PRODUCT RELEASE DOCUMENT

BIOVIA Draw

2021

Minor
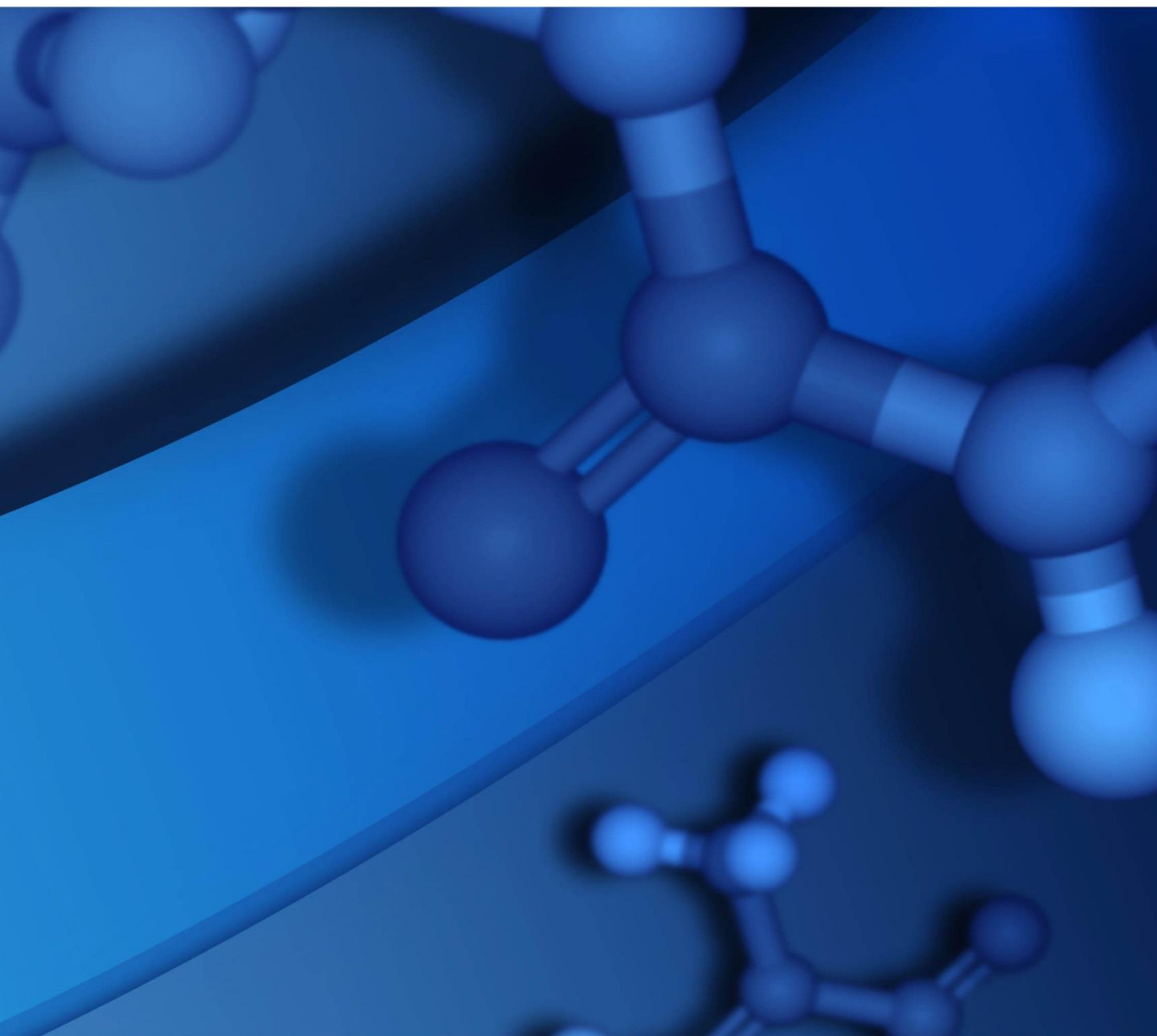
Third Party Notification

Your BIOVIA Draw 2021 installation contains third-party software components. For details, refer to the BIOVIA Program Directory at https://media.3ds.com/support/progdir/.

Acknowledgments and References

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Contents

Customer Release Details

Release of BIOVIA Draw 2021

Release Type: Minor

23 Oct 2020

Key Technical Points

- This release contains the following installers:
  - 32-bit for Enterprise Edition, Desktop, and Portable versions.
  - 64-bit for Enterprise Edition, Desktop, and Portable versions.

  For details about installers and supported environments, see the *BIOVIA Draw 2021 System Requirements* document.
- **BIOVIA Draw 2021** is a complete replacement for earlier versions of Accelrys Draw.
- Earlier standalone versions of **BIOVIA Draw** or Accelrys Draw must be uninstalled before installing **BIOVIA Draw 2021**.
- **BIOVIA Draw 2021** installs assembly redirect policies for earlier versions of Draw such that **BIOVIA Draw 2021** acts as the sole standalone editor for these versions. The redirection equally affects applications developed using Draw API.

> **Note:** Installation of BIOVIA Draw 2021 requires earlier versions of BIOVIA Plugin or Desktop Connector to be uninstalled and replaced by BIOVIA Desktop Connector 2021.

BIOVIA Desktop Connector

The BIOVIA Desktop Connector replaces the BIOVIA Plugin included in Pipeline Pilot releases before version 2019. The Desktop Connector can be configured to run in a new "Messaging Service" mode, which has several advantages over the previous "HostProcess" Plugin legacy mode, including improved security and better support for the Edge browser. The Messaging Service, which is the recommended mode of operation, requires a Windows server. The legacy mode will be supported for a limited time only, until the security certificates shipped with Pipeline Pilot 2021 expire.

The Desktop Connector must be installed and configured by a Pipeline Pilot administrator by following the directions in the **Set Up BIOVIA Desktop Connector** page, which is accessible from the Pipeline Pilot Server Home page.

When users run Pipeline Pilot protocols or applications that create Chemistry Sketcher windows in web pages, a Desktop Connector application will run on the user's client. If the Desktop Connector client is not installed, or if the connection between the browser and the Desktop Connector client cannot be established, users will be prompted to install the Desktop Connector client. Once the Desktop Connector client is installed, a new icon is displayed in the system tray. Users can click this icon to show the Desktop Connector and view the current connections, to restart or exit the Desktop Connector, and to access Help for further information.

DrawBridge Web Component

DrawBridge provides components for integrating web applications with BIOVIA Draw. With DrawBridge, you can open Draw from a web application and transfer structures between them. For developer documentation and coding examples see "Getting Started with DrawBridge" in the *Draw Developer Guide*.

The DrawBridge executable is included with all installations of Draw.

> **Note:** BIOVIA Draw 2021 will be the last release that contains the legacy Draw ActiveX control (see "Internet Explorer Examples" in the *Draw Developer Guide*). As announced by Microsoft, IE11 has reached its end of life and will be replaced by the Edge Browser.

Support Dates

- For information regarding currently supported releases and the dates on which mainstream support ends, see https://www.3ds.com/support/policies-offers/lifecycle-policy/.

- For complete details about support policies, see https://www.3ds.com/support/policies-offers/.

Getting Help

If you have questions, visit Dassault Systèmes Customer Support at https://www.3ds.com/support and click either **Call us** or **Submit a request**.

System Requirements and Installation

System Requirements

The system requirements for BIOVIA Draw are identified in the document *BIOVIA Draw System Requirements*. This document is included in the **BIOVIA Draw** documentation zip file.

Installation

Validating the Draw License

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

Draw is supplied as a zipped file on Windows. This provides access to a Pre-Installation License Validation tool and supporting files. A license file is provided separately. When the Pre-Installation License Validation tool has validated your license, it provides your installation archives, which can then be used in the Draw installation procedure.
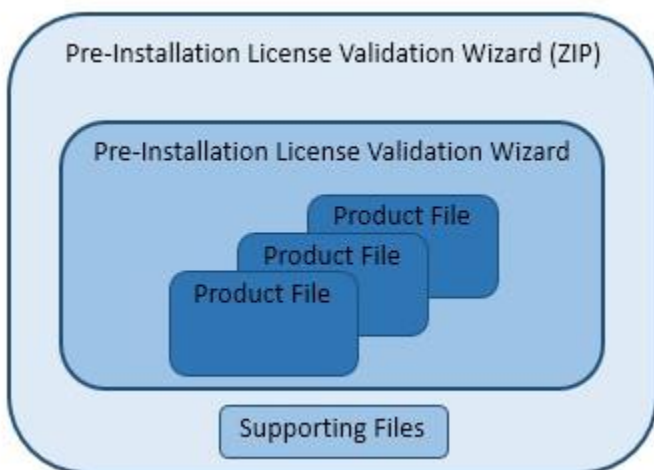
> **Tip**: When Pre-Installation License Validation has completed successfully you can distribute the installation archives to all systems where Draw should be installed. You do *not* need to re-validate the license for each system.

> **Note**: The Pre-Installation License Validation Wizard requires Visual C++ 12 runtime library or later on Windows systems. If this is not available on the system where you run the wizard, it will be installed automatically before license validation proceeds. If there are restrictions on installing additional libraries on the systems where Draw will be installed, you can perform the license validation on another system and subsequently transfer the resulting installer archives.

1. Log on to the destination computer as an administrator.
2. To unpack the Pre-Installation License Validation Wizard, do one of the following:
   - For the 32 bit EE version, extract **BIOVIA_Draw_32bit_2021_Package.zip**.
   - For the 64 bit EE version, extract **BIOVIA_Draw_64bit_2021_Package.zip**.

3. Navigate to the extracted directory.

4. Double-click on the **BIOVIA_Draw_2021_32-bit_Package.exe** to run the Pre-Installation License Validation Wizard.

5. Click **Next** to begin the license validation.

6. If the wizard detects that Visual C++ 12 runtime library or later is not available:

   a. Ensure that the "Visual C++ Redistributable for Visual Studio" checkbox is checked and click **Next** to install it.

   b. Review the terms and conditions and, if you are satisfied, check the "I agree to the License terms and conditions" checkbox and click **Install**.

   c. Wait for the installation of Visual C++ to runtime library complete, then click **Close**.

7. Click **Browse**, select your license file, and click **Next** to verify that you are licensed to install Draw.

   A message reports whether validation was successful or if it failed for one of the following reasons:

   ▪ License file does not apply to the product.

   ▪ The license file has expired.

   ▪ The file specified is not a valid license.

   > **Tip:** If you run the Pre-Installation License Validation Wizard without having extracted it from the ZIP or TGZ archive, the license file will fail validation.

8. To extract the installation archives to a location other than the default, click **Browse** and choose the destination folder.

9. Click **Next**.

10. Click **Extract** to complete the wizard and obtain the installation archives.

    The wizard reports its progress.

11. When the process is complete, click **Finish**.

The Draw Pre-Installation License Validation Wizard creates the installation archives in the specified directory. Use these archives to continue the installation procedure.

Setting up Authentication to a Pipeline Pilot server configured for BIOVIA Foundation Hub SSO Kerberos

Draw now supports Single Sign-On authentication using Windows credentials to a Pipeline Pilot server configured for Foundation Hub SSO Kerberos authentication. This feature is supported for connecting Draw 2021 to Pipeline Pilot server versions 2020 or 2021.

BIOVIA Draw 2021 – portable version

Draw Portable was introduced in Draw 4.1 for individual-level ease-of-deployment. Installation consists of extracting a zip to get a folder with subfolders, files, and the application executable, `BIOVIADraw.exe`. You do not need administrator privileges. No DLLs are registered in the Windows Global Assembly Cache (GAC). It can be run from any file structure on any device, including a portable thumb drive. The disk space required is 100 MB. Deployment can be automated with a batch file that uses the DOS or Windows XCopy command. Portable deployments can coexist with MSI installations. To uninstall, remove the folder. There is no need to use Windows Programs and Features.

> **Note:**
>
> Draw Portable does not support Object linking and embedding (OLE).
>
> To run Draw Portable on a system where the standalone version is not installed, make sure the following prerequisites are installed.
>
> MS Visual C++ 15 runtime (x86/x64)
> MS Visual C++ 17 runtime (x86/x64)

Silently Installing and Uninstalling Draw 2021

You can perform a silent installation, upgrade, or uninstallation of **BIOVIA Draw** using command line syntax. These methods require minimal user interaction, and the installation, upgrade, or uninstallation does not display messages or windows during its progress.

> **Note:** You must have administrator privileges to perform the silent installation. You must run the command line interpreter as an administrator.

To perform a fresh installation

The following is an example command to perform a silent installation of **BIOVIA Draw** with the usertype as the Application User and the CDX file association as Yes:

```
BIOVIADraw-2021 _EE.exe /s /v" USERTYPE=Application ADDLOCAL=ALL CDX_ASSOCIATION="Yes" /l*v
BIOVIADraw2021.log.txt /qn"
```

Syntax	Description
`BIOVIADraw-2021_EE.exe`	File name of the executable file.
`USERTYPE`	Type of user. It can be either "Developer" or "Application". If you do not specify the type of user, the default is Application.
`/l*v <path to log file>`	Path to the log file. It is optional, but when specifying a path, the path or directory must exist, otherwise the log file will not be created and the installation will be aborted.
`CDX_ASSOCIATION`	Whether to associate CDX format files with BIOVIA Draw. You can specify either Yes or No. The default is Yes.
	Command line for CDX_ASSOCIATION="No"
	`BIOVIADraw-2021_EE.exe /s /v" USERTYPE=Application ADDLOCAL=ALL REMOVE=File_Association_CDX_SymyxDraw CDX_ASSOCIATION="No" /l*v BIOVIADraw2021.log.txt /qn"`
	Command line for CDX_ASSOCIATION="Yes"
	`BIOVIADraw-2021.exe /s /v" USERTYPE=Application ADDLOCAL=ALL CDX_ASSOCIATION="Yes" /l*v BIOVIADraw2021.log.txt /qn"`

Syntax	Description

INSTALLDIR	Installation path for Draw. If you do not specify the installation path, the typical installation directory on Windows 10 is:
	
	`C:\Program Files (x86)\BIOVIA\BIOVIA Draw 2021`
	
	for 32 bit Draw
	
	And:
	
	`C:\Program Files\BIOVIA\BIOVIA Draw 2021`
	
	for 64-bit Draw.

Notes:

- All parameters and values are case-sensitive, including the name of the executable file.
- If the path has a space in the name, then pass double quotes (") escaped with the (\) character. You also need to escape the (\) character inside the path. For example:

  `INSTALLDIR=\"C:\\ Program Files (x86)\\BIOVIA\\BIOVIA Draw 2021\"`

- The command has been changed. The ADDLOCAL=ALL parameter must be passed to make sure all the features of the installer gets installed on the respective system.
- You must run the command line interpreter as an Administrator.

To perform an uninstallation

In the command line, run the following command:

```
<path to exe> /s /x /v"/qn"
```

For example:

```
BIOVIADraw-2021_EE.exe /s /x /v"/qn"
```

Configuring Citrix to Properly Paste Chemical Structures

Using Citrix-hosted structure editors, chemical structures are pasted as images without structure data. To resolve this problem, configure Citrix to correctly paste chemical structures as described in TechNote T13-2014: "Configuring Citrix to Properly Paste Chemical Structures".

To obtain this TechNote, contact Dassault Systèmes Customer Support at https://www.3ds.com/support.

Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in BIOVIA Draw 2021. For information about previous release of BIOVIA Draw2020, see the Product Release Document for the release

Change Advice

Per the GAMP 5 and ICH Q9 Guideline, BIOVIA understands the requirement to apply Quality Risk Management to computerized systems. The Release Notes include Change Advice information to aid in the risk assessment of changes to a validated environment and determines the required effort to validate the release of BIOVIA Draw. The Change Advice:

- Provides a measure of the potential harm of the issue in the environment
- Identifies the complexity of change

Risk Definition

- **High:** Update affects several distinct areas of the code or is in a complex area of the code
- **Medium:** Update affects a few distinct areas of the code or is in a stable area of the code
- **Low:** Update affects an isolated area of the code or is in a stable area of the code

New Features

- Reagent support – Create and open reaction files that store reagent information.
- Sequence Clean – To improve the layout and cleaning of sequences in structure view.
- Clean – Now uses Pipeline Pilot Chemistry SDK instead of Cheshire scripts.
- Save SCSR Template – Added support for saving a modified residue from a sequence chain.
- Added support for zooming by pressing Ctrl+ Mouse scroll wheel.
- Enhanced HELM monomer synchronization with Draw and the centralized library:
    - HELM monomers are now synchronized with the previously synchronized SCSR templates.
    - Centralized library folders are now grouped by library name and nolonger requires manual configuration of XML by an administrator.
- Added support for an administrator to add a registry key to customize the PipelinePilot Protocol Root folder.
- New option to set the CIP calculation timeout for highly symmetrical molecules with many stereo centers can time out. You can now extend the time out which re-runs the calculation with reduced accuracy. This may result in some stereo centers being marked as "C" (complex).

Enhancements

This release of BIOVIA Draw includes the following enhancements.

Description	Areas Affected	Risk	User Story
Users can create a new SCSR template from a modified residue in the sequence chain.	Sequence	Low	DRAW-15680
Draw now supports creation of Chimestring and SMILES string for reactions.	Copy/Paste	Low	DRAW-11642
Draw has improved usability for working with grouped objects.	GUI	Low	DRAW-14485
Improved the display of brackets in drawings.	GUI	Low	DRAW-3876
Added Chemistry > Sequence Clean to improve the layout and depiction of biological sequences in structure view and expanded form.	PPChem SDK, Sequence	Low	DRAW-13486
Clean functionality for small molecules is now using PPChem SDK instead of Cheshire scripts.	PPChem SDK	Low	DRAW-13880
Improved placement of linkers in structure view.	Sequence	Low	DRAW-14802
Improved depiction of biological sequences in structure view.	Sequence	Low	DRAW-14826
Added support for reagents in RXN format.	GUI	Medium	DRAW-14840
Added method for zoom using Ctrl + mouse wheel.	GUI	Low	DRAW-15750
Central library now does not require any manual xml configuration. Libraries are group based on the library names.	Central Monomer Library	Low	DRAW-15928
Added option to display long form or short form terminal groups for sequences.	GUI	Medium	DRAW-15966
Draw now allows copying only text object as text on to Office applications.	OLE	Low	DRAW-16205
Draw now supports single atom attachments for the sequence.	Sequence	Low	DRAW-16248

Description	Areas Affected	Risk	User Story
For molecules with complex stereochemistry, the CIP timeout dialog text was updated and an option to re-run the calculation faster but with reduced accuracy was added.	PPChem SDK	Low	DRAW-16250
Generating an SD file from canvas now prompts the user to include or expluce duplicates.	SDF Utility	Low	DRAW-16260
Draw now can support HELM operations with the custom templates downloaded from Central library.	PPChem SDK	Low	DRAW-16388
Atom numbers are now automatically displayed when using Chemistry > Auto Map Reactions.	GUI	Low	DRAW-16403
Draw can now use a custom Pipeline Pilot protocol folder, which can be set by an administrator.	PP Protocols	Low	DRAW-16417
Draw now supports connecting to different Pipeline Pilot servers for the central library and pipeline protocol dialog. This can be configured by an administrator.	Integration	Low	DRAW-16497

Fixed Defects

This release of BIOVIA Draw includes the following fixed defects.

Severity	Description	Areas Affected	Risk	Defect
Major	Draw now handles "clean" structures with multibonds, such as adamantine or zirconocenes.	PPChem SDK	Low	DRAW-14410
Major	Orientation is now maintained in both Sequence and Structure view after performing copy/paste sequences with linkers.	Sequence	Low	DRAW-16386
Major	Fixed an issue with display of chiral labels in reactions with single sequence residues.	Sequence	Low	DRAW-16433
Major	Draw can now handle structures with MUL group brackets while performing the Clean operation.	GUI	Low	DRAW-16468

Severity	Description	Areas Affected	Risk	Defect
Major	Draw now displays stereo labels for single sequence residues.	GUI	Low	DRAW-16500
Major	Draw now displays reactions from Workbook without distortion regardless of preference settings.	GUI	Low	DRAW-16501
Major	Draw can now read and display HELM files that contain BASE templates.	PPChem SDK	Low	DRAW-16568
Major	Fixed an issue where BIOVIA Draw would crash after HELM CHEM templates were downloaded from central library.	Templates	Low	DRAW-16578
Major	Draw now has better placement position for attachments in structure view.	Sequence	Low	DRAW-16617
Major	Workbook now shows the structure properly in the materials section grid.	Integration	Low	DRAW-16637
Major	BIOVIA Draw 64-bit academic and trial version now supports OLE operations.	Installation	Medium	DRAW-16644
Minor	The E and Q sequence template has been updated with better coordinates for a neater depiction on the canvas.	Templates	Low	DRAW-11591
Minor	Draw now always uses single bond irrespective of selected bond type in the toolbar while creating bonds between sequences.	GUI	Low	DRAW-12605
Minor	Edited residue labels are now correctly displayed in red in the sequence and structure views.	GUI, Sequence	Low	DRAW-12780
Minor	BIOVIA Draw now preserves settings/preferences when loading structures from or passing structures to other applications/OLE operations.	OLE	Low	DRAW-14842

Severity	Description	Areas Affected	Risk	Defect
Minor	Fixed an issue where modifying a cystine in an SCSR sequence would be converted to SUP groups.	Sequence	Low	DRAW-15026
Minor	Custom SCSR templates created from BIOVIA Draw now show an appropriate leaving group text instead of LG1 or LG2.	Sequence	Low	DRAW-15128
Minor	Text objects can now be deleted from a set a grouped objects.	GUI	Low	DRAW-15307
Minor	Improved the display of the aromatic rings in sequence view.	GUI	Low	DRAW-15311
Minor	BIOVIA Draw settings/preferences are now copied when copying and pasting the structure, and when using transfer.	OLE	Low	DRAW-15391
Minor	Improved user experience for deletion of grouped objects.	GUI	Low	DRAW-15544
Minor	Improved handling of structures with MUL brackets while performing a "clean" operation.	GUI	Low	DRAW-16021
Minor	Updated Chemical Representation 2021 guide with guidelines about Z, R, X, and M query atoms.	Documentation	Low	DRAW-16053
Minor	Added support for HELM/xHELM strings that consist only of sugar and phosphate.	PPChem SDK	Low	DRAW-16128
Minor	Draw now supports reading an SD file (with only one record) generated from Pipette sketcher.	SDF Utility	Low	DRAW-16220
Minor	Fixed an error that occurred when saving with Full-CTAB-ON for sequences with disulphide bridges.	Sequence	Low	DRAW-16227
Minor	Improved the canvas display of the Cystine sequence template.	Templates	Low	DRAW-16243

Severity	Description	Areas Affected	Risk	Defect
Minor	You can now copy HELM strings directly from an Excel cell and paste as structure.	GUI	Low	DRAW-16398
Minor	Fixed an issue that occurred when applying the Bracket Tool to a single (non-hydrogen) atom.	GUI	Low	DRAW-16399
Minor	Fixed an issue with the Map Residue option in the sequence view.	Sequence	Low	DRAW-16478
Minor	Fixed an issue where chimestrings differed when using Copy As and Chemistry > Generate text from structure.	Calculator	Low	DRAW-16479
Minor	Extended canvas size is preserved now while switching between the sequence and structure view.	GUI	Low	DRAW-16618

Known Issues

This release of BIOVIA Draw has the following known issues.

Severity	Description	Defect
Major	Copying and pasting of particular structures with nested abbreviations sometimes alters the structures, and can lead to BIOVIA Draw closing unexpectedly. Workaround: This issue might be related to conversion to and from SKC format, and can be avoided by copying and pasting the structures as MOL files instead.	DRAW-14131
Major	For reaction drawings where reactants and products have ABS stereochemistry and are enclosed in polymer brackets, the chiral flag is not properly set when the drawings are saved in rxn format. These stereo compounds are saved as "and enantiomer" (chiral flag off).	DRAW-14777
Major	The Renditor sometimes hangs during editing of an Sgroup bracket.	DRAW-15769
Minor	BIOVIA Draw can handle the Hydrogen query count feature, but has no tool to draw it.	DRAW-10681
Minor	When the Markush Bond tool is being used, an exceeded valence violation is not reported.	DRAW-12122
Minor	Draw sometimes incorrectly applies opaque and transparent fill styles for graphic objects.	DRAW-12855
Minor	Reaction schemes and information above or below the reaction arrows in CDX files are not always parsed and preserved exactly as in the original CDX files.	DRAW-12862

Severity	Description	Defect
Minor	When SKC files with nested abbreviations containing COOH are saved, the abbreviation is sometimes stored incorrectly.	DRAW-14000
Minor	Expanded sequence with attachments may have overlaps.	DRAW-14898
Minor	Calculations of chemical names using the OpenEye Lexichem libraries miss stereo marks (E/Z) for some double bonds.	DRAW-15019
Minor	The Japanese font setting for text elements is lost after saving into an SKC file.	DRAW-15123
Minor	The Clean tool does not always handle biopolymer sequences correctly. We recommend users use the Sequence Clean to clean sequences in Structure view.	DRAW-15154
Minor	The Clean tool resets structure display to use standard settings, but fails to reset atom label sizes.	DRAW-15318
Minor	The angle can be incorrect when a bond is sprouted from a ring.	DRAW-15401
Minor	The Bond tool and the All-Purpose Drawing tool sometimes edit bonds differently.	DRAW-15402
Minor	In some cases, terminal attachment groups of a sequence are not recognized as modifications.	DRAW-15425
Minor	The Rectangle tool + Shift does not correctly draw squares.	DRAW-15458
Minor	In some specific cases, flipping a sequence alters the stereo configuration of residues.	DRAW-15733