

Installing the Workbook Client Application

Note: BIOVIA supports using Ansible to manage installations and upgrades for Workbook client systems, Workbook vault servers, Pipeline Pilot, Compose and Capture, and CISPro. For more information, see the *Ansible Scripting Installation Guide for BIOVIA 2021*. This guide is included in the ULM documentation zip file on the Dassault Systèmes Download Platform.

This document explains how to uninstall an existing version of the BIOVIA Workbook client application, as well as how to install the Workbook 2021 version on an end-user system and on a Citrix server.

When you install the Workbook client application, the following client-related components are installed:

- BIOVIA Workbook Client Manager, which includes the Workbook client application
- Black Ice printer driver
- BIOVIA Draw

Note: The folder name and Windows Add/Remove Programs listing for the *Workbook client application* and *Workbook Client Manager* is *BIOVIA Workbook Client Manager*.

Installation Prerequisites

Perform the following steps before you install the Workbook client application:

1. Check the *Workbook System Requirements* document to verify that the client system meets all requirements.

Note: The BIOVIA Workbook 2021 client application requires BIOVIA Vault Server 2021, but you can install it before or after you install Vault Server.

2. Set the Microsoft User Account Control (UAC) to its lowest setting (**Never Notify**), and then reboot. Reset the UAC to your preferred setting after you finish the installation.
3. Ensure that the Windows Print Spooler service is running.
4. Ensure that the Windows Remote Procedural Call (RPC) services are running.

IMPORTANT! Some operating systems include built-in PDF readers that do not always handle experiment reports correctly. For example, they sometimes create reports that are missing the first page and that have data in the file section that should not be there. To circumvent these issues, install an Adobe PDF application and change the default PDF application to Adobe Acrobat.

Additional Prerequisites for Citrix Environments

To support Workbook in a Citrix environment, ensure that the following additional prerequisites are met:

- Provide each end user with a unique Citrix account and their own Citrix credentials to use each time they log on.
 - Anonymous users are not supported.

- Sharing of the same account by more than one user should not be allowed. If more than one scientist uses the same account, an experiment's file-section can get attributed to the incorrect scientist.
- The recent users list does not persist between sessions. Users must log on each time they access Workbook.
- The Citrix server must be configured to use the existing user session and sessions that are disconnected, rather than creating a new session.
- If the Citrix server uses a self-signed certificate, use the system account, not the user account, to install the BIOVIA Vault Server security certificate on the client system. The default method is to use the user account. For more information about security certificates, see your Administrator and the *BIOVIA Vault Server 2021 Installation Guide*.

For more information about Citrix, see the Citrix documentation.

Uninstalling the Previous Version of the Client Application

If a previous version of Workbook is installed, uninstall it, and then verify that the Black Ice printer driver was removed:

1. In the Windows Add or Remove Programs application, locate the BIOVIA Workbook Client Manager application, and then click **Uninstall**.
2. Check the C:\WINDOWS\system32 folder for the BiPrnDrv.ocx file and remove it if it exists.

Installing the Workbook 2021 Client Application

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To install the BIOVIA Workbook 2021 client application:

1. Log on to the destination computer as an Administrator.
2. Extract BIOVIA_Workbook_2021.zip to a temporary folder whose path contains no spaces.
After extraction, your temporary folder will contain a Client and Server Installers subfolder.
3. In the Client and Server Installers subfolder, double-click BIOVIA.Workbook.21.1.64bit.msi to start the Workbook client application installer.
4. After the installer finishes running, access the following folder and provide **Full Control** permissions to all users.

C:\Program Data\Symyx Technologies

Note: This step prevents log-on issues that can occur when a user other than the first user to access the application attempts to log on. It is critical if you are installing the client on a Citrix server for use by multiple users. It is also important for local installations if more than one user shares the same system and if usernames are subject to change.

After the installation completes, Microsoft Windows lists the Workbook client as **BIOVIA Workbook Client Manager**.

Excluding Workbook Folders from Anti-Virus Scans

To improve performance, exclude the following folders from virus scanning:

- Workbook client installation folder under c:\Program Files:
 \BIOVIA\BIOVIA workbook Client Manager
- Symyx Technologies folder:
 C:\ProgramData\Symyx Technologies

Verifying Access to the Vault Server

1. After the installation completes, start Workbook and attempt to log on to Vault Server, or just access the Vault Server URL directly from your browser.
2. If you get a certificate error, contact your Vault Server administrator for certificate installation instructions.

Changing the Default Structure Editor to ChemDraw (Optional)

Workbook supports two structure editors: BIOVIA Draw and PerkinElmer's ChemDraw. BIOVIA Draw is the default structure editor.

The default structure editor can be changed two ways:

- An administrator can change the global default from Draw to ChemDraw so that ChemDraw instead of Draw is initially selected in Workbook client deployments. For more information, see the *BIOVIA Workbook Administration Guide*.
- Each user can override the global default by using the Workbook client's Preferences screen.

Users with ChemDraw as their selected preference must activate it from within the Workbook client, as follows:

1. Start ChemDraw from within the BIOVIA Workbook client.

Note: If you launch ChemDraw directly from Windows instead of from within Workbook, you must use copy-and-paste instead of the structure **Transfer** function to copy structures from ChemDraw to Workbook.

2. Right-click the ChemDraw drawing pane.
3. Select **Help > Activate ChemDraw Plugin**.

Users who set ChemDraw as their preferred editor should be aware that when they work in a File section, Workbook opens the structure editor that is associated with the file extension instead of checking their preferences to see whether they specify BIOVIADraw or ChemDraw. Usually, .rxn files are associated with Draw and opened in Draw, whereas .cdx files are associated with ChemDraw and opened in ChemDraw.

ChemDraw Usage Notes

After installing ChemDraw and setting it as the preferred structure editor, access it from Workbook as follows:

- Double-click a Workbook structure or right-click the structure and choose **Edit** to open it in ChemDraw.

Note: When you work in a File section, Workbook opens the structure editor that is associated with the file extension instead of checking your preferences to see whether they specify BIOVIA Draw or ChemDraw. Usually, .rxn files are associated with Draw and opened in Draw, whereas .cdx files are associated with ChemDraw and opened in ChemDraw, but you can changes these

settings in Windows.

- Edit the structure as needed in the ChemDraw window and then click the ChemDraw **Transfer** button to transfer it back to Workbook and close ChemDraw.

If you opened ChemDraw directly from Windows or from a File section instead of by double-clicking a structure, you might have to use copy-and-paste instead of the Transfer function to get your changes into Workbook.

- To close the ChemDraw window without transferring the edited structure, click the ChemDraw window's **Close** button.

For information on setting ChemDraw as your default structure editor, see [Setting Preferences in the online help](#).

Be aware of the following when you use ChemDraw with Workbook:

- **Reactions that contain R-groups.** Reactions with R-groups created in ChemDraw must have the R-group variable box to be understood as R-groups by the Reaction Scheme section in Workbook. Without the R-group variable box, reaction enumeration is not possible. If this variable box was not used when the reaction was created, it must be cleared and re-drawn because you cannot copy/paste the original structure.
- **Polymer beads (polymer groups).** The Transfer function does not transfer polymer groups drawn in ChemDraw. If a ChemDraw structure has polymer groups, save it as a .rxn or .mol file, and then import it into Workbook by using the Import or Browse function instead of by using Transfer.
- **Reaction annotations.** Reaction annotations (chemicals above and below the arrow) are not transferred to Workbook or BIOVIA Draw.
- **Reaction wrapping.** Long reactions can appear wrapped when launching the ChemDraw editor from the Workbook Reaction Scheme section. Ensure that all reactants and products have a "+" between them before transferring them into Workbook. The "+" ensures that all molecules are transferred back to Workbook as expected.
- **Markush reactions.** You cannot import ChemDraw-generated Markush reactions into a Reaction Scheme section; attempts to do so result in the message "Error: loading structure to Cheshire has failed."
- **Salt/hydrates.** When you transfer ChemDraw reactions with a salt/hydrate (multi-component material) to Workbook, the components of the salt/hydrate are treated as multiple compounds, with a plus sign (+) between each compound. To avoid this issue, select the components and group them in ChemDraw before you transfer the reaction to Workbook. Note that such grouping is not necessary for the Synthetic Chemistry section.
- ChemDraw cannot open *.rxn or *.skc files created using early versions of Draw if they contain multiple fragment (grouped) structures. To work around this issue, open these files using Draw and ungroup the structures before reopening them in ChemDraw.
- If Workbook displays an error message from ChemDraw that indicates that your ChemDraw license might be missing or expired, try rebooting your system. This often resolves the issue.

Installing the Workbook SDK (Optional)

Note: The Workbook SDK must be licensed independently from Workbook. You cannot install it without a valid license.

The Workbook SDK is provided as a ZIP file that also includes a Pre-Installation License Validation Wizard and supporting files.

This chapter explains how to validate your Workbook SDK license and install it after validation.

Install the SDK on client systems that developers will use to create interfaces between Workbook and other applications.

For more information, see the *BIOVIA Workbook SDK Developers Guide*.

Installation Prerequisites

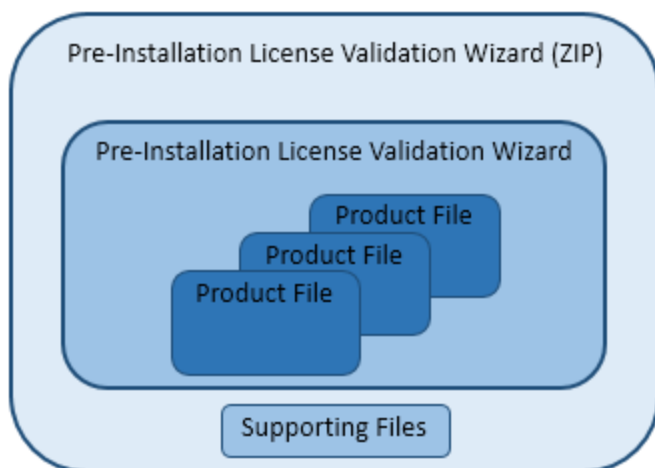
Check the *Workbook System Requirements* document to verify that the client system meets all requirements.

Note: You must install the Workbook client application before you can *use* the SDK, but you can *install* the SDK before or after you install the Workbook client application.

Validating the Workbook SDK License

Running Pre-Installation License Validation ensures that your license is valid and provides access to the installation archive.

Workbook SDK is provided as a ZIP file that includes the Pre-Installation License Validation Wizard and supporting files. A license file is provided separately. After the Pre-Installation License Validation tool has validated your license it provides your installation archive which can then be used in the installation procedure.



Tip: After the Pre-Installation License Validation Wizard has completed successfully, you can distribute the Workbook SDK installation archive to all machines where Workbook SDK should be installed. You do not need to re-validate the license for each machine.

Note: The Pre-Installation License Validation Wizard requires Visual C++ 12 runtime library or later and installs it if it is not already installed. If there are restrictions on installing additional libraries on the machines where Workbook SDK will be installed, you can perform the license validation on another machine and subsequently transfer the resulting installation archive.

1. Log on to the destination computer as an administrator.
2. Extract `BIOVIA_workbook_2021_SDK.zip` to unpack the Pre-Installation License Validation

Wizard.

3. In the extracted folder, double-click `BIOVIA_workbook_2021_SDK.msi` to run the wizard.
4. Click **Next** to start license validation.
5. If the wizard reports that Visual C++ 12 runtime library or later is not available:
 - a. Ensure that the "Visual C++ Redistributable for Visual Studio" checkbox is selected and then click **Next** to install it.
 - b. Review and agree to the terms and conditions and, if you are satisfied, check the "I agree to the License terms and conditions" checkbox, and click **Install**.
 - c. After the installation completes, click **Close**.
6. Click **Browse...** and select your license file, click **Next** to check that you are licensed to install Workbook SDK.

A message reports whether validation was successful or whether it failed.

Reasons for failure to validate include:

- License file does not apply to the product.
- The license file has expired.
- The file specified is not a valid license.

Tip: If you attempt to run the Pre-Installation License Validation Wizard without having extracting it from the ZIP archive, the license validation will fail.

7. To extract the installation archive to a location other than the default, click **Browse...** and choose the destination folder.
8. Click **Next**.
9. Click **Extract** to complete the wizard and obtain the installation archive.
10. When the process is complete, click **Finish**.

The Pre-Installation License Validation Wizard will create the installation archive in the selected folder. You should use this archive to continue the installation procedure.

Running the Workbook SDK Setup Program

To run the Workbook SDK setup program that was extracted by the Pre-Installation License Validation Wizard:

1. Log on to the destination computer as an administrator.
2. Start `BIOVIA_workbookSDK_2021_SDK.msi`.
3. Identify the destination for the installation, if other than the default (`c:\Program Files (x86)\BIOVIA\BOVIA workbook SDK 2021`), and then click **Next**.
4. Click **Install**.
5. Click **Finish**.

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Acknowledgments and References

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"Computational results were obtained by using Dassault Systèmes BIOVIA software programs. BIOVIA Workbook was used to perform the calculations and to generate the graphical results."

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