

# How to use Biologics Explorer Software

Biologics Explorer Software Quick Guide

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# Biologics Explorer Software

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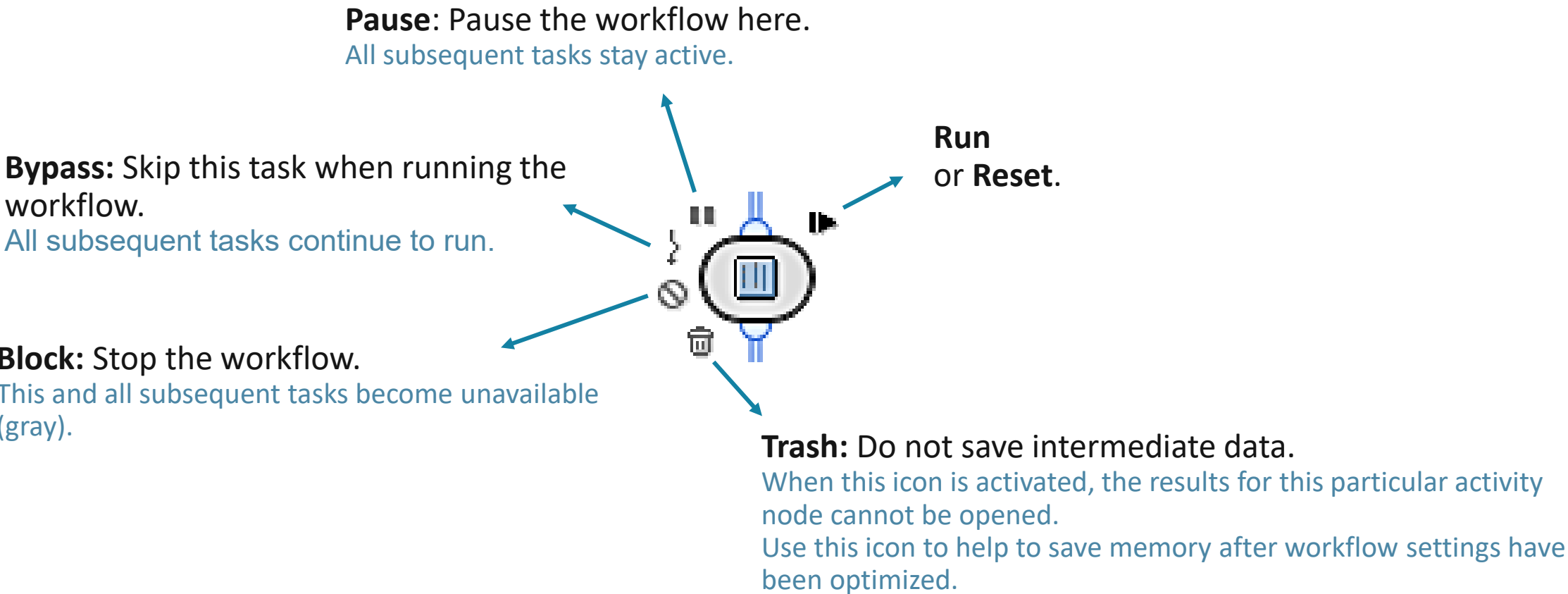
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## Part A

# General Features of Biologics Explorer Software

# A

# Activity Node Icons



# 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

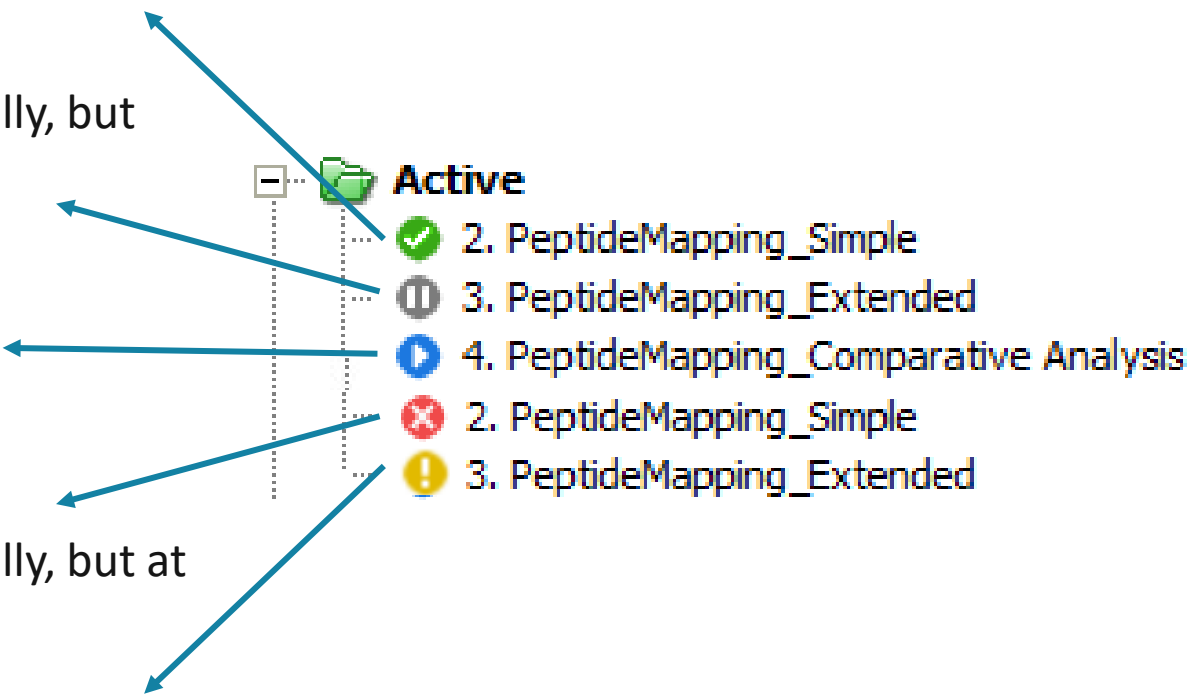
No activity nodes have been completed. The workflow is ready to start.

## Workflow Error

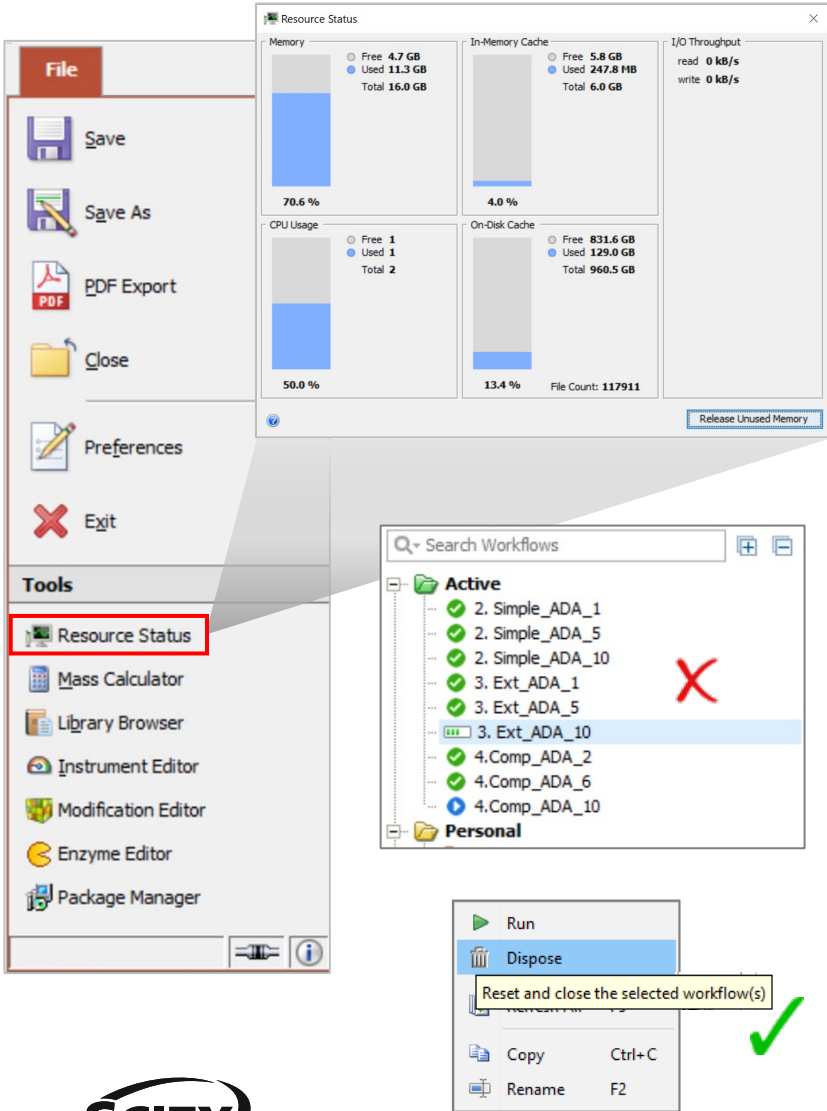
Some activity nodes have been completed successfully, but at least one activity node cannot run.

## Workflow Warning

Some activity nodes are not complete.



# Recommendations for Correct Use of the Resources



- Some activity nodes are very resource intensive. Processing multiple workflows might use up all of the resources.
  - Open the **Resource Status** from the **Tools** menu to monitor the resources.
- Obey 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 a new analysis is started.

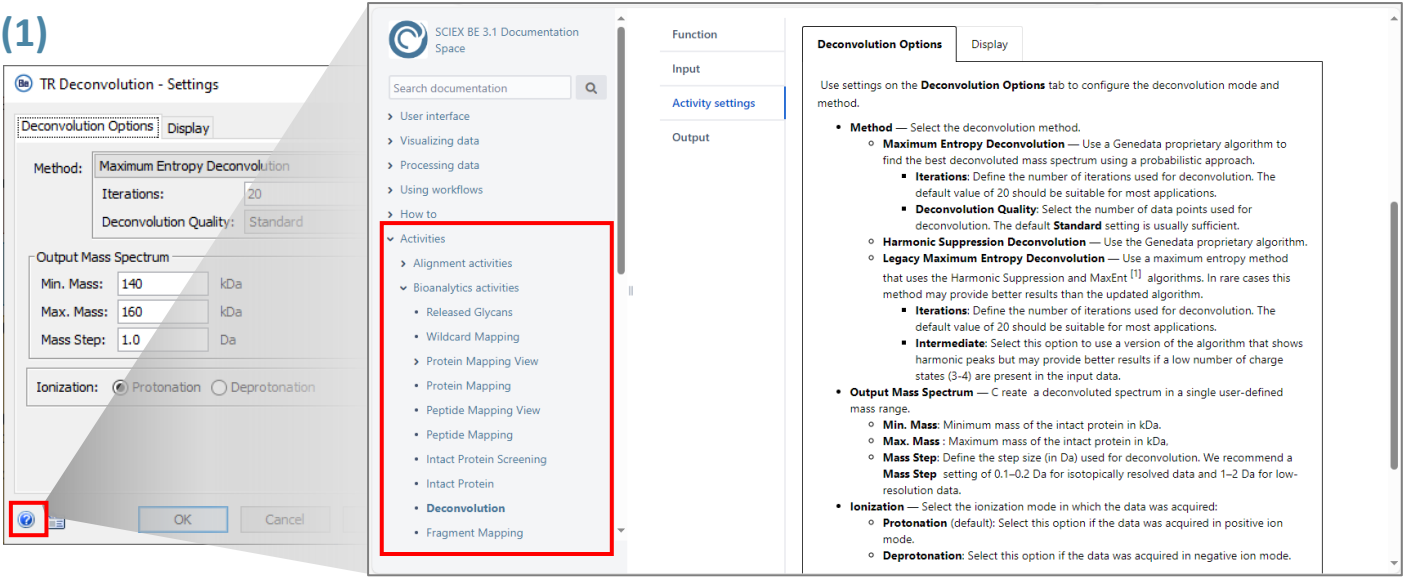
The processing computer should have at least 250 GB of free disk space and 6 GB of In-Memory Cache.


- Files processed for peptide mapping workflows (other than Batch Processing) should not add up to more than 4 GB.
- Files processed for intact protein workflows (other than Batch Processing) should not add up to more than 12 GB.




# How to Open the Online Help

(1)

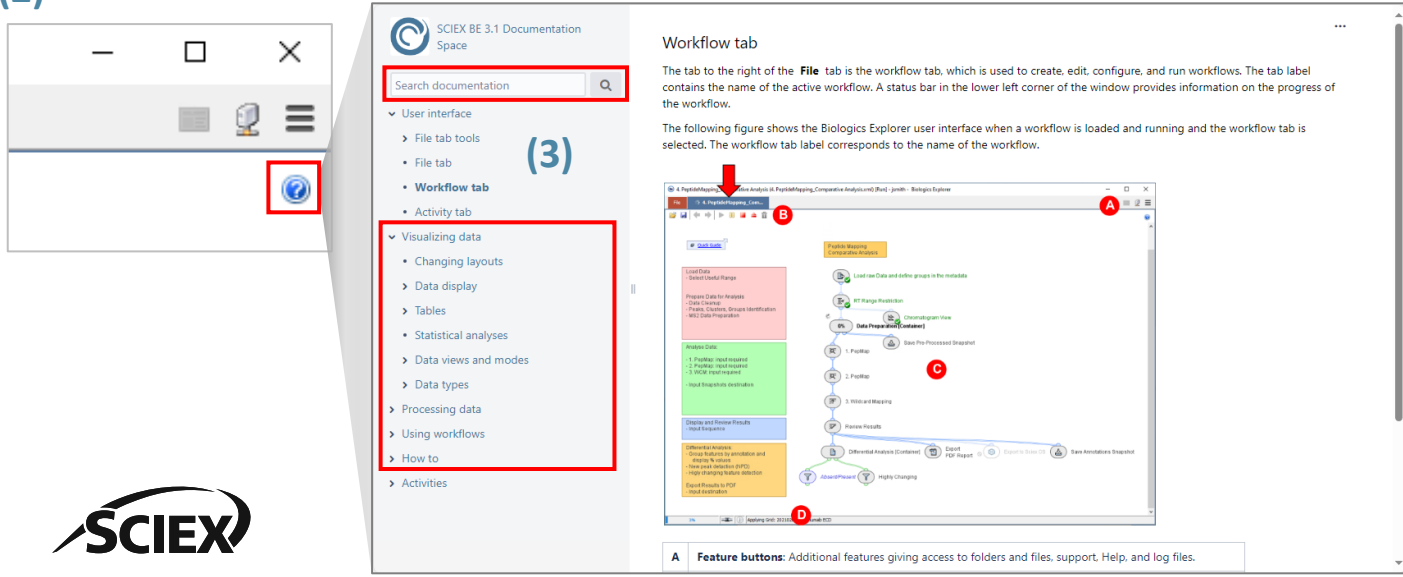


1. For information about individual activity nodes and their settings, click the  icon in the lower left corner of the settings window to open the applicable Help pages.

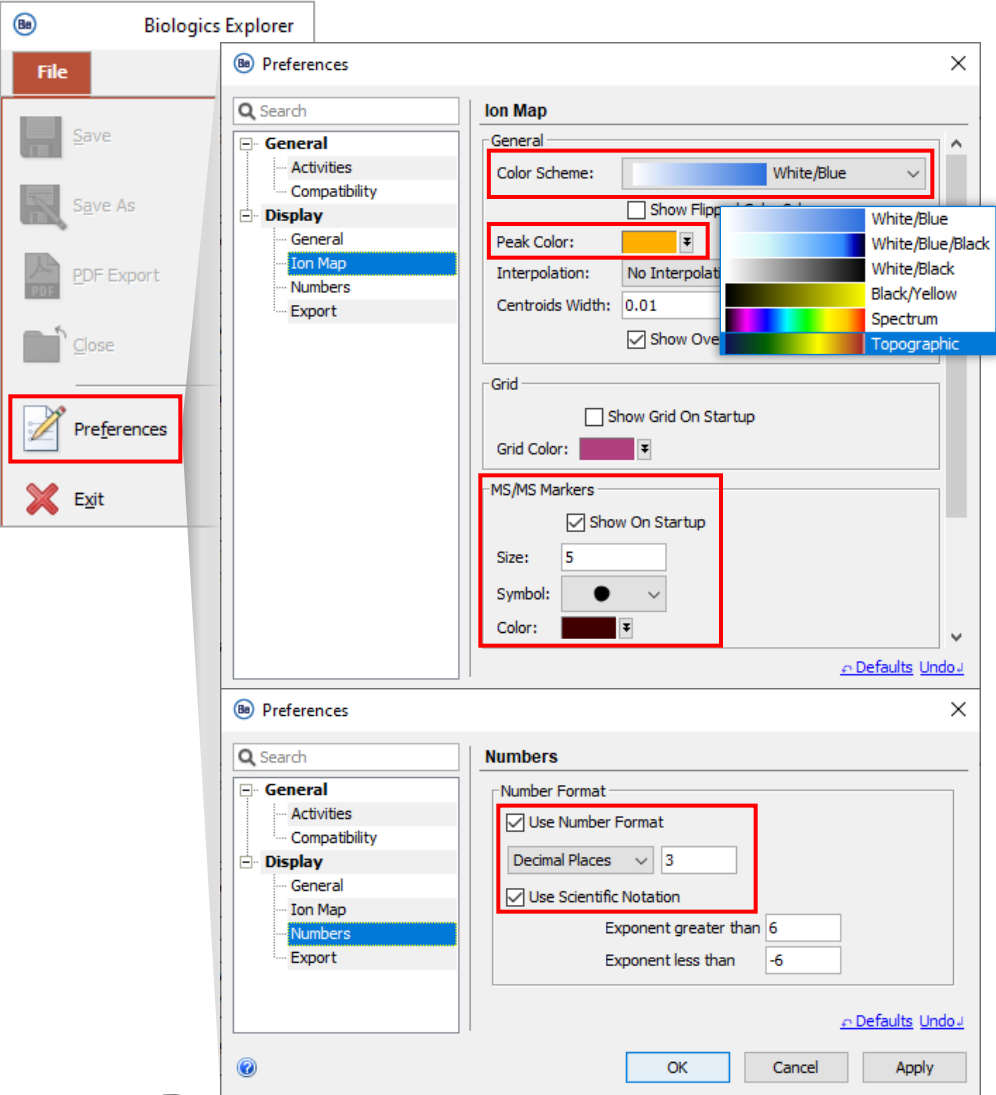
2. For information about the user interface, click the  icon in the upper right corner of the window to open the applicable Help pages.

3. For information about how to visualize data, use workflows, or any other topic of interest, expand the sections listed in the Online Help pages, or type into the Search bar.

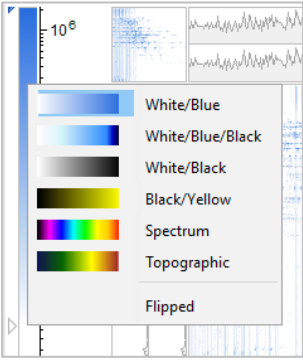
(2)



# How to Visualize Data: Preferences

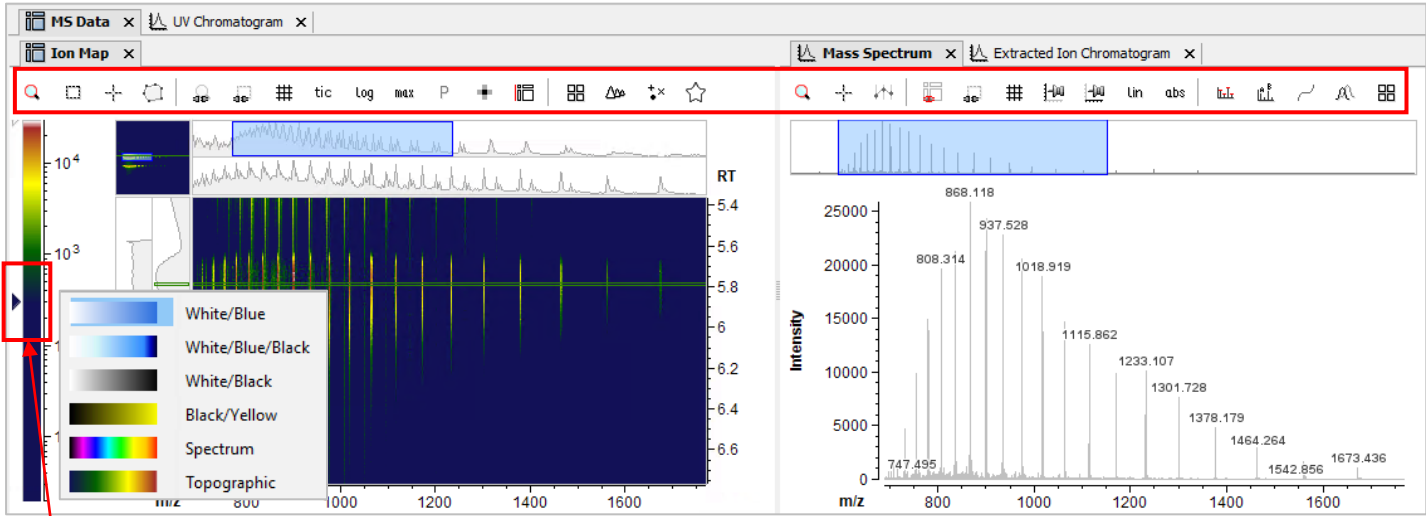


- To set how data is shown in Biologics Explorer software, select **Preferences** on the red **File** tab.
- **Display: Ion Map**
  - Select the ion map **Color Scheme** that is shown by default when a data file is opened.
    - To use a different color scheme for an ion map, right-click the color scale 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.

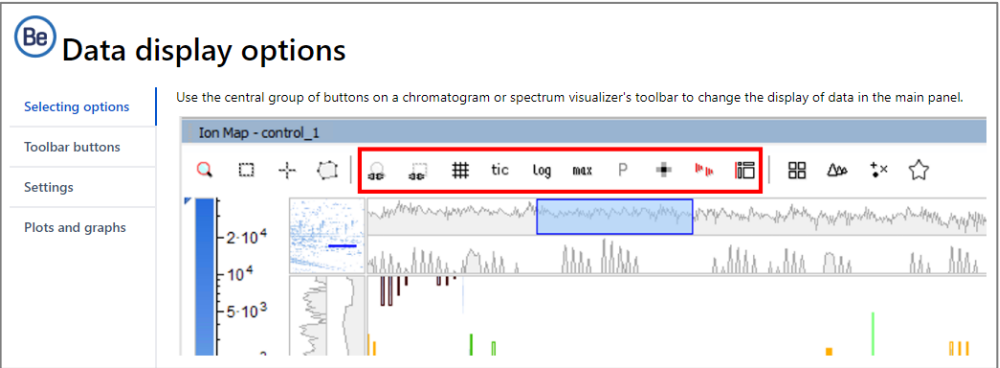




# How to Visualize Data: Useful Tools



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



- Use the Visualizer Tools to control the data display options.
  - The Tool icons are context dependent.
    - For example, the icon to **Show/Hide MS/MS Precursors** ( $\frac{MS}{MS}$ ) is only available if the raw data contains MS/MS data.

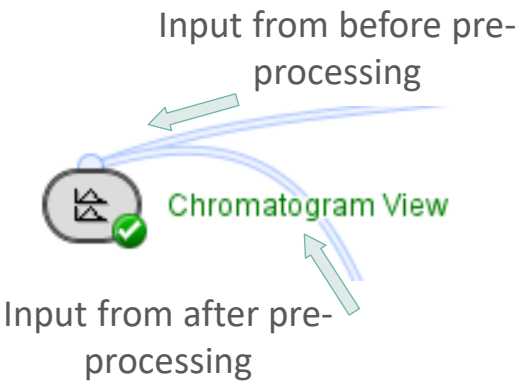
- Frequently used tools:

- Zoom Mode
- Measurement Tool
- Synchronize Zoom or Synchronize Selection
- Lock Vertical (y-axis) Scale or Horizontal (x-axis) Scale
- Show/Hide Data Points
- Show/Hide MS/MS Precursors
- Set Peak Visibility Mode (None, Peaks, Clusters, Groups)
- Bookmark: Save an area of interest

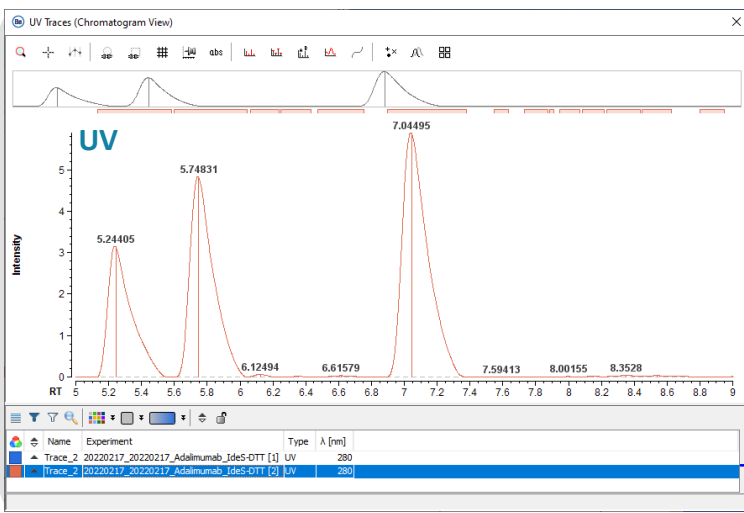
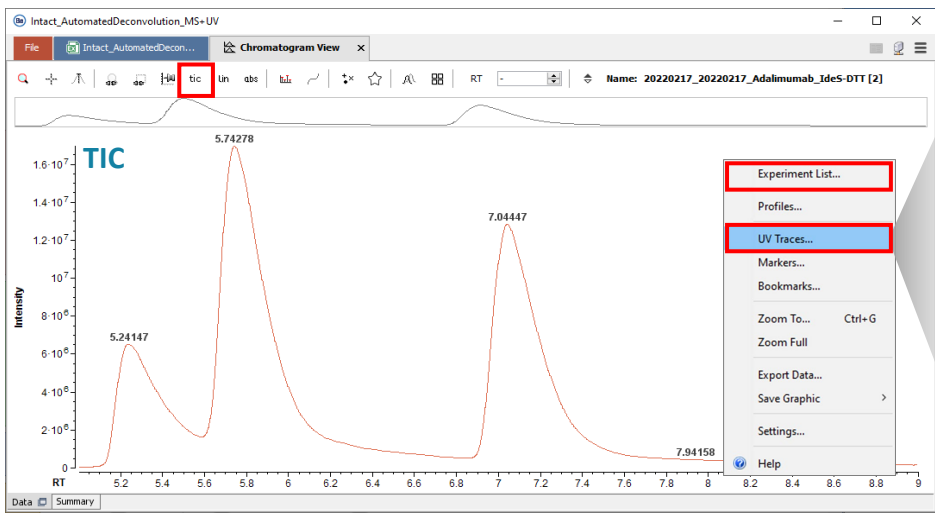


Note: For more information about data display options, use the [Online Help](#).

# How to Visualize Data: *Chromatogram View*



- Use *Chromatogram View* to see the Total Ion Chromatogram (TIC) or Base Peak Chromatogram (BPC) of the data before and after pre-processing.
  - To change between TIC and BPC, use the icon in the Tool bar.
- To see the **Experiment List** and **UV Chromatograms**, right-click the plot.



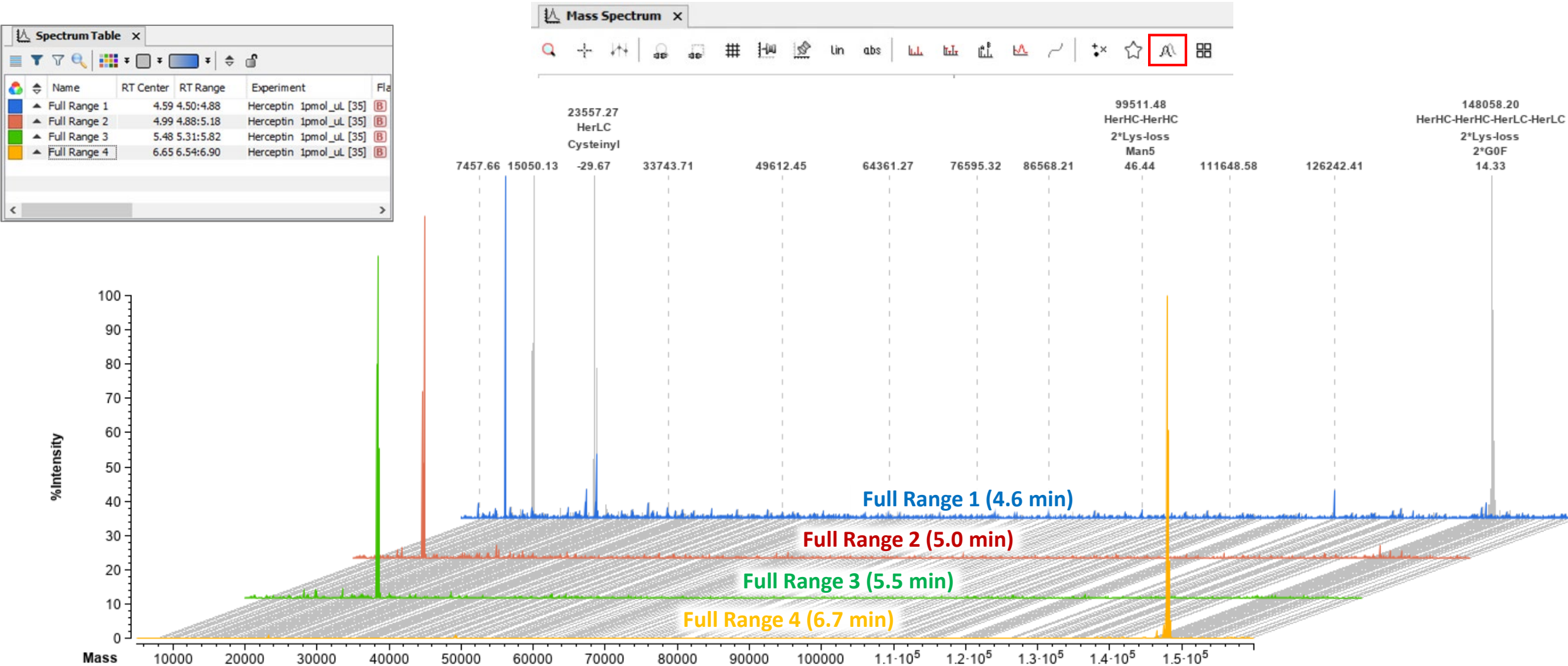
The screenshot shows the 'Experiment List' window with a table of experiments. The table has columns for Name, Scans, Method Name, Method Date, Source Type, Data Set, Flags, and UV Shift. Two rows are visible, with the second row selected.

Name	Scans	Method Name	Method Date	Source Type	Data Set	Flags	UV Shift
20220217_20220217_Adalimumab_IdeS-DTT [1]	455	MS_AdalimumAb_Subunit	Thu Feb 17 17:50:30 CET 2022	SCIEX WiffTwo	Intact Mass Analysis [1]		0.0
20220217_20220217_Adalimumab_IdeS-DTT [2]	455	MS_AdalimumAb_Subunit	Thu Feb 17 17:50:30 CET 2022	SCIEX WiffTwo	Intact Mass Analysis [2]		0.07755

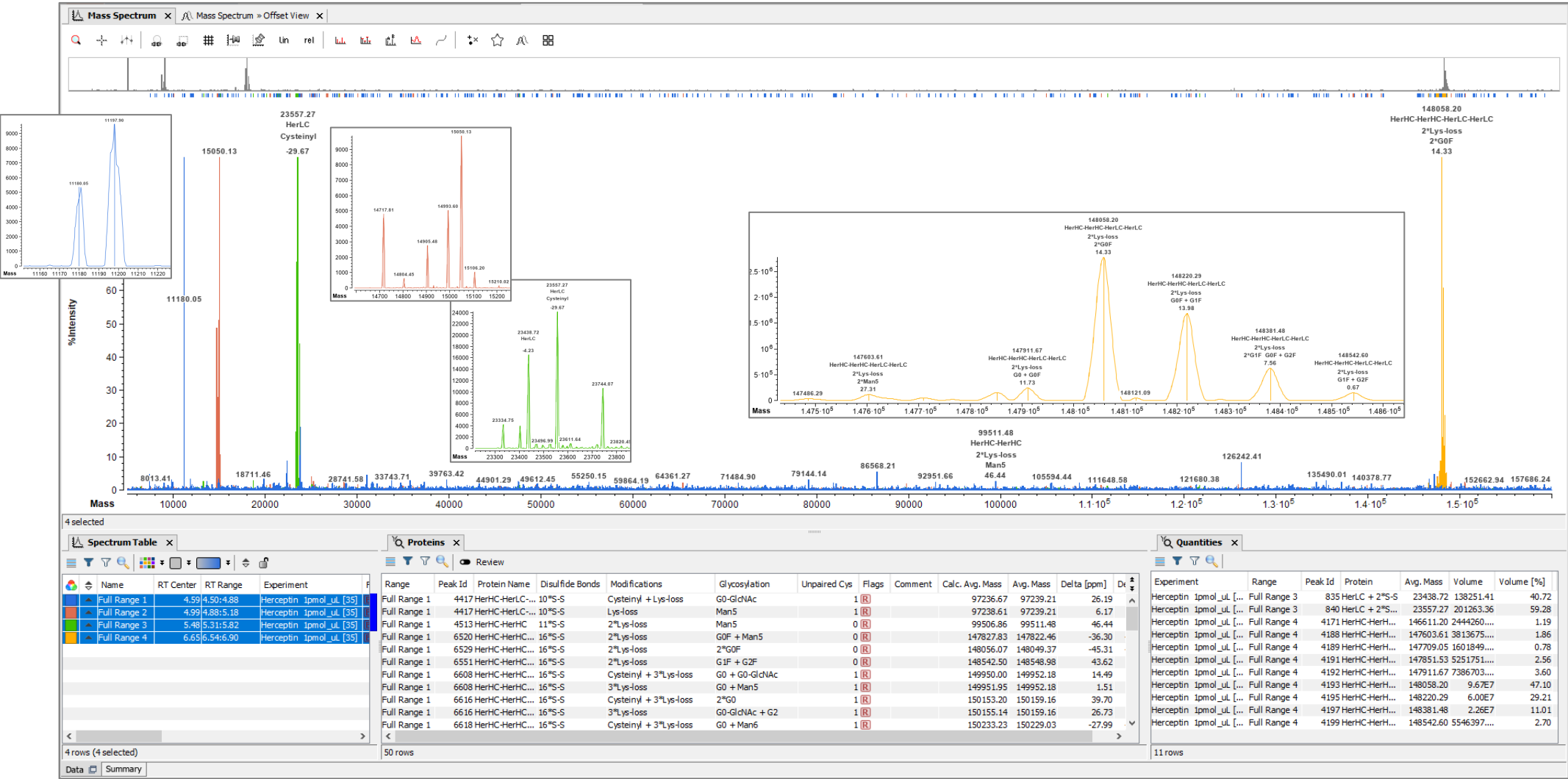
- Multiple chromatograms can be selected from the **Experiment List**, and then overlaid or flipped to show mirror views.



# How to Visualize Data: Spectrum Offset View



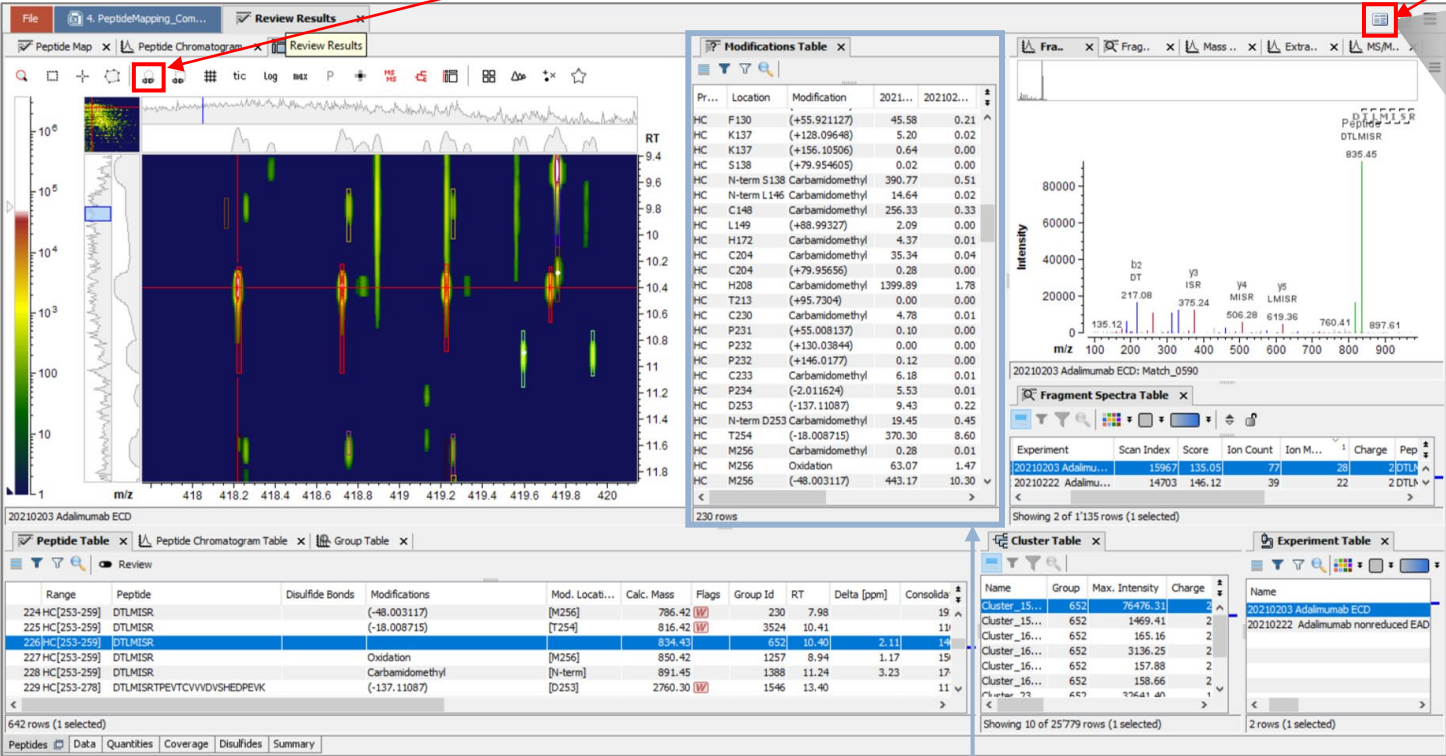
# How to Visualize Data: Spectrum Overlap View



# How to Create and Save Custom Layouts

Click to **Synchronize Zooms** across different tabs.

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




**Data Layout**

Intact Mass (raw)

Peptides\_Load Data

SavedResults\_Intabio

- Favorite layouts can be saved and opened.
  - When selected, a saved layout shows the available panes for the data type.
  - To open the default layout, click the  icon.

- To create a new layout:
  - Click and hold the name, and then 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 it is in the correct location.

Click to move panes from one tab to another.

- For example, to move useful tables from the **Data** tab to the **Peptides** tab.



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## Part B

# How to Use Biologics Explorer Workflows

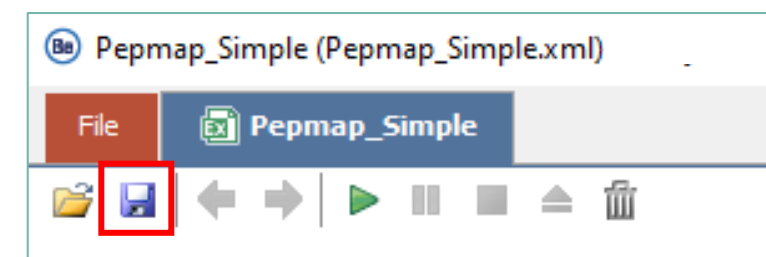
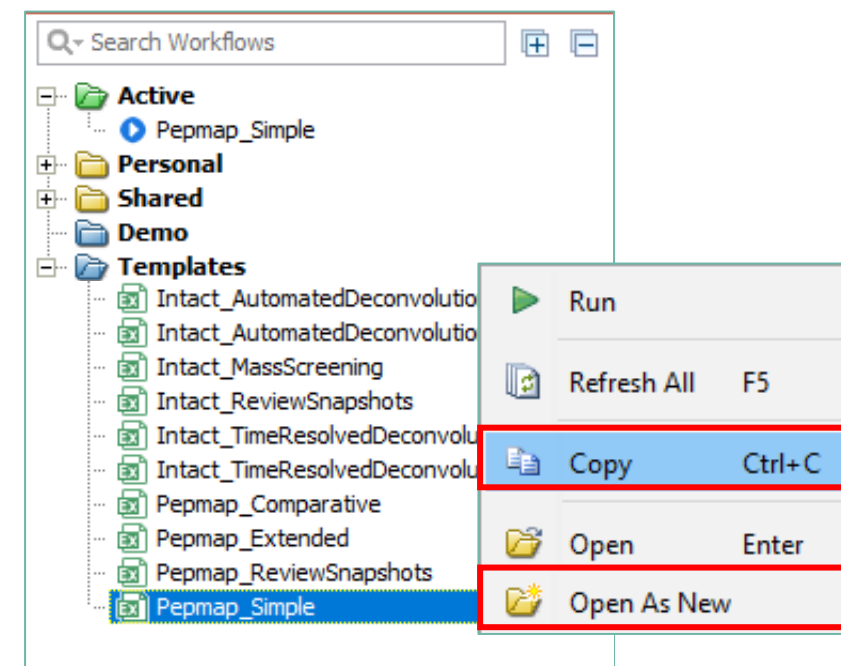
# B



# How to Start and Save Workflows

To start a new analysis, do one of these steps:


- 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.



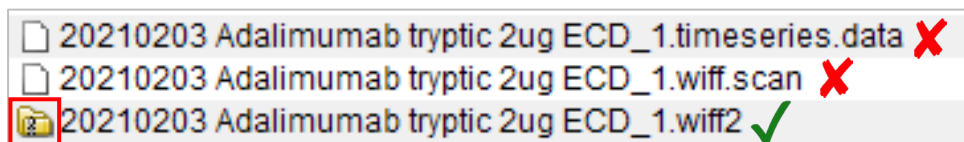
# How to Import Data



Load Raw Data

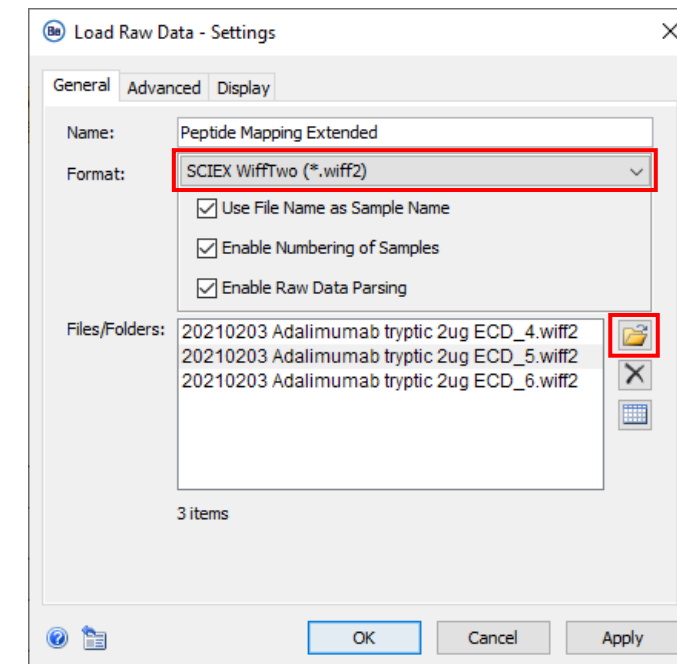
To upload raw data files, click the folder icon .

- Select container files with the format wiff or wiff2.
  - If data was acquired with the ZenoTOF 7600 system, then select only the wiff2 format.
  - Do not select the auxiliary files with the same name.



- To select samples in a wiff or wiff2 container file:
  - Double-click the wiff or wiff2 container to see the sample files.
  - Select the samples to upload.

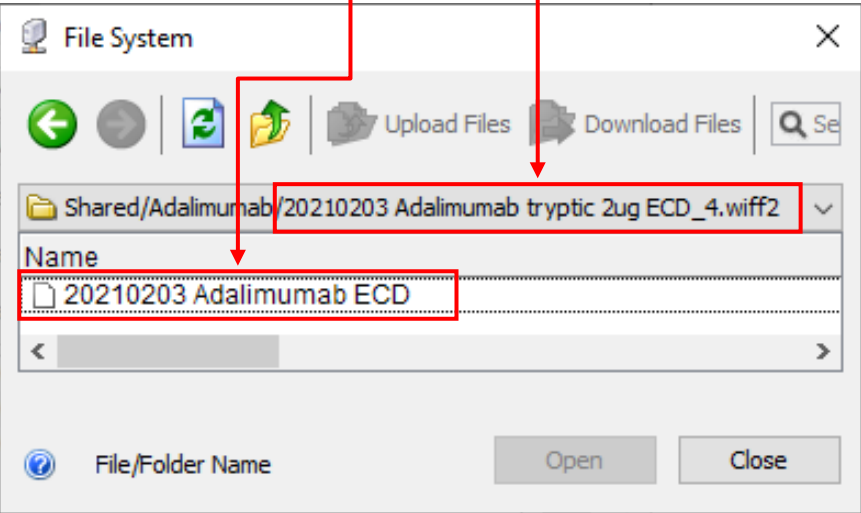
Note: For information about Batch Processing, refer to the document: [Peptide Mapping Demo Workflow Information](#).



# How to Import Data: Use File Name as Sample Name

- The **File Name** of the wiff or wiff2 container file might not be the same as **Sample Name** in the wiff or wiff2 container file.
  - The name of the **Data File** in the SCIEX OS software becomes the name of the wiff or wiff2 container file (**File Name**) in Biologics Explorer software.

	Sample Name	MS Method	LC Method	Rack Type	Rack Position	Plate Type	Plate Position	Vial Position	Injection Volume (ul)	Sample Type	Data File	Processing Method	Results File
1	Sample Name										File Name		

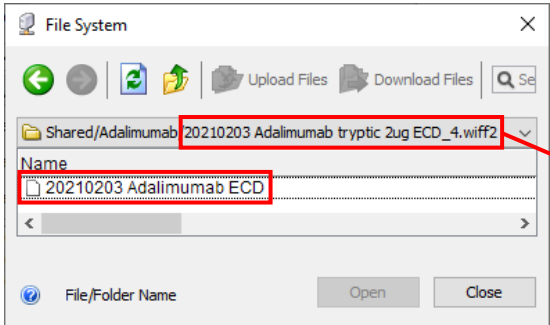


- Individual acquisitions with different wiff or wiff2 **File Names** might have the same **Sample Name**.

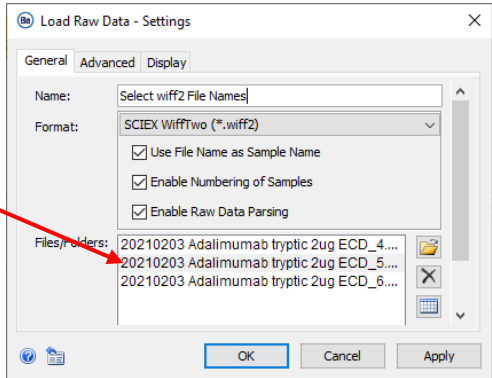
Note: If entries in the **Experiment Table** have the same **Sample Name**, then there can be an effect on the quantitative information reported.
- Select **Use File Name as Sample Name** in *Load Raw Data* to use the **File Name** in the **Experiment Table**.
  - If **Format: Auto Detect** is selected, then the **Sample Name** is used in the **Experiment Table**.

# How to Import Data: Use File Name as Sample Name

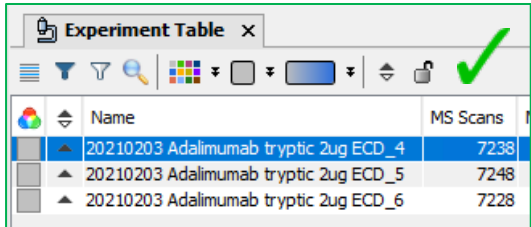
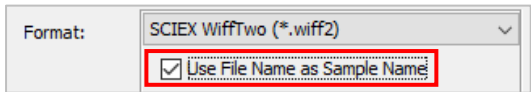
1. To load replicates that have one sample in each wiff or wiff2 container, select **Use File Name as Sample Name**:

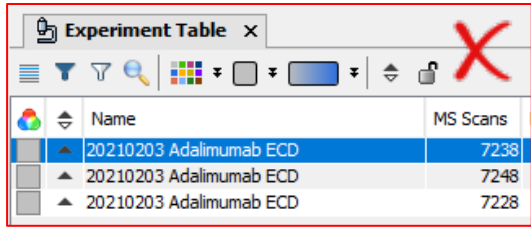
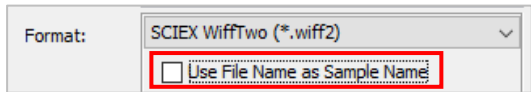


Single sample in a wiff2

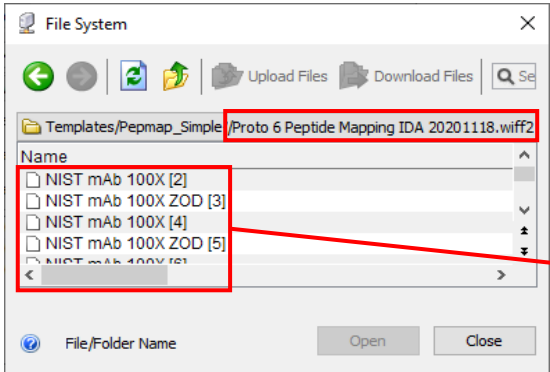


wiff2 container file selected

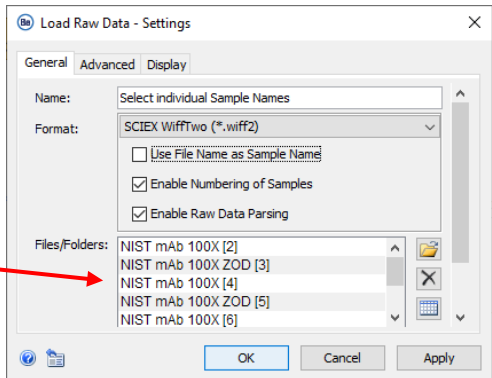




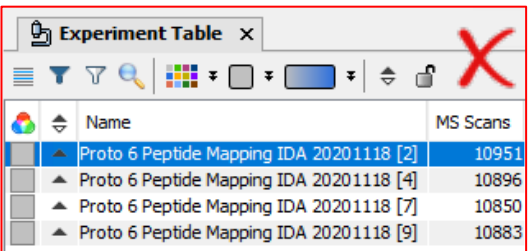
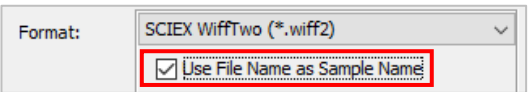
2. To load multiple samples from in the same wiff or wiff2 container, do not select **Use File Name as Sample Name**:

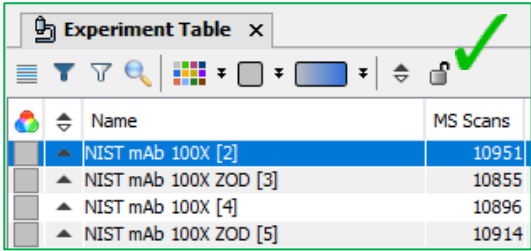
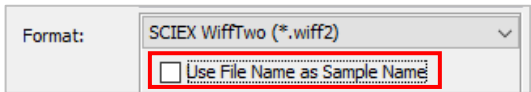


Multiple samples in a wiff2



Individual samples selected



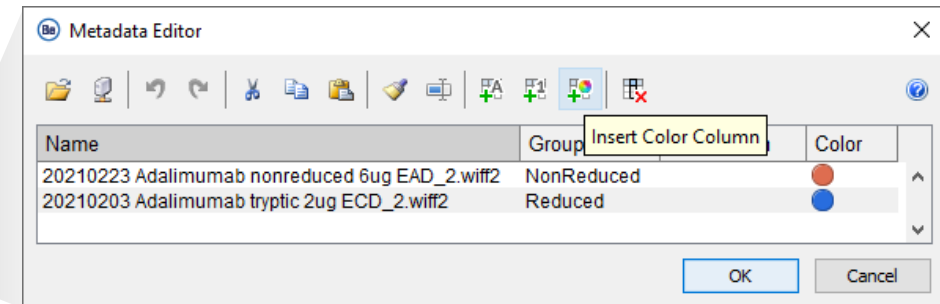
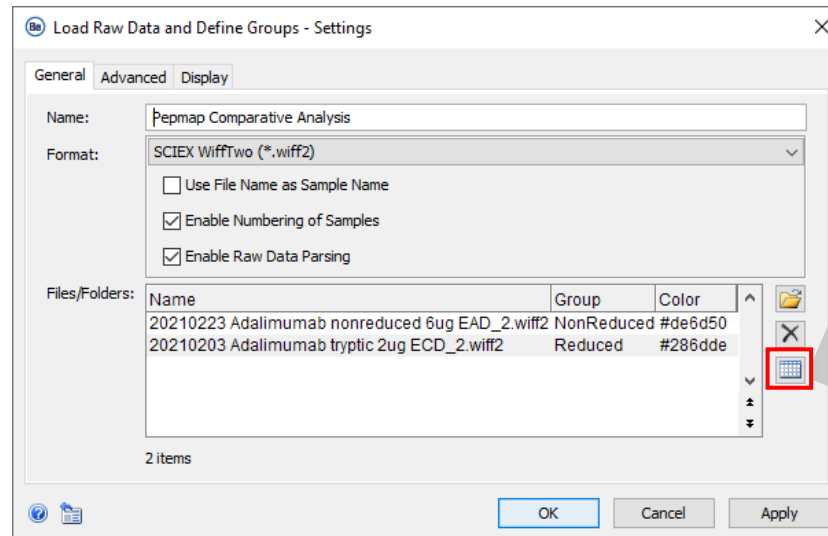




# How to Import Data: Define Groups

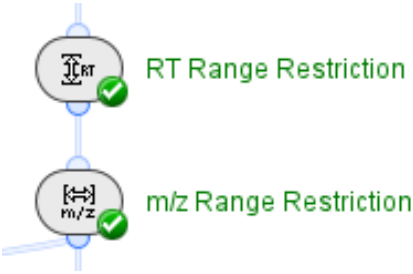


Load Raw Data

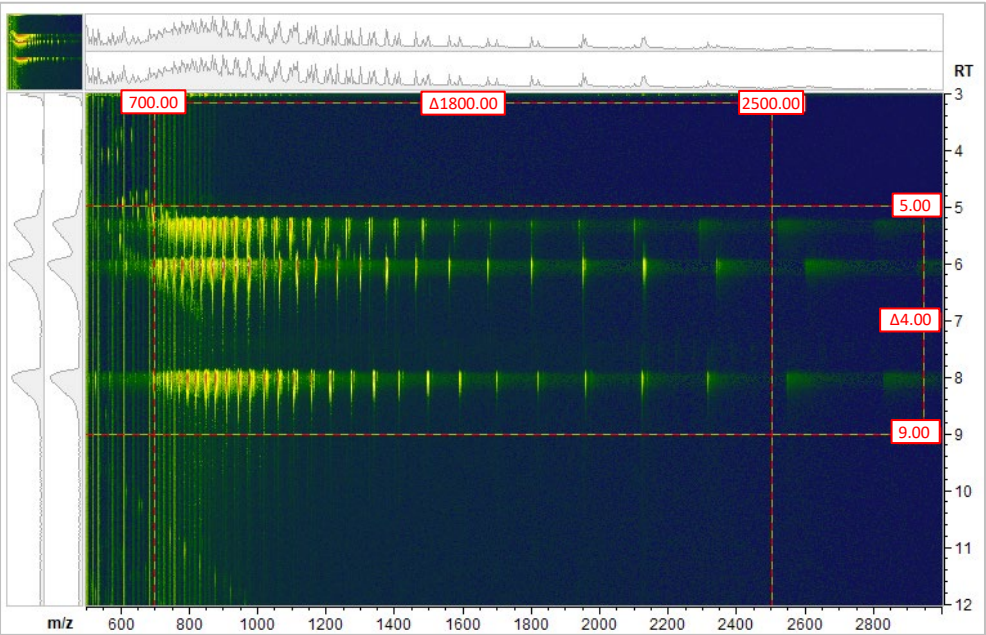


- Click the table icon to open the **Metadata Editor**.
  - Enter the **Group** names for the files to be compared.
  - Optionally, add a **Color** column and select a color for each group.

# How to use RT and $m/z$ Range Restrictions



- To identify the retention time (RT) and mass-to-charge ratio ( $m/z$ ) ranges that contain meaningful data, open (double-click) the results of *Load Raw Data*.
- If minor components or contaminants at lower masses are not of interest, then limit the RT and  $m/z$  ranges to the target protein.



RT Range Restriction - Settings

General Display

RT Minimum: 5 Minutes

RT Maximum: 9 Minutes

OK Cancel Apply

m/z Range Restriction - Settings

General Display

m/z Minimum: 700 Da

m/z Maximum: 2500 Da

OK Cancel Apply

Note: If the fields are blank, or if the **Bypass** icon is activated, then the full RT or  $m/z$  ranges are used.

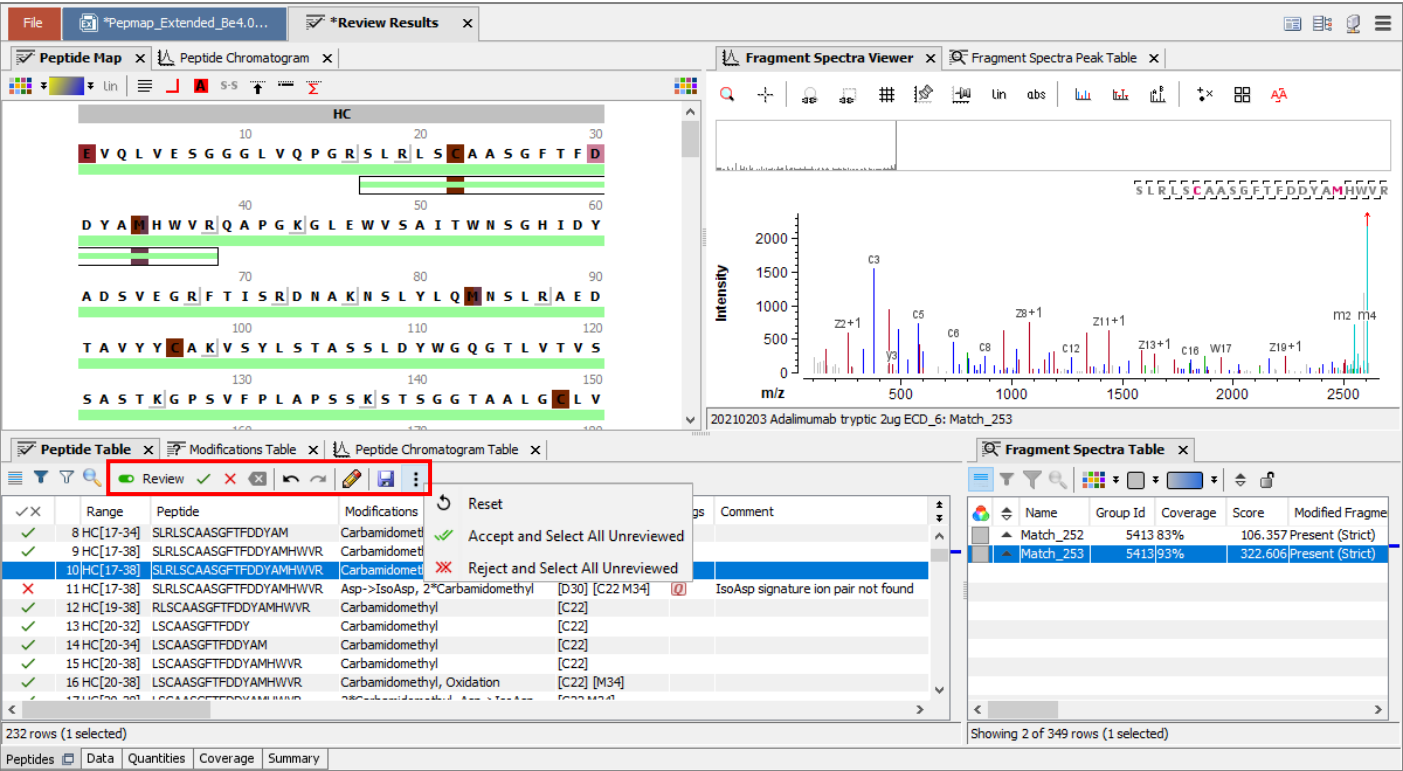


# How to Review Results: Accept and Reject Annotations

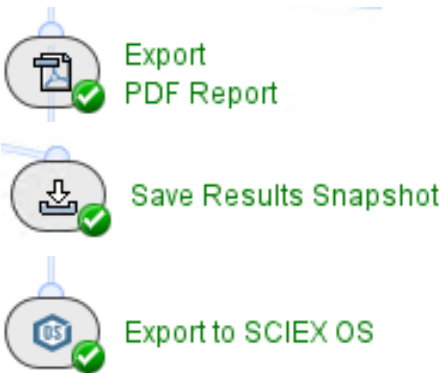


- Open the *Review Results* activity node to review the results of all the feature annotation (*Mapping*) activity nodes.

1. Activate the **Review** mode, and then **Accept** or **Reject** annotations.
  - To add a comment, type in the row in the **Comment** column or use the icon to add the same comment to multiple rows.
2. To apply the changes, click the **Save** icon, and then select **Save and Reload**.
  - Where applicable, the information in the **Quantities** tab is automatically updated.



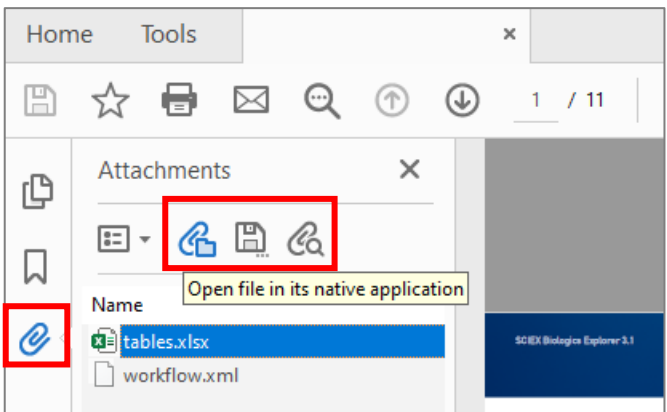
# How to Export Results




- There are different types of activity nodes to report or export results:
  - **Export PDF Report:** A summary of results is saved as a PDF.
  - **Save Snapshots:** Results are saved as sbf files that can be opened in applicable workflows.
  - **Export to SCIEX OS:** Peptide mapping results are saved as txt files that can be used for applications that use the SCIEX OS software.
- To use an export activity node:
  - Deactivate the Block icon.
  - Select or add the folders where the sbf files will be stored.

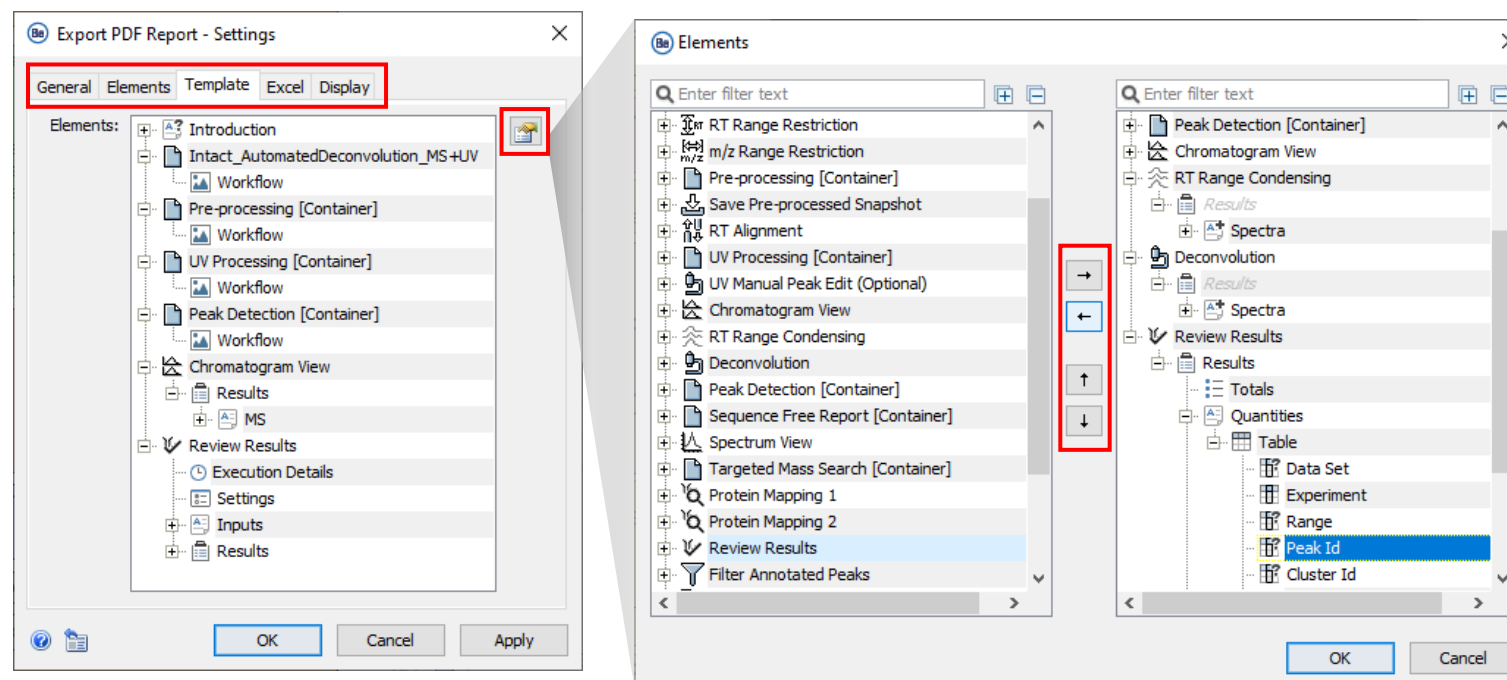


- The *Export PDF Report* activity node includes:
  - A PDF document: The layout of the tables in the report is controlled by the number of columns selected on the **Template** tab.
  - An Excel file: All columns in a selected table are included in the report.
  - A workflow xml file: The workflow includes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

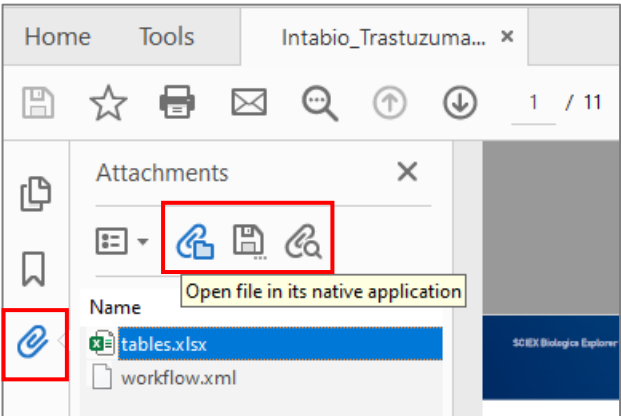
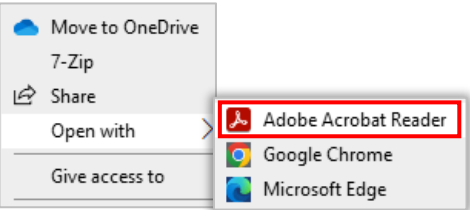
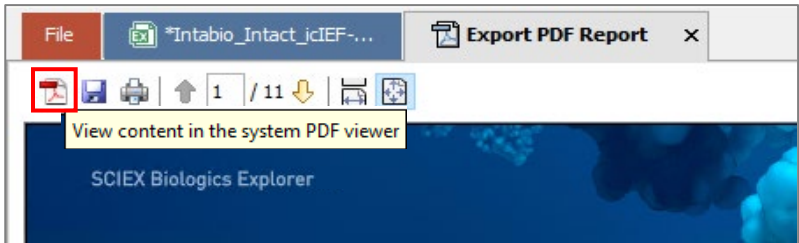


# How to Export Results: *Export PDF Report*


- **General** tab: Select the name and saved location of the exported report.
- **Template** tab: Use the **Edit Selection** icon to select the **Elements** to be included in the report.
  - To remove columns from a selected table, use the  icon.
  - The layout of the tables in the PDF report is controlled by the number of columns.
- **Excel** tab: Use the **Edit Selection** icon to select the **Tables** to be included in the report.
  - All columns in a selected table are included in the report.



# How to Open Saved Excel Tables from the PDF Report

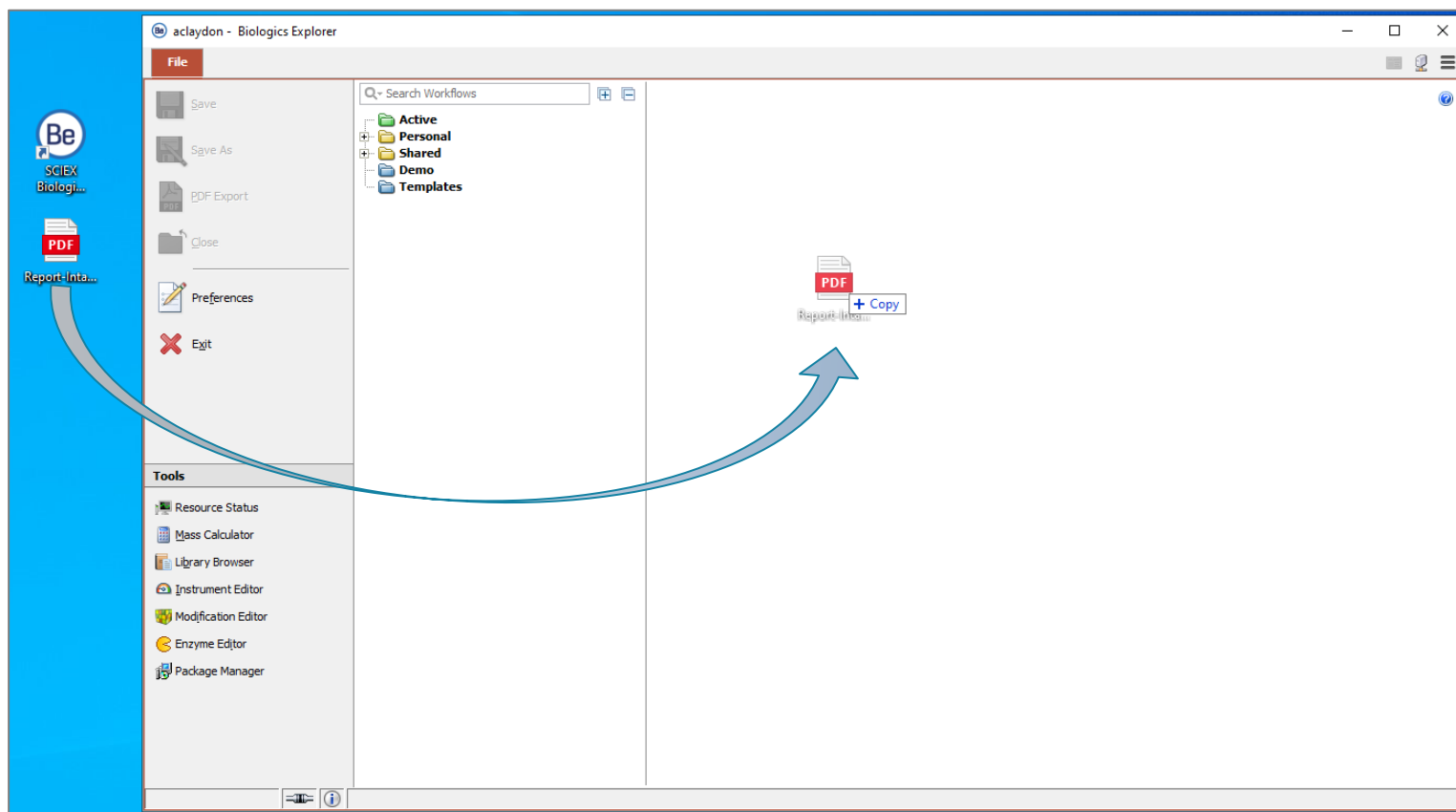


To open the Excel tables that were saved with the PDF report:

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

# How to Open a Saved Workflow File from a PDF Report

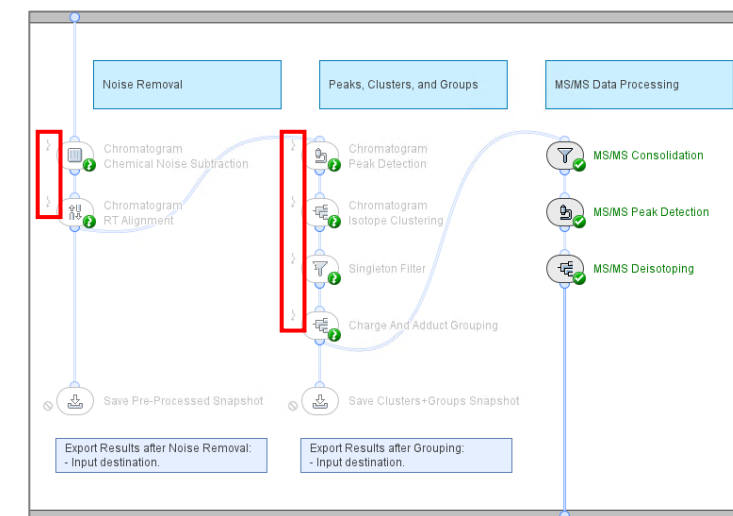
- To open the workflow xml file that was saved with the PDF report:
  - Drag the saved PDF into the workflow space in Biologics Explorer software.



# How to Use the *Save Snapshots* Activity Nodes

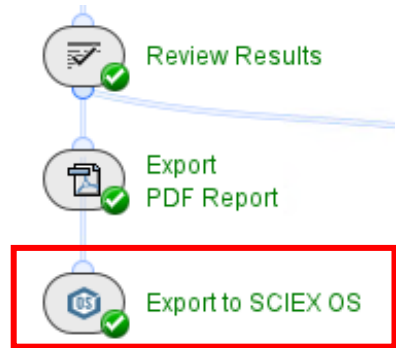
- The *Save Snapshot* activity nodes save intermediate results at different stages of a workflow.
  - A Snapshot (sbf file) is saved for each sample processed in the workflow.
  - The Snapshot (sbf file) contains the properties of the processed data that are required to continue analysis from that point in the workflow.
- To continue data analysis with Snapshots saved before feature annotation:
  - Select the sbf file to import into *Load Raw Data*.
  - Change the **Format** to **Snapshot (\*.sbf)** or **Auto Detect**.
  - Activate the **Bypass** icon on the activity nodes in the workflow that are before the Snapshot was saved.
    - For example: To use sbf files from *Save Clusters and Groups Snapshot* in a peptide mapping workflow, activate the **Bypass** icon for all activity nodes between *Load Raw Data* and *MS/MS Consolidation*.

Note: A [Container] shows a **yellow warning** if the **Bypass** icon is activated on activity nodes in it.
- To continue data analysis with Snapshots saved after feature annotation, use the applicable *\_Review Snapshots* workflow.





# How to *Export to SCIEX OS*



- *Export to SCIEX OS* creates a txt file of peptide mapping data that can be imported into the SCIEX OS software.

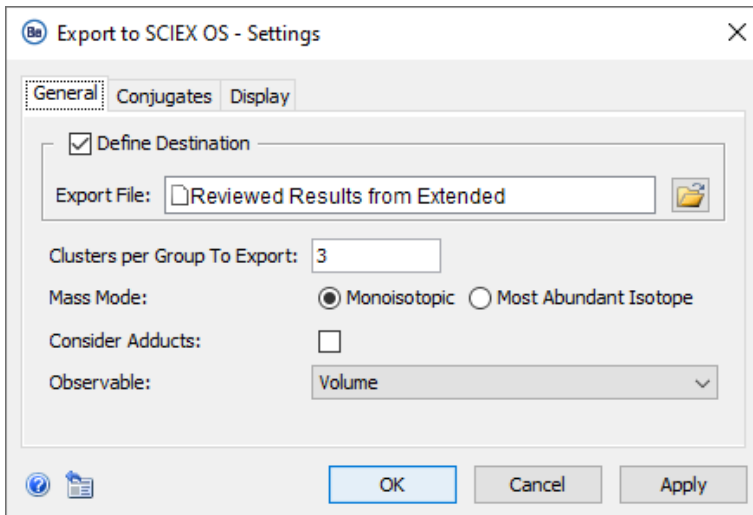
- **General** tab:

- Select the name and saved location of the exported report.
- Select the requirements of the export, for example, the number of clusters for each group, and if adducts are to be included.
- Use **Observable: Volume** for data that was acquired with a QTOF mass spectrometer.

Note: The modification position that is exported with the *Export to SCIEX OS* activity node is relative to the peptide, not the protein. For example, DTL[M]ISR would be M4, not M255.

- Do not use the *Export to SCIEX OS* activity node with the *Wildcard Mapping* activity node.

- Activate the **Bypass** icon on the *Wildcard Mapping* activity node when required.



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