Biologics Explorer Software

Biologics Explorer Software Quick Guide

Powered by Genedata Expressionist®

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Biologics Explorer Software

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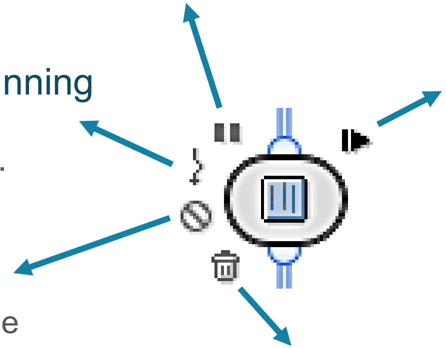
Activity Node Icons



Pause: Pause the workflow here.
All subsequent tasks stay active.

Run
or **Reset**.

Bypass: Skip this task when running the workflow.
All subsequent tasks continue to run.

Block: Stop the workflow.
This and all subsequent tasks become unavailable (gray).

Trash: Do not save intermediate data.
When this icon is activated, the results for this particular activity node cannot be opened.
Use this icon to help to save memory after workflow settings have been optimized.

Workflow Icons

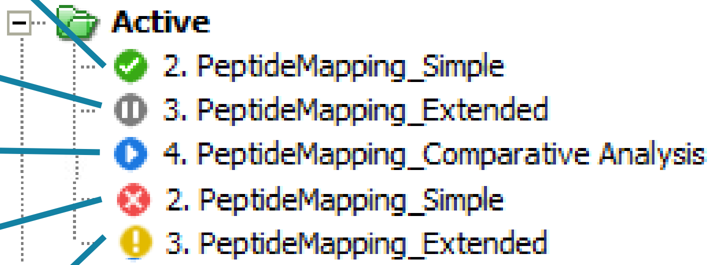
Workflow Completed
All activity nodes have completed successfully.

Workflow Paused
Some activity nodes have been completed successfully, but some have not yet started.

Workflow Ready
No activity nodes have been completed. The workflow is ready to start.

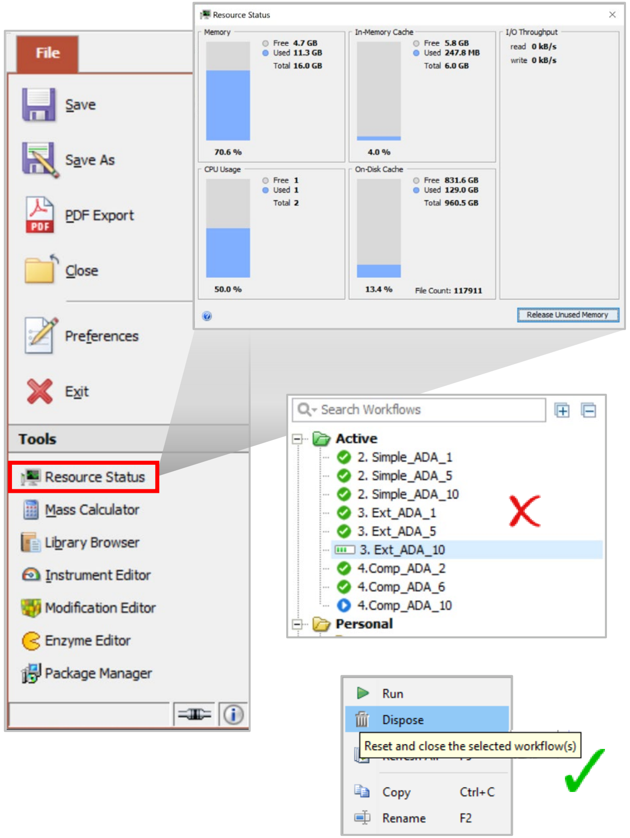
Workflow Error
Some activity nodes have been completed successfully, but at least one activity node cannot run.

Workflow Warning
Some activity nodes are not complete.



Active
- ✓ 2. PeptideMapping_Simple
- ⏸ 3. PeptideMapping_Extended
- ▶ 4. PeptideMapping_Comparative Analysis
- ✗ 2. PeptideMapping_Simple
- ! 3. PeptideMapping_Extended

Recommendations for Correct Use of the Resources



Memory: Free 4.7 GB, Used 11.3 GB, Total 16.0 GB, 70.6 %

In-Memory Cache: Free 5.8 GB, Used 247.8 MB, Total 6.0 GB, 4.0 %

I/O Throughput: read 0 kB/s, write 0 kB/s

CPU Usage: Free 1, Used 1, Total 2, 50.0 %

On-Disk Cache: Free 831.6 GB, Used 129.0 GB, Total 960.5 GB, 13.4 %, File Count: 117911

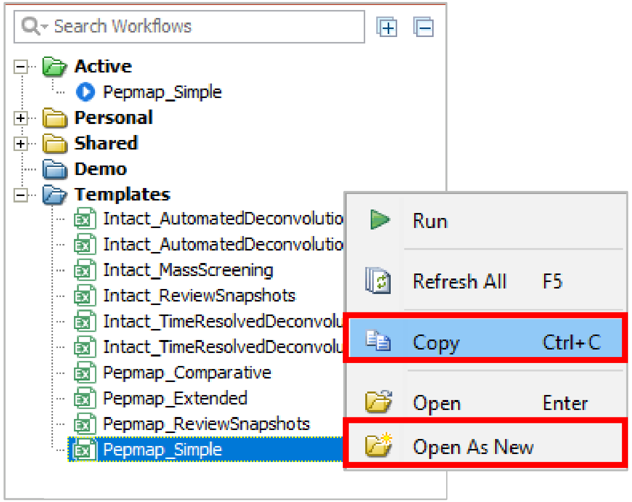
Reset and close the selected workflow(s)

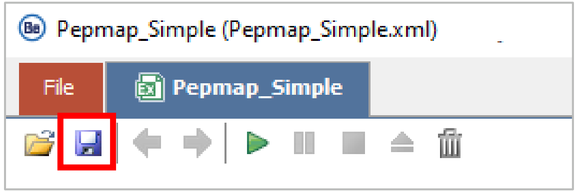
- Some activity nodes are very resource intensive. Processing multiple workflows might use up all resources.
  - Open the **Resource Status** from the **Tools** menu to monitor the resources.
- Follow best practices to make sure that Biologics Explorer software has sufficient memory and computing power:
  1. To save memory in optimized workflows, activate the **Trash** icon.
  2. To save intermediate results, use the *Save Snapshot* activity nodes.
  3. To review results, use the ReviewSnapshots workflows.
  4. Reset or dispose workflows before starting a new analysis.
- The processing computer should have at least 250 GB of free disk space and 6 GB of In-Memory Cache.
  - Files being processed for peptide mapping workflows (other than Batch Processing) should not add up to more than 4 GB.
  - Files being processed for intact protein workflows (other than Batch Processing) should not add up to more than 12 GB.

How to Start and Save Workflows

To start a new analysis, do one of the following:

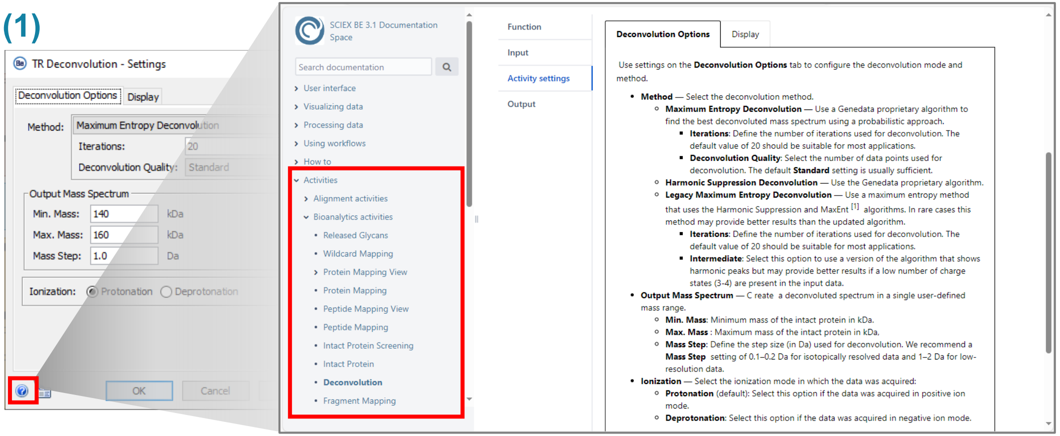
- Move a workflow from the ***Templates*** folder:
    1. Right-click the workflow, and then click **Copy***.*
    2. Right-click the ***Personal*** folder, and then click **Paste**.
- Open a workflow in the ***Templates*** folder:
    1. Double-click the workflow.
    2. To save the workflow in the ***Personal*** folder or the ***Shared*** folder, use the **Save** icon.
        - Any changed settings will be saved in this version of the workflow.
- Open a workflow from the ***Personal*** folder:
    1. Right-click the workflow, and then click **Open As New**.
    2. To save the workflow in the ***Personal*** folder or the ***Shared*** folder, use the **Save** icon.
        - Any changed settings will be saved in a new version of the workflow.





How to Access the Online Help

(1)



Method: Maximum Entropy Deconvolution
Iterations: 20
Deconvolution Quality: Standard

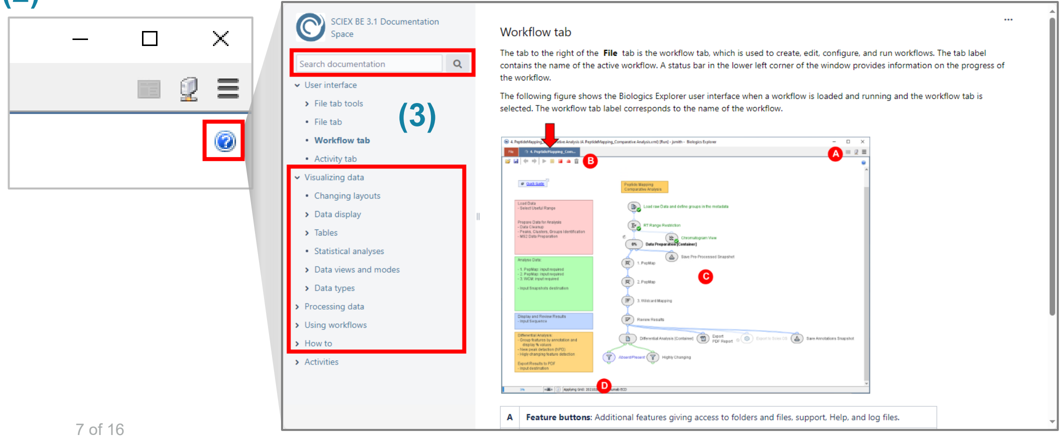
Output Mass Spectrum
Min. Mass: 140 kDa
Max. Mass: 160 kDa
Mass Step: 1.0 Da

Ionization: ● Protonation ○ Deprotonation

Use settings on the **Deconvolution Options** tab to configure the deconvolution mode and method.

- **Method** — Select the deconvolution method.
  - **Maximum Entropy Deconvolution** — Use a Genedata proprietary algorithm to find the best deconvoluted mass spectrum using a probabilistic approach.
    - **Iterations**: Define the number of iterations used for deconvolution. The default value of 20 should be suitable for most applications.
    - **Deconvolution Quality**: Select the number of data points used for deconvolution. The default **Standard** setting is usually sufficient.
  - **Harmonic Suppression Deconvolution** — Use the Genedata proprietary algorithm.
  - **Legacy Maximum Entropy Deconvolution** — Use a maximum entropy method that uses the Harmonic Suppression and MaxEnt [1] algorithms. In rare cases this method may provide better results than the updated algorithm.
    - **Iterations**: Define the number of iterations used for deconvolution. The default value of 20 should be suitable for most applications.
    - **Intermediate**: Select this option to use a version of the algorithm that shows harmonic peaks but may provide better results if a low number of charge states (3-4) are present in the input data.
- **Output Mass Spectrum** — C reate a deconvoluted spectrum in a single user-defined mass range.
  - **Min. Mass**: Minimum mass of the intact protein in kDa.
  - **Max. Mass** : Maximum mass of the intact protein in kDa.
  - **Mass Step**: Define the step size (in Da) used for deconvolution. We recommend a **Mass Step** setting of 0.1–0.2 Da for isotopically resolved data and 1–2 Da for low-resolution data.
- **Ionization** — Select the ionization mode in which the data was acquired:
  - **Protonation** (default): Select this option if the data was acquired in positive ion mode.
  - **Deprotonation**: Select this option if the data was acquired in negative ion mode.

(2)



Workflow tab

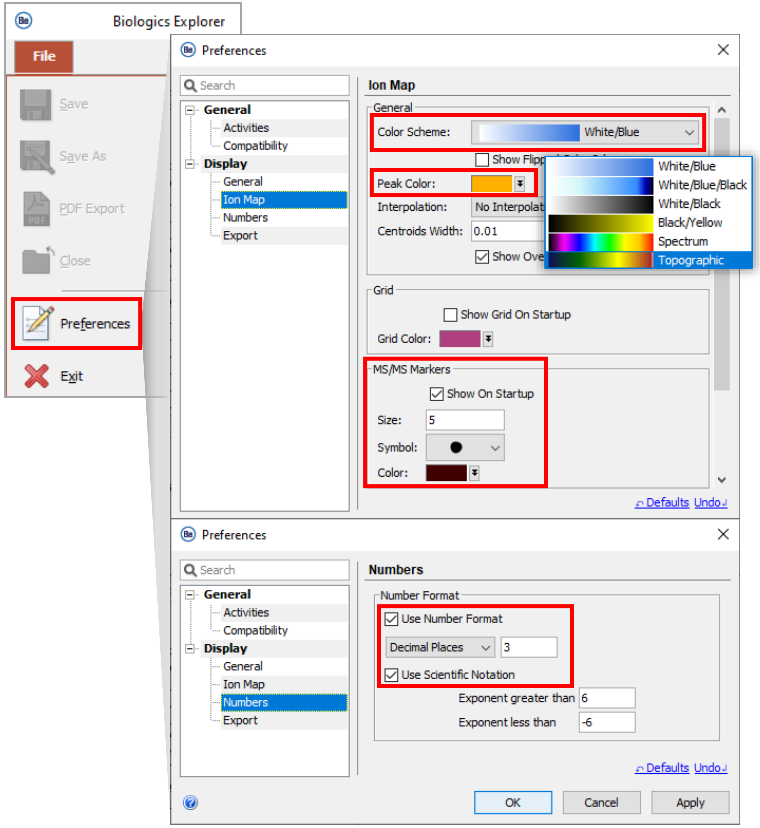
The tab to the right of the **File** tab is the workflow tab, which is used to create, edit, configure, and run workflows. The tab label contains the name of the active workflow. A status bar in the lower left corner of the window provides information on the progress of the workflow.

The following figure shows the Biologics Explorer user interface when a workflow is loaded and running and the workflow tab is selected. The workflow tab label corresponds to the name of the workflow.

A **Feature buttons**: Additional features giving access to folders and files, support, Help, and log files.

1. For information about individual activity nodes and their settings, click the **?** icon in the lower left corner of the settings window to open the applicable Help pages.
2. For information about the user interface, click the **?** icon in the upper right corner of the window to open the applicable Help pages.
3. For information about how to visualize data, use workflows, or any other topic of interest, expand the sections listed in the Help pages, or type into the Search bar.

How to Visualize Data: Preferences



Ion Map

General

Color Scheme: White/Blue

☐ Show Flipp

Peak Color:

Interpolation: No Interpolat

Centroids Width: 0.01

☑ Show Ove

Grid

☐ Show Grid On Startup

Grid Color:

MS/MS Markers

☑ Show On Startup

Size: 5

Symbol: ●

Color:

Numbers

Number Format

☑ Use Number Format

Decimal Places 3

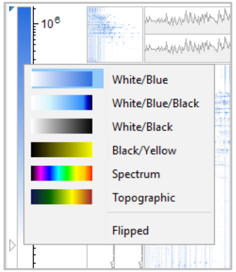
☑ Use Scientific Notation

Exponent greater than 6

Exponent less than -6

- To set how data is shown in Biologics Explorer software, select **Preferences** on the red **File** tab.

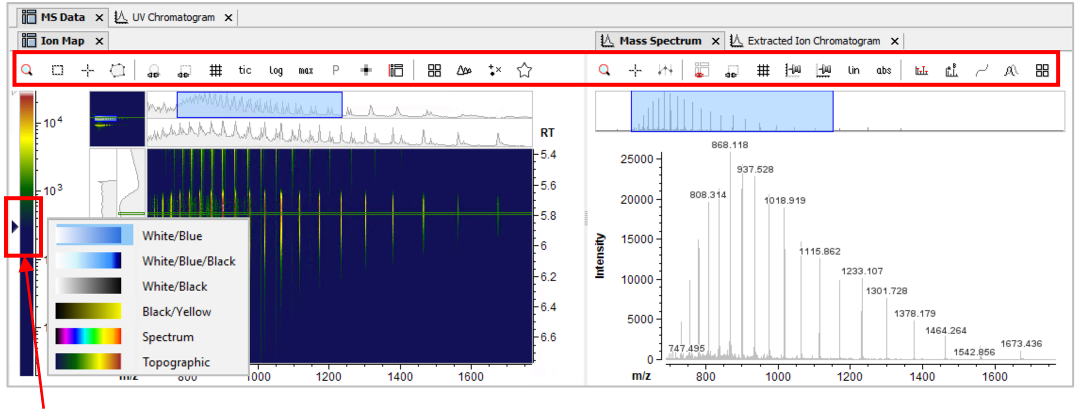
- **Display: Ion Map**
  - Select the ion map **Color Scheme** that is shown by default when a data file is opened.
    - To use a different color scheme for an ion map, right-click the color scale in the ion map window.



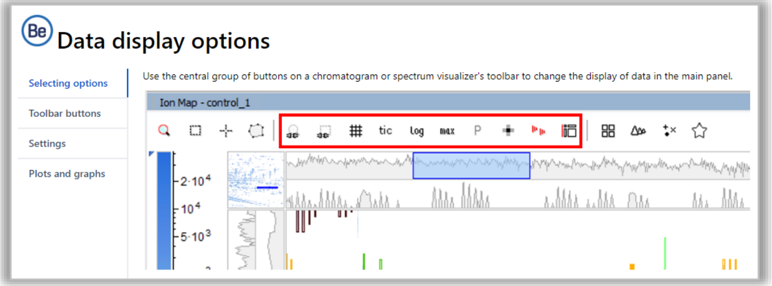
  - Select the **Peak Color** for the peak boundaries.
  - Select the color and symbol for MS/MS data and if they are shown by default when data is opened.

- **Display: Numbers**
  - Select the number format to be used by default.

How to Visualize Data: Useful Tools



- Move the slider to control the noise level that is seen in the ion map.
- Right-click to select the color-scheme.



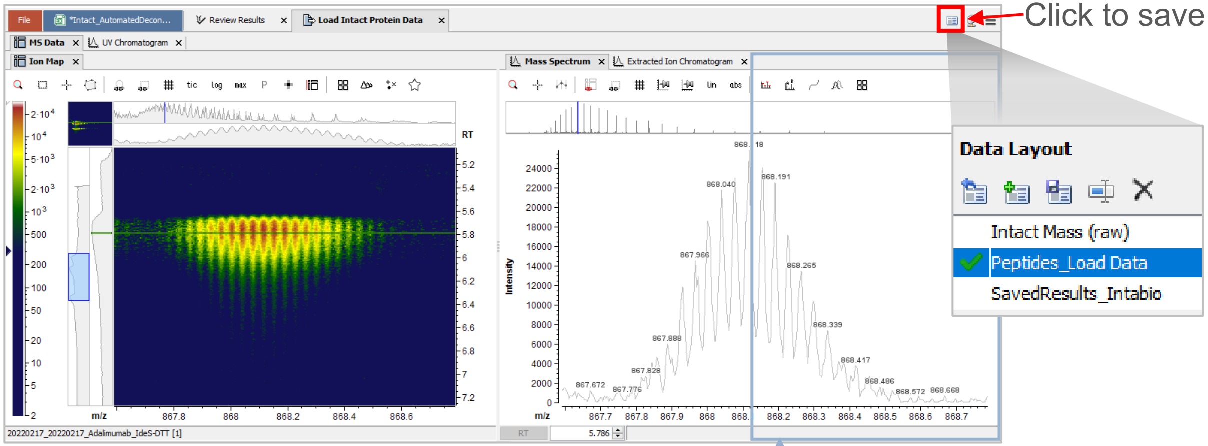
Data display options

Use the central group of buttons on a chromatogram or spectrum visualizer's toolbar to change the display of data in the main panel.

Note: For more information about data display options, use the Online Help.

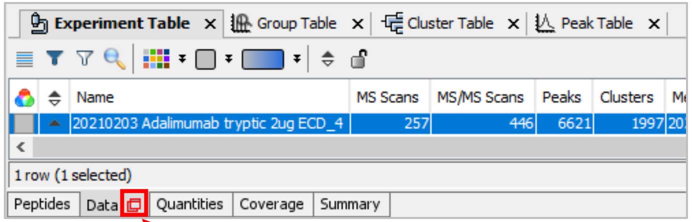
- Use the Visualizer Tools to control the data display options.
  - The Tool icons are context-dependent.
    - For example, the option to **Show/Hide MS/MS Precursors** (MS MS) is only available if the raw data contains MS/MS data.
- Frequently used Tools of interest:
  - Zoom Mode
  - Measurement Tool
  - Synchronise Zoom or Synchronise Selection
  - Lock Vertical (y-axis) or Horizonal (x-axis) Scale
  - Show/Hide Data Points
  - Show/Hide MS/MS Precursors
  - Set Peak Visibility Mode (None, Peaks, Clusters, Groups)
  - Save an area of interest as a Bookmark

How to Save Layouts



Click to save the active layout, or to open saved layouts.

- Favorite layouts can be saved and opened with the **Data Layout** icon.
  - When selected, a saved layout will show the available panes for the data type at that stage of the workflow.
  - To return to the default layout, click the icon.



Name	MS Scans	MS/MS Scans	Peaks	Clusters	Me
20210203 Adalimumab tryptic 2ug ECD_4	257	446	6621	1997	20

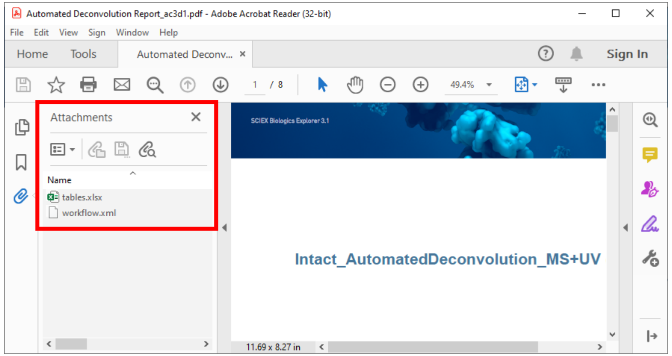
1 row (1 selected)

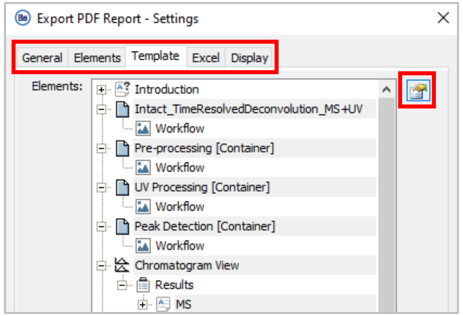
Click to move panes from one tab to another.

- To create a new layout:
  - Click the pane name tab and drag the pane to undock it.
  - Move the pane to the new location.
  - The location where the undocked pane will be docked is highlighted by a blue box.
  - Release the pane when is it in the correct location.
  - For suggested layouts for specific data types, refer to the General Guidelines of the workflow of interest.

How to Export Results

- The *Export PDF Report* activity node creates:
  - A PDF document.
    - The layout of the tables in the report is controlled by the number of columns selected on the **Template** tab.
  - An Excel file.
    - All columns in a selected table are reported.
  - A workflow xml file.
    - The workflow includes the settings that were used to produce the results.

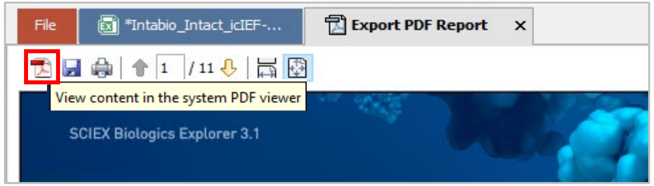




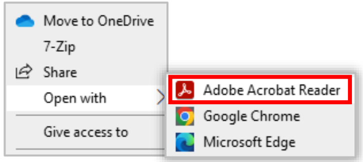
- **General** tab
  - Specify the name and saved location of the exported report.
- **Template** tab
  - Use the **Edit Selection** icon to specify the **Elements** to be included.
- **Excel** tab
  - Use the **Edit Selection** icon to specify the **Tables** to be included.

How to Open Saved Excel Tables from the PDF Report

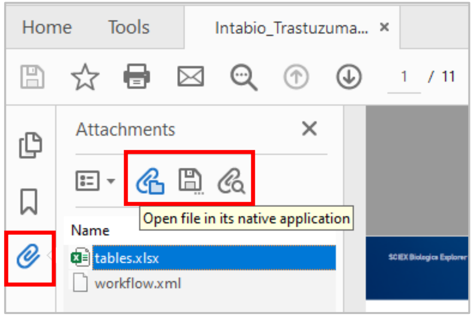
- To open the Excel tables that were saved with the PDF report:
  1. After the activity node is complete, open (double-click) *Export PDF Report*.



  2. Click the icon to show the report in the PDF viewer.
     - Note: Make sure that Adobe Acrobat (not an internet browser) is the default application.

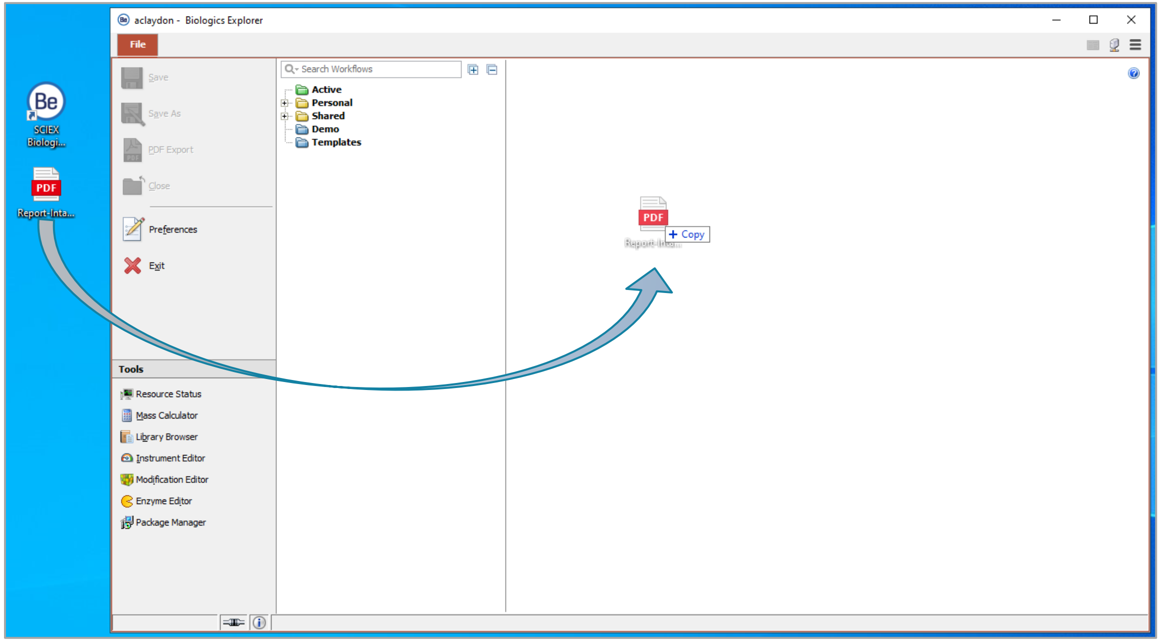


  3. To show the associated attachments, select the paper-clip icon in the opened PDF Report.
  4. To open or save the Excel document, click on the *tables.xlsx* attachment and use the applicable icon.



How to Open a Saved Workflow File from a PDF Report

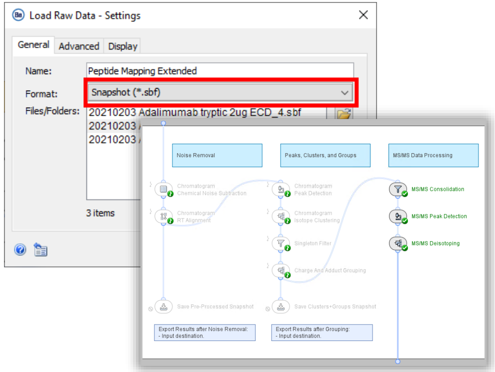
- To open the workflow xml file that was saved with the PDF report:
  - Drag the saved PDF into the workflow space in Biologics Explorer software.



How to Use the *Save Snapshots* Activity Nodes

- The *Save Snapshot* activity nodes store intermediate results at different stages of a workflow.
  - A Snapshot (sbf) file is saved for every sample processed in the workflow.

- To use a *Save Snapshot* activity node to store intermediate results:
  - Deactivate the **Block** icon.
  - Select or add the folders where the results will be stored.


Load Raw Data - Settings

Name: Peptide Mapping Extended

Format: Snapshot (*.sbf)

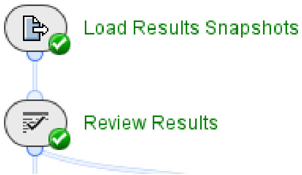
Files/Folders: 20210203 Adalimumab tryptic 2ug ECD_4.sbf
20210203
20210203

3 items

Export Results after Noise Removal:
- Input destination.

Export Results after Grouping:
- Input destination.

- To use intermediate results, such as from Pre-Processed snapshots:
  - Select the sbf file in the *Load Raw Data* or *Load Intact Protein Data* activity node, and then select **Format: Snapshot (*.sbf)**.
  - Activate the **Bypass** icon on the other activity nodes in the workflow that are before the point where the sbf file was saved.



- To review results after an applicable mapping step, such as *Peptide Mapping*, *Protein Mapping* or *Targeted Mass Search*:
  - Open the sbf file in the *Load Snapshots* activity node in a _ReviewSnapshots workflow.

The Power of Precision

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