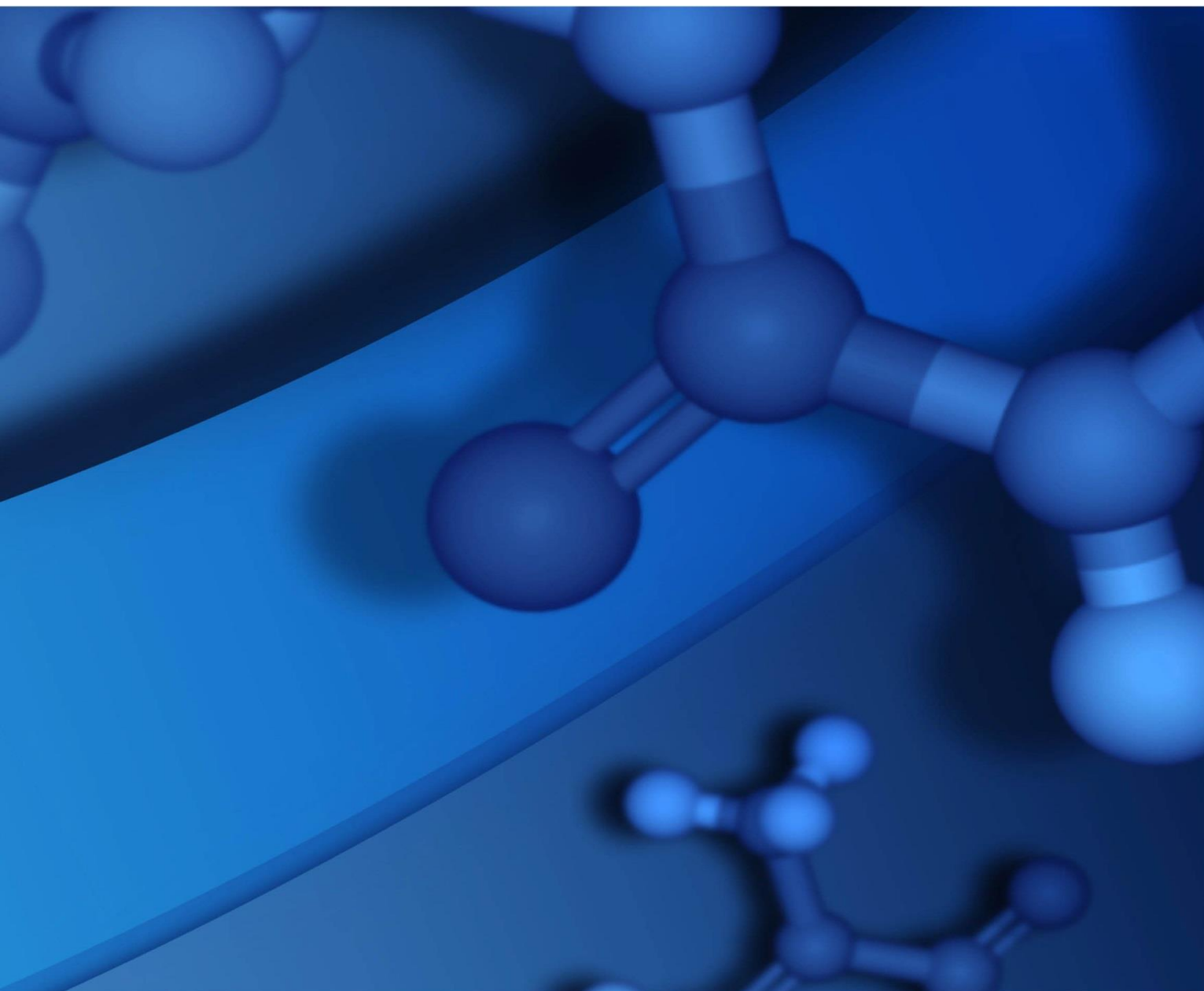


PRODUCT RELEASE DOCUMENT

BIOVIA Pipeline Pilot

2021

Major



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Third Party Notification

Your BIOVIA Pipeline Pilot 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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Dassault Systèmes Customer Support
10, Rue Marcel Dassault
78140 Vélizy-Villacoublay
FRANCE

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Customer Release Details

Release of BIOVIA Pipeline Pilot 2021

Release Type: Major

04 Nov 2020

Key Technical Points

- After upgrading to BIOVIA Pipeline Pilot 2021, users must also upgrade their Pipeline Pilot Client systems to 2021. Pipeline Pilot clients from version 2020 and earlier cannot connect to a 2021 Pipeline Pilot Server. This is true not only for the Professional Client, but also for clients that use Pipeline Pilot Client SDKs (.NET, Java). The Client Compatibility configuration file has been updated to reflect this change.
 - **What do I need to do?** If a client that uses an older SDK needs to connect to a 2021 or later Pipeline Pilot server, relink client code based on the old NALPP or JALPP Client SDK to the new 2021 version.
 - **What if I cannot update my client?** If it is not possible to update a client to the latest client SDK, you can use the “Client Version Support” configuration option in the Pipeline Pilot Administration Portal on the **Setup > Server Configuration** page. For new and upgraded servers, the default setting is "v2021 and Later". If you change this to "v2020" or "pre-v2020," you must also update the Client Compatibility configuration file. For details, contact Dassault Systèmes Support.
- To install Pipeline Pilot as part of a suite of BIOVIA applications, install or upgrade BIOVIA Foundation Hub before Pipeline Pilot. Install all other BIOVIA applications after installing or upgrading Pipeline Pilot.
- A trusted TLS/SSL certificate issued by a recognized Certificate Authority is now required, not just recommended, for production Pipeline Pilot servers. The Deployment Guide, Admin Portal Guide, and System Requirements Guide have been modified to state this requirement.
- When Pipeline Pilot is configured to use Foundation Hub for authentication, enable the Foundation Hub “Save user passwords for the duration of session” on the **Foundation Hub Admin and Settings > Applications > Application Settings > Foundation Hub** page. This setting enables several Pipeline Pilot capabilities including:
 - User impersonation
 - Use of the HTTP Connector set to 'Use Pipeline Pilot Credentials' to connect to a remote service
 - Setting up scheduled jobs
- A separate installer is required to install GPL-licensed third-party tools used by the Pipeline Pilot Biology Collections. Run the GPL installer after the standard Pipeline Pilot installer. There is no impact to functionality and no changes to existing components, protocols, or licenses are required.
- BIOVIA is aware of an issue where Trend Antivirus' behavioral monitoring functionality is incorrectly identifying the Pipeline Pilot Apache process (httpd.exe) as a malicious application and quarantines the executable. When this happens, Trend reports an "Unauthorized File Encryption" from httpd.exe. The action primarily occurs when Pipeline Pilot cleans the users' job folders to delete

expired job data. To avoid this problem, if your environment uses Trend Antivirus, add the Pipeline Pilot folders to Trend Antivirus' behavioral monitoring exclusion list. Minimally, the Apache folder located in `apps/scitegic/core/packages_win64/apache` and the Pipeline Pilot job folder location should be excluded. There may be a similar issue with other antivirus products.

Developer note about Java upgrades and security levels:

To keep up with evolving security technology and standards, BIOVIA Pipeline Pilot 2021 includes several server enhancements. These enhancements relate to OpenJDK 11, TLS, and other security standards.

Because of these enhancements, this release is not completely backward-compatible. Adaptations might be required to enable existing customer components and application code to function correctly after an upgrade to BIOVIA Pipeline Pilot 2021. To help mitigate this situation, several new administration settings are available to revert specific behaviors, if necessary. For more information, contact Dassault Systèmes Customer Support.

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 Pipeline Pilot 2021 are identified in the document *BIOVIA Pipeline Pilot System Requirements*. This document is included in the BIOVIA Pipeline Pilot zip file.

Other BIOVIA Applications

If you are installing other BIOVIA applications, install the following applications before you install BIOVIA Pipeline Pilot:

- Foundation

Installation

Refer to the *BIOVIA Pipeline Pilot Server Installation Guide*.

Pipeline Pilot Release Notes

This section provides cumulative information about all new features, enhancements, and fixed defects since the last major BIOVIA Pipeline Pilot release, which was Pipeline Pilot 2020. It also identifies known issues in this release.

New Features

General

- Improved scripting usability. You can now have multiple script dialog boxes open simultaneously for most of the scripting components and custom manipulators, enabling you to compare and copy between dialog boxes.
- Improved server stability and overall resource usage.
- Updated internal tools such as Perl, Java, OpenSSL, Apache HTTPD, Python and Apache POI libraries.
- Support for protocol database backup without locking the database to other users.

Working with external resources

- Added support for interacting with SharePoint Online and AWS S3 external resources.
- Added a new component, *Resource Connection*, for interacting with external resources such as SharePoint Online and AWS S3.

Working with Python

- Enhanced support for Python Jupyter Notebook.
- Added a new component, *Python Script*, to facilitate working with dataframes in Pipeline Pilot.
- Added a new component, *Declare Python Environment*, to define an external Python environment to use in a protocol.
- You can now define an external Python environment as a Tagged Resource in the Administration Portal and use it with the *Python Jupyter Notebook* or *Python Script* components.

Enhancements

This release of BIOVIA Pipeline Pilot 2021 includes the following enhancements.

Administration

Description	User Story
<p>SharePoint/single sign-on: A new capability has been added for managing credentials to access external systems and resources (specifically, Amazon S3 and SharePoint Online) independently of PLP protocols.</p> <p>Components that write, read, and list files have been enhanced to access these resources in a seamless way (using a new “resource” URI) that automatically pulls in the credentials needed for access.</p> <p>This is achieved with new capabilities for administrators to add Pipeline Pilot’s tagged resource to define the information needed to connect to the external system.</p> <p>In addition, for SharePoint Online, access tokens and refresh tokens using OAUTH2 flow initiated by individual users in a new "Resource Authorization" webpage are acquired to authorize Pipeline Pilot to access SharePoint Online on the user's behalf.</p>	PPP-40052
<p>The “Legacy” format option has been removed from the administration report summary page. This option should no longer be relevant to any Pipeline Pilot installations.</p>	PPP-44155
<p>You can refresh Data Source Name (DSN) information on Pipeline Pilot Server. If you make any change to the set of ODBC DSNs defined on the Pipeline Pilot Server operating system:</p> <ul style="list-style-type: none">• Navigate to the bin or linux_bin directory in the server installation, and run the command <pre>dbutil -dsn</pre> <p>to effect the immediate refresh of the set of data sources configured for Pipeline Pilot to use. The changes to the DSN list are reflected in the Select Data Source dialog box in Pipeline Pilot Client, among other places.</p> <div style="border: 1px solid gray; padding: 5px;"><p>Note: You can also trigger an automatic update of the list of known DSNs from the operating system by viewing the Setup/Data Sources page in the Administration Portal.</p></div>	PPP-45889
<p>JDBC data sources can be configured in the Administration Portal to use specific Kerberos and JAAS configurations. Previously, these items were configured the same way for all data sources. This capability was added primarily for connection to Hive and Impala data sources, but it can be used with any JDBC data sources.</p>	PPP-44780 PPC-9418[IR]
<p>In the Tagged Resource Administration UI, any field with a name ending in "_password" is obfuscated and shown as "*****".</p>	PPP-45699

Description	User Story
A Tagged Resource Template for Amazon S3 connection credentials has been added in the Administration Portal.	PPP-45429
A Tagged Resource Template for Microsoft Sharepoint Online connection credentials has been added in the Administration Portal.	PPP-45140 PPP-44553
A Resource Authorization UI page has been added to Pipeline Pilot Server that allows Oauth2 grant authorization tokens to be obtained for Microsoft Sharepoint Online connections. A link to the new page is provided on the Pipeline Pilot Server Home Page.	
Protocol database scalability has been improved, and the protocol database is no longer exclusively locked during protocol database backup operations.	PPC-9030

Developers

Description	User Story
<p>REST URL mapping in package definitions: A new Response parameter is supported called \$defaultformat.</p> <p>When used as a parameter declaration within a package.conf url section, \$defaultformat defines the default format for the response results of the mapped URL, and takes the same value options as the \$format parameter. Within a package.conf file, unlike the \$format parameter, \$defaultformat can be overridden by a client computer connecting to the URL. For instance, if the \$defaultformat is set to "xml", but the client instead requests a JSON response, the client can provide its own \$format parameter in the query string. For example:</p> <p>[https://myserver:9943/mypath?\$format=json]</p> <p>However, if \$format is not specified by the client, the \$defaultformat setting is used from the package.conf entry. The order of precedence for formats is: \$format, \$defaultformat, HTTP Accept header, implementation-defined default, text/plain. The Accept header has lower precedence than \$defaultFormat in order to handle situations where browsers add default Accept headers.</p>	PPP-45483
\$validationstate has been added as an optional parameter for the POST-based /xinfo/api/v1/validate/ REST endpoint. This parameter allows the caller to preserve the state of the validation from one validate call to the next. The current state is returned as a result property in the REST call.	PPP-45224
A property, legal-values-are-enforced, has been added as a result property of the /xinfo/api/v1/validate/ REST endpoint.	PPP-45222
A new REST endpoint, GET /xinfo/api/v1/calculable, has been added to return the list of calculable properties by category.	PPP-45238

Generic Components

Description	User Story
The Excel Reader can now read sheet names based on wildcards. For example, if a workbook contains sheets named xyz123, xyz234, and xyz345, specifying xyz* as the value for the <i>SheetName</i> parameter results in those three sheets being read.	PPP-39374
The library used for reading and writing Microsoft Office documents to a newer version has been updated. The old version had been released in 2012 (poi-3.8). The new version is poi-4.1.0, which was released in early 2019.	PPP-44305
<p>The Location components have been removed from the scitegic/scmobile collection. In previous versions of Pipeline Pilot, these were shipped, and marked as "Deprecated". However, since changes in Google Maps API requirements, the Location components no longer function at all.</p> <p>Revised versions of these components are now available through the scitegic/report2 package (HTML5), which use the revised Google APIs.</p> <p>If you have any existing protocols that use the Location components, you must replace them with the scitegic/report2 components. These are available in Components\Reporting and Visualization\Dashboards\Utilities\Location.</p>	PPP-43548
There are improvements to Unicode character handling of DateProposeFormat for several international locales with regard to months and weekdays.	PPC-9478

Grid

Description	User Story
A new Grid option, <i>Number of GPUs</i> , is available for scheduling GPU usage for Grid integration with SLURM and PBS Pro.	PPC-9732

Internal Libraries

Description	User Story
OpenSSL has been updated to the latest available 1.1.1 release.	PPC-9636 PPC-9486 PPC-9345
The Pipeline Pilot Apache web server has been updated to version 2.4.41.	PPC-9345
<p>The version of Python used in the <i>Python (on Server)</i> component has been updated to Python 3.8.1. Please see https://docs.python.org/3.8/ for more information on changes to Python. Notably, on Windows, there are changes to how DLLs are located by the ctypes module (see https://docs.python.org/3/whatsnew/3.8.html#bpo-36085-whatnews).</p> <p>Versions of the packages in Python Essentials libraries have also been upgraded to the following: pandas 1.0.0, numpy 1.18.1, scipy 1.4.1, matplotlib 3.1.2, and scikit-learn 0.22.1.</p>	PPC-9346

Description	User Story
The Perl installation used for the <i>Perl (on Server)</i> component has been updated to Perl 5.30.0. For information relating to changes in the Perl language, see https://www.perl.org/ .	PPC-9344
Java had been updated from Open JDK8 to Open JDK11, and all third-party Java libraries have been updated to work in the new version. All third-party Java libraries have been named with the convention <i>libraryname_version.jar</i> , so that the versions are easily visible.	PPP-43686 PPP-43685 PPP-44579
Tomcat has been updated to v8.5.55.	PPC-9677
The library used for reading and writing Microsoft Office documents to a newer version has been updated. The old version had been released in 2012 (poi-3.8). The new version is poi-4.1.0, which was released in early 2019.	PPP-44305
The internal Chromium Embedded Framework (CEF) browser, used in the Pipeline Pilot Professional Client, has been updated to version 79.1.31+chromium-79.0.3945.117.	PPP-44303
Hadoop related Java libraries in the scitegic/integration package have been updated, as follows. commons-configuration2-2.1.1.jar commons-io-2.5.jar commons-lang3-3.3.2.jar commons-logging-1.1.1.jar guava-11.0.2.jar hadoop-auth-3.1.1.3.1.0.0-78.jar hadoop-common-3.1.1.3.1.0.0-78.jar hadoop-hdfs-3.1.1.3.1.0.0-78.jar hadoop-hdfs-client-3.1.1.3.1.0.0-78.jar hadoop-hdfs-httpfs-3.1.1.3.1.0.0-78.jar hadoop-hdfs-native-client-3.1.1.3.1.0.0-78.jar hadoop-hdfs-nfs-3.1.1.3.1.0.0-78.jar hadoop-hdfs-rbf-3.1.1.3.1.0.0-78.jar htrace-core4-4.1.0-incubating.jar re2j-1.1.jar woodstox-core-5.0.3.jar	PPP-44815
ODBC drivers have been updated as follows: The <i>BIOVIA Oracle</i> driver has been updated to version 8.00.02.2289. The <i>BIOVIA SQL Server</i> driver has been updated to version 8.00.02.269.	PPP-44309

Professional Client

Description	User Story
A new component, <i>Resource Connector</i> , allows reuse of credentials when a resource is called in a protocol.	PPP-44544

Description	User Story
File access components can now interact with Amazon S3 external resource for file storage.	PPP-45429 PPP-44343
File access components can now interact with the Microsoft Sharepoint Online external resource for file storage.	PPP-45140 PPP-44547
<p>Pipeline Pilot script editors are now modeless. This means that users can now open multiple script editor dialog boxes simultaneously, and interact with the rest of the Pipeline Pilot UI while the dialog boxes are open. The script editors for PilotScript (for example <i>Custom Manipulator</i> and <i>Custom Filter</i>), <i>Perl (on Server)</i>, <i>Python (on Server)</i>, <i>Dynamic Java (on Server)</i>, <i>Dynamic .NET (on Server)</i>, and a few other components that use the same editors have been converted to allow modeless editing.</p> <p>The modeless dialog boxes have several consistent behaviors:</p> <ul style="list-style-type: none"> • When the dialog box has mouse and keyboard focus, the component associated with the dialog box is highlighted in a lime green color in the protocol. If the component is in a subprotocol, the subprotocol is highlighted. • If the text in the dialog box has been modified, an asterisk (*) is appended to the dialog box title, and the Apply button is enabled. • The title of the dialog box updates if the component's display caption is changed. • If a protocol is run while modeless dialog boxes for its components are open with unsaved changes, the user is asked to choose whether or not to apply the changes, or to cancel protocol execution. The user can save this preference. If the user wants to restore dialog box alerts, they can use the new menu option View/Restore View Settings/Dialog Alerts. • While the protocol is running, a warning caption is displayed in the dialog box, and the dialog box's Apply and OK buttons are disabled. The user can still edit the script in the dialog box, but cannot apply their edits to the component until the protocol completes execution. After the protocol stops, the buttons are enabled and the warning caption is removed. • Saving the protocol does <i>not</i> apply changes from open dialog boxes. Moreover, Pipeline Pilot Client does not alert the user to unsaved changes. • If the dialog box's component is deleted as a result of an action in the protocol (deletion of the component, collapsing of the component to a subprotocol, pressing of Ctrl-X/CUT, closure of the protocol, and so on), the dialog box closes, and any changes are discarded. 	PPP-18178
An alert and a notification have been added to the Pipeline Pilot Client status bar for the current server's SSL/TLS certificate expiration. The tool tip for the server name on the status bar now includes the server's certificate expiration. When expiration is less than 1 month away, the background color of the server name on the status bar turns yellow, and when expiration is less than 14 days away, it turns red. Expiration is only checked on connection to a server during client startup, and on changing of the primary server.	PPP-21472

Description	User Story
In old versions of Pipeline Pilot, when Pipeline Pilot Client was still using an integrated Internet Explorer window to display HTML data, the Pilotscript Guide information could be opened into a new Internet Explorer window from the context menu in the PilotScript editor dialog box. When Pipeline Pilot Client was converted to use embedded Chromium windows, this functionality disappeared. The behavior has now been restored. Clicking the background of the guide window in the PilotScript editor now opens a context menu to open the current page in a new window, and clicking a link opens a menu to open the link in a new window. In both cases, the link target opens in the Windows-defined default browser.	PPP-44116

Python and Jupyter Notebook

Description	User Story
Versions of the packages in Python Essentials Libraries have been upgraded to: pandas 1.0.0, numpy 1.18.1, scipy 1.4.1, matplotlib 3.1.2, and scikit-learn 0.22.1.	PPC-9346
A new component, <i>Python Script</i> , has been added. It converts incoming data records to a pandas DataFrame, applies the user's Python script to the DataFrame, and converts any data in the DataFrame back to Pipeline Pilot data records. The behavior is the same as the <i>Python Jupyter Notebook</i> component, except that <i>Python Script</i> features a plain Python script editor instead of the Jupyter notebook editor, and therefore does not require the Jupyter server.	PPP-44502
A utility protocol <i>Install Python Packages Using Built-in Python</i> is provided for Pipeline Pilot users to more easily install additional Python packages for use in the <i>Python (on Server)</i> component.	PPP-45065
Environment variables can be specified when an external Python environment is launched, using the <i>Environment Variables</i> parameter of the <i>Declare Python Environments</i> component, or the <i>EnvVarsJSON</i> parameter of the Python Environment tagged resources in the Administration Portal.	PPP-45161
Protocols containing the <i>Python Jupyter Notebook (on Server)</i> component from the 2020 release should be updated to instead use the <i>Python Jupyter Notebook</i> component. The <i>Python Jupyter Notebook (on Server)</i> component from the 2020 release is deprecated. Note that Replace With Latest Version does not update the component. Protocol authors must replace instances of the deprecated component manually.	PPP-45159
Clicking OK in the <i>Python Jupyter Notebook</i> script editor dialog box automatically saves the Jupyter notebook. It is no longer necessary to save the notebook first manually.	PPP-44858

Description	User Story
<p>Example protocols using the <i>Python Jupyter Notebook</i> and <i>Python Script</i> components have been added to Protocols/Examples/Integration/Programming/Python/Jupyter Notebook and Protocols/Examples/Integration/Programming/Python/Python Script, respectively.</p>	PPP-45231
<p>Example protocols using the <i>Python (on Server)</i> component have been renamed to begin with "Python (on Server)" so that they are more readily identifiable in searches.</p>	PPP-43777
<p>External Python environments can be declared using either a <i>Declare Python Environment</i> component or as a Tagged Resource in the Administration Portal. The environments can then be used to run Python code in the <i>Python Jupyter Notebook</i> or <i>Python Script</i> components.</p>	PPP-44897
<p>External Python environments such as those created in Anaconda or using venv can be used to run cells in the <i>Python Jupyter Notebook</i> component's interactive script editor.</p>	PPP-44760
<p>In the <i>Python Jupyter Notebook</i> component, Pipeline Pilot global parameters containing path tokens such as UserDir and JobDir can now be used in the Python script, by means of their entries in the plp_globals dictionary (for example, plp_globals["UserDir"] or plp_globals["JobDir"]).</p>	PPP-45322
<p>In the <i>Python Jupyter Notebook</i> component, the initialization cell required to load Pipeline Pilot data and perform other setup tasks is now run automatically when the Jupyter Notebook script editor is opened.</p>	PPP-44893
<p>Jupyter Notebooks (.ipynb files) on a client computer can now be imported into the <i>Python Jupyter Notebook</i> component. Users can do this by opening the Jupyter notebook script editor and selecting File > Import Notebook. The required Pipeline Pilot initialization cell in the notebook is inserted automatically if it does not already exist.</p>	PPP-44630
<p>Pipeline Pilot URIs with prefixes such as userdata:/ can be used in the <i>PythonPath</i> parameter of the <i>Python (on Server)</i> component. The paths are internally resolved to their absolute paths.</p>	PPP-45084
<p>Plotting in the Python components using matplotlib from the Python Essentials Libraries now works immediately, without the user having to set the backend to "Agg".</p>	PPP-44146
<p>The Cancel button in the <i>Python Jupyter Notebook</i> script editor window now opens a dialog box warning the user if there are unsaved changes. Included in the dialog box is a button that the user can click to stay in the editor.</p>	PPP-44903
<p>The ability to use external Python environments such as those created using Anaconda or Python's venv tool has been added to the <i>Python Jupyter Notebook</i> component. This facility is also incorporated into the new <i>Python Script</i> component. See the <i>Python Development Guide</i> for more details.</p>	PPP-44632

Description	User Story
The Python libraries that are shipped with Pipeline Pilot are now included in the Core package rather than the Integration package. Therefore, both the Core and the Integration packages are now required to use the <i>Python (on Server)</i> component.	PPP-44876
The <i>Python Jupyter Notebook</i> and <i>Python Script</i> components now, by default, unmerge data before outputting it. Users can keep data records merged by setting the <i>Keep Output Data Merged</i> parameter to True.	PPP-45521
The <i>Python Jupyter Notebook</i> component now always treats missing values and Pipeline Pilot NullValues as numpy.nan, improving consistency between the Jupyter notebook editor and the behavior of the component when it is run in a protocol. Pandas DataFrame columns containing mixed types are also now converted to StringArrayValues in a better way.	PPP-44509
When import statements are evaluated in the <i>Python (on Server)</i> component, the paths in the <i>PythonPath</i> and <i>Use Pipeline Pilot Package</i> component parameters are now searched before any paths in the <i>PythonPath</i> integration package global that is set in the Administration Portal.	PPP-45582
In paths to external Python environments in the <i>Conda Base Path</i> and <i>Path to Python</i> parameters, URIs with prefixes such as shortcut:// can now be used.	PPP-45135

Fixed Defects

This release of BIOVIA Pipeline Pilot 2021 includes the following fixed defects.

Administration

Severity	Description	Defect
Minor	Fixed the case when an administrator chose a different backup path to the default backup folder, the restore would fail.	PPP-42340
Minor	<p>Disabled support for certain characters that cause problems in shortcut names within the Administration Portal File Browsing page:</p> <ul style="list-style-type: none"> - Forward and backward slash characters (\ and /) - Greater than and less than characters (< and >) - Single and double quote characters (' and ") were already disabled via the admin portal, but are now also disabled via configutil <p>Existing File browsing shortcuts with any of these characters can be removed.</p>	PPP-40570
Minor	Fixed an issue with admin-created user names that included double quote characters that caused the user list to not appear correctly in the Security > Users page of the Administration Portal.	PPP-44394

Severity	Description	Defect
Minor	Fixed an issue where non-alphanumeric characters in user names would result in errors in the various server web pages. These html/javascript errors would prevent the user from logging out or subsequently accessing the login page, preventing the user from reauthenticating.	PPP-44873
Minor	Fixed an issue with DbUtil -s when run with the -batched option where items that claimed to be registered in the output from the command would not be properly indexed into the Protocol Database if there were empty folders within the tab. DbUtil -s run without the -batched option worked fine.	PPP-44724
Minor	Fixed issues with SAML configuration and authentication: <ul style="list-style-type: none"> ■ Fixed an issue present in version 2020 with the Import Key action of the Security/SAML Configuration Administration Portal page. ■ Fixed an issue where SAML-based authentication would fail in Web Port when the Pipeline Pilot "Server Port Usage" setting was set to "SSL Only". 	PPP-44515 PPC-9421[IR] PPC-9396[IR]
Minor	Fixed an issue where the Pipeline Pilot Apache service process (httpd.exe) would continually grow in memory over time in situations where the server was set to use Domain-based authentication and at least one Pipeline Pilot group was defined to include members of an External Claim (Domain Group).	PPC-9508
Minor	Fixed an issue where occasionally Kerberos authentication to the Pipeline Pilot server would result in a log message of the form "Cannot dereference a NULL pointer". Authentication would proceed successfully, but the server log files would include the error.	PPC-9719
Minor	Fixed an issue where protocols executed as either the service account or a user defined within the Pipeline Pilot Administration Portal would fail on Linux when impersonation was enabled. In particular, this affected tasks scheduled from packages.	PPP-44722 PPC-9480 [IR]
Minor	Removed access to the Solr Admin UI from.	PPP-44885

Developers

Severity	Description	Defect
Minor	Fixed an issue where Pipeline Pilot Web Service REST Requests (including Protocol launching via URL requests such as /auth/launchjob, runjob.pl) did not properly URL decode short query string parameter values (1 or 2 characters) that contained "+" URL encodings of the space character. Longer query string parameter values were unaffected by the issue. However, the fix to this issue could possibly impact applications that relied on the defective behavior.	PPP-45365
Minor	Fixed an issue where the server would respond with a 500 Internal Server Error when a request to a REST API included an invalid \$bodyref parameter. The error response is now more appropriate to the circumstances.	PPC-9726
Minor	Fixed an issue where slash characters ('/' and '\') were not properly URL decoded when passed through the package defined REST URL interfaces to the running protocol as parameter values. The characters would appear as %2F for '/' and %5C for '\'. On Linux servers, only forward slash characters were affected. The characters now appear correctly when passed through to the protocol. This change affects package defined URL directives where the request field includes "request" directives containing either "{+ParamName}" or "*ParamName" or entries where a custom "constraint" is defined for the element.	PPC-9473
Minor	Fixed display of Unicode (international) characters within error messages from blocking launch calls to the Job REST endpoints (such as /auth/launchjob and /protocols/myProtocolName).	PPC-8852
Minor	Added \$clienttype to the GET /jobs/ REST API to support returning jobs only associated with the given client type.	PPP-45197
Minor	Fixed an issue in the .NET Client SDK where the RemoteFileManager::DoesFileExist() method would not return the correct result for job folder URLs when Job Folder Restriction is enabled on the server.	PPP-44990

Generic Components

Severity	Description	Defect
Minor	Fixed the <i>Array Property Merge</i> and <i>Array Property Resize</i> components to work as documented.	PPP-45366
Minor	Fixed an issue with the <i>Copy to Client</i> component where specifying the source using "job:" did not work correctly for remote Pipeline Pilot servers	PPP-44489
Minor	Fixed an issue where writing .zip files using the <i>Delimited Text Writer</i> would fail if the incoming data records has variable property lists, the data is moderately lengthy (at least 80 characters per line), and the output character encoding is set to either ANSI or UTF-8 with no Byte Order Mark.	PPP-44907 PPC-9578 [IR]
Minor	Fixed the behavior of the <i>Extract Protocol Components</i> component when handling Owner Access Only (OAC) subprotocols. If Recursive is "true" and an item within the requested protocol or subprotocol is marked as OAC where the registrant does not match the executing protocol's username, the component will be output, but the OAC subprotocol's nested components will not. If an OAC protocol or subprotocol is requested, the incoming data record will be output to the Fail Port of <i>Extract Protocol Components</i> .	PPP-45589
Minor	Fixed an issue where the <i>Excel Reader</i> failed to read sheets containing a single row of data.	PPP-43758
Minor	Fixed an issue where the <i>Excel Reader's</i> array column recognition system created a false positive hit for a column name of the form ABC[XYZ]. Now, only numbers are allowed within the '[' tokens for the array detection to trigger.	PPP-43865
Minor	Fixed an issue where the <i>Excel Reader</i> was ignoring background color and comments in cells that were perceived as containing an array.	PPP-43413
Minor	Fixed an issue where the <i>File Reader</i> would crash when trying to read files with the extension ".file".	PPP-36608
Minor	The <i>List Files</i> component now reports file paths using the job: and userdata: URIs.	PPP-44689
Minor	The "Show Distance" option is now functional on the <i>HTML Cluster Viewer</i> component.	PPP-41349
Minor	Fixed an issue with the <i>Table (HTML5)</i> component where a clickable table would not respond correctly when images contained within the table were clicked.	PPP-44431
Minor	Fixed an issue where setting Socket Debugging to true on the <i>Http Connector</i> component running on a Linux server could result in the component failing to run successfully with an error of the form "Invalid or incomplete multibyte or wide character".	PPC-9750

Severity	Description	Defect
Minor	Fixed an issue with the Pipeline Pilot JSON parser used by the <i>JSON Reader</i> and the <i>Data from JSON</i> components where attempting to parse invalid JSON would result in a memory leak within the executing Protocol process. This was especially noticeable when processing large quantities of data records containing JSON where the readers' error handling is set to catch the error and send the data record out to the fail port.	PPC-9682
Minor	Fixed an issue where certain safe file URIs such as "allusers:" and "alljobs:" were not correctly translated by <i>Run Program (on Server)</i> components. Starting in Pipeline Pilot version 2020, the <i>List Files</i> component outputs safe file URIs where possible. When listing files in the user directory or jobs folder, the output was in the form of allusers: and alljobs: paths. Passing these paths into <i>Run Program (on Server)</i> component command lines would often result in failures within the external application. In Pipeline Pilot 2021, each of these file URI types is correctly translated within the <i>Run Program (on Server)</i> component. See PPP-44689 for related enhancements to the <i>List Files</i> component.	PPP-44612
Minor	Fixed an issue where double-clicking on the <i>Sharepoint List Reader</i> components would result in an error message of the form "Unable to open this shortcut. Unable to find subprotocol "Sharepoint List Reader" in the Database".	PPP-45724
Minor	Fixed an issue where the <i>SMTP Mail Writer</i> component would halt with an error after sending the message when the component receives an unexpected response from the SMTP server following the SMTP QUIT command.	PPP-45549 PPC-9756 [IR]
Minor	Fixed an issue with the prototype <i>Search Protocol Database</i> component where the component would fail when running in Debug Mode.	PPP-44739 PPC-9497 [IR]
Minor	Fixed an issue in Bar Charts where drawing an object with height 0 would create an exception. The fix is to not draw objects with width or height of 0.	PPP-39393
Minor	Writing dashboards as pdf files will now work on Linux systems without an installed libpng library. The libpng embedded in Pipeline Pilot is used instead.	PPP-43615
Minor	Fixed an issue with HTML5 collection components that internally make use of the Highcharts Data Series, where certain data sets would cause the components to halt with a memory access error.	PPP-45001

Severity	Description	Defect
Minor	Fixed a problem where the SQL components were generating an exception when using an ODBC driver and executing a statement that contained a comment with a single quote in it.	PPC-9385[IR]
Minor	Fixed the parsing of PilotScript date formats of the form "%c %Z", to show the national representation of date and time, followed by the time zone, if known.	PPP-45156
Minor	Fixed an issue where turning on error handling for a Run To Completion subprotocol and having at least 4096 errors caught within the subprotocol and sent to either the fail or pass port could result in subsequent components failing with an error of the form "CScopeData: Maximum number of properties exceeded"	PPC-9698

Professional Client

Severity	Description	Defect
Minor	Dragging a source file (.txt, .xlsx, .sd, etc.) onto a protocol now creates an appropriate reader component within the existing protocol rather than opening a new protocol.	PPP-45074
Minor	Fixed an issue where the return value of the "OnEvent" api within Custom parameter javascript implementations was not properly handled by the Professional Client dialog. When the onEvent handler returns false, the dialog is now correctly prevented from closing.	PPP-44849
Minor	Fixed an issue that caused the Professional Client to crash when opening other copies of a local shortcut after saving one of the copies of the local shortcut as a regular Protocol Database based shortcut.	PPP-44708
Minor	Fixed an issue since version 2017 where HTML based dialogs displayed during running protocols would frequently appear with the browser offset from the dialog window rendering the dialog unviewable. In particular, this frequently affected the Global Data Tree Viewer and Data Record Tree Viewer components.	PPP-44785
Minor	Fixed an issue where the automatic Professional Client update process would fail when connecting an older Professional Client version to a 2020 server where the "Enable Full Server Configuration Listing" admin portal Server Configuration setting was set to the default value of "No".	PPP-44705
Minor	Fixed an issue in the Professional Client where pressing Enter when the Protocol Error Dialog was displayed would often result in the client crashing.	PPP-44593 PPC-9461 [IR]

Severity	Description	Defect
Minor	Fixed an issue where exporting a folder of components or protocols could cause the files to be named with .xml extensions instead of .ppxml.	PPP-44826
Minor	Fixed an issue where the parameter "promote" menu option would incorrectly appear within the top-level protocol edit dialog.	PPP-45090
Minor	Fixed an issue where the Server File Browser was no longer showing the correct icons for each file extension (.txt, .xlsx, .pdf, etc.)	PPP-44412
Minor	Fixed handling of client-side Windows OS directory shortcuts (.lnk files) in the Professional Client file browser. The icons now show as directories when the shortcut points to a windows folder and double clicking on folder targeted .lnk files will navigate correctly.	PPP-44944 PPC-9585 [IR]
Minor	Restored the functionality of the "Show Folding" option within the Professional Client's script editor dialogs.	PPP-44615
Minor	Fixed the behavior of parameters when switching the "Initialize Using" state back to "Initialize Using/Parameter Value" after setting it to a different state and renaming the parameter.	PPP-44971
Minor	In the Professional Client, when right clicking on a job result from the jobs tab and choosing "Save As...", the client will now report errors that occur while trying to save the file.	PPP-44978
Minor	Fixed an error in the Professional Client that would occur when loading the File Browser for DirectoryType parameters when the parameter value was set to the name of a server shortcut (shortcut:/my shortcut name).	PPP-44485
Minor	Fixed an error in the Last Data Record window of the Error Dialog when certain Reporting components failed. The window now shows the error that resulted from the attempt to render an invalid reporting object rather than a separate javascript error dialog.	PPP-42625

Python

Severity	Description	Defect
Minor	All IronPython example protocols have been removed because the IronPython Script (on Server) component is deprecated.	PPP-44884
Minor	In the Python Jupyter Notebook component, <code>__future__</code> import statements in the Python code such as <code>"from __future__ import division"</code> now work.	PPP-44727
Minor	In the Python Jupyter Notebook component, output pandas DataFrames with column names that are not of string type (for example, integers) are now handled correctly and converted to string property names.	PPP-44536

Severity	Description	Defect
Minor	On Linux, Python code in the Python (on Server) component can now use urllib.request to make HTTPS requests without SSL certificate verify errors.	PPP-45810
Minor	Temporary runtime files created by the Jupyter Notebook server are now deleted when the Jupyter Notebook server service is stopped.	PPP-45465
Minor	The "assert" statement in Python (on Server) will now raise an error if the assert expression evaluates to False. This default behavior can be overridden by setting the PYTHONOPTIMIZE environment variable to 1 before starting the Pipeline Pilot server. See the Python documentation for more information.	PPP-45075
Minor	The close button of the Python Jupyter Notebook (on Server) component's script editor was disabled so that only the OK or Cancel buttons can be used to close the dialog. This prevents users from clicking the close button and then losing changes that appeared to be saved in the Jupyter notebook but were not actually saved yet.	PPP-44401
Minor	The Jupyter notebook script editor now works for Jupyter notebook components nested at least two deep in subprotocols.	PPP-44824
Minor	The Python Jupyter Notebook component script editor window now only has one scrollbar	PPP-44819
Minor	The Python package bottleneck (version 1.3.2) has been added to the Python Essentials Libraries. The pandas shipped with Pipeline Pilot will automatically use bottleneck to improve the performance of certain computations. To disable the use of bottleneck by our built-in pandas, the following code can be added: <pre>import pandas as pd pd.set_option('compute.use_bottleneck', False)</pre>	PPP-45550
Minor	Unicode characters can now be passed to Python's print() function in the Python (on Server) component without causing an error.	PPP-44997
Minor	When an empty data record is passed into a Python Jupyter Notebook component containing no added Python code, an empty data record now is sent out the pass port. Previously, no data record exited the component.	PPP-44680
Minor	When exporting a Jupyter notebook from within the Jupyter notebook script editor, an extra blank window no longer pops up. Also, only file formats that can be successfully exported to are shown in the File > Download As menu.	PPP-44631

Web Port

Severity	Description	Defect
Minor	Fixed an issue with the Web Port file browser where attempting to rename an uploaded file after the system had determined that the file already exists in the target directory would result in a failure of the form "Uncaught TypeError: Cannot read property 'name'"	PPP-44404
Minor	Extra error handling has been added to the Web Port client code to better handle any errors in network connections to the server.	PPP-42814

Other Fixed Defects

Severity	Description	Defect
Minor	Removed the unused Apache Derby database from the Pipeline Pilot server environment, along with GEMS examples that depended upon it.	PPP-44854
Minor	Updated the mechanism used to recover when Linux protocol process launching breaks down. This should allow the Pipeline Pilot server to quickly and automatically recover when the internal Linux cross process communication system stops working.	PPC-9537 PPP-44813[IR]
Minor	Fixed an issue on Linux where temporary files for various tasks would be written to the TMPDIR location instead of the desired temp folder when the Linux TMPDIR OS environment variable was enabled within the Pipeline Pilot server. This affected a number of systems within the server including the Cache Writer component.	PPC-9781
Minor	While it is always preferable to sign into the Pipeline Pilot server to ensure the best experience, this release does correct some issues in the Help Center for unauthenticated users where some PDF documents could not be downloaded, and other related to differences in experience from that of authenticated users.	PPP-44082
Minor	PDF documents in the Help Center have alternative HTML document links. Internal document links (for example, in the table of contents) in the HTML documents no longer open in a new browser tab when the Pipeline Pilot Server is not configured to use only HTTPS navigation.	PPP-44904
Minor	Updated the Administration help for the Catalog Settings to reflect recent enhancements.	PPC-9546[IR]
Minor	It is now possible to use SAML-based authentication for browser-only sessions. Previously, users had to log in using the Pro Client first, before being able to log in via a web client.	PPC-9396

Known Issues

This release of BIOVIA Pipeline Pilot 2021 has the following known issues.

Professional Client

Severity	Description	Defect
Minor	The Pipeline Pilot client administrator mode is not functional when the Pipeline Pilot server is connected to Foundation Hub.	PPP-44504
Minor	Under full impersonation with File Browsing set to Restricted, accessing a remote shared folder can result in an error in the Professional Client file browser when automatically resetting to the folder previously used to select a file. The workaround is to navigate again to the remote shared folder to select the additional file.	PPC-9527[IR]

Excel

Severity	Description	Defect
Minor	If you have a data record property that is a scalar on some records and an array on others, the Excel Writer (Cross platform) component writes one column with that property name to contain the scalar values. It writes column names with suffixes [1], [2], etc. to contain the array values. However, when reading the file back with Excel Reader (Cross platform), the original data format is recovered.	PPP-22221
Minor	Pipeline Pilot only supports those functions that are supported in the POI libraries used for cross-platform Excel file processing. Spreadsheet cells containing certain Excel functions show up as value "#ERROR", when reading with the Excel Reader (Cross platform) component. Functions known to display the problem include CORREL(), SLOPE(), and INTERCEPT().	PPP-25524
Minor	If an Excel sheet contains more than one column with the same name, Excel Reader (Cross Platform) outputs only the value in the last column of that name. By contrast, Excel Reader (on Client) outputs all of the values as an array.	PPP-37051
Minor	Excel Reader may exhibit rounding errors for some borderline numeric values.	PPP-43244

Reporting

Severity	Description	Defect
Minor	For Reporting Components: because the Format and Position parameters are linked, inside a sub-protocol it is not possible to promote the Format parameter of one component and the Position parameter of another.	PPP-27491

Severity	Description	Defect
Minor	For the Reporting Collection, protocol Link parameters on aggregating components (for example, Paragraph, Tile Vertical, Tile Horizontal) do not work in HTML reports. They may work when used with the PDF Report Viewer.	PPP-27589
Minor	For the Reporting Collection, if an HTML attribute is set to the same value as the value of the ParameterToMap parameter, no formatting will be applied to the form element.	PPP-29023
Minor	For the Reporting Collection, charts containing non-existent data properties may still attempt to render, rather than throwing an error when the protocol is run.	PPP-34439
Minor	Displaying a report with multiple tabs in an HTML report viewer may result in tabs being cut off if the display window is initially too small to show all tabs prior to being maximized.	PPP-35315
Minor	In a report containing a Table element that is displayed in the Excel Report Viewer, Excel treats columns of numeric data containing 50% or more blank cells as if they were text columns.	PPP-36907
Minor	If multiple Report viewers of different types (for example, PDF Report Viewer and HTML Report Viewer) are connected to the same pipeline with an XY Chart component, the lower viewer in the pipeline shows the markers displaced from their correct location on the chart.	PPP-42379
Minor	In the Visual Selector Reporting component, if the property specified in the Value parameter is blank or undefined for a data record, the image associated with that data record will always be selected.	PPP-38399
Minor	For the Cross Tab component, using an Image as one the Row or Column Levels and specifying an absolute size in the Header Position causes the PDF Report Viewer to display the image across multiple cells. The workaround is to use the HTML Report Viewer and print the HTML as PDF from the browser.	PPP-26927
Minor	A maximum of 100 tab groups can be created by the Tab Group component.	PPP-41526
Minor	For the XY Chart, if both scalar and array data is used as input to the XY Chart, setting the Line Color to be read from a property will result in an error.	PPP-32280
Minor	The XY chart's automatic axis range determination may require some manual adjustment when the values to plot are very small.	PPP-34288
Minor	When plotting array data with dates as X values using the XY Chart, if the Tickmark Label Orientation is Vertical, tickmark values may be repeated multiple times.	PPP-37254

Severity	Description	Defect
Minor	In charts produced by the Line Chart component, the legend always shows a circle as the symbol, even if a different symbol is used for points in the chart. However, the color of the circle reflects the color of the line.	PPP-37556
Minor	In charts created by the Bar Chart component with labels on the bars, setting the label location to Above the Bar may cause all bars except for the first to be shifted slightly downward. Other label locations do not have this effect.	PPP-37755
Minor	In a report containing a chart created by a Bar Chart component with the Bar Layout parameter set to Stacked, labels within the stacked bars might be vertically misplaced.	PPP-37821
Minor	When sending many data points to the XY Chart component (>1M) the JVM for the scisvr process may have excessive memory usage.	PPP-38398
Minor	In the XY Chart (Categorical X), if the same X-axis category value appears more than once per data series, that category value will be duplicated on the X-axis.	PPP-38423
Minor	When using the Symbol font within a reporting Canvas component, symbols might not be displayed if the report is output in PDF format. However, the display may work if you use a Unicode symbol with the default font setting.	PPP-38426
Minor	Overlaying a moderate number of Line (Canvas) reporting elements on an XY Chart with a large number of data points (10s of thousands) may result in a Java error.	PPP-39402
Minor	When the Display Type parameter in the XY Chart component is set to Interactive, internal links specified by the Link parameter may fail. The links succeed if Display Type is set to Image.	PPP-39879
Minor	Links are ignored on images used as part of the Canvas Reporting elements.	PPP-41212
Trivial	In the XY Chart component, when you create a chart with more than one data series that uses the same value for the X-axis, the automatic label that is generated treats property names in a case-sensitive way. For example, if you specify "IDNUMBER" for one of the X values and "IDNUMBER" for the other, then the label is "IDNUMBER". However, if you specify "IDNUMBER" and "IDNumber", then the label is "IDNUMBER, IDNumber".	PPP-27419
Minor	For the PDF Report Viewer, a memory leak may occur when generating a large number of PDF reports in a single protocol.	PPP-28707
Minor	The PDF Cross Tab display does not show an image of a molecule if the orientation is set to 'landscape' and the image's cell spans multiple rows.	PPP-32844

Severity	Description	Defect
Minor	In PDF reports whose elements are arranged using Tile Horizontal, a small amount of space may appear between elements, even when the margins and padding are set to zero. The space does not appear in HTML reports.	PPP-37575
Minor	When displaying a canvas in a PDF viewer, all fonts are Helvetica regardless of specification.	PPP-40390
Minor	Using SVG format images in the Reporting Collection Header component for output to the PDF Report Viewer will result in a protocol error.	PPP-41735
Minor	The Searchable List Box cannot be initialized with multiple items selected unless the first data record is one of the selected items.	PPP-26985
Minor	In the cells of a table created by the Editable Table component, if a property has a value of "0" and is of String type, then "0" is displayed in the cell. However, if a property has a value of 0 and is of Integer type, a blank is displayed in the cell.	PPP-36486
Minor	If multiple checkboxes are included in a report with long string values for the Checked Value parameter, an error may occur if attempting to display the report in PDF format. Displaying the report as HTML does not result in an error.	PPP-37574
Minor	The Image From File component is unable to fetch files through a proxy. The workaround is to read the image via another method and use Image From Data.	PPP-29498
Minor	For the Bulleted List component, padding is ignored when the report is rendered as a Word document.	PPP-32052
Minor	Justification of a checkbox in a Report Table cell is ignored and is always left-justified.	PPP-34190
Trivial	In the Reporting File Chooser component, when File Type is set to Select to Single Source File, there is a refresh problem with the displayed file when changing one file to another.	PPC-9725[IR]

Generic Components

Severity	Description	Defect
Minor	When an SMTP Mail Writer message body contains an unprintable ASCII character (value below 32) an error will occur when you run the protocol.	PPP-25588
Minor	When using the SOAP Connector with a Username parameter override, you might receive an unauthorized response.	PPC-9327
Minor	Enabling the subprotocol parameter "Parallel Processing Options" based on the value of another parameter is not working as expected.	PPP-36391
Minor	The Keep Properties dialog on file reader components may display misaligned data for properties whose values contain the newline character.	PPP-38243
Minor	In the Wrap Elements (HTML5) component, multiple CSS classes are not supported.	PPP-43326
Minor	If a protocol is stopped while either the global or data record tree viewer window is open, and then restarted without closing the tree viewer window first, the protocol does not initialize and the Client program needs to be closed and reopened to restart.	PPP-44908 PPC-9571[IR]

Web Port

Severity	Description	Defect
Trivial	For Web Port, tool tips showing parameter help display raw HTML rather than the formatted text.	PPP-33159

Other Known Issues

Severity	Description	Defect
Major	When the Pipeline Pilot server uses Foundation Hub for authentication, Pipeline Pilot protocols that are executed anonymously succeed on the first attempt, but fail on subsequent attempts.	PPC-9423
Minor	There is a limitation on saving a file to a remote shared folder with a file path longer than 260 characters.	PPC-9291[IR]
Minor	If a protocol function is invoked more than once via JavaScript, checkbox groups used with dynamic content containers no longer work after the second and subsequent invocations. The workaround is to manually check individual boxes.	PPP-26946
Minor	When trying to read in a string property in a .NET component (Dynamic C# (on Server) for example), Unicode characters are not properly carried through.	PPP-36351

Severity	Description	Defect
Minor	Run As Anonymous does not work with Protocol Links on Dashboard Collection components.	PPP-42877
Minor	When a protocol that is embedded within a protocol that is also embedded in another protocol, and is copied to a second server using the network tab and then edited on the first server, the parent layer and child layer changes made on server the first server are not reflected on the other server. However, if a change is made to the 'grandchild' layer, then that change is seen on the second server. This is only apparent when viewing the protocols using the network tab on the server where the changes are made. The workaround is to work independently on each server.	PPP-43727
Minor	Users whose username contains Unicode characters are not able to see checkpoint data in the Auto Watch window. Instead, the error message "Check Point Information Doesn't Exist" is shown.	PPP-43892
Minor	After running Backup and Purge operations on the Protocol database, a blank page is displayed in the Administration Portal.	PPC-8535 PPC-9545[IR]
Minor	3DPassport authentication is not working with 3DExperience 2020x when 3DPassport is configured for SAML.	PPC-9817 PPC-9813[IR]
Minor	When using the Run Program (on Grid) component targetting a SLURM grid, problems have been observed in some cases with the LD_BIND_NOW environment variable. A workaround is to add a line to 'unset LD_BIND_NOW' to SLURM scripts in apps/scitegic/integration/bin/scripts.	PPC-9814 PPC-9822[IR]
Minor	When the User Directory location is modified to reside on an Amazon FSx share, there are reports that the List Caches component can fail with a "No Server Process" error.	PPP-45953 PPC-9834[IR]

Analytics and Machine Learning Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in the BIOVIA Pipeline Pilot 2021 Analytics and Machine Learning Collection. For information about previous interim releases of BIOVIA Pipeline Pilot 2020, see the Product Release Documents for the interim releases Pipeline Pilot 2020 HF2, Pipeline Pilot 2020 HF3 and Pipeline Pilot 2020 HF4.

New Features

- None.

Enhancements

This release of the BIOVIA Pipeline Pilot Analytics and Machine Learning Collection includes the following enhancements.

None.

Fixed Defects

This release of the BIOVIA Pipeline Pilot Analytics and Machine Learning Collection includes the following fixed defects.

None.

Known Issues

This release of the BIOVIA Pipeline Pilot Analytics and Machine Learning Collection has the following known issues.

Severity	Description	Defect
Minor	Error models built from R-based models with the <code>_Learn Quality Model (RP Forest)_ learner</code> are unable to make use of the <code>#MDpvalue</code> output property of the original model. This is the p-value for the Mahalanobis distance from the centroid of the training data. Workaround: Use the <code>#MD</code> property, which represents the Mahalanobis distance itself.	PSM-2368
Minor	The <i>R Robust Dose Response Fit</i> component can become stuck in an apparent infinite loop and hang in certain cases when no or poor initial coefficient estimates are provided for the <i>Initial Coefficients Property</i> parameter. In such situations, use the "Robust IRLS" option of the <i>Least Squares Curve Fit</i> as an alternative way to perform a robust fit of dose-response data.	PSM-2369
Minor	In any of the R-based smoother components, if you inadvertently leave a space at the end of the specified property name, the property is correctly smoothed, but the spurious space is retained in the name of the smoothed property (with suffix " <code>__Smoothed</code> ").	PSM-2355

Biology Collections Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in the BIOVIA Pipeline Pilot 2021 Biology Collections. For information about previous interim releases of BIOVIA Pipeline Pilot 2020, see the Product Release Documents for the interim releases Pipeline Pilot 2020 HF2, Pipeline Pilot 2020 HF3 and Pipeline Pilot 2020 HF4.

New Features

- New components have been added for calculating the sequence extinction coefficient, counting the number of residues present at each position of an alignment, and listing and downloading NCBI BLAST databases.
- Many third-party tools have been upgraded to newer versions, including BLAST+ and GATK.
- The search parameters of Entrez EUtilities and other online NCBI components now automatically update to include the latest search options.

Enhancements

This release of the BIOVIA Pipeline Pilot Biology Collections includes the following enhancements.

Gene Expression Collection

Description	User Story
Components and protocols have been modified to utilize user-entered email addresses for parameters such as FTP passwords rather than pre-populated generic email addresses.	PBIO-5455
Updated the Biology collections to be compatible with Pipeline Pilot infrastructure changes.	PBIO-6307 PBIO-6326 PBIO-6317

Mass Spec for Proteomics Collection

Description	User Story
Components and protocols have been modified to utilize user-entered email addresses for parameters such as FTP passwords rather than pre-populated generic email addresses.	PBIO-5455
Updated biology collections to work with Pipeline Pilot infrastructure changes.	PBIO-6307 PBIO-6326 PBIO-6317

Next Generation Sequencing Collection

Description	User Story
Enhanced Create Sequence Repository. You can now optionally add an user-defined prefix to reference sequence names.	PBIO-6356
Updated the search options for EBI and NCBI online components.	PBIO-6364
Components and protocols have been modified to utilize user-entered email addresses for parameters such as FTP passwords rather than pre-populated generic email addresses.	PBIO-5455
Updated the Biology collections to be compatible with Pipeline Pilot infrastructure changes.	PBIO-6307 PBIO-6326 PBIO-6317 PBIO-5786
SAMtools, HTSlib, and BCFtools are upgraded to version 1.10.	PBIO-6328
Picard is upgraded to version 2.23.0.	PBIO-6286
Color space is no longer supported by the Pipeline Pilot NGS collection. Color space components and third-party tools have been removed.	PBIO-6284 PBIO-6018
The Internal Download NCBI Setting component is no longer used and has been removed.	PBIO-6270
GATK is upgraded to version 4.1.6.0.	PBIO-6162
Added a parameter, Merge All Input Regions, to Variant Calling for Region (SAMtools), Joint Variant Calling for Region (GATK), and Variant Calling for Region (GATK) components. If True, all input regions are merged for improved performance.	PBIO-5867
Components that modify BAM files have been renamed to indicate that they also work with CRAM files.	PBIO-4953
Entrez EUtilities and NCBI download components now automatically update search parameters with the latest options.	PBIO-5340

Sequence Analysis Collection

Description	User Story
Entrez EUtilities and NCBI download components now automatically update search parameters with the latest options.	PBIO-5340
Removed the Internal Download NCBI Setting component is no longer used and has been removed.	PBIO-6270
Updated the search options for EBI and NCBI online components.	PBIO-6364

Description	User Story
Components and protocols have been modified to utilize user-entered email addresses for parameters such as FTP passwords rather than pre-populated generic email addresses.	PBIO-5455
Updated the Biology collections to be compatible with Pipeline Pilot infrastructure changes.	PBIO-6307 PBIO-6326 PBIO-6317 PBIO-5786
Added prototype components to list and download BLAST databases provided by NCBI.	PBIO-6399
Added a prototype component that counts the number of residues present at each position in a sequence alignment.	PBIO-6378
Updated NCBI Online BLAST components to use the latest NCBI BLAST options.	PBIO-6374
The Linux version of HMMER3 was updated to 3.3 and moved from the GPL installer to the standard Pipeline Pilot installer.	PBIO-6349
Some EMBOSS components now allow batch processing for faster performance.	PBIO-6335
BLAST+ is upgraded to version 2.10.1.	PBIO-6331
Updated how EMBOSS components handle temp files. If "Use Braces in Job Directory Names (Compatibility)" is selected in the admin portal, EMBOSS components create temp files in the PP_SAC_TEMP folder in the user directory. Otherwise, temp files are written to the standard job directory. Temp files are deleted after the EMBOSS program is run.	PBIO-6330
Modified BLAST output parsing so the accession number no longer contains database names. This makes the components compatible with downstream usage of the EUtilities components.	PBIO-6188
UniGene has been removed as an option in the Entrez EUtilities components because the database has been retired by NCBI. Example protocols have been updated accordingly.	PBIO-6163
You can now use the SAC_NCBI_API_Key global parameter to specify a NCBI API key instead of setting the "NCBI Account API Key" parameter multiple times in a protocol. If both are set, the parameter value is used.	PBIO-6032
Improved control over prolonged searches in the NCBI Online BLAST components by adding parameters for Polling Time, Time Out, and Batch Search.	PBIO-5979
Updated descriptions of online BLAST databases in the component help text.	PBIO-5904
Updated the BED Reader and BED Writer components to support the use of GFF-style attributes in the Name field.	PBIO-5725
Added a component, Calculate Sequence Extinction Coefficient.	PBIO-5543

Fixed Defects

This release of the BIOVIA Pipeline Pilot Biology Collections includes the following fixed defects.

Gene Expression Collection

Severity	Description	Defect
Minor	Updated the Check BioConductor Installation example protocol to be compatible with newer versions of R.	PBIO-6388

Mass Spec for Proteomics Collection

None.

Next Generation Sequencing Collection

Severity	Description	Defect
Major	Updated the URL for the Saccharomyces Genome Database.	PBIO-6359
Minor	Updated the example protocol, 01 Create Human Repository for GATK, to use the current FTP location.	PBIO-6355
Minor	Fixed broken links in component help text.	PBIO-6385
Minor	Updated the list of available genome builds for the Download NCBI Features and Download NCBI Genome Sequences components.	PBIO-6363
Minor	Updated the Biology collections to be compatible with Pipeline Pilot infrastructure changes.	PBIO-6354
Minor	Download NCBI SRA FASTQ Files now uses NCBI's prefetch to download experiments.	PBIO-6310
Minor	Components that use GPL third-party tools now check that the required GPL packages are installed.	PBIO-6016
Minor	Variant Calling for Region (GATK) now uses HaplotypeCaller instead of HaplotypeCallerSpark for multiple-threads.	PBIO-5924
Minor	Moved RunToCompletion and Parallel Processing Options parameters to the Runtime component tab.	PBIO-5827
Trivial	Improved the performance of the Create Sequence Repository from Files component.	PBIO-6373

Sequence Analysis Collection

Severity	Description	Defect
Major	The Download and Process NCBI Taxonomy Files protocol no longer uses unzip to decompress files.	PBIO-6332
Major	Updated the Biology collections to be compatible with Pipeline Pilot infrastructure changes.	PBIO-6379
Major	Added a component, Get BLAST Database Information, to retrieve database information from v5 BLAST databases.	PBIO-6398
Major	Updated Biology collections to work with Pipeline Pilot infrastructure changes.	PBIO-6345
Minor	Improved error messages for the Download and Process NCBI Taxonomy Files protocol.	PBIO-6308
Minor	Improved Perl variable checking, reducing warning messages.	PBIO-6402
Minor	Moved RunToCompletion and Parallel Processing Options parameters to the Runtime component tab.	PBIO-5827
Minor	NCBI Online BLASTp now uses "pataa" instead of "pat" to conform with NCBI standards.	PBIO-6450
Minor	Fixed the warning messages for the BLAST+ DB Specifier Fetcher (blastdbcmd) and BLAST+ DB Sequence Fetcher (blastdbcmd) components.	PBIO-6441
Minor	Reserved property names now undergo a case-insensitive check when creating features.	PBIO-6434
Minor	Entrez EFetch can now handle sequence IDs with no GI number.	PBIO-6366
Minor	Improved sequence ID handling of rare formats.	PBIO-6365
Minor	Components that use GPL third-party tools now check that the required GPL packages are installed.	PBIO-6016
Minor	Entrez EFetch can now handle PubMed results with an empty abstract.	PBIO-6362
Minor	Search options for EB-eye Search Update Legal Values are now automatically updates.	PBIO-6361
Minor	The Alphabet parameters of Add Reverse Complement Sequence and Reverse Complement Sequence are now case-insensitive.	PBIO-6358
Minor	Open Targets components are updated to use the current API.	PBIO-6314
Minor	By using an API key, Entrez ESearch and Entrez ESearch for Each Data can now send up to 10 requests per second.	PBIO-6306
Minor	Updated the Biology collections to be compatible with Pipeline Pilot infrastructure changes.	PBIO-6296

Severity	Description	Defect
Minor	Moved the Entrez Query parameter of NCBI Online BLASTp and NCBI Online BLASTx to the Implementation tab.	PBIO-6265
Minor	The Destination parameter now supports writing BLAST databases to both the default job directory drive and other Windows drive locations.	PBIO-6262
Minor	Added a parameter, First High Scoring Pair Only, to Convert All Hits to Alignment and Covert Each Hit to Alignment. The default value is True (the original behavior) and will only use the first high scoring pair for each hit. If False, all high scoring pairs will be used to create the output alignment.	PBIO-5933
Minor	Updated the Biology collections be compatible with Pipeline Pilot infrastructure changes.	PBIO-5919
Minor	Updated the BLAST DB Information, BLAST DB Sequence Fetcher, Local PSI-BLAST (BLAST+), Local MegaBLAST (BLAST+), and Add Sequence to BLAST Hit components to work when the database path contains a space.	PBIO-5789
Minor	Enhanced the online BLAST components to no longer produce excessive warning messages.	PBIO-5699
Trivial	Added a parameter, Keep PubMed Abstract HTML Tags , to Entrez EFetch to provides control over HTML tag parsing of PubMed results.	PBIO-6325

Known Issues

This release of the BIOVIA Pipeline Pilot Biology Collections has the following known issues.

Gene Expression Collection

None.

Mass Spec for Proteomics Collection

None.

Next Generation Sequencing Collection

None.

Sequence Analysis Collection

None.

Chemistry Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in the BIOVIA Pipeline Pilot 2021 Chemistry Collection. For information about previous interim releases of BIOVIA Pipeline Pilot 2020, see the Product Release Documents for the interim releases Pipeline Pilot 2020 HF2, Pipeline Pilot 2020 HF3 and Pipeline Pilot 2020 HF4.

New Features

- Added a new component, Clean SCSR Sequence, to improve the layout of the residues in molecules with SCSR sequences or sequences represented by SUP Sgroups.
- Added Unified Data Model (UDM) reader and writer components.
- You can now overrule the internal perception rules in Pipeline Pilot Chemistry for Atropisomers.
- Reagents stored in the RXN file format are now interpreted and displayed correctly, and you can now write RXN files with the reagent information.
- Added Python support for the Molecular Toolkit and Software Development Kit (SDK).

Enhancements

This release of the BIOVIA Pipeline Pilot Chemistry Collection includes the following enhancements.

Description	User Story
Applications launching Pipette Sketcher can now control the output formats returned by using the following URL parameters: <ul style="list-style-type: none">▪ chemistryformat: sd (default), mol▪ reactionformat: rd (default), rxn▪ macromoleculeformat: helm1 (default), helm2 Some sketcher features are disabled by default, but the highlight feature can be enabled by using the enablefeatures URL parameter: enablefeatures=highlight	PCHE-7925
The Generate RGroups, and Generate SAR Information components can now process an input core molecule which contains a doubly-connected R atom. Previously these could not be processed and were ignored.	PCHE-5134
Updated the formats for Molecule to HELM, HELM Writer, Molecule from HELM, HELM Reader components. When HELM version 2 is selected in the HELM writer components, inline SMILES notation will contain R atoms in HELM2 OpenSMILES format rather than CXSMILES format. HELM version 1 will still be written in CXSMILES format. The HELM reader components will accept and process either format for inline SMILES. Added new method to the MolIO class, setUseHELM2Format(boolean flag), for Chemistry Java, .NET, and Python SDK. Calling this method with the argument True selects HELM version 2 output when writing HELM strings. The default (False)	PCHE-7933

Description	User Story
writes HELM strings as version 1, the old behavior of the SDK.	
<p>Added Python molecular toolkit, which supports the same molecular objects and methods in the Perl toolkits.</p> <p>Added Python molecular toolkit example components and protocols, similar to the Perl examples.</p>	PCHE-6068
<p>Added Python as a supported language in the Pipeline Pilot Chemistry SDK. This Python SDK covers all PP Chemistry modules and methods as in the Java and .NET C# chemistry SDK.</p> <p>The SDK python files (*.py) are located in SCIROOT/apps/scitegic/chemistrysdk/bin/lang/python3/ppchemsdk</p> <p>Two new scripts, run_python3.sh and run_python3.bat, are located in SCIROOT/apps/scitegic/chemistrysdk/examples. These will run the same examples that Java runs, these example python scripts are located here: SCIROOT/apps/scitegic/chemistrysdk/python3</p>	PCHE-6069
<p>Pipeline Pilot Chemistry now includes the 2D coordinate calculation algorithm used by the legacy MDL Cheshire product. The chemistry component 2D Coords (Advanced) and the three chemistry SDKs (.NET, Java, and Python) include new options to select and control Cheshire computation of 2D coordinates.</p>	PCHE-6135
<p>The original format of the molecule, V3000 or V2000, is now preserved after processing by the Chemistry Sketcher.</p>	PCHE-6807
<p>Added support for Nextmove reagents.</p>	PCHE-6883
<p>Enhanced the Pipeline Pilot Chemistry depiction components. Improved the layout of the sequence chains found in "Perceive Sequence from Structure". The atomic coordinates of the atoms in the sequence are displayed better now when setting "Show Sequence View" to False and "Display Inter-Residue Bonds in NonSequence View" to True.</p>	PCHE-7420
<p>Changed the names of some of the Hub Centralized Libraries protocols to clarify and reflect better the action that they perform.</p>	PCHE-7752
<p>The Java, .NET, and Python SDK MolIO class now provide all of the same functionality as the Molecule To InChI, Reaction to InChI, and Reaction from InChI components in Pipeline Pilot. All of the conversion options are available and reactions can be created from both InChI and InChI AuxInfo strings.</p>	PCHE-7757
<p>Added two components XD Reader (Hierarchical) and XD Writer (Hierarchical).</p> <p>XD Reader (Hierarchical) creates the hierarchy record represented in the XD file.</p> <p>XD Writer (Hierarchical) creates XD files with hierarchy in the input records.</p>	PCHE-7766
<p>When the StereoChemistry option SUCF (use Chiral Flag, non-standard InChI) is selected and the Chiral flag is On, the InChI will be a Absolute Stereo (\s1). If the Chiral flag is Off, the inChI is Relative Stereo (\s2). The default, UseMolToInChI = false, always generates relative stereo (/s2). InChI cannot pick up the Chiral flag correctly and create the desired InChI. UseMolToInChI = true can pick up the Chiral</p>	PCHE-7784

Description	User Story
flag correctly and create the desired InChI.	
In BIOVIA Draw, display of modified RNA and DNA nucleotides is improved both when converting from HELM and when making a modification to the base, sugar, or phosphate.	PCHE-7793
Enhanced the ChemDraw CDX reader component. When the ChemDraw bracket is SRU, it is converted to the PPChem SRU instead of GEN SGroup.	PCHE-7796
Added support for reagent molecules to the RXN and RD file formats and updated the corresponding reader and writer components in Pipeline Pilot to parse the reagent information.	PCHE-7807
Modified the internal molecular data model in Pipeline Pilot Chemistry to include zero-order bonds (Coordination bonds, Hydrogen bonds) as standard bond types, which is in addition to Single, Double, and Triple bonds. Zero-order bonds are now taken into account in chemical perception operations such as counting of fragments and rings, and in Molecular Toolkit and PPChem SDK scripts that loop over the bonds in the molecule. It is no longer necessary to have separate counters and loops to manipulate zero-order bonds.	PCHE-7808
Enhanced the perception of atropisomer centers. Added two methods for specifying atropisomer centers in a molecule, overruling the internal perception rules in Pipeline Pilot Chemistry.	PCHE-7810
You can add wedges to both sides of the atropisomers center. The wedges must be on one of the single bonds attached to the atoms that bound the atropisomers center. The atoms are not required to be sp ² , but they cannot be valid tetrahedral stereo centers.	
You can also add a DAT Sgroup named ATROP_ST to the atropisomer bond. If you set ATROP_STE to "On", "True", or "Ste", the bond is always perceived as a atropisomer center. If you set ATROP_STE to "Off", "False", or "NoSte", the bond is prevented from being perceived as an atropisomer center.	
Added Reagent as a molecule array in the vcReaction.	PCHE-7811
Added support for reagents.	PCHE-7812
V2000 RXN:	
Updated the COUNT line format: rrrpppggg (when there is reagent in the reaction), rrrppp (when there is no reagent in the reaction).	
The reagent MOL follows the REACTANT and PRODUCT MOLS.	
V3000 RXN:	
RXN COUNT line format: M V30 COUNTS r p g (when there is reagent in the reaction), M V30 COUNTS r p (when there is no reagent in the reaction). The "M V30 BEGIN REAGENT M V30 END REAGENT" block following the REACTANT and PRODUCT blocks when there is reagent in the reaction.	
In the V3000 RXN, the V3000 format CTAB for Reagent uses the optional NAME and	

Description	User Story
<p>COMMENTS keywords for reagent name and reagent role (Catalyst, Solvent ...).</p> <p>Updated RXN Reader to read reagents from V2000 and V3000 format, including RXN file format output from Nextmove and ChemAxon.</p> <p>Updated RXN Writer to write reagents in the RXN file when there are reagents in the reaction.</p>	
<p>Added five methods to support reagents in reactions to the ppchemapi, PPChem SDK, and Molecular Toolkits:</p> <ul style="list-style-type: none"> ■ getNumReagents ■ addReagent ■ addReagents ■ getReagent ■ getReagents 	PCHE-7821
<p>Added "Reagent" as a reaction role to the "Molecules from Reaction" and "Reaction from Molecules" components.</p>	PCHE-7822
<p>Added support for displaying reagents. Added a parameter, "Display Reagents", in "Depiction Options/Reactions" to control the display of reagents in reaction images. "Display Reagents" can display any combination of the reagent name, comments and structure above/below the reaction arrow. The default is all three options are selected.</p> <p>Added a new method: SetReactionDisplayReagents(bool displayName, bool displayComment, bool displayStructure) in the PPChemAPI and SDK.</p>	PCHE-7825
<p>Added a new Java and .NET PPChem SDK method to the Tautomer Generation class, estimateNumTautomers() to estimate the number of tautomers that would be generated for the specified molecule without performing enumeration. The result is returned as a double to cover cases where the estimated number is very large. Calls to this method should be made before calling generateTautomers() or getCanonicalTautomer(). If you call this method after tautomers are generated you would need to generate the tautomers again, as this method reinitializes the tautomer generation engine.</p>	PCHE-7830
<p>Added a new component, Bad Entry Filter, to filter entries with bond query features in \\Chemistry\Utilities\Centralized Library (Hub)\Utilities\.</p> <p>Added the filter to:</p> <ul style="list-style-type: none"> ■ Add Entry To Library (Hub) component, which is used for all protocols to add SCSR or HELM into library ■ Create Configuration Files from SCSR Template File example protocol ■ Create Configuration Files from HELM Monomer File example protocol 	PCHE-7835
<p>Modified perception of hybridization of Nitrogen atoms to harmonize with DiscoveryStudio and to be in better agreement with generally accepted rules.</p> <ul style="list-style-type: none"> ■ Neutral Nitrogen with only single bonds 	PCHE-7843

Description	User Story
<ul style="list-style-type: none"> ■ In PLP 2020 and earlier: only Nitrogens attached to atom with terminal double bond to non-Carbon atom is sp2 ■ In PLP 2021: any Nitrogen attached to an atom with a double bond is sp2 ■ Positively charged Nitrogen with two or fewer single bonds connected to atom with double or triple bonds <ul style="list-style-type: none"> ■ In PLP 2020 and earlier: Nitrogens are sp2 ■ In PLP 2021: Nitrogens are sp3 	
Molecular properties that can be affected by these changes	
<ul style="list-style-type: none"> ■ Num_H_Acceptors ■ Molecular_SurfaceArea, Molecular_FractionalPolarSurfaceArea ■ QED Drug likeness ■ Atom Stereo: Some Nitrogen atoms in rings were perceived as sp3 in PLP 2020 and considered valid stereo centers because of the constrained geometry. The same Nitrogen atoms are now perceived as sp2 and are not stereo centers ■ Num_TerminalRotomers ■ pKa, logD, Ionize at pH: Some pKa queries use “sp”, “sp2”, “sp3” labels as query features Molecules with Nitrogens with different hybridization might match different queries and/or have different calculated pKa ■ 3D Properties: 3D Coords, Conformations, Minimized Energy ■ Pharmacophore Fingerprints ■ Different Sybyl Mol2 format atom types ■ Output from learned regression or classification models that use any of the molecular descriptors that are affected 	
<p>Note: Extended Connectivity Fingerprints (ECFP, FCFP) are not affected.</p>	
Chemdraw version19 is a supported version in Sketcher Integration.	PCHE-7869
<p>Added a parameter, Direct Version Compatibility, to the Create Direct Database and Add to Direct Database components. By default this parameter is set to allow the components to work with Direct 2021 and previous versions of Direct such as 2019. This default setting requires the use of JDBC as the connection protocol—using ODBC results in an error.</p> <p>The parameter can also be set to allow updates only to the current version of Direct (2021). With this setting, either JDBC or ODBC can be used for the connection to Oracle, and performance (speed of registering records) is better.</p> <p>This change was required due to modifications made to the binary molecule format used in Pipeline Pilot and Direct—the 2021 format is not compatible with any previous versions of Pipeline Pilot or Direct.</p>	PCHE-7870
Added a component, UDM Reader, to read Pistoia Alliance's Unified Data Model	PCHE-7873

Description	User Story
(UDM) files and create a reaction record with hierarchical properties for each reaction in the input file. UDM files are supported up to Version 5, with an option to output Citation, Molecule, or Reaction records. UDM formatted files has a defined hierarchy and vocabulary (UDM documentations in https://www.pistoiaalliance.org/projects/current-projects/udm).	
Created a component, UDM Writer, that writes a Pistoia Alliance's Unified Data Model (UDM) formatted file with input reaction records. UDM files are supported up to Version 5. UDM formatted files has a defined hierarchy and vocabulary (UDM documentations in https://www.pistoiaalliance.org/projects/current-projects/udm).	PCHE-7874
Pipette Sketcher version 3.2.8 includes a fix to preserve the original bond types in haptic ring systems instead of marking them as query aromatic bonds.	PCHE-7898
Updated the CTFile format document to include the extensions added to support the representation of reagents in reactions.	PCHE-7901
The PPChem Java SDK is now compatible with JVM versions 8 and higher.	PCHE-7915
Included protocols used internally by BIOVIA Draw to connect to the Hub centralized library and to run from the Draw Pipeline Pilot protocols interface in standard packages in the Pipeline Pilot Chemistry collection (scitegic/chemistry and scitegic/chemistryhub)	PCHE-7916
The PPChem SDK folder is no longer created by the Pipeline Pilot installer when the PP Chemistry Collection is installed. The PPChem SDK is now available only as a separate download, requiring its own license.	PCHE-7919
Added three functions to the PilotScript implementation of the Molecular Toolkit: MolRingAssemblyAtoms, MolRingAssemblyBonds and MolRingAssemblyRings. In previous versions, these functions were only available in the Perl, Java and Python implementations.	PCHE-7934
Removed the Full Data option from the Enumerate Bioisosteres, Identify Bioisosteres, Enumerate Metabolites, and Identify Metabolites components. Only the partial subsets of the data from the Bioster and Metabolism databases are now available. Access to the full data requires a valid license to the Bioster and Metabolism databases, which is no longer available from BIOVIA.	PCHE-7937
Added support for subscript "\s" and superscript "\S" in the Name and Comment field of the reagent molecule CTAB in molecular depictions.	PCHE-7963
Added two methods to the .NET, Java, and Python SDKs that allow you to define more than one HELM-SCSR monomer map file used when converting between HELM string and molecule.	PCHE-7974
Updated the Sketcher Integration dependency for JQuery to 3.5.1.	PCHE-7981
Added "21.1" to the default list of supported versions of BIOVIA Draw.	PCHE-7989
Fixed a problem in the depiction of molecules with adjacent MUL Sgroups sharing the same link bond. The link bonds, which were not being displayed, are now	PCHE-7994

Description	User Story
correctly displayed.	
Pipette 3.3.0 now supports RXN and RD file formats with reagent extensions, and supports adding and modifying reagents above and below the reaction arrow.	PCHE-8032
The PPChem SDK folder can now be downloaded to any location.	PCHE-8038
Updated the "Set Up BIOVIA Desktop Connector" page with information on how to use a non-default web service port configured on the Messaging Service server.	PCHE-8061
Added a component, Clean SCSR Sequence, to improve the layout of the residues in molecules with SCSR sequences or sequences represented by SUP Sgroups. The atomic coordinates of each residue in the sequence, both contracted and expanded, are recalculated, translated, and rotated in order to connect each residue to the previous residue in the sequence, leaving enough space to display the expanded residues. This generates an extended linear conformation for the sequence when visualized as a structure in molecular depictions ("Show Sequence View" set to False in the Pipeline Pilot Chemistry depiction components). This functionality is also exposed in the PPChem .NET SDK, and is used by BIOVIA Draw.	PCHE-8063

Fixed Defects

This release of the BIOVIA Pipeline Pilot Chemistry Collection includes the following fixed defects.

Severity	Description	Defect
Major	Fixed the Bond.setStereo() method in the Java PPChem SDK to correctly assign the specified stereo state (Up, Down, Cis, Trans) instead of changing the bond type (Single, Double, Triple).	PCHE-7832
Major	Added two parameters to the Calculate CIP Chirality component and corresponding PPChem SDK APIs. Maximum Number of Shells: Sets the maximum number of shells allowed before the CIP calculation stops for the stereo atom being processed. The number of shells is related to the depth of the molecular graph followed from the stereo atom. If the maximum number of shells is reached, the CIP value ComplexMaxShells is assigned to the atom. Maximum Number of Nodes: Sets the maximum number of nodes allowed before the CIP calculation stops for the stereo atom being processed. The number of nodes is related to the number of possible paths to follow in the molecular graph starting from the stereo atom. If the maximum number of nodes is reached, the CIP value ComplexMaxNodes is assigned to the atom.	PCHE-7880
Major	When using the Molecule to CTAB component, the CTAB in the input molecule is kept unchanged.	PCHE-7906
Major	Fixed the Help button Pipette Sketcher to point to the appropriate page.	PCHE-7908
Major	Fixed an issue with Enumerate Repeat Units that could cause a crash for molecules with more than one multiple groups (MUL Sgroups) in previous	PCHE-7941

Severity	Description	Defect
	releases.	
Major	Fixed issue in Perceive Sequence from Structure to avoid crashes when processing some structures with unusual connections.	PCHE-7977
Major	Fixed a problem in the Molecular Toolkit and PPChem SDK method used to define new MUL Sgroups in a molecule. In previous releases, this method did not correctly handle cases where the MUL Sgroup consisted of one atom. Also, even for MUL Sgroups with more than one atom, sometimes the connectivity of the atoms in the MUL duplicate copies was not assigned correctly, creating molecules with multiple disconnected fragments.	PCHE-8000
Major	Improved the parsing of DAT Sgroups FIELDDISP lines in V3000 mol files to make it more robust and handle cases where the line is not in exactly the same fixed-string format used in V2000 mol files.	PCHE-8008
Major	The XD Reader now uses the original date string if applying the meta data format to the date results in "**/**/**".	PCHE-8014
Major	Removed the "Create SCSR Template Library From BIOVIA Draw Template Definition File" example protocol. Its function is covered by the "Create Configuration Files from SCSR Template File" example and "Create SCSR Library from Template File" in Web Port.	PCHE-8021
Major	Fixed an issue with XD writer and XD writer (Hierarchical). The <XDfile> tag is changed to <XDfile> in the output XD files.	PCHE-8028
Major	Changed the default format for transferring reactions from Pipette Sketcher to the sketcher window in browser pages from RD format to RXN format.	PCHE-8031
Minor	Fixed an issue where an oxygen in the cross-link was removed by mistake when expanding cross-linked residues. This only affects unusual cross-links. The example was between the oxygen in glutamic acid and a carbon in the phenylalanine phenyl ring.	PCHE-5292
Minor	Pipeline Pilot data for isotopic mass and composition have been updated to the latest values from the NIST website (http://physics.nist.gov). Half life data have been updated to the latest (2016) values from the AMDC website (http://amdc.in2p3.fr/web/nubase_en.html). The affected file is in chemistry data, IsotopeData/IsotopeData.txt.	PCHE-6086
Minor	The Remove Hydrogens component no longer removes hydrogen atoms that are the sole leaving atom in sequence superatoms. Peptide superatoms now retain their N-terminus hydrogen leaving atom, plus any cross-link hydrogen leaving atoms (such as in histidine).	PCHE-6986
Minor	The Mol2 Reader component now correctly computes the kekule form for all histidines.	PCHE-7239
Minor	Fixed a problem drawing Pi Systems with a -1 negative charge using the EMF format in molecular depictions. The negative symbol didn't appear in the depictions in previous releases.	PCHE-7569

Severity	Description	Defect
Minor	Fixed an issue with Perform Reaction on Each Molecule and Perform Reaction from Tag. Reactions from SMIRKS strings with aromatic atom types now generate the appropriate pattern of single and double bonds in the modified input molecules.	PCHE-7795
Minor	Improved usability for Enumerate using RGroups, which does not support cases where the core molecule has two R atoms connected to the same atom and the fragment has the corresponding two Z atoms connected to the same atom. Molecules enumerated for this combination of core and fragment had bad connectivity (duplicate bonds connecting the same atoms), which caused problems downstream. Added a check to catch this case and throw an exception saying "ExchangeBonds given atoms to bond which are already bonded". Users can configure the component to send these cases to the Fail port.	PCHE-7797
Minor	Fixed handling of X atoms (query feature representing any halogen atom) in the Query Features Filter and Check and Normalize Structure components. X atoms are now correctly perceived as query features, and can be allowed by listing them in the Allow These Non-Standard Elements parameter.	PCHE-7809
Minor	Pipette sketcher version 3.2.7 has a fix for an issue observed in previous versions when loading V2000 molfiles with molecules with one stereo center marked as AND ENANTIOMER (chiral flag Off). The configuration of the stereo center was being changed to ABS. This is no longer the case in the new version, the AND ENANTIOMER configuration is preserved.	PCHE-7828
Minor	Pipette sketcher can correctly perceive stereo labels for V2000 files, the "AND Enantiomer" is no longer displayed as Absolute stereo.	PCHE-7829
Minor	Improvements have been made converting legacy SCSR sequence structures containing modifications to HELM strings.	PCHE-7837
Minor	The Java, C#, and Python SDK function MolIO.findMolecularFormat() now returns the correct format when presented with a HELM string as input. Previously the function returned the format as Unknown.	PCHE-7860
Minor	The Replace Murcko Assemblies component now makes sure that fragments connected to the original scaffold by double bonds are connected to replacement scaffolds also by double bonds instead of by single bonds as in previous releases. Added a new parameter, Include Exocyclic and Exolinker Double Bonds in Scaffold, to control whether or not to include terminal double bonds connected to rings or to linkers as part of the original scaffold. The new parameter is set to True by default to preserve the previous behavior.	PCHE-7863
Minor	Added checks for isotopes in the Perceive Sequence from Structure component to prevent standard residues to map substructures with isotopes, which are identified as unknown residues.	PCHE-7875
Minor	Modified the depiction of structures that combine biological sequences and unattached small molecules. When the depiction parameter Show Sequence	PCHE-7878

Severity	Description	Defect
	View is set to True and Show Expanded Sequence Structure is set to False, the unattached small molecule atoms and bonds are not displayed. When both parameters are set to True, the unattached small molecule atoms and bonds are displayed. In previous releases the unattached small molecules were always displayed.	
Minor	Updated the Direct Database component so that it only updates those columns in the Direct table in Oracle that have corresponding properties in the Pipeline Pilot data record. This change is required to support Oracle 19c, and also prevents the component from overwriting existing column data with NULL when the data record does not include a property for that column.	PCHE-7894
Minor	Updated the .NET PPChemSDK examples to use a Visual Studio solution file that is compatible with Visual Studio 2017.	PCHE-7913

Severity	Description	Defect
Minor	<p>Fixed an issue where a molecule or reaction containing a symmetrically tetra-substituted double bond (one that cannot be cis or trans) might not match itself with a FLEXMATCH search. The same symmetrically tetra-substituted structure with an "either" double bond might not match the structure with the normal double bond.</p> <p>Newly inserted molecules or reactions will search correctly, structures in existing databases must be updated to correct the problem. Locate these structures using mdlaux.scanindex with the 'CTAB' argument. Any structures that do not find themselves, but which do find themselves when ignoring stereochemistry, should be updated.</p> <p>For example:SQL> execute mdlaux.scanindex('mdctestix', 'ctab'); BEGIN mdlaux.scanindex('mdctestix', 'ctab'); END; * ERROR at line 1: MDL-1152: Molecule CTAB scan has errors, use MDLAUX.LOGTABLE to view errors MDL-1112: MDLAUX.SCANINDEX has warnings or errors, use MDLAUX.LOGTABLE to view them ORA-06512: at "C\$DIRECTS2021.MDLAUXOP", line 4895 ORA-06512: at "C\$DIRECTS2021.MDLAUXOP", line 4885 ORA-06512: at line 1 SQL> select msg from table(mdlaux.logtable('mdctestix', 'asc')); MSG</p> <hr/> <p>Scanning molecule index MDCTESTIX on table MDCTEST.MDCTEST Scanning ROWID conversion table ROWID conversion table scan complete, there are 2 rows Scanning molecule CTABs Molecule at ROWID=AANqImAAPAAAADmAAA cannot find itself with FLEXMATCH Molecule at ROWID=AANqImAAPAAAADmAAA does find itself with FLEXMATCH when ignoring stereochemistry and data Sgroups (IGNORE=STE,DAT) Previous message occurred at ROWID=AANqImAAPAAAADmAAB Molecule CTAB scan has errors SQL> update mdctest set ctab=mol(molfile(ctab)) where rowid = 'AANqImAAPAAAADmAAB'; 1 row updated. SQL> commit; Commit complete.</p>	PCHE-7935

Severity	Description	Defect
Minor	Fixed a problem with molecular depictions to ensure that the query operator in DAT Sgroups attached to GEN Sgroups is displayed in the depictions when it is defined. Also, removed the display of "eu" as bracket type for GEN Sgroups.	PCHE-7944
Minor	BIOVIA Draw can now import HELM or XHELM strings that contain sugars such as am6 which can not have a connection to a base, for example: RNA1{{am6}P.R(C)}\$\$\$\$	PCHE-7945
Minor	Fixed issue in molecular depictions that prevented the brackets from being displayed correctly for some GEN Sgroups where one of the brackets has no link bonds crossing it.	PCHE-7967
Minor	Fixed an issue with the Perform Reaction on Each Molecule component where it might assign a valence of (IV) to the modified nitrogen when transforming a charged nitrogen to an uncharged nitrogen.	PCHE-7978
Minor	The "Calculate CIP Chirality" component now skips the calculation of E/Z configuration for double bonds adjacent to other double bonds, such as in A-N=P=N-A substructures.	PCHE-7984
Minor	The SD Writer component now includes crossing bonds to MER polymer subunits when writing an SDFFile.	PCHE-7987
Minor	You are now warned when running the HUB protocols from Web port and there is no library of the selected type.	PCHE-8006
Minor	When converting a reaction with reagents to RInChI string, the conversion now ignores the reagents and creates RInChI with reactants and products only. RInChI v 1.0 does not support reagents in reaction.	PCHE-8026
Trivial	When deleting one or more atoms from a molecule containing a MUL sgroup the coordinates of the brackets surrounding the MUL group of atoms are no longer removed. The molecule is now displayed correctly in BIOVIA Draw.	PCHE-7754
Trivial	Fixed an issue that occurred when reading a MOL2 file containing a thiophosphate that has explicit hydrogens on the thiophosphate oxygens. Charges or double bonds are no longer added to the oxygens.	PCHE-7871
Trivial	Provided a Pipeline Pilot protocol as a workaround to process and preserve name-value properties attached to structures in ChemDraw files after reading them with the ChemDraw Reader in Pipeline Pilot.	PCHE-7979

Known Issues

This release of the BIOVIA Pipeline Pilot Chemistry Collection has the following known issues.

Severity	Description	Defect
Major	In the depiction code in Pipeline Pilot Chemistry, when 2D Coords are calculated for a molecule with MUL groups, the atoms in the MUL groups that overlap in the original file are expanded. To indicate that there is still a MUL group present the MUL group brackets are drawn with a repeat count of 1. This can be confusing and not consistent with the display of the expanded structure in other applications such as BIOVIA Draw.	PCHE-6488
Major	The SD Reader does not correctly read structures with bracket Sgroups that include Markush bond definitions.	PCHE-7774
Minor	Stereochemical perception of stereo centers in highly symmetrical caged molecules, such as adamantyl derivatives, might produce the wrong values for counters, such as Num_UnknownTrueStereoatoms.	PCHE-5116
Minor	The ChemDraw Reader can only read the first level of grouping in CDX files. If there are multiple levels of grouping, it cannot see the chemistry. To work around this issue, open the structures in ChemDraw and remove the nested grouping.	PCHE-6108
Minor	The Query Features Filter component does not see *-atoms as query features. Although a *-atom is a wildcard feature in the SMARTS format, it is often used as a non-query attachment point marker in MDL formatted files (for example, in polymers).	PCHE-6309
Minor	The Molecule to Chemical Name component, which uses OpenEye libraries, does not output the correct chemical name if there is mixed enhanced stereochemistry. OpenEye is aware of this issue.	PCHE-6330
Minor	The RD Writer only adds the extra \$MFMT tag to \$DATUM fields containing molecular structure information if the property name is "MOLSTRUCTURE". This does not affect the behavior of subsequent RD reads in Pipeline Pilot; these fields are read in as text with or without the \$MFMT marker. Some third-party products might rely on the \$MFMT marker.	PCHE-6347
Minor	The SKC Reader component converts abbreviation labels into deprecated atom aliases.	PCHE-7087
Minor	The Molecule from Chemical Name component fails on simple halogen names, such as Iodine and Chlorine.	PCHE-7342
Minor	In Pipette Sketcher, editing and display of complementary RNA strands and converting to SCSR format for display in applications such as Insight and Biological Registration are not fully supported.	PCHE-7454

Severity	Description	Defect
Minor	Components that check structures and the corresponding PilotScript functions sometimes generate different results.	PCHE-7546
Minor	The Calculate CIP Chirality component returns "NotApplicable" for one of two pseudochiral centers when there is another meso/pseudochiral center in other parts of the molecule.	PCHE-7561
Minor	Pipette Sketcher does not display the 'ABS' or "Chiral" label.	PCHE-7615
Minor	Some symmetric ring systems and relative stereochemistry, such as 1,4 cyclohexanes and other systems with a plane of symmetry, are not named correctly by the OpenEye OEChem toolkit, which is called by the Molecule to Chemical Name component.	PCHE-7663
Minor	The creation of SMILES from structures with enhanced stereochemistry in BIOVIA Direct, BIOVIA Draw, and PPChem is inconsistent. While BIOVIA Direct smiles and mdlaux.smiles operators return NULL for such molecules, BIOVIA Draw and PPChem convert the enhanced stereochemistry to absolute stereochemistry, and then they create the SMILES from the results.	PCHE-7841
Minor	Polymer structures sketched in ChemDraw might show incorrect searching behavior when converted to mol files with bracketed Sgroups (SRU, GEN and others) by the Pipeline Pilot ChemDraw Reader.	PCHE-7868

Documents and Text Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in the BIOVIA Pipeline Pilot 2021 Documents and Text Collection. For information about previous interim releases of BIOVIA Pipeline Pilot 2020, see the Product Release Documents for the interim releases Pipeline Pilot 2020 HF2, Pipeline Pilot 2020 HF3 and Pipeline Pilot 2020 HF4.

New Features

- Search SharePoint Online/Office 365
- Tweets now returned by the “Search Twitter” component

Enhancements

This release of BIOVIA Pipeline Pilot Documents and Text includes the following enhancements.

Description	User Story
New components allow searching of SharePoint Online/Office 365.	TXT-1007
The <i>Search Twitter</i> component now returns extended tweets.	TXT-1041

Fixed Defects

This release of BIOVIA Pipeline Pilot Documents and Text includes the following fixed defects.

Severity	Description	Defect
Minor	The <i>HTML Table Reader</i> now handles embedded tables better.	TXT-1040
Minor	The example protocol <i>08 Browse MeSH Concept Dictionary</i> now loads PubMed results in a new browser tab.	TXT-1044
Minor	The <i>Search SharePoint</i> components are now <i>Owner Access Only</i> , so the components cannot be expanded in the Pipeline Pilot Client.	TXT-1042
Minor	The example protocol <i>03 Simple Crawler using Web Harvest</i> now displays web pages crawled from the 3DS website.	TXT-1033

Known Issues

This release of BIOVIA Pipeline Pilot Documents and Text has the following known issues.

None.

Imaging Collection Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in the BIOVIA Pipeline Pilot 2021 Imaging Collection. For information about previous interim releases of BIOVIA Pipeline Pilot 2020, see the Product Release Documents for the interim releases Pipeline Pilot 2020 HF2, Pipeline Pilot 2020 HF3 and Pipeline Pilot 2020 HF4.

New Features

- Added a component, Learn CNN Image Segmenter, that trains a segmentation model from labelled data.

Enhancements

This release of the BIOVIA Pipeline Pilot Imaging Collection includes the following enhancements.

Description	User Story
Added a new component, Learn CNN Image Segmenter.	IMG-2783
Tensorflow 2.2 is included in shipped libraries.	IMG-2773
Exposed TensorFlow "Batch Size" as a parameter in the Learn CNN Image Classifier component.	IMG-2728

Fixed Defects

This release of the BIOVIA Pipeline Pilot Imaging Collection includes the following fixed defects.

Severity	Description	Defect
Minor	Fixed a broken link in the parameter help for the Learn CNN Image Classifier component.	IMG-2727
Minor	Fixed a minor "globals leak" by declaring <code>_togglerID_</code> to be a local variable in the Image Toggler Viewer component.	IMG-2633

Known Issues

This release of the BIOVIA Pipeline Pilot Imaging Collection has the following known issues.

Severity	Description	Defect
Major	Models built with Learn CNN component do not follow data modeling output naming standard.	IMG-2725

Laboratory Analytics Collection Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in the BIOVIA Pipeline Pilot 2021 Laboratory Analytics Collection. For information about previous interim releases of BIOVIA Pipeline Pilot 2020, see the Product Release Documents for the interim releases Pipeline Pilot 2020 HF2, Pipeline Pilot 2020 HF3 and Pipeline Pilot 2020 HF4.

New Features

This is a maintenance release. There are no new features.

Enhancements

None.

Fixed Defects

None.

Known Issues

None.

Material Studio Collection Release Notes

Customers will not be able to access Materials Studio Collection's components from Pipeline Pilot 2021 client until the release of Materials Studio 2021 at a later time.

Note: The Pipeline Pilot Admin Portal nevertheless lists "Materials Studio Collection version 21.1.0.2519" as present. This is a consequence of dependencies that Discovery Studio 2021 has on some Materials Studio executables that are therefore installed. This does not indicate availability of Materials Studio Collection 2021.

Notebook Collection Release Notes

This section provides information about the new features, enhancements, fixed defects, and known issues in the BIOVIA Pipeline Pilot Notebook Collection 2021. For information about previous interim releases of BIOVIA Pipeline Pilot 2019, see the Product Release Documents for the interim releases Pipeline Pilot 2020 HF2, Pipeline Pilot 2020 HF3, and Pipeline Pilot 2020 HF4.

New Features

- **None.**

Enhancements

Description	User Story
It is now possible to create and delete groups using the Notebook Component Collection.	ANC-246
The Get Current User Info component now retrieves all the groups for which the current user has administrative privileges.	ANC-245
A component now exists to retrieve groups and users that are members of another group.	ANC-244
Project administration is now possible by means of the Notebook Component Collection.	ANC-243
You can now add and edit PowerPoint Presentation sections to Notebook experiments using the Notebook collection for Pipeline Pilot. You must update your protocols with the new version of these components to access the new section type. Note: The Extract Sections from Experiment and Section Query component interfaces and behavior have changed. For new and existing protocols, these components now only retrieve sections of all types if you set the new What To Extract parameter to All Section Types.	ANC-242
Users can add and edit user-defined references and site-specific lookup sections from Pipeline Pilot, using the Add/Edit Local Lookup Section and Add/Edit Site Specific Lookup Section components.	ANC-233

Fixed Defects

Severity	Description	Defect
Minor	The flag for a limiting reagent is now preserved when the content of a Chemical Reaction section is updated.	ANC-251
Minor	Files are now written to individual folders to avoid overwriting when two or more files have the same name.	ANC-250
Minor	The Experiment Query component now retrieves experiments in projects with commas in their names.	ANC-212

None. See above.

Known Issues

This release of the BIOVIA Material Studio Collection has the following known issues.

None.