

Compound Discoverer 3.2 Installation Instructions

Thermo Compound Discoverer™ is a licensed application. After you install the application, you can use it for up to 60 days without activating the software license.

After you order the Compound Discoverer 3.2 application, you will receive a software media kit that includes a key-shaped USB flash drive with the installation executable. In addition, you will receive an email from Thermo MS Licensing providing you with the information that you need to activate the software license.

If you are upgrading the software from a previous version of the application, you can find the software installer and a license on the LSMS Software Download and Licensing Portal.

IMPORTANT Read the following:

- The installation requires the Windows 7 SP1 64-bit or Windows 10 64-bit operating system.
- The Compound Discoverer 3.2 licensing process requires an Internet connection to validate the software license. You can install the application on a computer without Internet access and complete the activation process on a computer with Internet access.
- The Compound Discoverer application is supported for US-English Only locale.

Note The following versions of the Compound Discoverer application can coexist on the same computer: 1.0, 2.0, 2.1, 3.0, 3.1, and 3.2

The installation executable includes three installers. The Thermo Compound Discoverer 3.2 installer installs the Compound Discoverer application. The Thermo mzCloud™ Offline Library installer installs four mzVault libraries that are July 2020 snapshots of the online mzCloud mass spectral database, and the Thermo mzVault installer installs the mzVault application.

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❖ **To install the Compound Discoverer application**

1. Do one of the following:
 - a. Insert the Compound Discoverer USB flash drive into a USB port on your computer.
 - b. Open Windows Explorer and select the USB drive to view its contents.
 - c. Locate the executable: XStart_Compound Discoverer.exe.

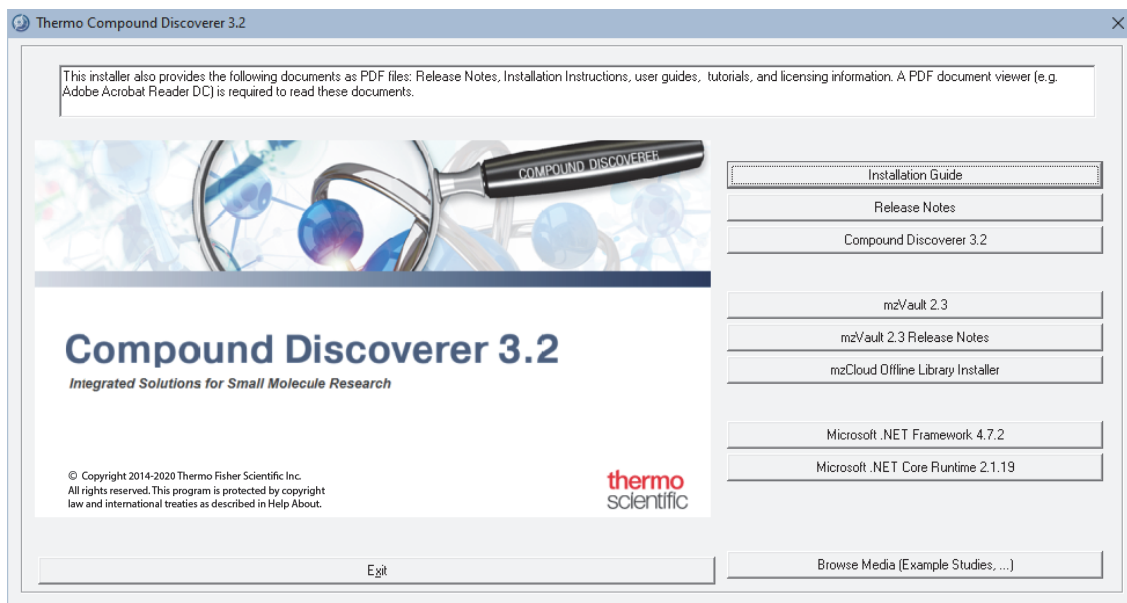
Installing the Compound Discoverer application

—or—

- a. Go to the following website address: <https://thermo.flexnetoperations.com>.
 - b. Log in to your account. If you do not have an account, click **Register** and create one.
 - c. On the left side of the Life Sciences Mass Spectrometry Software Download and Licensing Portal, click **Product List** under Software and Services.
 - d. On the Product List page, click the **Demo** hyperlink.
 - e. On the Product Information page, click the **Compound Discoverer 3.2** hyperlink.
 - f. On the Product Download page, in the File Name column, click the down arrow to the left of Compound Discoverer 3.2.zip, click **Save As**, and then save the compressed zipped folder to your computer.
 - g. Extract the contents of the zipped folder, and locate the executable: XStart_Compound Discoverer.exe.
2. Double-click **XStart_Compound Discoverer.exe**.

The installation wizard starts.

Figure 1. Compound Discoverer installation wizard



3. Click **Compound Discoverer 3.2**.
4. When the installer opens, click **Next** and follow the instructions.

The Minimum Product Requirements screen appears with a product requirements scan summary. If the computer meets the system requirements, the summary states the following:

All the system minimum requirements checks passed.

5. At the Installation Qualification prompt, click **Yes** if you want to view the Installation Qualification report. Otherwise, click **No**.
6. When the installation is complete, select whether you want the installer to restart your computer, and then click **Finish**.

Installing the mzCloud Offline libraries

❖ To install the mzCloud Offline libraries

1. If the installer restarted your computer, double-click **XStart_Compound Discoverer.exe** to restart the installer.
2. Click **mzCloud Offline Library Installer** to install the mzCloud Offline libraries.
3. When the installation is complete, restart your computer if you did not restart it after installing the Compound Discoverer application.

To create mass spectral libraries from your own data acquired with a high-resolution accurate-mass (HRAM) Thermo Scientific mass spectrometer, install the mzVault 2.3 application. The Compound Discover installer includes an installer for the mzVault application.

❖ To install the mzVault application

1. If the Compound Discoverer installer is not open, open it as follows:
 - a. Locate the XStart_Compound Discoverer executable.

You can find the executable on the USB drive provided in the Compound Discoverer application media or in the zip folder that you downloaded from the product download web site.

- b. Double-click **XStart_Compound Discoverer.exe**.

2. Click **mzVault 2.3**.

The Thermo mzVault Installshield Wizard opens.

Note If you have an earlier version of the application, follow the instructions to remove it, and then restart the mzVault 2.3 installer.

If your computer meets the minimum requirements, the Next button becomes available.

3. Click **Next** to continue.
4. When the installation is complete, click **Finish**.

To process GC EI Orbitrap data with the Compound Discoverer application, Thermo Fisher Scientific recommends that you install at least one NIST MS Search formatted EI MS library on the processing computer. The Compound Discoverer installer does not include any NIST formatted libraries. You can purchase them from third-party vendors and install them separately within the NIST MS Search folder.

To activate your Compound Discoverer 3.2 software license, see these topics as necessary:

1. [Entering the product ID and the activation Code](#)
2. Follow one of these topics:
 - [Activating the license on an online computer](#)
 - [Activating the license on an offline computer](#)

To activate your Compound Discoverer 3.2 license, you must know the product ID (XCALI-XXXXXX) and the activation code. Within one week of ordering the software, you should receive an email from Thermo MS Licensing with the subject line “Your Order Is Ready.” This email contains the product ID and activation code information.

Installing the mzVault 2.3 application

NIST libraries for GC EI Orbitrap data

Activating the software license

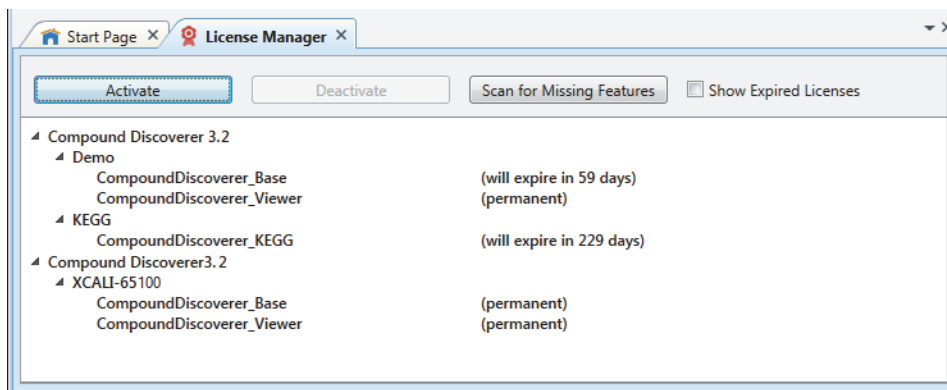
Entering the product ID and the activation Code

❖ **To enter the licensing information**

1. From the application menu bar, choose **Help > License Manager**.

The License Manager opens as a tabbed document in the application window.

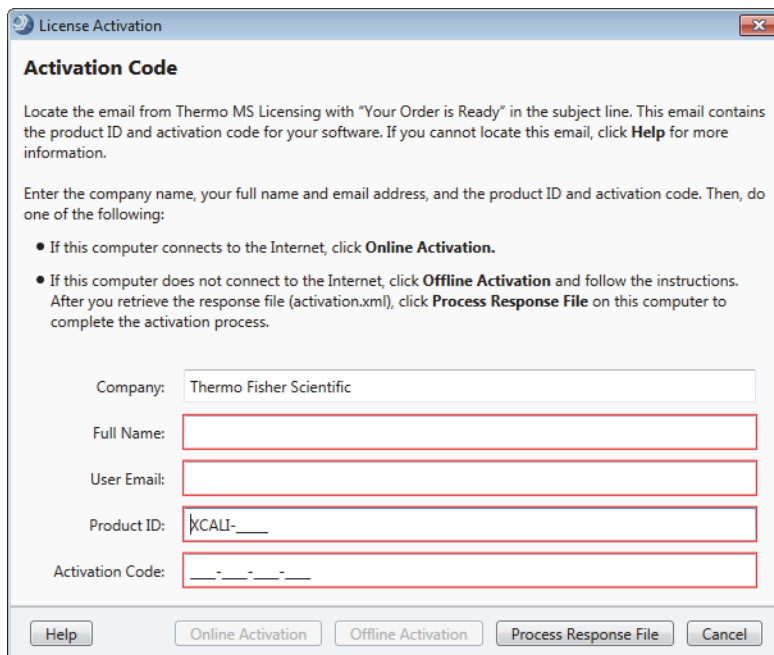
Figure 2. License Manager page



2. On the License Manager page, click **Activate**.

The License Activation dialog box opens to the Activation Code view.

Figure 3. License Activation dialog box opened to the Activation Code view



3. If you have not already received your activation code, do the following:
 - a. Check your Junk Email folder.
 - b. If the email is not in your Junk Email folder, log in to your account at the following URL. In the left navigation pane, under Software & Services, click **Order History**. Then, in the list of ordered products, click the order number.

<https://thermo.flexnetoperations.com>

- c. If you cannot find your account, send an email message to Licensing at ThermoMSLicensing@thermofisher.com.

Provide the following information in the body of the message:

- Software application: Compound Discoverer
- Sales order number or purchase order number: _____
- End user name: _____
- End user email: _____

4. In the License Activation dialog box (Figure 3), enter the following:

- Your company name
- Your full name
- Your contact email address
- The product ID for the Compound Discoverer 3.2 application.

There are five possible product IDs. Four of the product IDs are for software upgrades (see Table 1).

- The activation code. You can type or paste the activation code.

Table 1. Product IDs for the Compound Discoverer 3.2 software

Material Order No.	Product ID	Description
OPTON-31055	XCALI-65100	SW, Compound Discoverer 3.2 (single license)
OPTON-31056	XCALI-65100	SW, Compound Discoverer 3.2 (2–5 licenses)
OPTON-31057	XCALI-65100	SW, Compound Discoverer 3.2 (6–10) licenses
OPTON-31058	XCALI-65101	SW, Compound Discoverer 3.2 upgrade from MetWorks (MW) or Mass Frontier (MF)
OPTON-31059	XCALI-65102	SW, Compound Discoverer 3.2 upgrade from Sieve
OPTON-31060	XCALI-65103	SW, Compound Discoverer (CD) 3.2 upgrade from CD 1.0, CD 2.0, CD 2.1
OPTON-31061	XCALI-65104	SW, Compound Discoverer 3.2 upgrade from Compound Discoverer 3.1
OPTON-31062	XCALI-65105	SW, Compound Discoverer 3.2 and Mass Frontier 8.0 SR1 with Curator
OPTON-31063	XCALI-65106	SW, Compound Discoverer 3.2 and Mass Frontier 8.0 SR1 with Curator (2 or more licenses)

5. Depending on whether your processing computer is connected to the Internet, continue with one of these topics:

- [Activating the license on an online computer](#)
- [Activating the license on an offline computer](#)

Activating the license on an online computer

Follow these instructions if your processing computer has an Internet connection.

❖ To activate the software license on an online computer

1. If you have not already entered the licensing information, enter it in the Activation Code view of the License Activation dialog box.
2. Click **Online Activation** to process the activation code.
3. At the confirmation prompt, click **OK**.
4. At the “new features” prompt, click **OK**.

This completes the online license activation process.

Activating the license on an offline computer

Follow these instructions if your processing computer is not connected to the Internet.

Note Activating the license on an offline computer is a three-step process that requires access to an online computer.

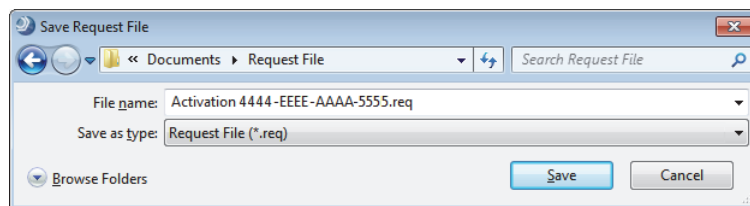
1. Create an activation request file (Activation-*Activation Code*.req) on the offline computer.
2. Transfer the activation request file to an online computer where you upload it to the licensing portal to obtain a response file (activation.xml).
3. Transfer the response file (activation.xml) to the offline computer, and then process it by clicking Process Response File in the License Activation dialog box.

❖ To activate the software license on an offline computer

1. If you have not already entered the licensing information in the Activation Code view of the License Activation dialog box, enter it now.
2. In the License Activation dialog box, click **Offline Activation**.

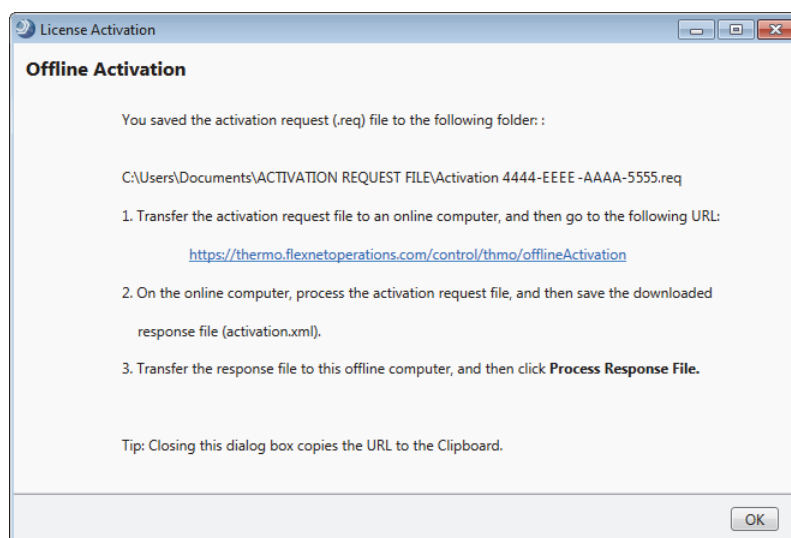
The Save Activation Request File dialog box opens.

3. Save the activation request file (Activation-*Activation Code*.req).



The Offline Activation instructions appear.

Figure 4. Offline activation instructions



4. Click **OK**.

The Activation Code view of the License Activation dialog box reappears.

Tip When you close the Offline Activation dialog box, the application automatically saves the URL to the Clipboard, so that you can save the URL to a file for use on an online computer.

5. (Optional) Save the URL to a file.
6. Keep the License Activation dialog box open on this offline computer.

IMPORTANT If you accidentally close the License Activation dialog box, start over at [step 1](#).

7. To download the response file (activation.xml) from the licensing server, do the following on an online computer:
 - a. Transfer the activation request file ((Activation-*Activation Code*.req) to the online computer.
 - b. Go to the following URL (case sensitive):

<https://thermo.flexnetoperations.com/control/thmo/offlineActivation>

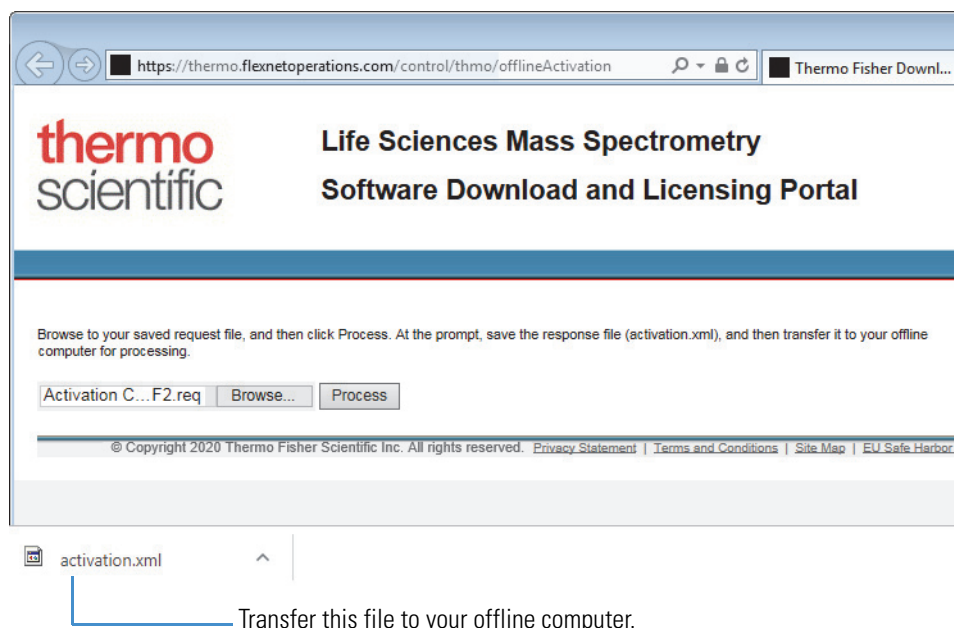
The Life Sciences Mass Spectrometry Software Download and Licensing Portal opens.

- c. Click **Choose File** or **Browse**, browse to and select the request file (**Activation *Activation Code*.req**), click **Open**, and then click **Process**.

Note Whether the page includes a Choose File button or a Browse button depends on the web browser.

The server downloads the activation file.

Figure 5. Software licensing portal with a view of a downloaded response file



- d. Save the response file (activation.xml).
8. To activate the license on the offline computer, do the following:
 - a. Transfer the response file (activation.xml) to this computer.
 - b. In the License Activation dialog box that you left open, click **Process Response File**.
The Open Response File dialog box opens.
 - c. Browse to and select the response file (activation.xml), and then click **Open**.
 - d. At the “license response processed” prompt, click **OK**.
 - e. At the “new features” prompt, click **OK**.

This completes the offline license activation process. The License Manager indicates that the license for the specified product (XCALI-XXXXX) is permanent.

Trademarks

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