installed with the NIST libraries. See [“Library Maintenance”](#) on page 56 for details.
- 7 For libraries which are to be stored and used locally, copy them into the local library folder designated at installation (**C:\NIST20\MSEARCH by default**) on each Workstation, Workstation Plus, AIC, or Client which should have access to them.
- 8 For libraries which are to be utilized on a network share, copy the library to the network share location. On each Client, AIC, Workstation, or Workstation Plus 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.

## Installation

- 9 Rename the copied folder to the name of the additional library being mapped. Edit the ALIAS.MSD file in Notepad to update it to the location of the additional library. Place the copied folder in the PC's local library folder (C:\NIST20\MSSEARCH by default). Repeat this procedure for each additional library. Once all libraries have been linked, copy the updated folders containing the links to the libraries to a location where they can be accessed for subsequent installations.

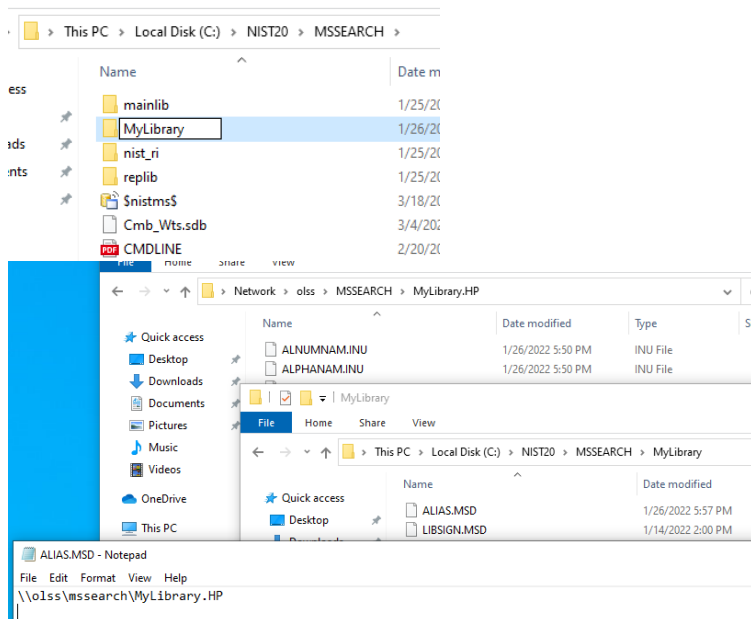
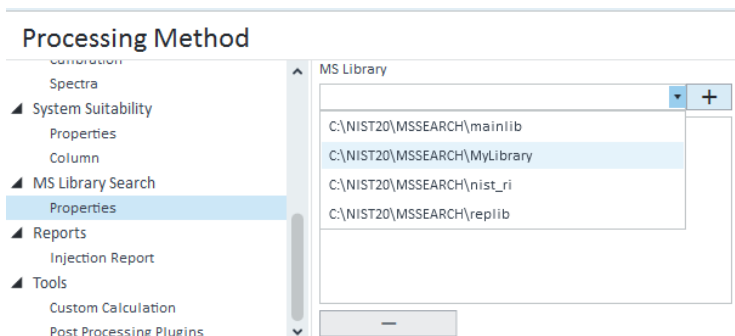


Figure 27 Library folder

## Installation

- 10 Copy these linking folders to each Workstation, Workstation Plus, AIC, or Client which should have access to these libraries.
- 11 Open CDS Data Analysis and load an MS method. The libraries should now be available for selection from the drop-down list.



**Figure 28** MS Library

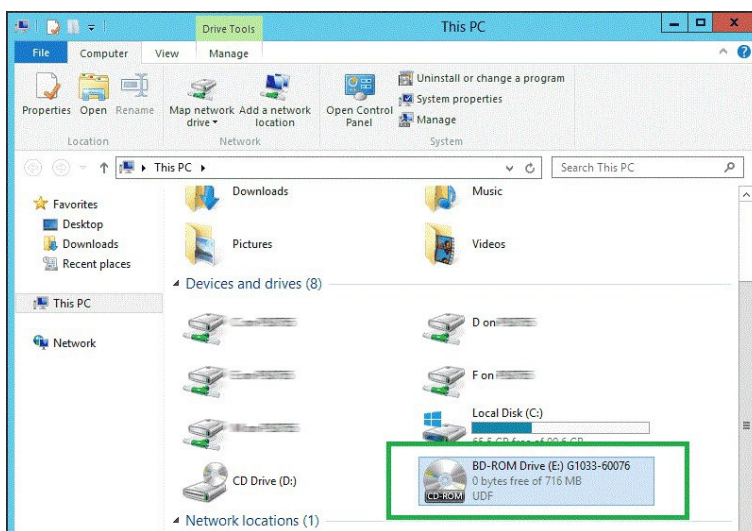
- 12 When searching the libraries in CDS, if the library name does not populate the library search window or reports generated, open the ALIAS.MSD file within that library's folder and delete the '\' at the end of the network path.

# Single Citrix/Terminal Server, Libraries Installed Locally

### NOTE

In this configuration, the AICs must have NIST MS Search and all applicable libraries installed locally on each AIC, following the instructions in “[Standalone Workstation](#)” on page 6 in order to enable library searching in processing methods which are executed from data acquisition. It is recommended that libraries and MS Search should be the same version on all AICs and Citrix/Terminal Servers 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.

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



**Figure 29** Example: ISO image mounted as drive E:

## Installation

- 2 Start the installation via **Install Application on Remote Desktop**.

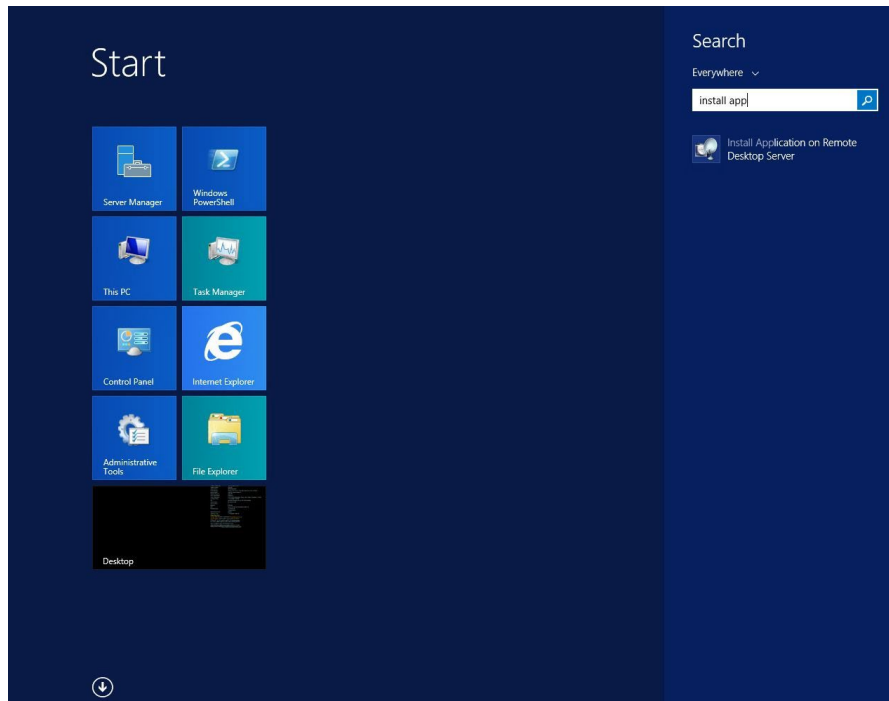


Figure 30 Start screen

- 3 Run the installation program from the mounted ISO image.

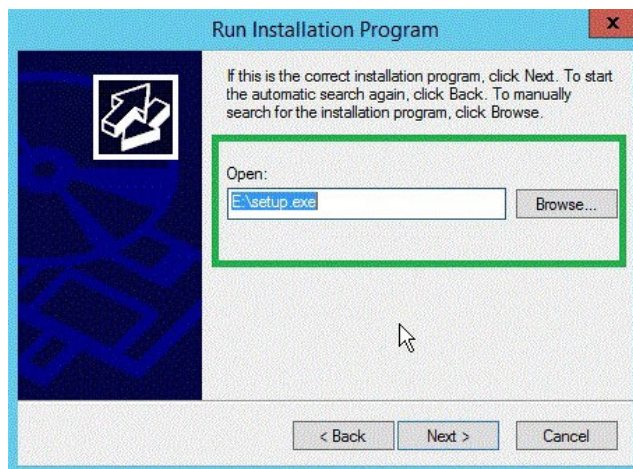


Figure 31 Installation program



## Installation

The NIST installation wizard opens.

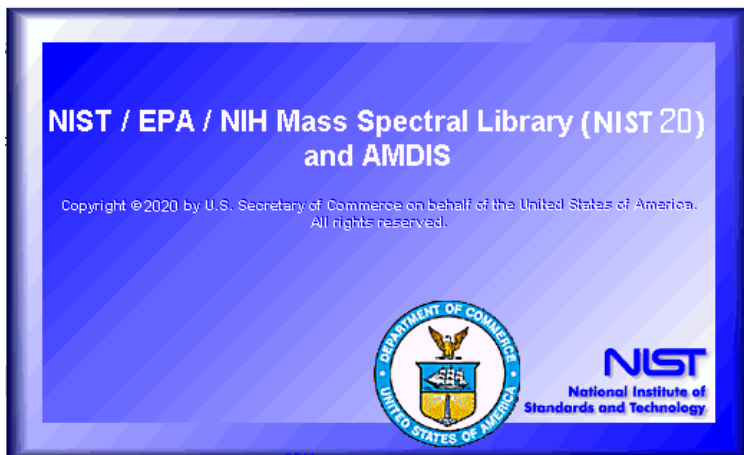


Figure 32 Installation wizard

4 Click **Next**.

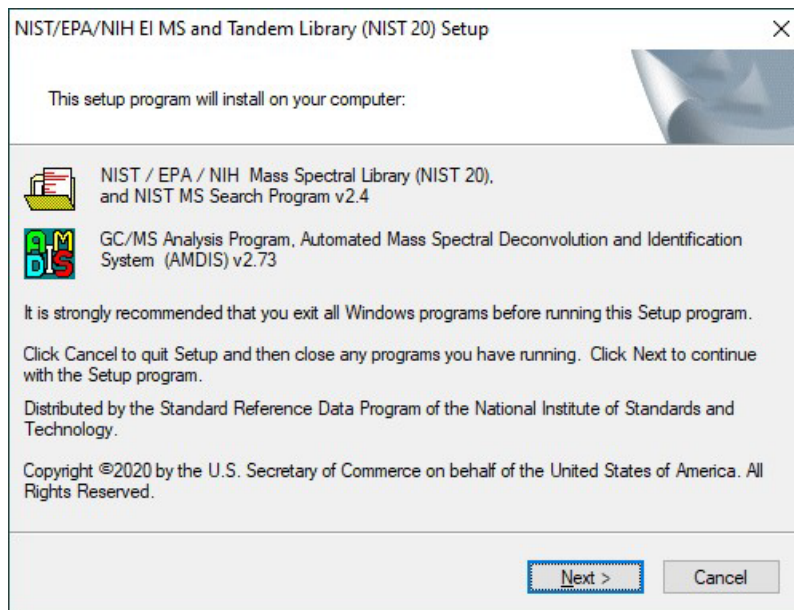


Figure 33 Setup screen

## Installation

- 5 Accept the license.

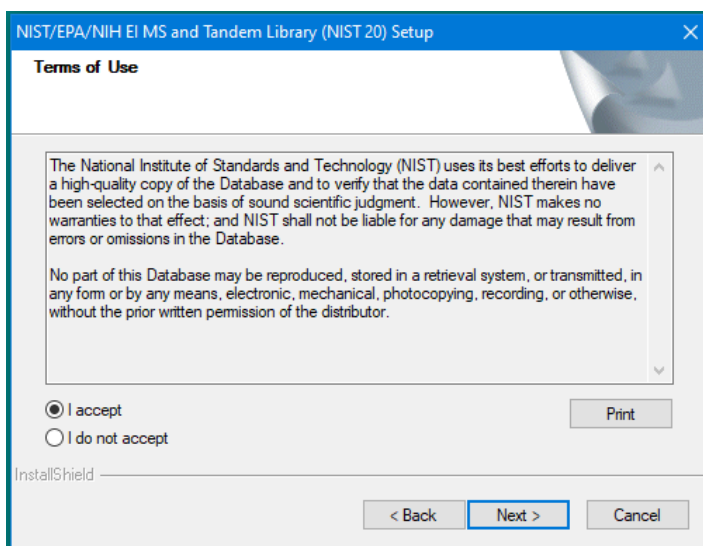


Figure 34 Terms of Use

- 6 From here, the **Typical** setup may be selected, or **Custom** may be chosen in order to save disk space by skipping libraries which are not needed (for example, the MS/MS libraries).

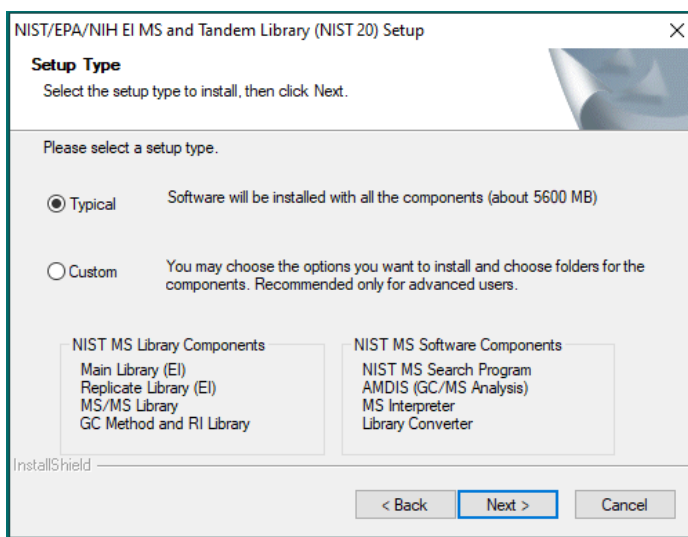


Figure 35 Setup type – Typical

## Installation

Or

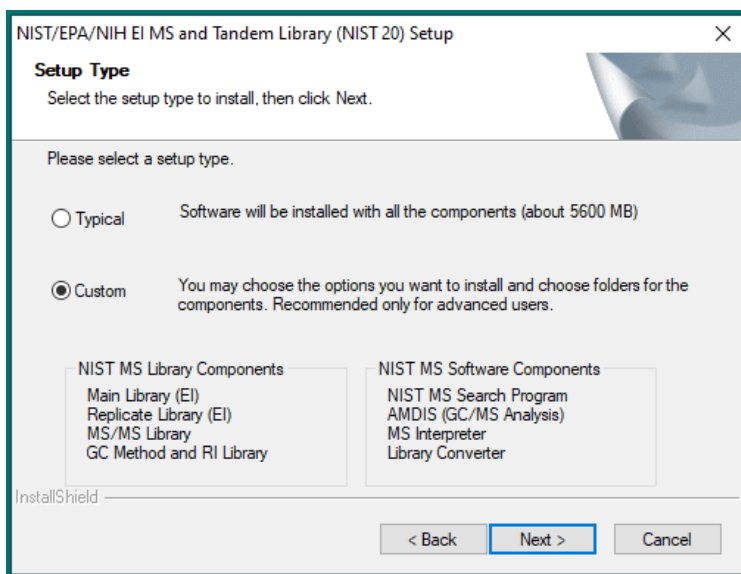


Figure 36 Setup type – Custom

- 7 Specify the folder to install the NIST MS Software (by default it is your local C drive). Make sure the check box has been selected. Click **Next** to continue.

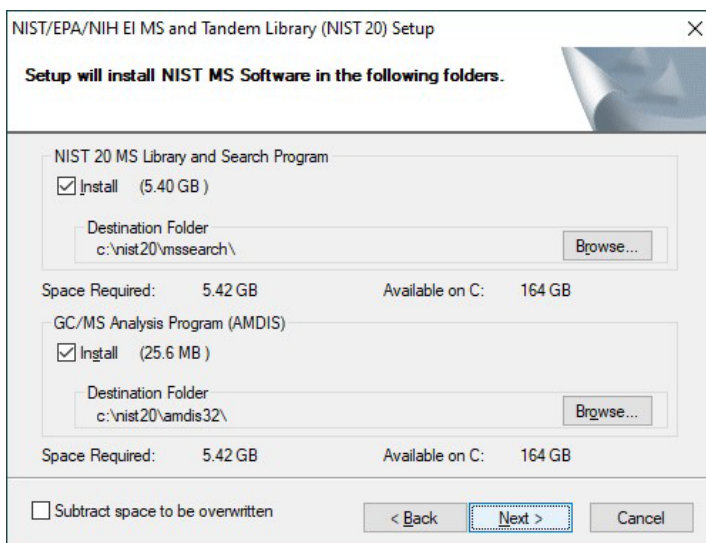
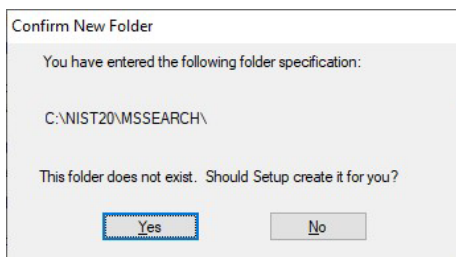


Figure 37 Installation folder screen

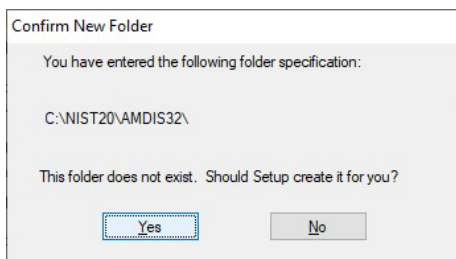
## Installation

- Click **Yes** to confirm the creation of the new folder for the NIST MS Search Program.



**Figure 38** Folder confirmation

- Click **Yes** to confirm the creation of the new folder for the GC/MS Analysis Program (AMDIS).



**Figure 39** Folder confirmation

## Installation

- 10 Select the program folder where the NIST shortcuts will be placed, then click **Next**.

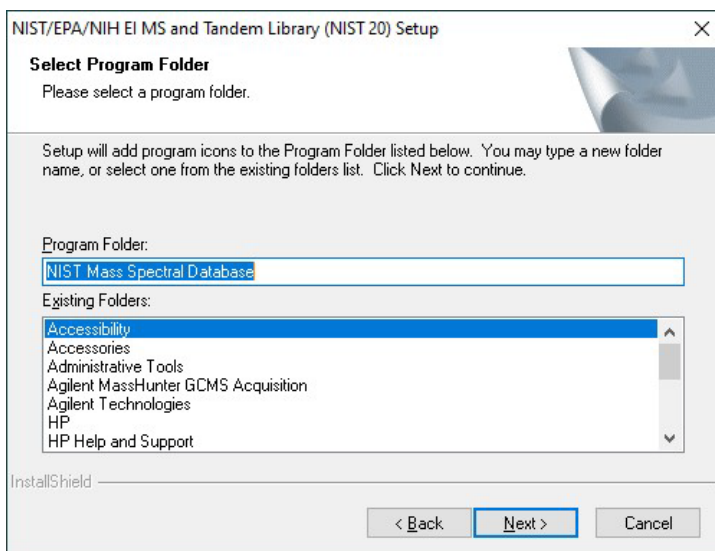


Figure 40 Program folder selection

- 11 Click **Next** to confirm the installation summary.

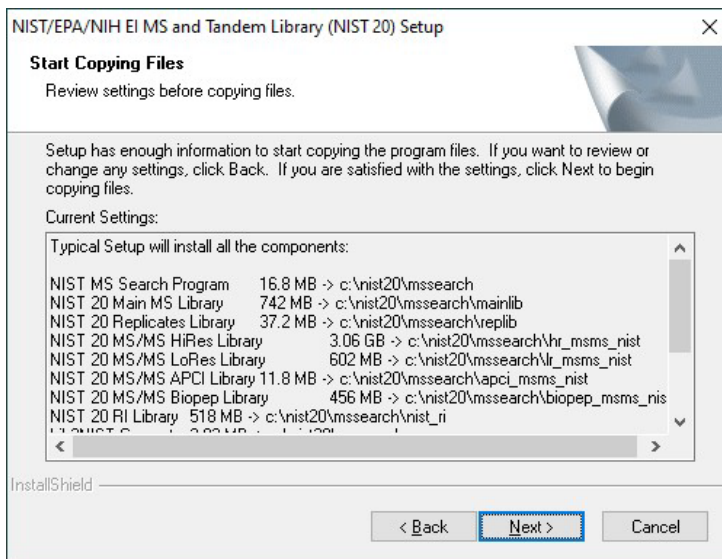
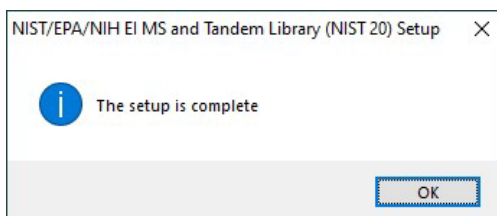


Figure 41 Installation summary

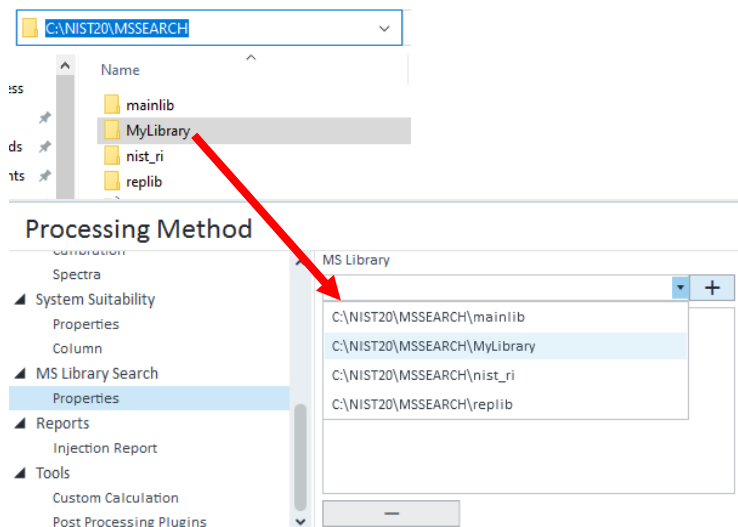
## Installation

- 12 After installation, click **OK** to close the wizard.



**Figure 42** Confirmation window

- 13 To use additional existing user-created or commercial libraries, they must be in NIST library format, and they should be copied to the local NIST library location (**C:\NIST20\MSSEARCH** by default).



**Figure 43** MS library

- 14 Libraries may be converted to NIST format using the Lib2NIST tool which is installed by default when the NIST installer is run. See "[Library Maintenance](#)" on page 56 for more information.
- 15 Publish the application from Citrix/Terminal Server setup.
- 16 From a thin client, access the Citrix/Terminal Server published link.

## Multiple Citrix/Terminal Servers, Shared Libraries

### NOTE

In this configuration, the AICs will need to have NIST MS Search installed locally on each AIC. Libraries may be installed locally on each AIC (as in “[Standalone Workstation](#)” on page 6), or they may link to libraries on a network share as described in “[On a Network Shared Drive](#)” on page 14, in order to enable library searching in processing methods which are executed from data acquisition. It is recommended that libraries and MS Search should be the same version on all AICs and Citrix/Terminal Servers 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.

### NOTE

MS Search and the link to the shared libraries needs to be installed locally on each Citrix/Terminal Server. Repeat this process for each Citrix/Terminal Server.

- 1 First, create and configure the network shared drive.
  - a Share the folder containing the libraries with **Everyone (Full Control)**.

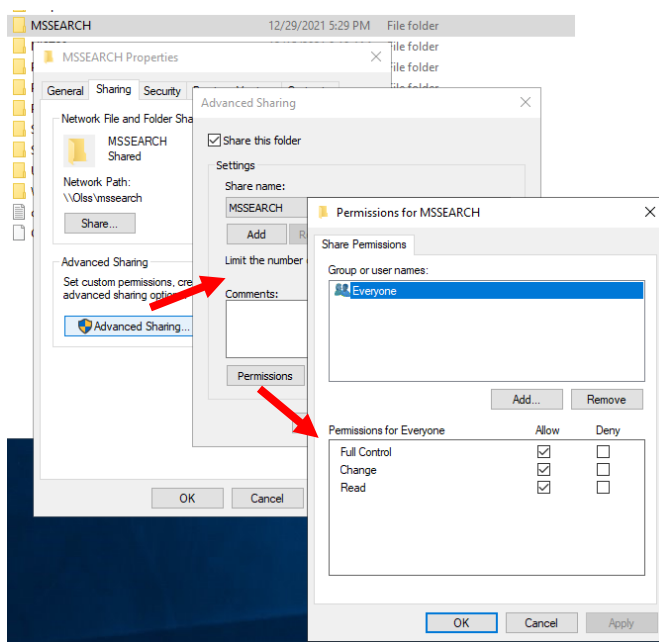


Figure 44 Share permissions settings

## Installation

- b** If it is necessary to limit the ability to modify the libraries to specific users or user groups, this should be done 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, as needed.

### NOTE

Commercial NIST libraries cannot be user edited.

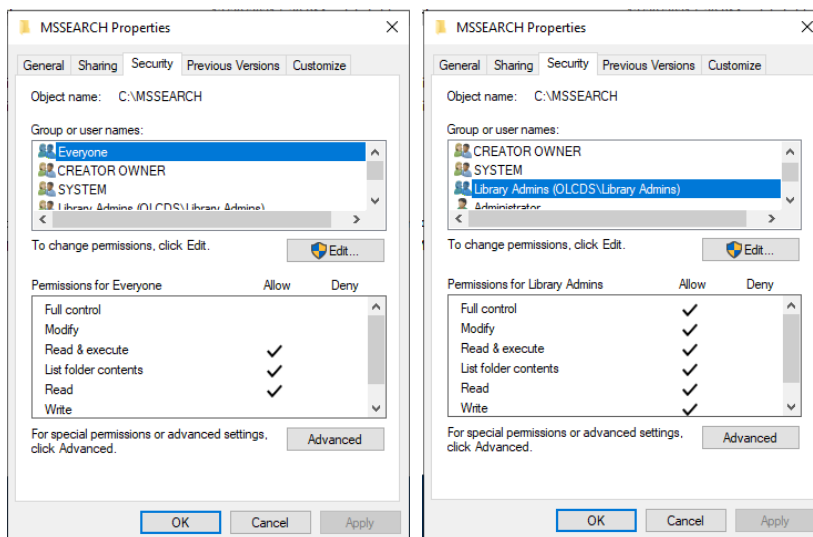


Figure 45 MSSEARCH properties

- c** 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 the Modifying Libraries sections in “[Library Maintenance](#)” on page 56 for more information.

- Copy any existing user-created libraries in NIST format (use the Lib2NIST conversion tool if needed) to the share – see step 2 in “[On a Network Shared Drive](#)”. If libraries exist which need to be converted, but the Lib2NIST tool has not yet been installed, they can be added later.
- NIST’s MS Search program (installed as part of the NIST20 installation) must be installed on every Workstation, Workstation Plus, Client, and AIC which will perform library searching. MS Search does not need to be installed on the server hosting the share, although it can be to allow local use of the libraries on the server.

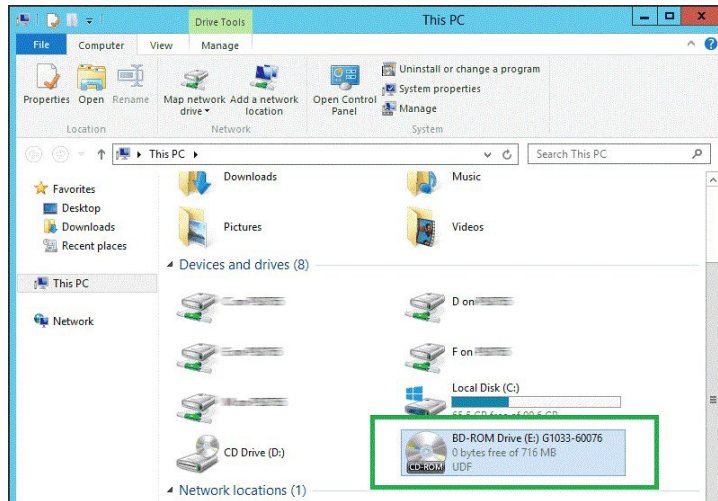


## Installation

### Installation on Citrix/Terminal Servers

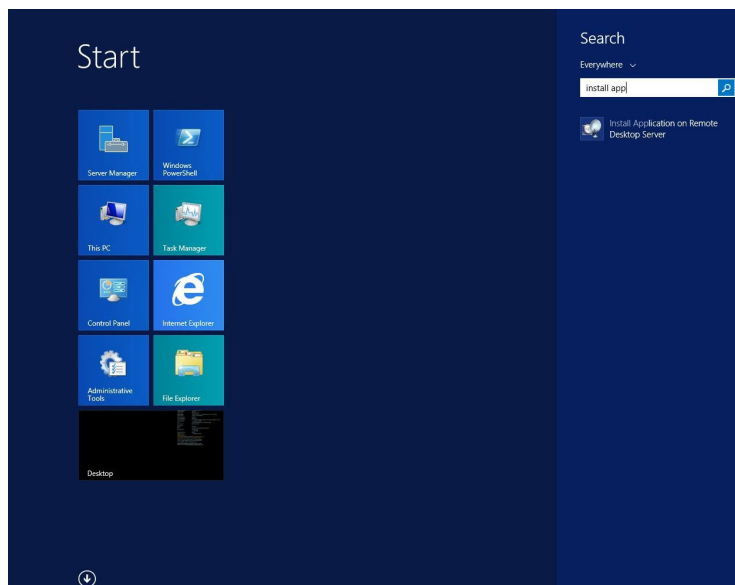
Proceed with the installation of the NIST software on each Citrix/Terminal Server:

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



**Figure 46** Example: ISO image mounted as drive E:

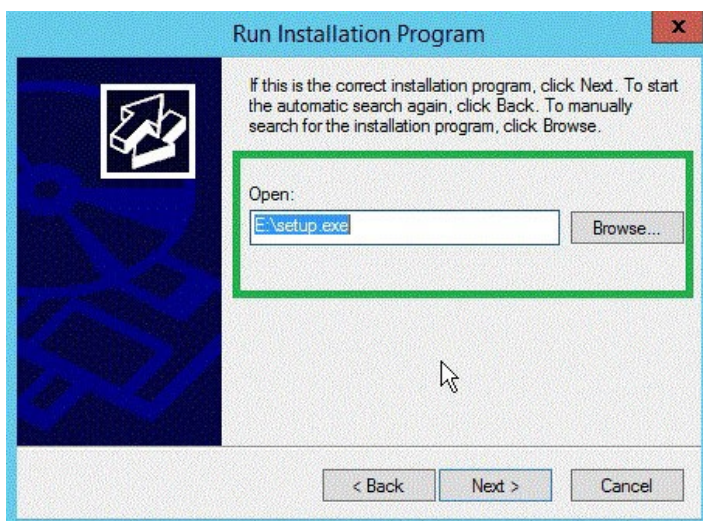
- 2 Start the installation via **Install Application on Remote Desktop**.



**Figure 47** Start screen

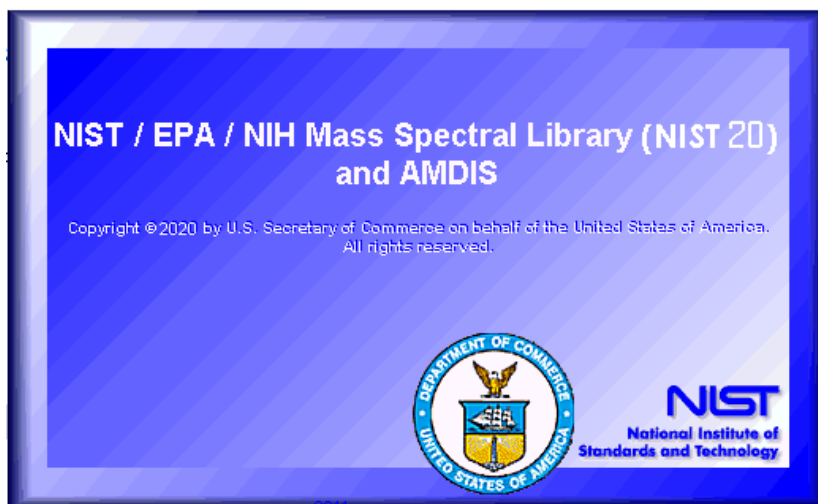
## Installation

- 3 Run the installation program from the mounted ISO image.



**Figure 48** Installation program window

The NIST installation wizard opens.



**Figure 49** Installation wizard

## Installation

### 4 Click **Next**.

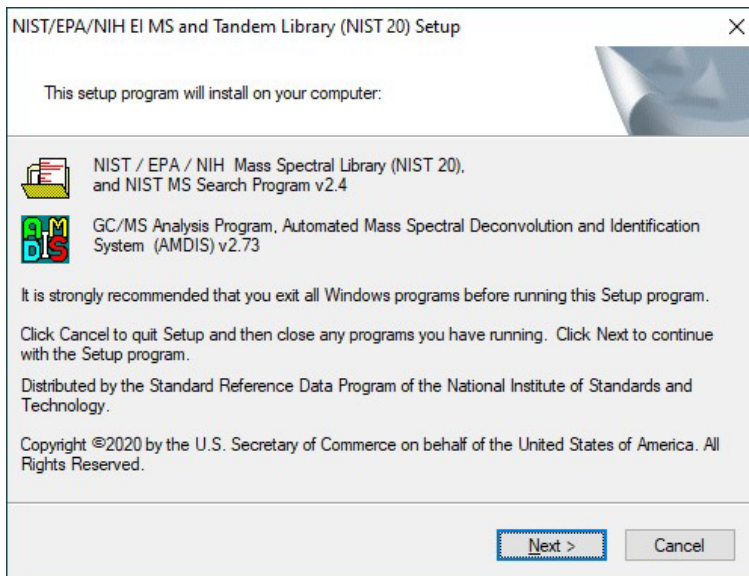


Figure 50 Setup window

### 5 Accept the license.

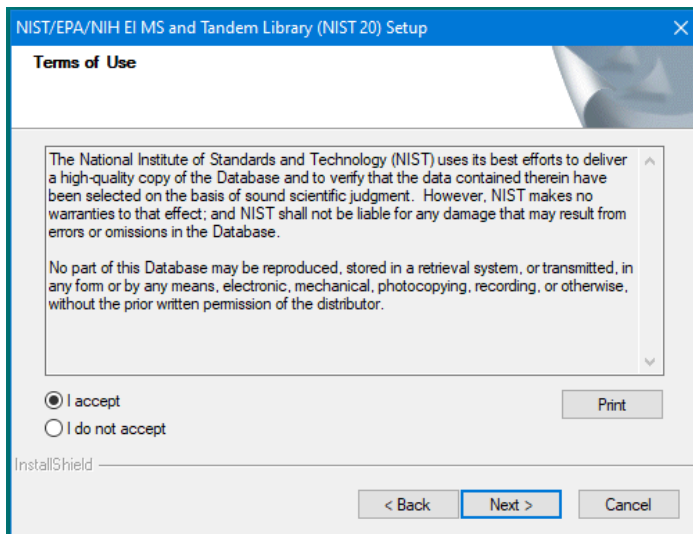


Figure 51 Terms of use

## Installation

- Choose the setup type **Custom**.

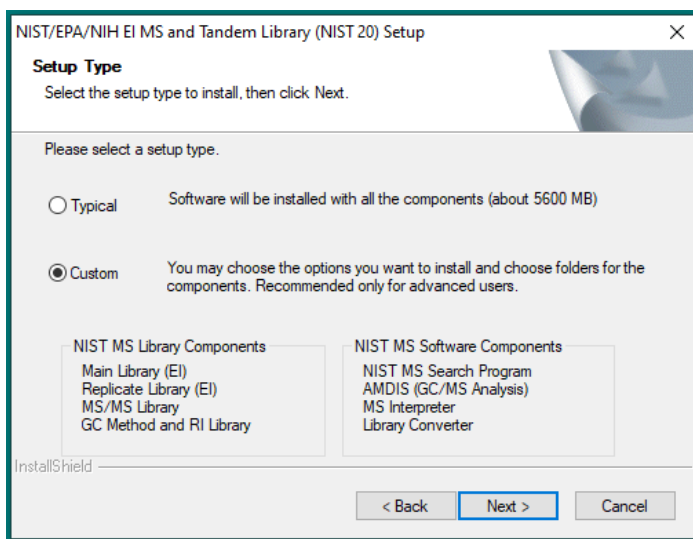


Figure 52 Setup type – Custom

- The NIST MS/MS libraries may be deselected in order to save disk space, if desired.

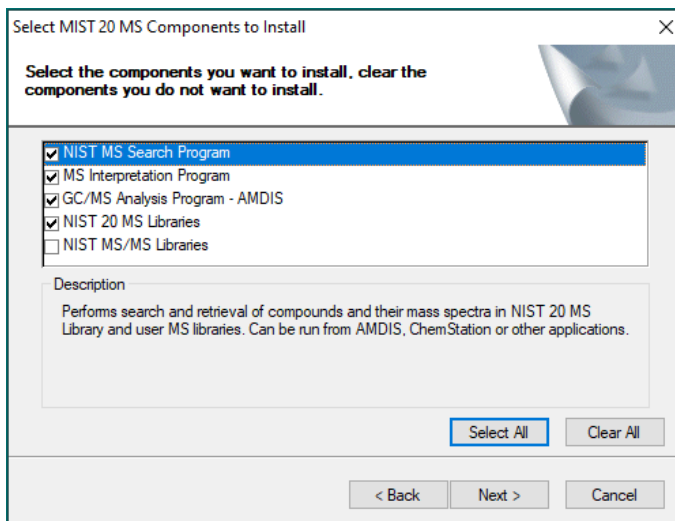
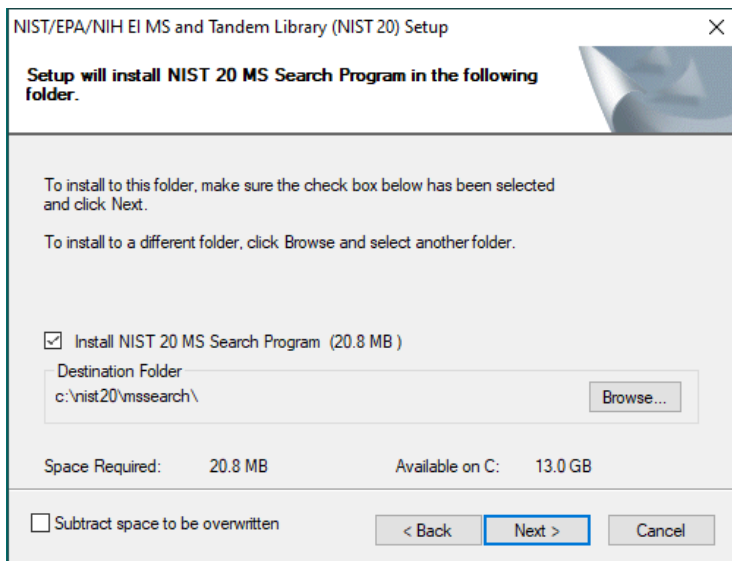


Figure 53 Component selection window

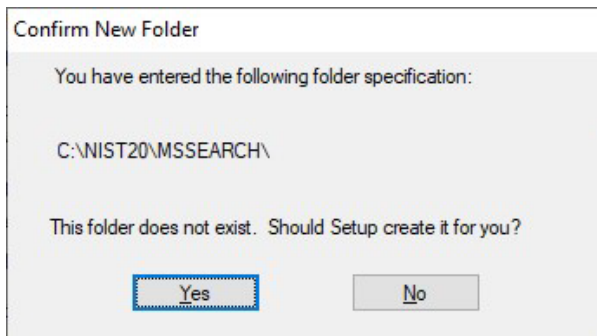
## Installation

- Specify the folder to install the NIST MS Search software (by default it is your local C drive – this must be installed on a local drive). Make sure the check box has been selected. Click **Next** to continue.



**Figure 54** Installation folder selection

- Click **Yes** to confirm the creation of the new folder for the NIST MS Search Program.



**Figure 55** Confirmation window

## Installation

10 For the *first installation* of the NIST libraries ONLY:

For subsequent installations, skip to step 11.

- a Browse to or type the location of the network share as the installation path of the NIST 20 Main Library and all other NIST libraries which are to be installed.

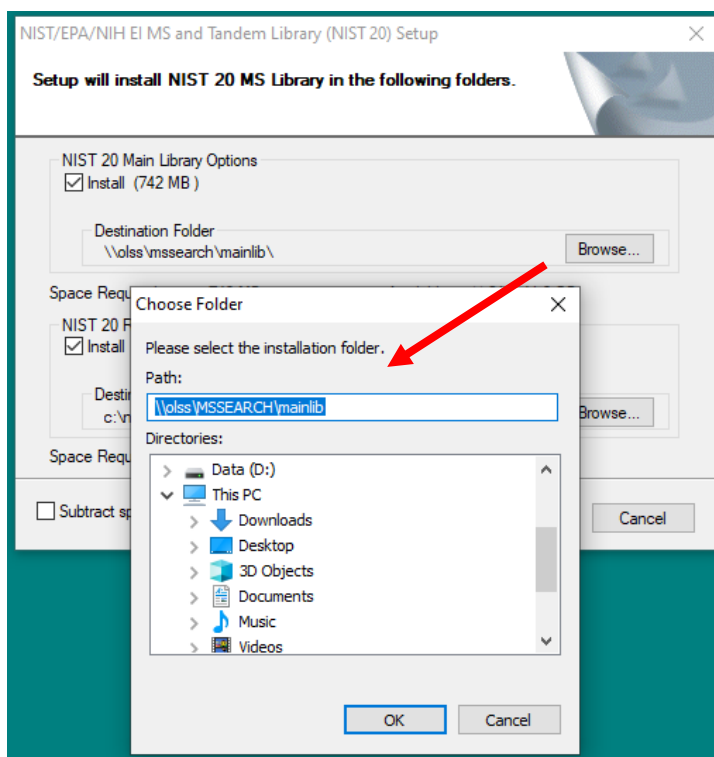
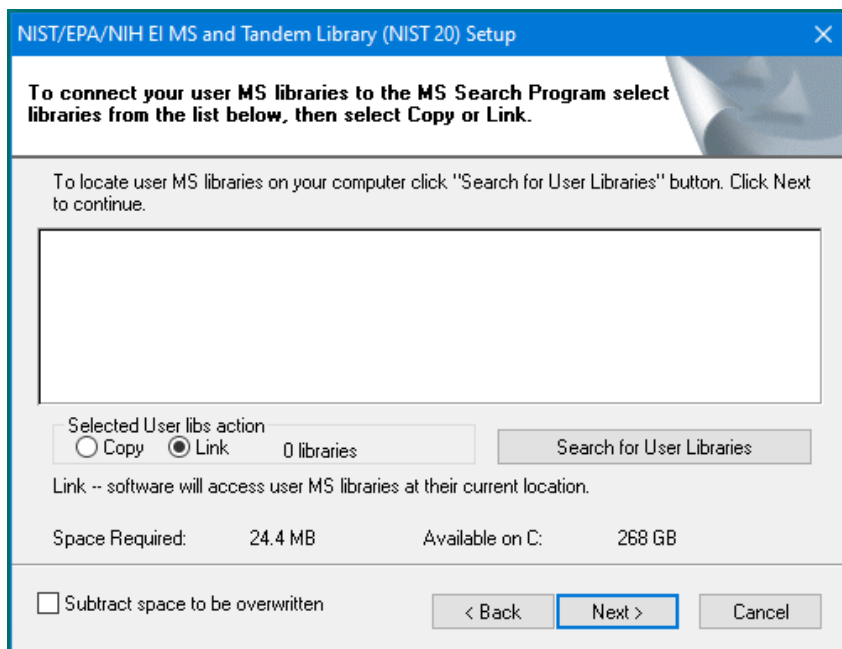


Figure 56 Folder selection

## Installation

- b** If the installer locates the other libraries on the network share, you may link (not copy) to them – but if they are not found, this can be done later.



**Figure 57** MS libraries connections

## Installation

- c The MS Interpretation Program and AMDIS may be installed if desired; they should be installed *locally*.

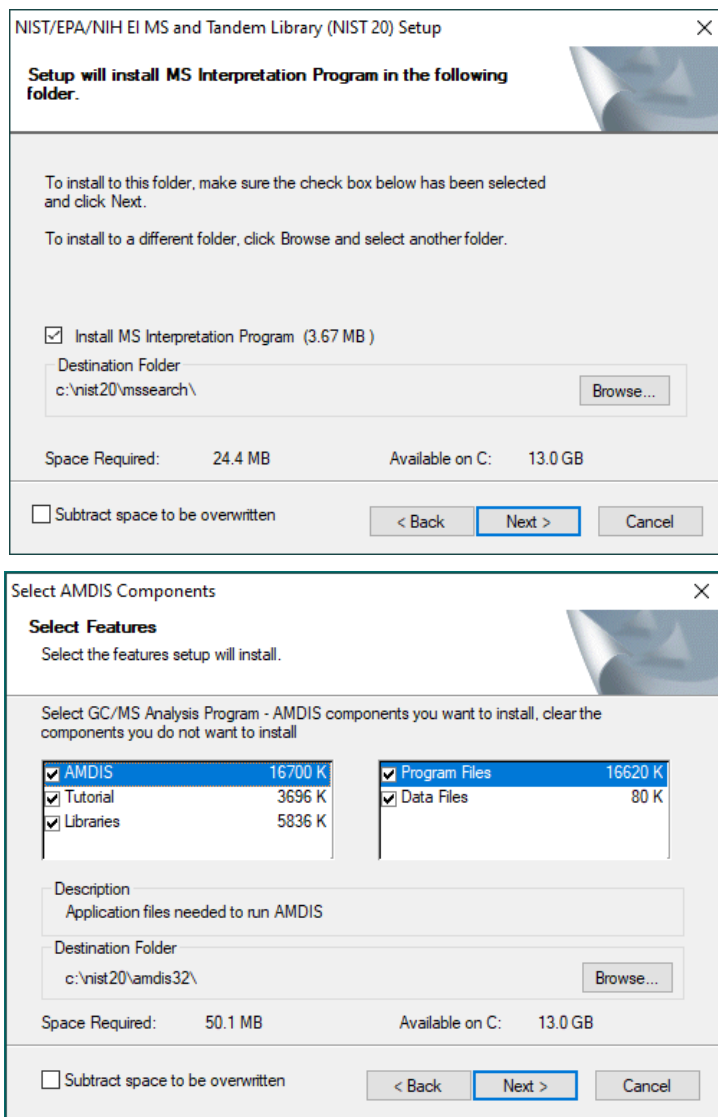


Figure 58 Feature selection



## Installation

- d Select a program folder for program icons.

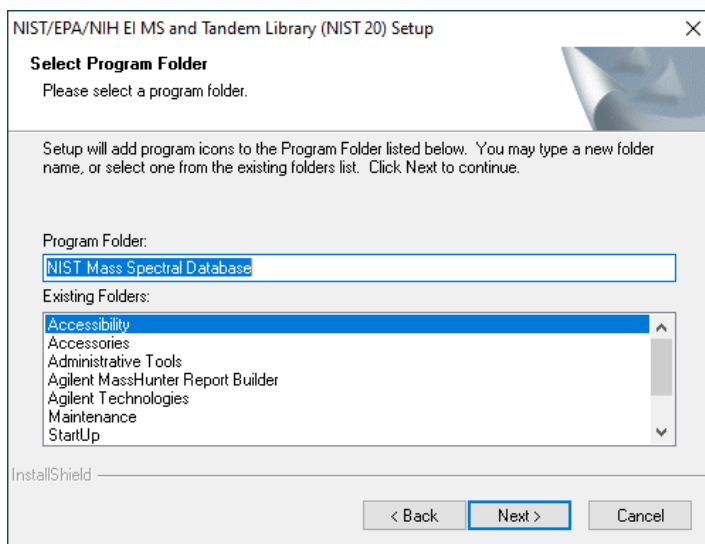


Figure 59 Program folder selection

- e The installation settings should be as follows:

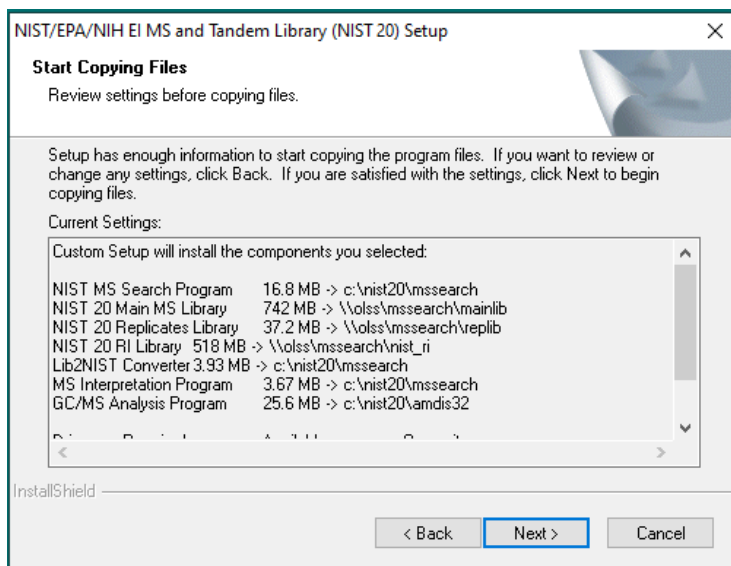
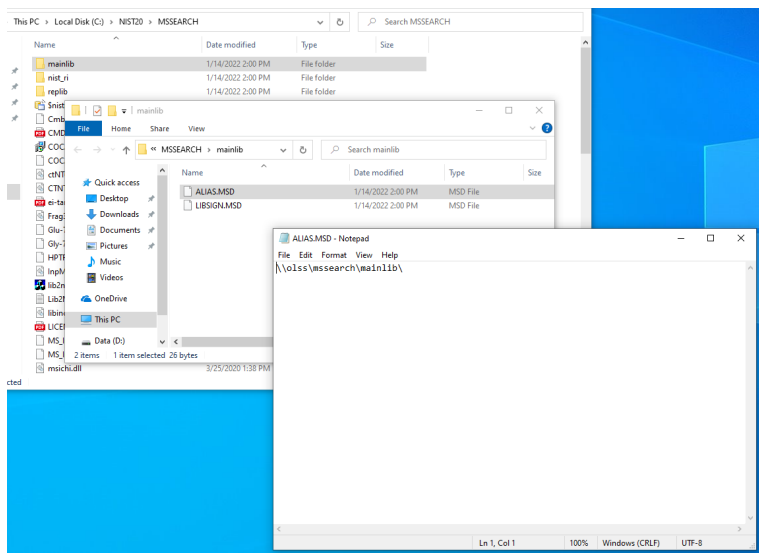


Figure 60 Installation settings

## Installation

- f Complete the installer. NIST MS Search is now installed. The NIST libraries selected have installed on the network share drive. They have also installed links to the shared libraries on the local machine:



**Figure 61** NIST libraries

- g This link, via the ALIAS.MSD file is how both CDS Data Analysis and MS Search find the libraries on the network share. It may be edited from a plain text editor like Notepad.

## Installation

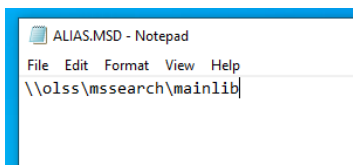
### NOTE

On the first installation of the NIST libraries, when the link files are created, the installer will create the network path with a final '\' at the end. This '\' must be removed for CDS to read the name of the library correctly. In the above example, the file will need to be edited so the path reads: **\\olss\mssearch\mainlib**. If this is not done, the library name will be empty in CDS data analysis and on generated reports:

#### MS Lib Search Results

Compound Name	Match Score	Reverse Match Score	Probability %	Library Name	CAS #	NIST #
Naphthalene-D8	890	892	91.99		1146-65-2	

ALIAS.MSD reads \\olss\mssearch\mainlib\



#### MS Lib Search Results

Compound Name	Match Score	Reverse Match Score	Probability %	Library Name	CAS #	NIST #
Naphthalene-D8	890	892	91.99	mainlib	1146-65-2	

ALIAS.MSD reads \\olss\mssearch\mainlib

- h All **ALIAS.MSD** files generated by the installer should be updated to remove the final '\' and saved. Copies of all the linking folders – containing **ALIAS.MSD** and **LIBSIGN.MSD** – should also be placed in a location which can be accessed during all future NIST library installations.

## Installation

- 11 For all *additional* installations of the NIST libraries:
- Once the first connection to the shared libraries has been created, all additional Citrix/Terminal Servers should be installed as follows.
  - Run the NIST installer as above. Choose the **Custom** installation.

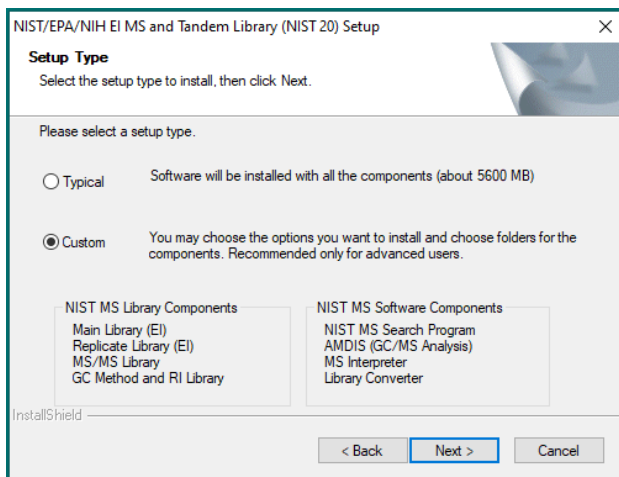


Figure 62 Setup Type – Custom

- c Deselect the NIST libraries so they are not installed.

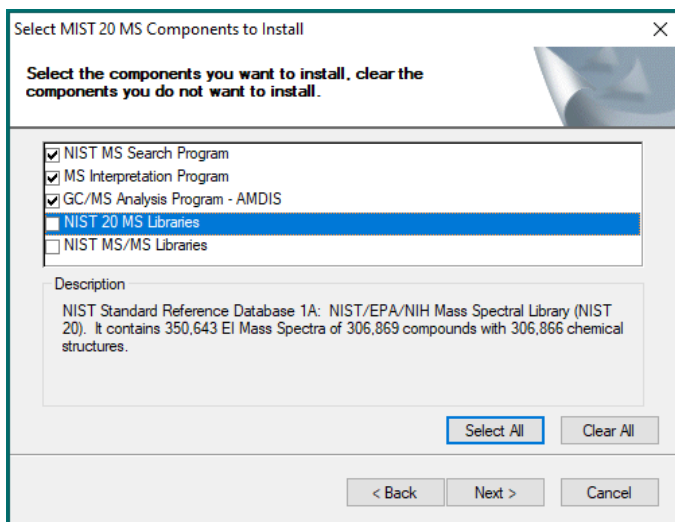


Figure 63 Component selection screen

## Installation

- d Install the NIST MS Search program locally (default is on the local C: drive).
- e The installer will pop up a warning about not finding the main and replicates libraries – select **Yes** to continue without them.

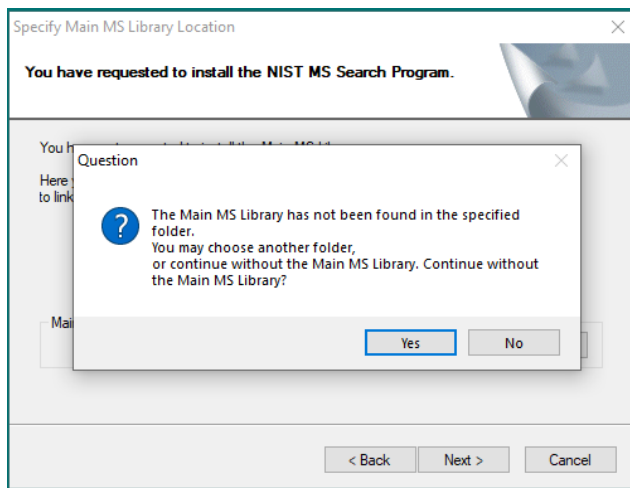


Figure 64 Warning pop-up

- f Unless locally installed libraries are intended to be used along with libraries on a network share, do not select any libraries to link or copy on the next installer screen.

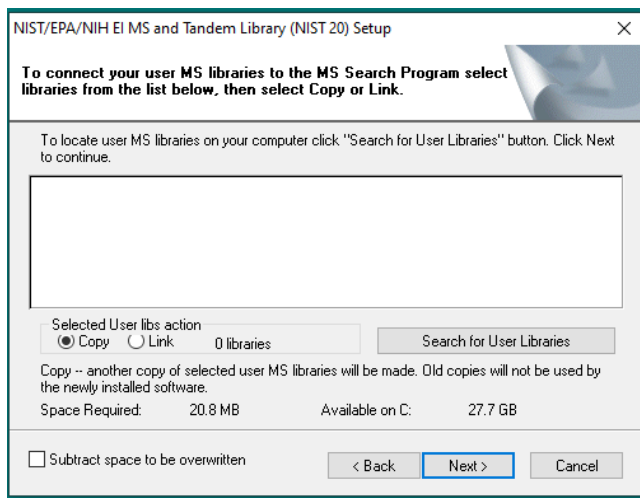
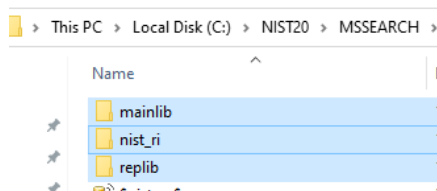


Figure 65 Library selection screen

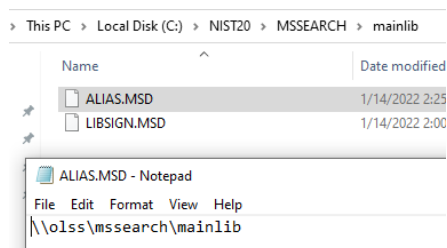
## Installation

- g** Click through the rest of the prompts and complete the installer.
- h** Navigate to the network location where the copies of the library link folders are saved, from step 10h above. Copy these folders into the **C:\NIST20\MSSEARCH** folder (or the local folder where MS Search was installed).



**Figure 66** Library link folders

- i** These folders contain the **ALIAS.MSD** file, which points to the network location of the library.



**Figure 67** ALIAS.MSD

## Installation

- 12 To use additional existing user-created or commercial libraries, they must be in NIST library format, and they should be copied to the shared NIST library location. See “[Library Maintenance](#)” on page 56 for details.
- 13 Ensure permissions for the additional library on the network share are set as in step 1a.
- 14 Make a copy of one of the “shortcut” folders created above, containing **ALIAS.MSD** and **LIBSIGN.MSD**. Rename this copied folder with the name of the additional library. Modify **ALIAS.MSD** to reflect the path of the additional library. Be sure not to include a final ‘\’. Place this copied folder on each Citrix/Terminal Server which will need access to the library.

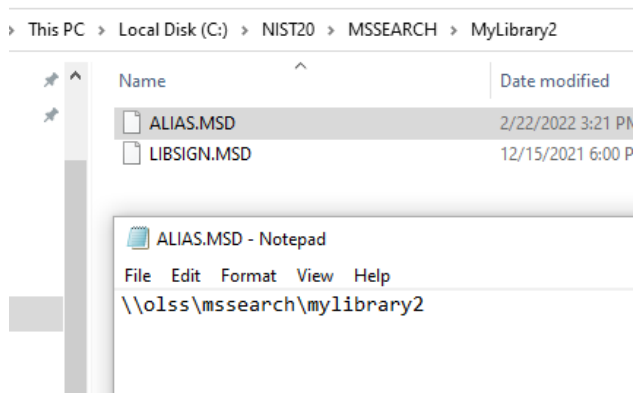


Figure 68 ALIAS.MSD

- 15 Publish the application from Citrix/Terminal Server setup.
- 16 From a thin client, access the Citrix/Terminal Server published link.

## 5 Library Maintenance

### To 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.

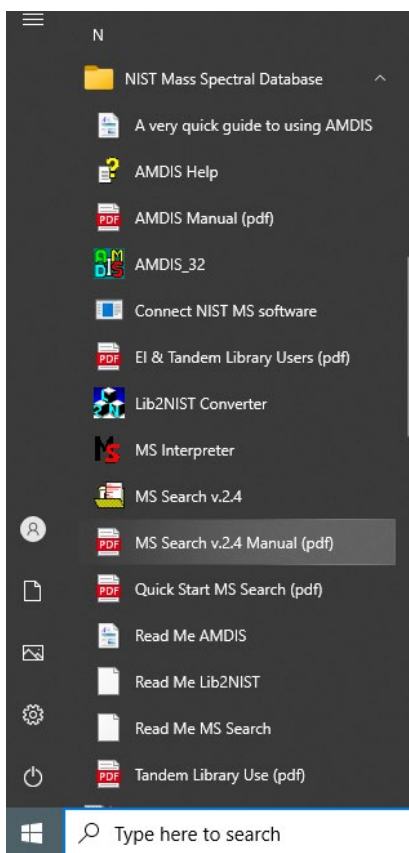
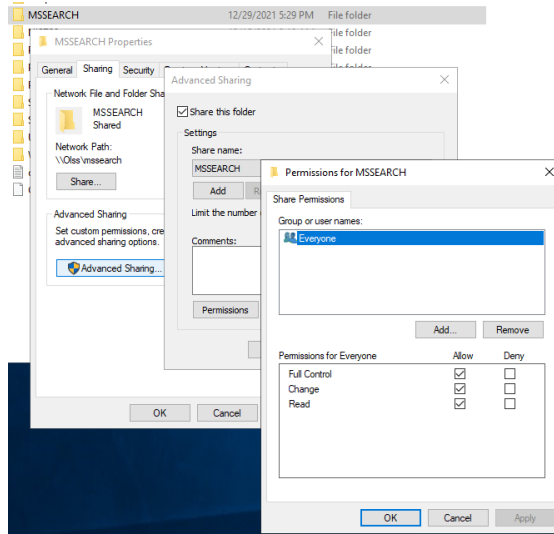


Figure 69 MS Search manual



## To Modify a Library in a Shared Configuration

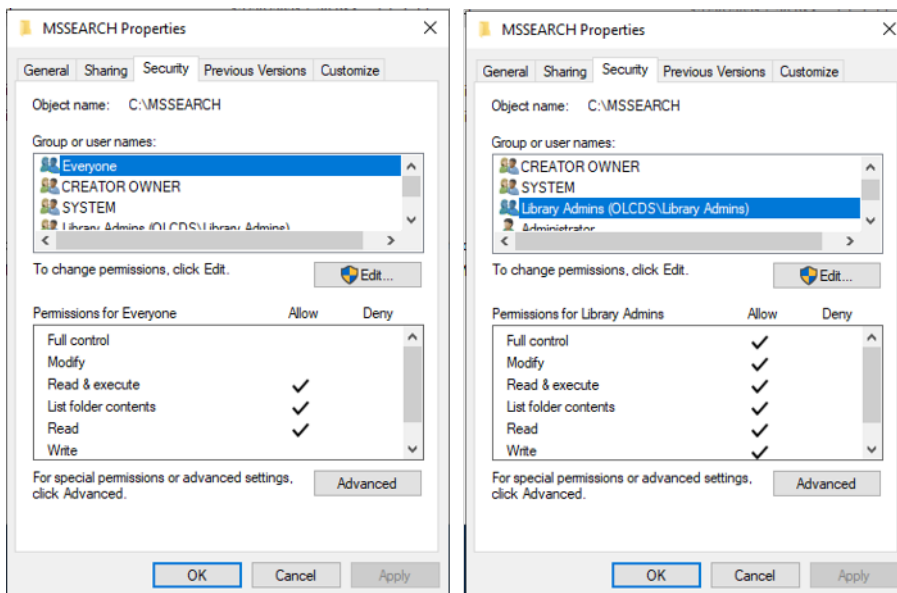
- The NIST commercial libraries are not user editable.
- The network share on which the library resides must be set to full control for everyone.



**Figure 70** Permission settings

## Library Maintenance

- 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 below example, only members of the Library Admins group can modify the libraries.



**Figure 71** 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.

### To 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 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 and LIBSIGN.MSD, modify **ALIAS.MSD** to point to the new library, and copy the link folder to each Client, Workstation, Workstation Plus, or AIC which should have access.

### To Convert an Existing Library to NIST Format

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

## Library Maintenance

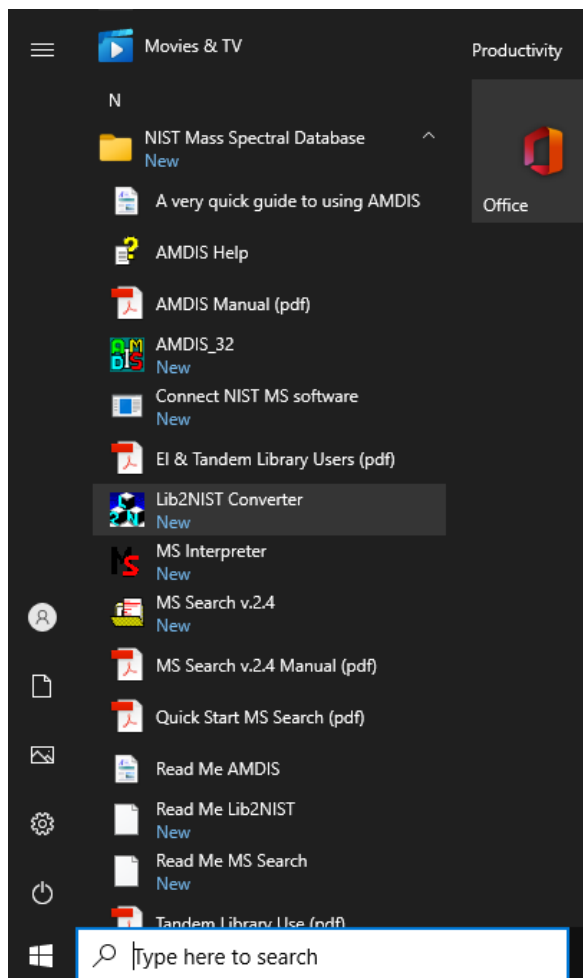
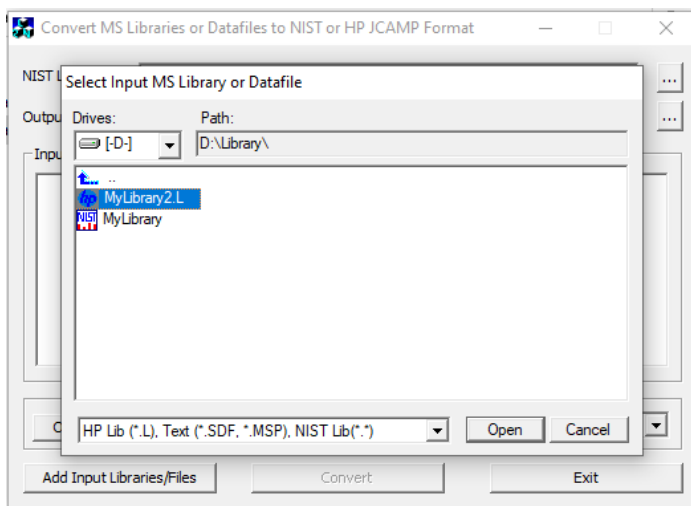


Figure 72 Lib2NIST Converter

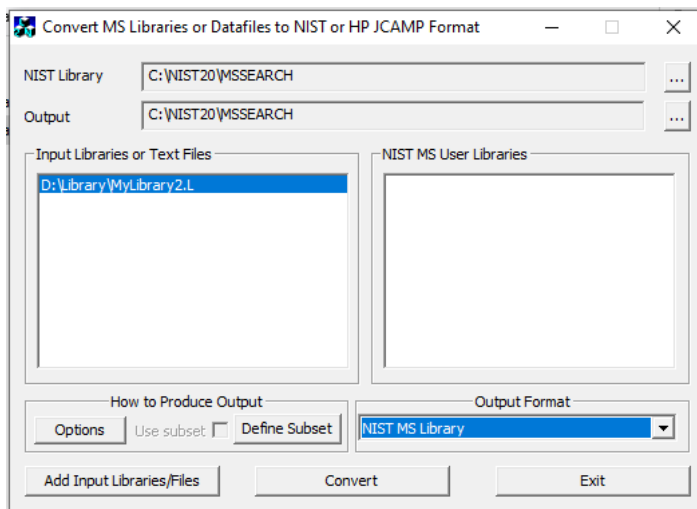
## Library Maintenance

- 1 Launch the Lib2NIST tool. Navigate to and select the library to be converted.



**Figure 73** Library selection

- 2 Select the NIST output format and the output folder.



**Figure 74** Output format and folder

- 3 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 finds the newly converted libraries.

## 6 Use of MS Libraries Within OpenLab CDS

In order 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.

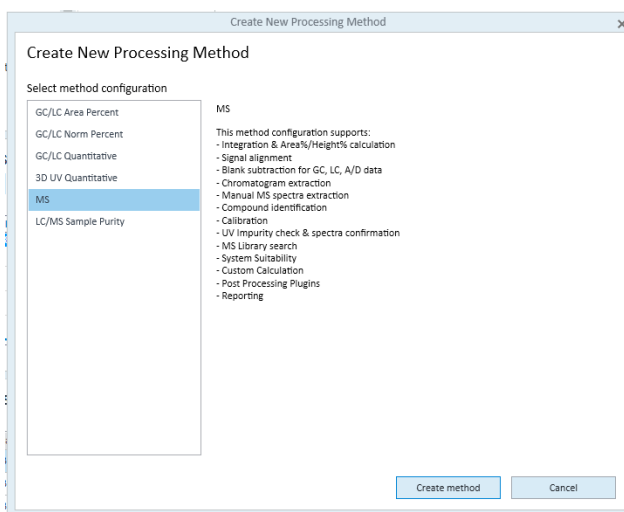


Figure 75 Processing method creation screen

- 3 Under **MS Library Search > Properties**, enter the common shared library paths, and click the + icon to add the libraries. For details, search for “Use the MS library search” in OpenLab Help and Learning.

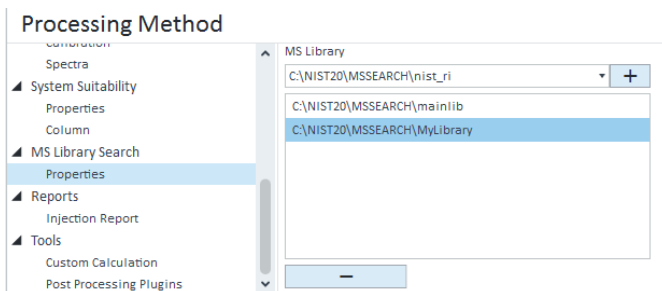


Figure 76 MS library properties

## Use of MS Libraries Within OpenLab CDS

- 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.

## 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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