



# Reporting

## User's Manual

December 2025

5.12

Protein Metrics LLC, Boston, Massachusetts USA

# Contents

Introduction.....	3
Data Flow .....	3
Creating Reports .....	4
Report Menu Overview .....	5
Report File Menu .....	6
Report Edit Menu .....	8
Report Tabs Menu .....	9
Report Toolbar .....	10
Report and Tab Templates .....	10
Report Tab Management .....	13
Summary Tab .....	14
Pivot Tab.....	17
Tour of Pivot Table Areas.....	19
Rendering Options .....	19
Aggregator Options.....	20
Field Management .....	21
Filters .....	23
Sorting .....	25
Show/Hide Configuration .....	26
Pivot Tab Current Tab Settings: Common .....	27
Pivot Tab Current Tab Settings: Chart specific .....	30
Pivot Tab Current Tab Settings: Modification specific .....	33
Pivot Tab Heatmap.....	34
Pivot Tab Error Charts.....	36
Pivot Tab Principal Component Analysis (PCA) Plots.....	38
Pivot Tab Pie Chart .....	39
Pivot Tab Protein 3D Plots.....	41
Pivot Tab Treemap Diagram .....	45
Pivot Tab Venn Diagram .....	45
Pivot Tab Volcano Plot.....	47
Pivot Tab Protein Map.....	48
Plots Tab .....	49
Plots Tab Current Tab Settings.....	49
Plots Tab Sorting .....	53
Plots Tab Filtering.....	54
Plots Tab Template Editor .....	55

Template Editor and Short Codes.....	55
Summary Tab Template Editor.....	56
Summary Tab Short Code Reference .....	56
Dynamic Columns: Pre-Pivot and Post-Pivot JavaScript .....	66
Pre Pivot JavaScript Reference .....	67
Post Pivot JavaScript Reference .....	70
Editing Pre or Post Pivot JavaScript.....	71
Tour of JavaScript Add New Column Dialog.....	72
Multi-Document Report.....	74
Customize Report.....	75

## Introduction

Protein Metrics applications have common Reporting features:

- Review all plots on the same page through the Plot Tab.
- Export the report into PDF, Microsoft Excel workbook, or CSV (common separated values) format.
- Perform further data analysis through the Pivot Table.
- Organize project information into a Summary.
- Reuse the report design saved as a template on future data sets.
- Time-saving – Reports are automatically generated through Byos workflows.

This manual will focus on reporting capabilities of the Byos suite of applications (mainly Peptide Analysis, Intact Analysis, and Chromatogram Analysis).

## Data Flow

When the user creates a report, application data is passed into the Report Module as a Flat Input Table. The Flat Input Table is a table of rows and columns, similar to the CSV format or an Excel worksheet. The user can add Dynamic Columns to further analyze data through the Pivot Tables. A simplified diagram detailing the data flow is shown below:

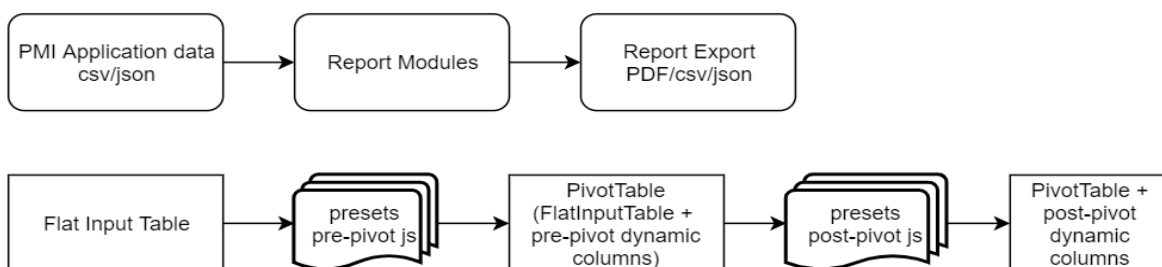



Figure 1: Data flow module for report generation

## Creating Reports

To create a report, select **File > Export > Report** or simply click the report icon  below the Help menu.

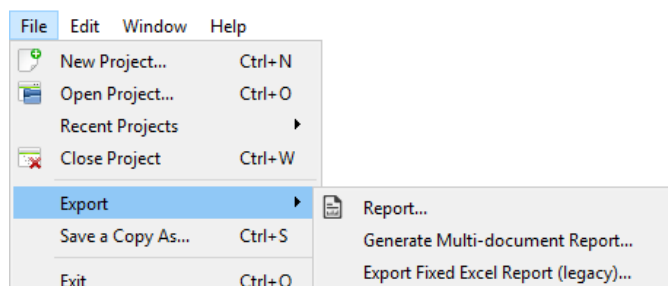


Figure 2: Generating a report from the project File menu

A report opens with tabs defined by the default report template as shown in Figure 3 and Figure 4:

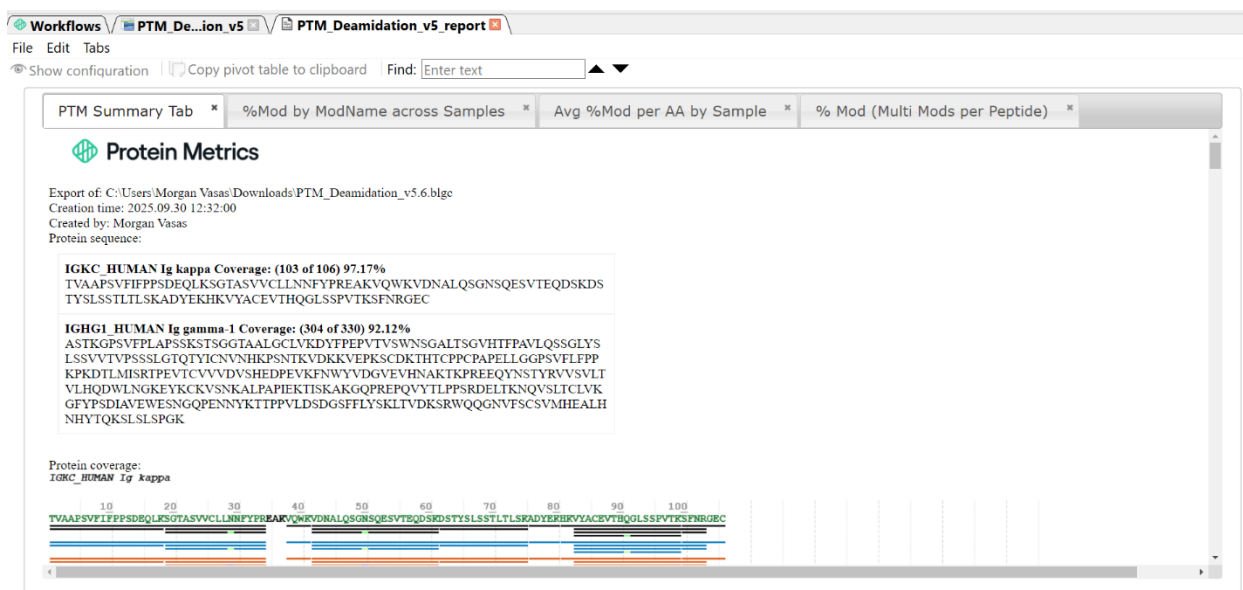


Figure 3: A default report.

In the legacy products, the report opens in a separate window. By toggling over the legacy product icon in the task bar, the user can select to view the project or associated report.

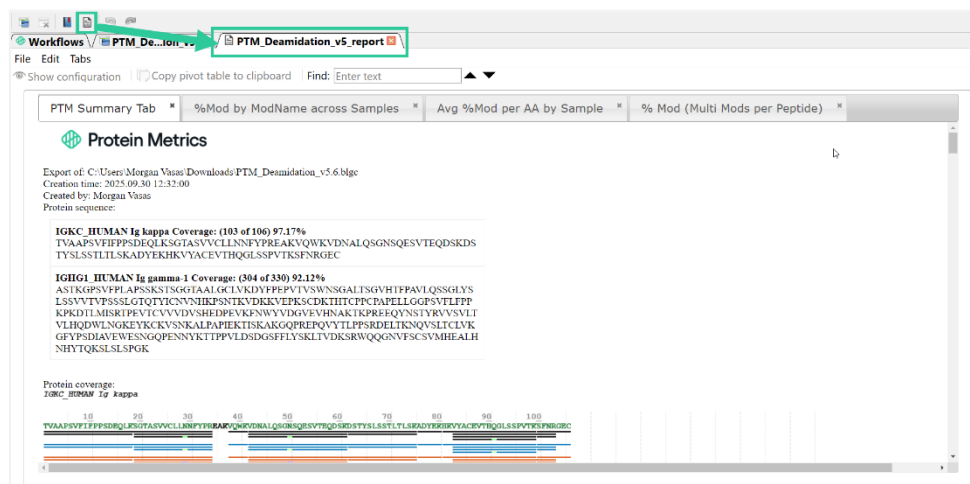


Figure 4: A default report template from Byos

In Byos, the report opens as an additional tab to right of the associated project. All default Byos workflows contain a report template specifically designed to support that type of analysis. This is included in the Processing nodes > Report section.

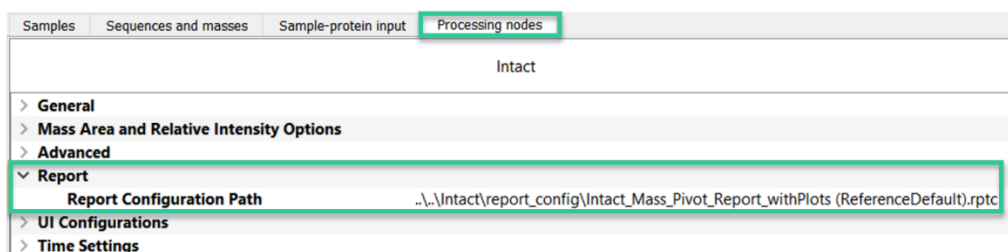


Figure 5: Set the report configuration in the Processing nodes tab during project creation

For details about the report template, see the **Report Template and Default Report Template** section.

To create a report based on data in multiple projects, please refer to the **Multi-Document Report** section.

**File > Export > Fixed Excel report (legacy)** exports the project to an Excel file in the same way that **File > Export > Export to Excel workbook** exports from within a report.

## Report Menu Overview

Menu	Sub Menu	Action and Notes
File	Load from File	Load a Report Template from the file system and create the tabs as defined in the Report Template. This action replaces all current tabs.
	Save to File	Save current tabs into a Report Template.
	Save to Document	Save current report as associated with the current analysis. When the project is next opened, the saved report will be attached to the associated file.
	Export	Export all or part of the report as PDF, Excel workbook, images, or CSV. Refer to the Export section for additional details.

	Preset	Load predefined Report Template, Tab Template, or Dynamic Columns. Refer to the Preset section for additional details.
	Close	Close the Report.
Edit	Current Tab Settings	Tab configuration settings. Refer to each tab section for additional details.
	Edit dynamic column	Add, edit, or delete a dynamic column. Refer to the Dynamic Column section for additional details.
	Copy pivot table to clipboard	Enabled for the Pivot tab only. Pivot table content is copied to the clipboard as tab separated values.
Tabs	Add pivot table	Add a pivot table tab. Refer to the Pivot Tab section for additional details.
	Add summary	Add summary tab. Refer to the Summary Tab section for additional details.
	Add plots	Add plot tab. Refer to the Plot Tab section for additional details.
	Add flat input table	Add a tab displaying the contents of the flat input table. The flat input table tab can be added only once. This option can be of use to examine the data that goes into the Report Module.
	Duplicate current tab	Make a copy of the current tab. The flat input table cannot be duplicated.
	Update tab content	Application changes, such as column filtering, will be updated and reflected in all Report tabs.

## Report File Menu

The File sub-menu contains various options to process reports:

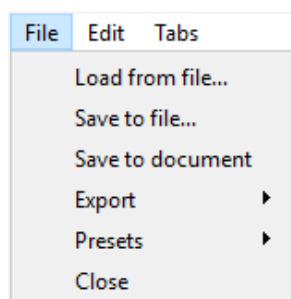


Figure 6: File Menus

**Load from file** loads in a previously saved report template and updates the report accordingly. **Save to file** saves the current report template format. **Save to document** attaches the generated report to the associated project.

**File > Export** includes five sub-menu items:

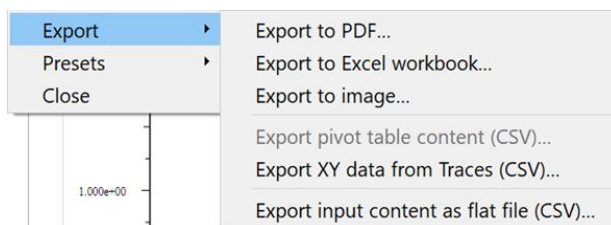


Figure 7: File &gt; Export menus

**Export to PDF** generates a .pdf document version of the report:

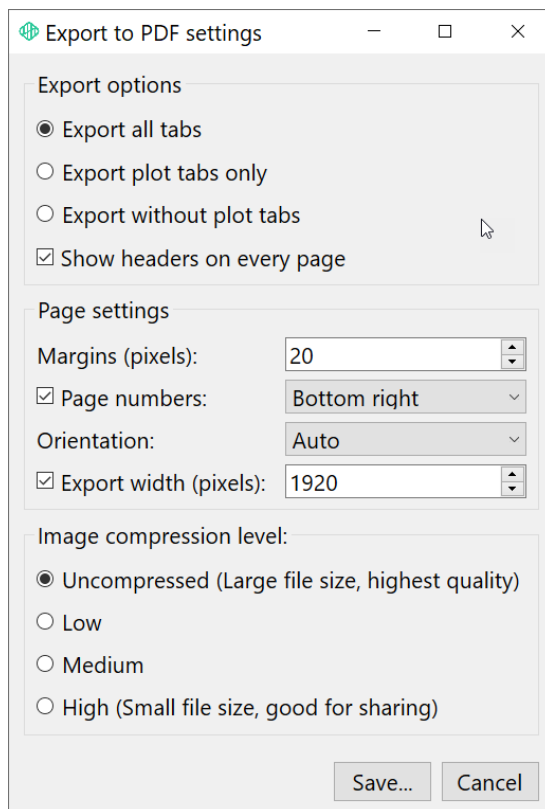


Figure 8: Export to PDF settings

The Export to PDF settings includes:

- **Export options** to choose to export all tabs, only plots, or all tabs except plots.
- **Page settings** to set page margins, visibility and placement of page numbers, page orientation (**Auto** uses a combination of portrait and landscape as suits each tab), and total document width.
- **Image compression level** to set the image resolution quality, and thus, size of the exported file. The higher the compression, the smaller the size but the lower the image quality.

**Export to Excel workbook** generates a \*.xlsx file of all tabs. The PTM Summary tab, charts and plots are rendered as images, while pivot tables are rendered as spreadsheets.



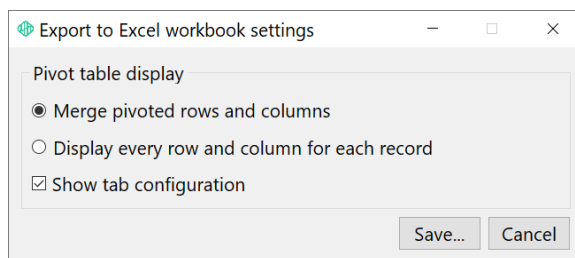


Figure 9: Export to Excel workbook settings

**Export to image** generates one \*.png file for each of the tabs. **Export to pivot table content (CSV)** writes the pivot table to a \*.csv file. **Export input content as flat file (CSV)** writes a pivot table to a flattened \*.csv file (common values are repeated for all pivoted fields). **Export XY data from traces (CSV)** exports the underlying XY data used to create the trace plot.

**File > Presets** refers to files that configure report formats:

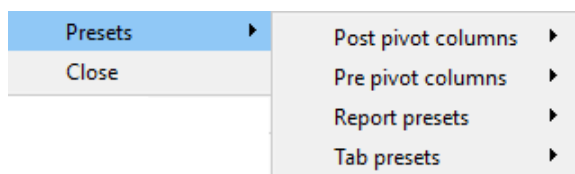


Figure 10: File &gt; Presets menus

**Post pivot columns** and **Pre pivot columns presets** load columns into the pivot tables. **Report presets** lists the default report templates provided to support different types of projects. The list is different when opening a \*.blgc, \*.ntms, and \*.bmap project type. **Tab presets** loads additional default tab types into an existing report. For more information, see the section [Report and Tab Templates](#).

**Close** closes the report without closing the project. However, closing the Project will also automatically close the associated Report.

## Report Edit Menu

The **Edit** menu contains three sub-menus:

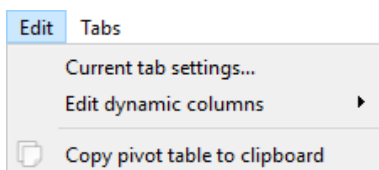


Figure 11: Edit menus

**Current tab settings** allow edits on certain tab properties; each tab type has a different set of properties that can be edited. See the sections on the tab types for the kinds of edits allowed through the **Current tab settings** dialog.

**Edit dynamic columns** allows the editing, addition, or removal of pivoted dynamic columns:

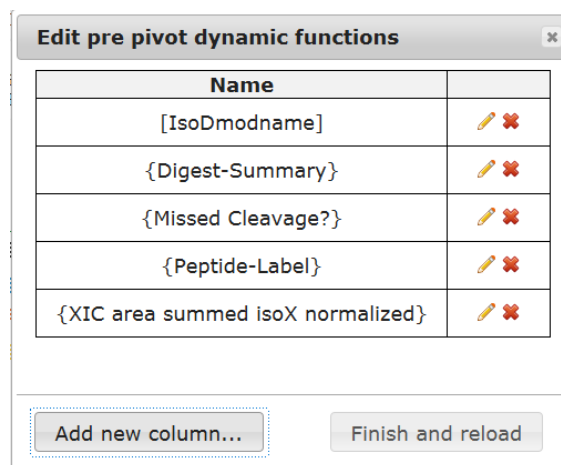




Figure 12: Edit dynamic columns for Peptide Analysis project report

Click the  icon to edit the displayed name. Click the  icon to delete the pivot field. Click the **Add new column** button to add another pivot field. Click the **Finish and reload** button to reload these edits. Please contact [support@proteinmetrics.com](mailto:support@proteinmetrics.com) for support working with dynamic columns.

**Copy pivot table to clipboard** copies the pivot table data as tab separated values.

## Report Tabs Menu

The **Tabs** sub-menus add additional tabs to an existing report:

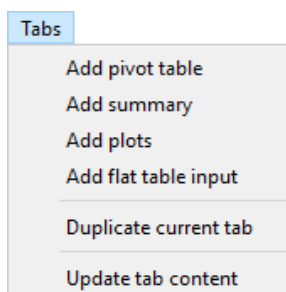


Figure 13: Tabs menus

**Add pivot table** adds a new **Pivot** tab that can be edited using **Edit > Edit dynamic columns**. **Add summary** adds a new **Summary** tab that defaults to the same format as the Summary tab included in many reports. **Add plots** adds a new **Plots** tab (as well as **File > Presets > Tab presets > Bmap\_Plots**) that creates a report of all the project plot types. **Add flat table input** adds a new **Flat Table Input** tab that contains data in many fields as a flattened pivot table. Right-click the header to see a list of available fields; uncheck the checkboxes to hide unneeded field columns.

**Duplicate current tab** makes a copy of the selected tab with the same name; this can be useful to explore altered layouts and displayed data fields. Please note the duplicated tab will appear at the very end of the set of tabs in the current report (to the far right). The user can simply drag the tab to the desired location. Double click the tab name to insert a cursor for editing.

**Update tab content** updates all the report tabs based on any new changes made to the project. Changes to the project are not automatically reflected to the report.

## Report Toolbar

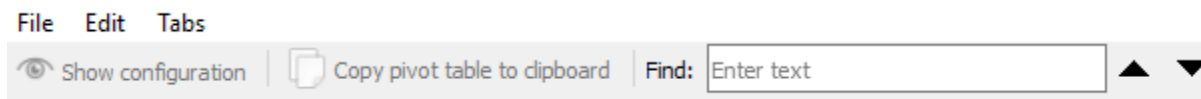


Figure 14: Report toolbar

The **Show configuration** button displays the available pivot fields and all rendering and aggregation options for the tab (for Pivot tabs only). When pressed again, these configuration options are hidden (to make printed or exported reports more condensed, for example). The configuration settings are still displayed in the report footer at the bottom left of the tab.

**Copy pivot table to clipboard** copies the pivot table data as tab separated values.

**Find** locates all occurrences of an entered text string within the current tab:

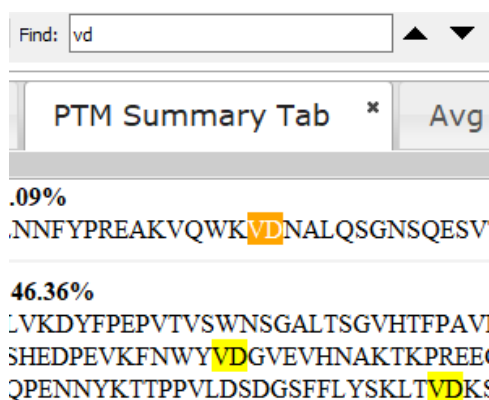


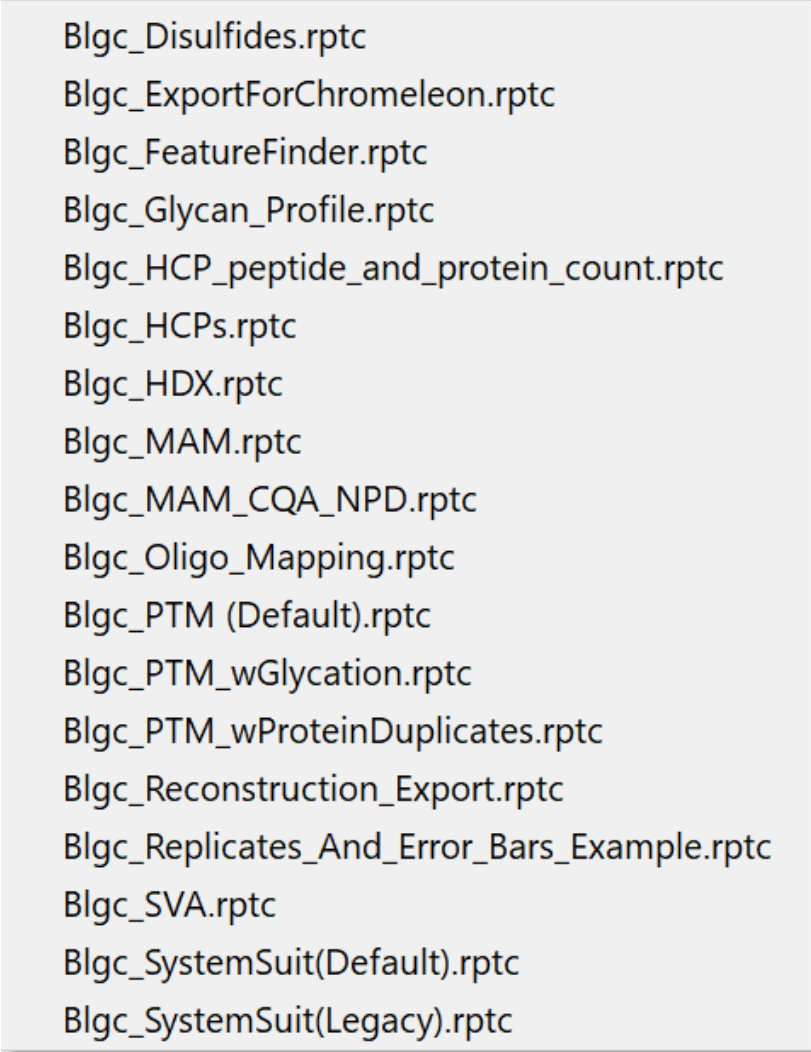
Figure 15: Find function

## Report and Tab Templates

A report template, with \*.rptc extension, contains the tabs and configurations, as well as both pre- and post-pivot dynamic columns, for the generated report. When generating a new report from an application, a default report template, with the name appended with "(Default)", is read from installed configurations. Other useful configurations are available in the same directories. To load a non-default report configuration file from within a report, choose **File > Presets > Report presets**.

Users can also add new Pivot and Plot tabs to existing reports. There are a number of default tab templates available for Pivot and Plot tabs. To load a new tab from within a report, choose **File > Presets > Tab presets**.

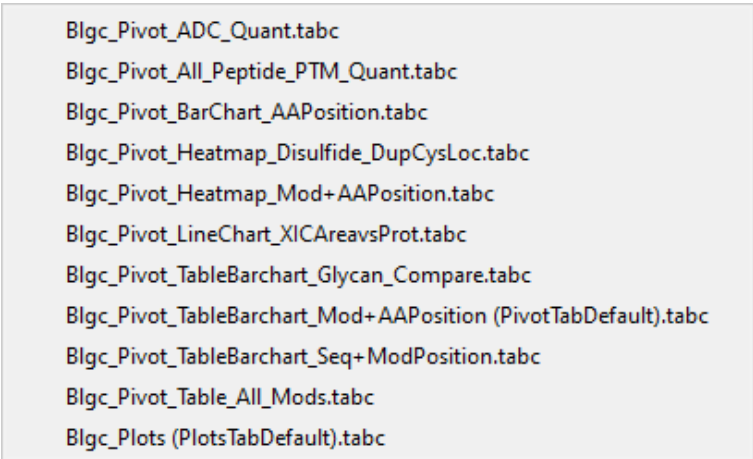
Peptide Analysis contains the following report templates available in File > Presets > Report presets:



Blgc\_Disulfides.rptc  
Blgc\_ExportForChromeleon.rptc  
Blgc\_FeatureFinder.rptc  
Blgc\_Glycan\_Profile.rptc  
Blgc\_HCP\_peptide\_and\_protein\_count.rptc  
Blgc\_HCPs.rptc  
Blgc\_HDX.rptc  
Blgc\_MAM.rptc  
Blgc\_MAM\_CQA\_NPD.rptc  
Blgc\_Oligo\_Mapping.rptc  
Blgc\_PTM (Default).rptc  
Blgc\_PTM\_wGlycation.rptc  
Blgc\_PTM\_wProteinDuplicates.rptc  
Blgc\_Reconstruction\_Export.rptc  
Blgc\_Replicates\_And\_Error\_Bars\_Example.rptc  
Blgc\_SVA.rptc  
Blgc\_SystemSuit(Default).rptc  
Blgc\_SystemSuit(Legacy).rptc

Figure 16: Peptide Analysis report templates

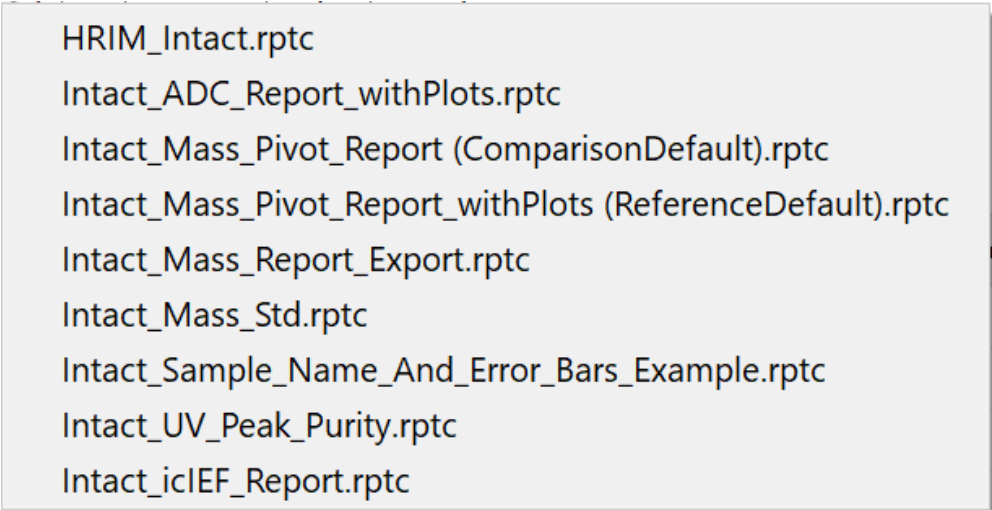
Peptide Analysis contains the following tab templates available in File > Presets > Tab presets:



Blgc\_Pivot\_ADC\_Quant.tabc  
Blgc\_Pivot\_All\_Peptide\_PTM\_Quant.tabc  
Blgc\_Pivot\_BarChart\_AAPosition.tabc  
Blgc\_Pivot\_Heatmap\_Disulfide\_DupCysLoc.tabc  
Blgc\_Pivot\_Heatmap\_Mod+AAPosition.tabc  
Blgc\_Pivot\_LineChart\_XICAreavsProt.tabc  
Blgc\_Pivot\_TableBarchart\_Glycan\_Compare.tabc  
Blgc\_Pivot\_TableBarchart\_Mod+AAPosition (PivotTabDefault).tabc  
Blgc\_Pivot\_TableBarchart\_Seq+ModPosition.tabc  
Blgc\_Pivot\_Table\_All\_Mods.tabc  
Blgc\_Plots (PlotsTabDefault).tabc

Figure 17: Peptide Analysis tab templates

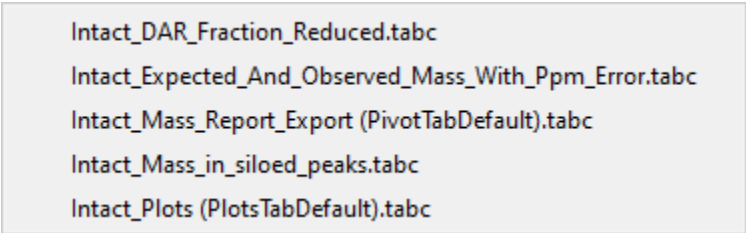
Intact Analysis contains the following report templates available in File > Presets > Report presets:



HRIM\_Intact.rptc  
Intact\_ADC\_Report\_withPlots.rptc  
Intact\_Mass\_Pivot\_Report (ComparisonDefault).rptc  
Intact\_Mass\_Pivot\_Report\_withPlots (ReferenceDefault).rptc  
Intact\_Mass\_Report\_Export.rptc  
Intact\_Mass\_Std.rptc  
Intact\_Sample\_Name\_And\_Error\_Bars\_Example.rptc  
Intact\_UV\_Peak\_Purity.rptc  
Intact\_icIEF\_Report.rptc

Figure 18: Intact Analysis report templates

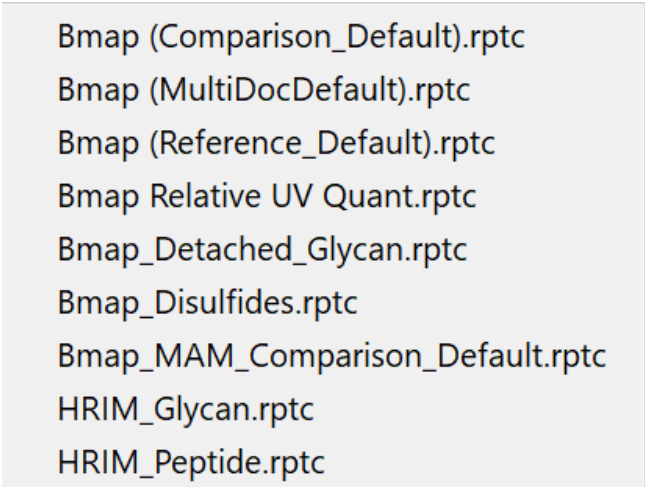
Intact Analysis contains the following tab templates available in File > Presets > Tab presets:



Intact\_DAR\_Fraction\_Reduced.tabc  
Intact\_Expected\_And\_Observed\_Mass\_With\_Ppm\_Error.tabc  
Intact\_Mass\_Report\_Export (PivotTabDefault).tabc  
Intact\_Mass\_in\_siloed\_peaks.tabc  
Intact\_Plots (PlotsTabDefault).tabc

Figure 19: Intact Analysis tab templates

Chromatogram Analysis contains the following report templates available in File > Presets > Report presets:



Bmap (Comparison\_Default).rptc  
Bmap (MultiDocDefault).rptc  
Bmap (Reference\_Default).rptc  
Bmap Relative UV Quant.rptc  
Bmap\_Detached\_Glycan.rptc  
Bmap\_Disulfides.rptc  
Bmap\_MAM\_Comparison\_Default.rptc  
HRIM\_Glycan.rptc  
HRIM\_Peptide.rptc

Figure 20: Chromatogram Analysis report templates

Chromatogram Analysis contains the following tab templates available in File > Presets > Tab presets:

```
Bmap_Fold_Change.tabc
Bmap_Plots (PlotsTabDefault).tabc
Pivot_BarChart_EndAA.tabc
Pivot_TableBarchart_Mod+AAPosition (PivotTabDefault).tabc
```

Figure 21: Chromatogram Analysis tab templates

Oligo Analysis contains the following report templates available in File > Presets > Report presets:

```
OligonucleotideReport.rptc
Oligonucleotide_Purity_byOpticalTrace.rptc
```

Figure 22: Oligo Analysis tab templates

Once a report has been modified, a report configuration file can be saved and used by another project. To save a report template, select **File > Save to file**. To load a custom report template, select **File > Load from file**, navigate to the directory and file containing the report configuration file, and click **Open**.

A custom report configuration file can be set to be the updated default report template loaded with a new report. The new default report template must be named a specific way and the old default report template renamed so it is no longer loaded. To create a new default report template:

- For Peptide Analysis, add (Default) at the end of the \*.rptc filename to create a default report. For example, `Blgc_Std_PTM Report(Default).rptc`. Paste the file into the directory: `\Program Files\ProteinMetrics\PMI-Suite\Base\presets\Byologic\report_config`. Rename the file `Blgc_PTM (Default).rptc` so that it is no longer a default report template. These actions require administrator privileges.
- For Chromatogram Analysis, add (Comparison\_Default) or (Reference\_Default) at the end of the \*.rptc filename to create a default report template for comparison or reference projects.. Paste the file into the directory: `\Program Files\ProteinMetrics\PMI-Suite\Base\presets\Byomap\report_config`. Rename the file `Bmap (Comparison_Default).rptc` or `Bmap (Reference_Default).rptc` so they are no longer the default report templates.
- For Intact Analysis, add (ComparisonDefault) or (ReferenceDefault) at the end of the \*.rptc filename to create a default report template for comparison or reference projects. Paste the file into the directory: `\Program Files\ProteinMetrics\PMI-Suite\Base\presets\Intact\report_config`. Rename the file `Intact_Mass_Pivot_Report (ComparisonDefault).rptc` or `Intact_Mass_Pivot_Report_withPlots (ReferenceDefault).rptc` so they are no longer the default report templates.

## Report Tab Management

The user can add Summary, Pivot Table, Plot, or Flat Input Tables as tabs in the Report.

To add a tab, select the **Tab** menu and select either **Add pivot table**, **Add summary**, **Add plots**, or **Add flat table input**.

The user can add a custom logo to a report tab by dragging and dropping an image onto a report tab. The customized image will be placed at the top left corner. The customization will apply to all tabs.

To remove the customized image, hover over the image until a red X appears at the top right corner of the image. Click on the red X to remove the image from all tabs.

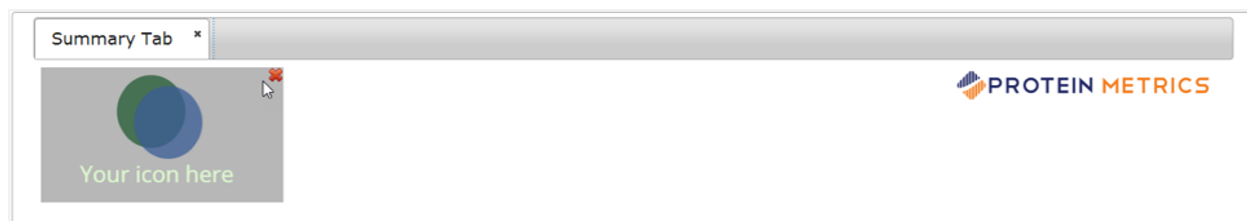


Figure 23: Customizing the report logo

To rename a tab, double click the tab name to insert a cursor for editing.

To remove the tab, click on the black X to the right of the tab name.

## Summary Tab

The Summary Tab includes some of the important table data from the project. An example Summary Tab from a peptide analysis appears as follows:

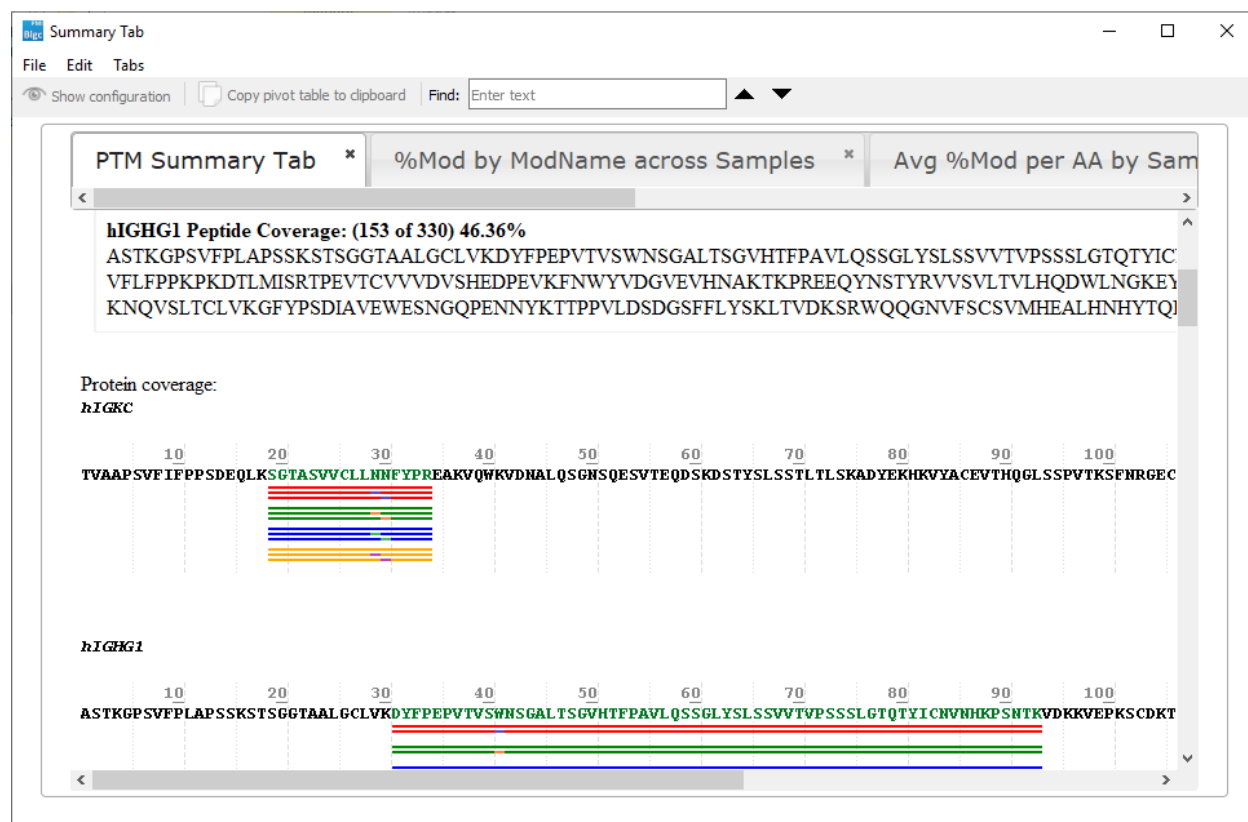


Figure 24: Summary tab

To edit the Summary Tab, select **Edit > Current tab settings**:

Current tab settings

General options

☒ Color code sample name

Project table options:

☐ Show predefined columns  
(Undesired, Unexpected, Desired, Status, Sample name)
 ☒ Show columns visible in application project table
 ☐ Show customized columns

Font options

Font size :

16

Font weight:

Normal

Font style:

Normal

Font name:

Times New Roman

Font color:

#000000

AaBbCcDdKk13.13-HKN

Edit summary template...

OK

Figure 25: Editing the Summary tab in Current tab settings

Current tab settings for the Summary tab have three sections:

- General options** contains **Color code sample name** which color codes the Project table text with the sample colors.

PTM Summary Tab

%Mod by ModName across Samples

Avg %Mod per AA by Sample

% Mod (Multi M

Project table:

Alias Name	Name	Type	Digestion Type	Dynamic Exclusion	MS Id	MS2 Id	Search Type	Search Server URL
Day0	P:\PMI-Demo\Managed\rawData\FD_Series\JH121614_ProtMet1_T0_Tryp_01.RAW	RAW	Tryptic		1			
Day1	P:\PMI-Demo\Managed\rawData\FD_Series\JH121614_ProtMet1_pH8p5_1Day_Tryp_01.RAW	RAW	Tryptic		2			
Day3	P:\PMI-Demo\Managed\rawData\FD_Series\JH121614_ProtMet1_pH8p5_3Day_Tryp_01.RAW	RAW	Tryptic		3			
Day7	P:\PMI-Demo\Managed\rawData\FD_Series\JH121614_ProtMet1_pH8p5_7Day_Tryp_01.RAW	RAW	Tryptic		4			

Figure 26: Project table in Summary tab color-coded by sample name

- Project table options** determines which columns are displayed in the report Project table. The user may choose between pre-defined table columns, all table columns (primarily applicable to Intact Analysis), and customized columns. When **Show customized columns** is selected, the **Edit columns** button appears.



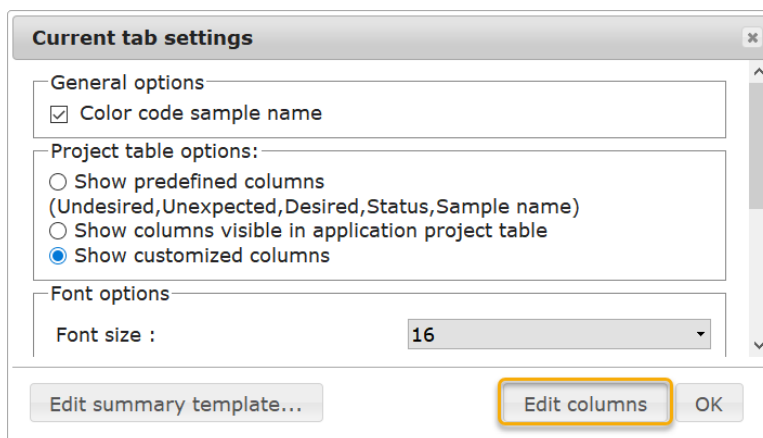


Figure 27: Current tab settings with **Show customized columns** selected

To edit the visibility and order of columns in the Project table, click the **Edit columns** button.

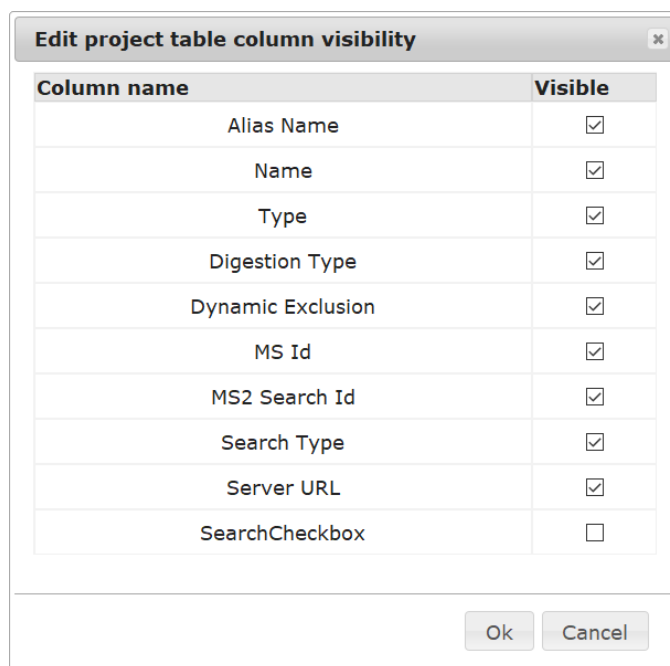


Figure 28: Setting Project table column visibility and order in the Summary tab

To remove a column from the Project table, uncheck the column name. To reorder a Project table column, click the column, drag it to the new position, and release it.

- **Font options** allows the user to adjust the size, weight (Normal or Bold), style (Normal or Italic), name and color of the font. An example of the formatted text is displayed in the dialog.

Advanced users can further edit the Summary tab by clicking the **Edit summary template** button to open the Template Editor:

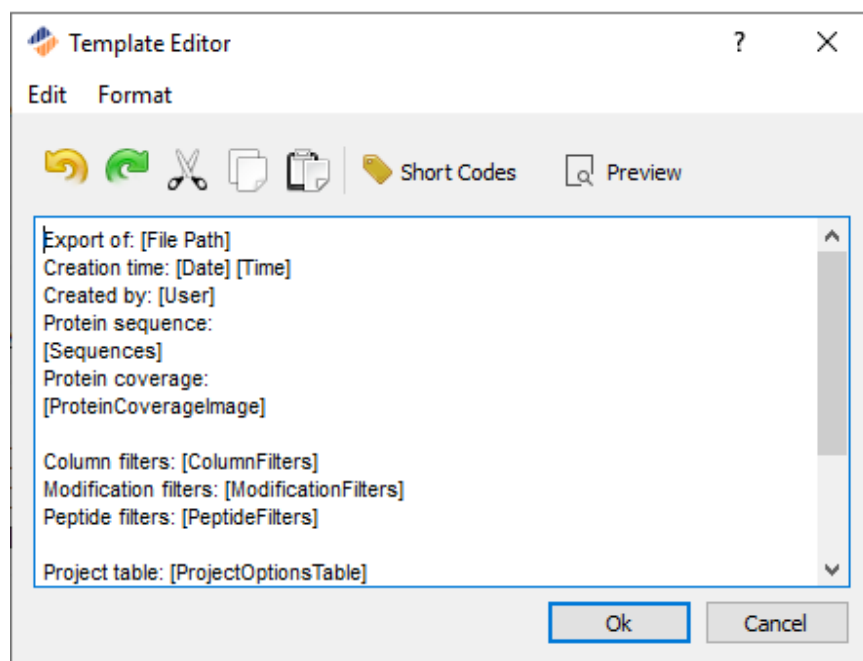


Figure 29: Summary tab template editor

See the [Summary Tab Template Editor](#) section for additional details.

## Pivot Tab

According to Wikipedia:

A pivot table is a table of statistics that summarizes the data of a more extensive table (such as from a database, spreadsheet, or business intelligence program). This summary might include sums, averages, or other statistics, which the pivot table groups together in a meaningful way.

Pivot tables are a technique in data processing. They enable users to arrange and rearrange (or "pivot") statistics in order to draw attention to useful information. By grouping hierarchical data (with one-to-many relationships) under multiple column headings, complex data can be organized and condensed into a simpler table.

For example, the data in the flat table in the figure below displays across 64 rows:

Sample name ▾	Sample name ↓	Peak # ↑	Name ↓	Expected mass ↑	Delta mass from calc. ↑
Peak # ▾	ADC 1000ug-ml_2-D_2_01_1185.d	4	ADC_linker , Drug(6)	151150	-3.85755
Name ▾			ADC_linker , Drug(5)	150191	-3.16754
Expected mass ▾			ADC_linker , Drug(4)	149227	2.85268
Delta mass from calc. ▾			ADC_linker , Drug(3)	148274	-0.653685
			ADC_linker , Drug(2)	147316	0.814321
			ADC_linker , Drug(1)	146357	0.876487
			ADC_linker , Drug(0)	145399	2.68384
			ADC , Drug(8)	152835	-2.57572
			ADC , Drug(7)	151877	-3.16825
			ADC , Drug(6)	150918	-1.79026
			ADC , Drug(5)	149960	-1.57985
			ADC , Drug(4)	148996	4.49659
			ADC , Drug(3)	148043	0.235289
			ADC , Drug(2)	147084	0.93887
			ADC , Drug(1)	146126	2.87699
			ADC , Drug(0)	145167	2.84894

Figure 30: Flattened table data

The same data can be reorganized in a much more intelligible structure using a pivot table, as show in the figure below:

Sum ▾						
Delta mass from calc. ▾						
Name ▾						
Expected mass ▾						
		Sample name ← Peak # ←	ADC 100ug-ml_2-C_7_01_1182.d	ADC 200ug-ml_2-C_8_01_1183.d	ADC 500ul-ml_2-D_1_01_1184.d	ADC 1000ug-ml_2-D_2_01_1185.d
	Name ↓ Expected mass ↑		1	2	3	4
	ADC_linker , Drug(6)		-5.656011	-3.029556	-2.168420	-3.857550
	ADC_linker , Drug(5)		-1.071813	-1.647766	-1.129801	-3.167542
	ADC_linker , Drug(4)		6.420644	4.485616	4.504757	2.852682
	ADC_linker , Drug(3)		-0.600375	-0.012828	1.830595	-0.653685
	ADC_linker , Drug(2)		2.353646	1.420844	1.655275	0.814321
	ADC_linker , Drug(1)		2.775643	3.045493	3.821059	0.876487
	ADC_linker , Drug(0)		1.843527	4.306960	8.389733	2.683840
	ADC , Drug(8)		-2.388330	2.832138	1.282910	-2.575723
	ADC , Drug(7)		-3.638739	-2.834629	-2.215001	-3.168253
	ADC , Drug(6)		1.376561	-0.239236	0.395879	-1.790259
	ADC , Drug(5)		0.335146	0.753834	-0.627207	-1.579847
	ADC , Drug(4)		7.586617	6.335042	7.026441	4.496590
	ADC , Drug(3)		1.324480	1.237413	1.530265	0.235289
	ADC , Drug(2)		2.879652	2.299738	2.770845	0.938870
	ADC , Drug(1)		3.820522	3.596316	3.437995	2.876987
	ADC , Drug(0)		5.236307	4.782913	4.458601	2.848939

Figure 31: Pivoted table data

In the above example, the fields “Sample Name” and “Peak” were dragged above the table to create two levels of pivoting. The numeric field “Delta mass from calc.” is removed from the field list in the left column, and instead is selected in the drop-down at top left. The “Delta mass from calc.” field is now displayed for the combination of the pair of row fields “Name” and “Expected mass” and the pair of column fields “Sample Name” and “Peak”.

## Tour of Pivot Table Areas

File Edit Tabs Debug  
 Show configuration Copy pivot table to clipboard

Pivot Tab

Table **1** Sum **2** MS Id MS Alias name **5**

Apex Time (Posit) **3** Mod. Names **4**

GlycanFamily  
 Glycans  
 Glycoform  
 Labels  
 Mod. AAs  
 Score  
 Sequence (unformatted)  
 Validate  
 Var. Pos. Peptide  
 XIC AUC  
 [runAliasName]  
 XIC Ratio%  
 XIC area summed  
 Z

Protein name  
 Var. Pos. Protein

Mod. Names	Protein name	Var. Pos. Protein	MS Id	MS Alias name	1	2	3	4	Totals
					Day0	Day1	Day3	Day7	
	hIGHG1				0	0	0	0	257
	hIGKC				0	0	0	0	
Ammonia-loss/17.0265	hIGHG1	169			0.351	0.237	0.404	0.392	
		198			3.43	3.69	3.76	3.76	
Deamidated/0.9840	hIGHG1	169				0.246	1.08	2.77	
		198			1.04	1.6	1.97	2.66	
		267			2.56	8.44	19.2	37.1	
		272			1.41	8.84	20.7	37.9	
	hIGKC	29			0.321	0.429	0.407	0.49	
		30			0.03	0.0437	0.0466	0.0548	
Dioxidation/31.9898	hIGHG1	196			0.135	0.278	0.252	0.214	
Oxidation/15.9949	hIGHG1	41			1.71	1.78	1.58	1.64	
		138			12.1	14.3	14.6	22.5	
		196			0.0107	0.014	0.0133	0.0137	
		311			4.41	4.39	4.99	6.43	
									257
									257
									257

**6** Level 0 Totals

**7** Level 0 Totals

Figure 32: The regions in a Pivot Table

1. View type
2. Aggregator options
3. Show unused fields
4. Show row fields
5. Show column fields
6. Show row total
7. Show column total

## Rendering Options

Pivoted data is not limited to tables; a variety of charts and plots can display pivoted data. To change the data display type (rendering option), click the drop-down option at the top-left:

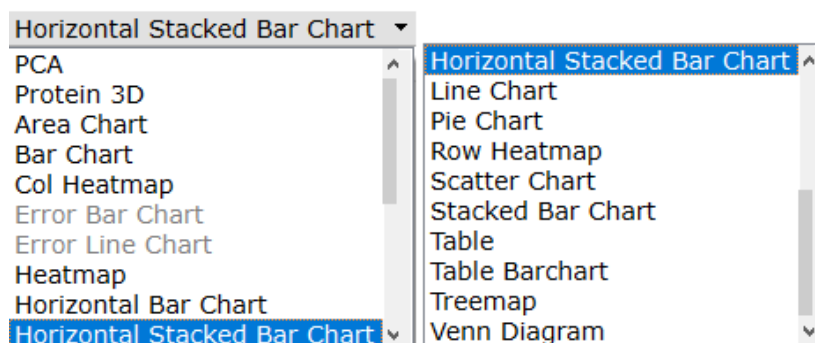


Figure 33: Pivot tab rendering options

Category	Rendering Options	Current tab settings and notes
Chart	Area Chart, Bar Chart, Horizontal Bar Chart, Horizontal Stacked Bar Chart, Line Chart, Pie Chart, Protein Map, Scatter Chart, Stacked Bar Chart, Table Barchart	Common settings and Chart-specific settings. Line Chart also has an option to Show R2, slope and intercept values.
Error Chart	Error Bar Chart, Error Line Chart	Common settings and Error Chart settings. Error Chart is enabled only if the post-pivot dynamic column AllErrorColumns or StdDevErrorColumns are added into the Pivot Table.
Heatmap	Col Heatmap, Heatmap, Row Heatmap	Common settings and Color settings. Col/Row Heatmap defines the color range based on values within each column/row. Heatmap will consider all values of columns and rows.
PCA	PCA	Common settings and PCA-specific settings.
Protein 3D	Protein 3D	Common settings and protein 3D-specific settings.
Treemap	Treemap	Common settings only.
Venn Diagram	VennDiagram	Common settings and Chart-specific settings.

## Aggregator Options

Aggregators are the statistical method used to display sets of pivoted numeric data. To change the aggregator, click the drop-down option to the right of the rendering option:

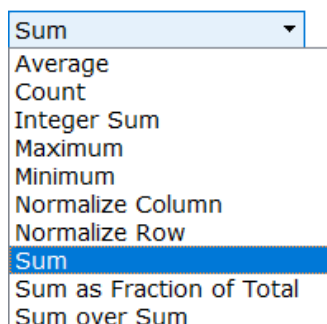
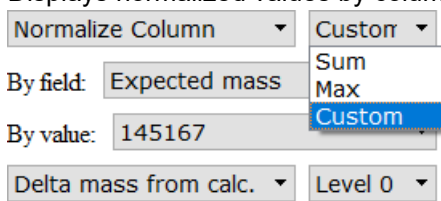
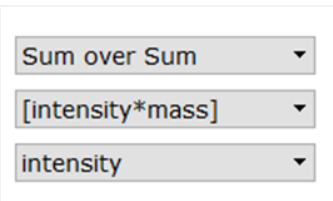


Figure 34: Pivot tab Aggregator options

Aggregator	Description
Average	Displays average values.
Count	Displays number of values. This function does not require a parameter.
Integer Sum	Displays summed values for integers.
Maximum/Minimum	Displays maximum or minimum values.
Normalize Column/Row	<p>Displays normalized values by column or row.</p>  <p>To normalize based on a specific value other than Sum or Max of all values in a column (or row), select Custom. Normalize By field will list all eligible fields. Normalize By value will list all values of the selected field. Level defines the pivot level to normalize against. Level 0 normalizes to the selected value. Level 1 and 2 normalizes by the first or second field values, respectively.</p>
Sum	Display summed values.
Sum as Fraction of Total	Display summed value as a percentage of all values in column/row/table.
Sum over Sum	<p>For example: <math>Mn = \text{Sum}(\text{intensity} * \text{mass}) / \text{Sum}(\text{intensity})</math>.</p> 

## Field Management

To change the numeric data field to pivot, click the drop-down option below the aggregate method:

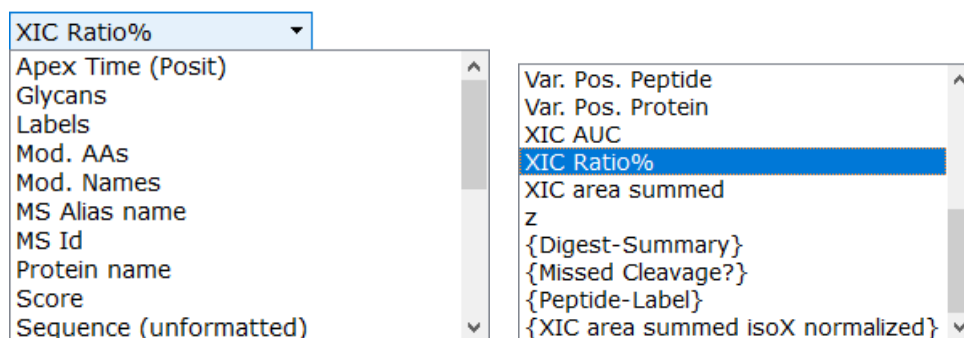


Figure 35: Data field to select for the pivoting

To add a new field to the table, click the field name from the available fields in the first column, and drag it to the desired order of the displayed fields in the second column. To reorder a table field column, click the field name in the second list, and drag it to the new order position:

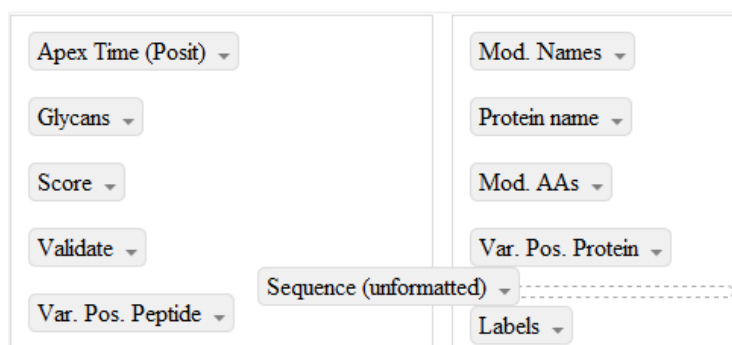


Figure 36: Drag-and-drop new fields into the table

To add a new field to the pivoted value columns, click the field name from the available fields in the first column, and drag it to the desired order of the pivot fields above the table:



Figure 37: Drag-and-drop new fields into the pivoting

The pivot table editing as in the Figure above updates to reflect the new layer of pivoting shown in the Figure below:

MS Id ←	1					2				
MS Alias name ←	Day 0					Day 1				
Var. Pos. Peptide ←	4	11	12	14	19	4	11	12	14	19

Figure 38: Pivoted results after the table edit

## Filters

Data values can be filtered from the report in two ways. **Include/Exclude** filters, where unchecked values are removed from the report and from all aggregate calculations, can be set for pivot row and column fields, but also for unused fields. **Show/Hide** filters, where unchecked values are not removed from aggregate calculations, but they are not displayed in the report, can be set for pivot row and column fields. The user can only Show or Hide values that are included in a pivot tab. A value that is excluded from the report will be disabled from Show/Hide selection. To open the filters, click the down arrow following the field name. Both filter types will open:

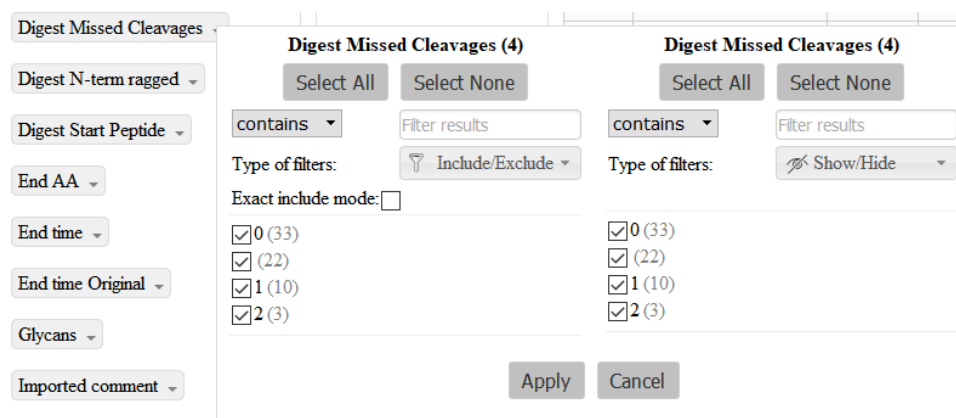




Figure 39: Included/Exclude and Show/Hide Data filters

Click **Select All** to check all unique values and **Select None** to uncheck all values. If any values are unchecked, the pivot field name is moved to the top of the field list and is marked in red with an exclude filter  or a hide filter  icon, as shown in Figure 40 below.

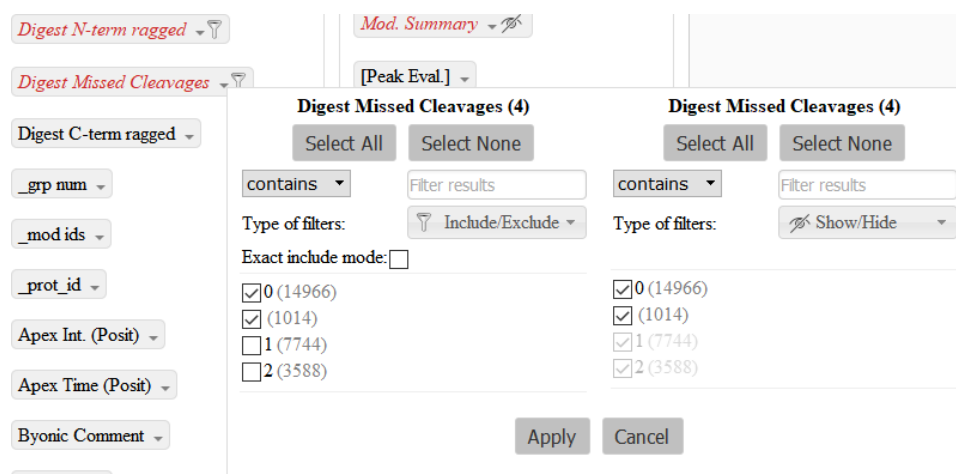


Figure 40: Filtered data is marked in red and shown with filter type icons

For numeric data, the filters apply to the aggregator calculation. Unchecked Include/Exclude filter values are excluded from the calculation, while unchecked Show/Hide filter values are included in the calculation:



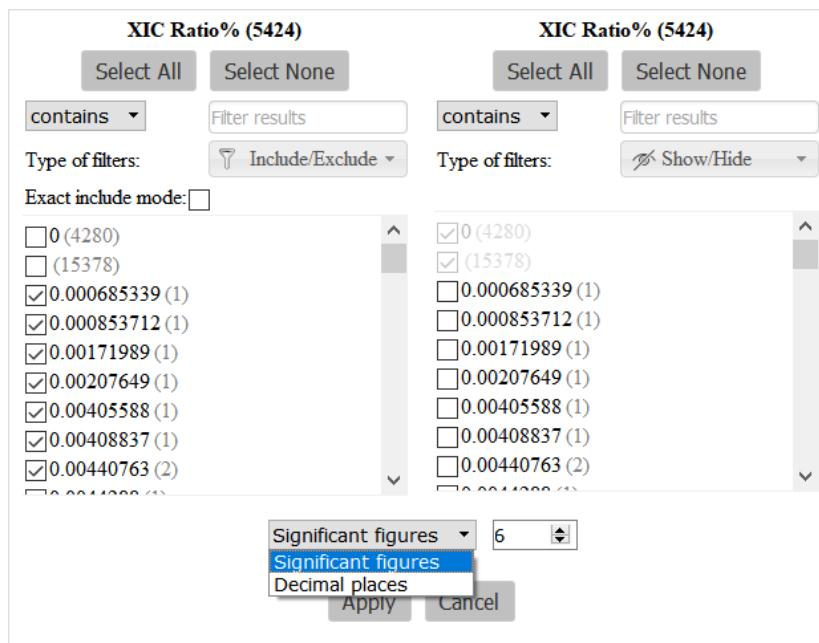


Figure 41: Filtering data from the aggregator calculation

To modify the data format for either the pivot column or pivot row fields, set the Significant figures or Decimal place to be displayed. Note the displayed data format does not change the calculation result for aggregator values.

To filter by string values or numeric ranges, select **Contains** for string values or a numeric operator. Then enter the string or numeric value:

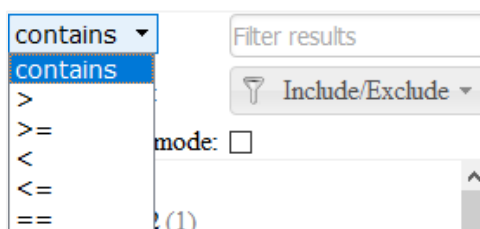


Figure 42: Text filters using operators

The available list of values updates as the value is typed in:

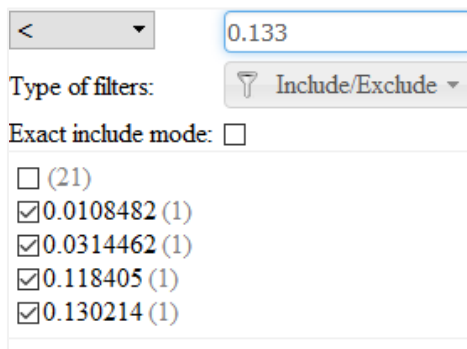


Figure 43: Numeric filters using operators

To reorder how the values of a pivot field is displayed, set **Type of filters** to **Custom order**, and drag and drop the values to reorder them. Reordering does not affect the aggregation calculation:

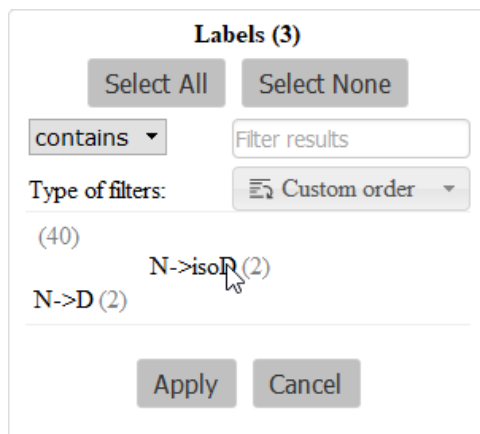


Figure 44: Reordering labels by drag-and-drop

Pivoted data can also be filtered inside the pivot table directly. To filter from within the pivot table, right-click the lower-level pivot field to open the filter dialog:

		Sample name ←	ADC 100ug-ml_2-C,7_01_1182.d	ADC 200ug-ml_2-C,8_01_1183.d	ADC 500ul-ml_2-D,1_01_1184.d	ADC 1000ug-ml_2-D,2_01_1185.d
		Peak # ←				
Name ↓	Expected mass ↑		1	2	3	4
ADC_linker , Drug(6)	151150			029556	-2.168420	-3.857550
ADC_linker , Drug(5)	150191			647766	-1.129801	-3.167542
ADC_linker , Drug(4)	149227			485616	4.504757	2.852682
ADC_linker , Drug(3)	148274			012828	1.830595	-0.653685
ADC_linker , Drug(2)	147316			420844	1.655275	0.814321
ADC_linker , Drug(1)	146357			045493	3.821059	0.876487
ADC_linker , Drug(0)	145399			306960	8.389733	2.683840
ADC , Drug(8)	152835			832138	1.282910	-2.575723
ADC , Drug(7)	151877			834629	-2.215001	-3.168253
ADC , Drug(6)	150918			239236	0.395879	-1.790259
ADC , Drug(5)	149960			753834	-0.627207	-1.579847
ADC , Drug(4)	148996			335042	7.026441	4.496590
ADC , Drug(3)	148043			237413	1.530265	0.235289
ADC , Drug(2)	147084			299738	2.770845	0.938870
ADC , Drug(1)	146126			596316	3.437995	2.876987
ADC , Drug(0)	145167					
			5.236307	4.782913	4.458601	2.848939

Figure 45: Filtering data in the pivot table through a right-click in the second pivot level

## Sorting

To sort data in the display fields, click once to sort ascending (down arrow), twice to sort descending (down arrow), and a third time to remove the sort (no arrow):

				MS Id ←	1
				MS Alias name ←	Day 0
Mod. Names ↓	Protein name ↑	Mod. AAs ↑	Var. Pos. Protein ↑		
<b>Oxidation/15.9949</b>	<b>hIGHG1</b>	<b>M</b>	<b>135</b>		98.3
			<b>311</b>		262
		<b>W</b>	<b>41</b>		135
			<b>196</b>		117
<b>Dioxidation/31.9898</b>	<b>hIGHG1</b>	<b>W</b>	<b>196</b>		234
<b>Deamidated/0.9840</b>	<b>hIGHG1</b>	<b>N</b>	<b>198</b>		351
			<b>267</b>		270
			<b>272</b>		180
	<b>hIGKC</b>	<b>N</b>	<b>29</b>		115
			<b>30</b>		115
<b>Ammonia-loss/-17.0265</b>	<b>hIGHG1</b>	<b>N</b>	<b>169</b>		160
			<b>198</b>		234

Figure 46: Table sorting

## Show/Hide Configuration

When the report tab is fully configured, the configuration controls can be hidden to maximize the display of the data. To hide the data and field configuration controls, click the selected **Show configuration** button at the top left:

☒ Show configuration 
 ☐ Copy pivot table to clipboard 
 Find:

PTM Summary Tab \* 
 %Mod by ModName across Samples \* 
 Avg %Mod per AA by Sample \* 
 % Mod (Multi Mods per Peptide) \*

**Protein Metrics**

						MS Id ←	1	2	3	4
						MS Alias name ←	Day 0 (P0)	Day 1 (P1)	Day 3 (P3)	Day 7 (P7)
Sequence (unmodified) ↑	Mod. Names ↑	Protein name ↑	Mod. AAs ↑	Var. Pos. Protein ↑	Label ↑					
DILMDSR EQVYNTYK	Oxidation/15.9949	hIGHG1_HUMAN Ig gamma-1	M	135			5.41	7.54	6.9	10.9
	Deamidated/0.9840	hIGHG1_HUMAN Ig gamma-1	N	180			0.0773	0.173	0.543	0.985
	Nitrosylation/1079.4017	hIGHG1_HUMAN Ig gamma-1	N	180			1.71	0.754	1.48	1.44
	Nitrosylation/1116.4129	hIGHG1_HUMAN Ig gamma-1	N	180			1.46	0.953	1.78	1.44
	Nitrosylation/1241.4545	hIGHG1_HUMAN Ig gamma-1	N	180			9.49	6.4	10.9	10.9
	Nitrosylation/1378.4757	hIGHG1_HUMAN Ig gamma-1	N	180			0.0811	0	0.0812	0.0815
	Nitrosylation/1402.5073	hIGHG1_HUMAN Ig gamma-1	N	180			2.18	2.27	2.86	2.26
	Nitrosylation/1444.5339	hIGHG1_HUMAN Ig gamma-1	N	180			22.5	52.8	22.1	22.7
	Nitrosylation/1606.5967	hIGHG1_HUMAN Ig gamma-1	N	180			22.9	22	22.2	22.6
	Nitrosylation/1768.6395	hIGHG1_HUMAN Ig gamma-1	N	180			3.7	2.6	3.63	3.46
	Nitrosylation/1809.6661	hIGHG1_HUMAN Ig gamma-1	N	180			0.689	0.298	0.737	0.662
	Nitrosylation/1897.6821	hIGHG1_HUMAN Ig gamma-1	N	180			0.16	0.0458	0.166	0.131
	Nitrosylation/2055.7349	hIGHG1_HUMAN Ig gamma-1	N	180			0.713	0.0404	0.735	0.7
	Ammonia-loss/-17.0265	hIGHG1_HUMAN Ig gamma-1	N	169			0.187	0.2	0.218	0.187
FNWYVGVETSTK	Deamidated/0.9840	hIGHG1_HUMAN Ig gamma-1	N	169			0.00492	0.00639	0.0076	0.0108
				169			0.000639	0.0077	1.22	2.26
	Ammonia-loss/-17.0265	hIGHG1_HUMAN Ig gamma-1	N	267			1.96	1.89	1.49	1.06
GYPIDIANLWLNQKPNNTYK	Deamidated/0.9840	hIGHG1_HUMAN Ig gamma-1	N	267		N → D	0.362	1.11	2.23	2.29
				272		N → ind	1.82	5.93	11.8	19.4
							1.28	1.82	17.3	29
	Dioxidation/31.9898	hIGHG1_HUMAN Ig gamma-1	W	264			0.0776	0.0554	0.0753	0.0713
NQVETCTYK	Deamidated/0.9840	hIGHG1_HUMAN Ig gamma-1	N	244			0.0572	0.178	0.415	1.07
	Deamidated/0.9840	hIGKC_HUMAN Ig kappa	N	29			0.308	0.412	0.386	0.409
IGTASVYCLINNTYK	Deamidated/0.9840	hIGKC_HUMAN Ig kappa	N	50			0.0585	0.011	1.39	3.18
VYNAIQGNQSTTTQDAK	Deamidated/0.9840	hIGKC_HUMAN Ig kappa	N	198			3.26	3.32	3.39	3.38
VYVLTLLDQWLNQK	Ammonia-loss/-17.0265	hIGHG1_HUMAN Ig gamma-1	N	198			0.198	0.411	0.839	1.28
	Deamidated/0.9840	hIGHG1_HUMAN Ig gamma-1	N	198		N → D	0.188	0.731	0.878	1.08
							0.127	0.25	0.229	0.191
VYVCTYTRQLDQVYK	Deamidated/0.9840	hIGKC_HUMAN Ig kappa	Q	91			0.00088	0.00094	0.00093	0.00093
	Ammonia-loss/-17.0265	hIGHG1_HUMAN Ig gamma-1	N	317			0.415	0.402	0.865	0.825
	Deamidated/0.9840	hIGHG1_HUMAN Ig gamma-1	N	317			0.998	0.475	0.574	0.648
WQQGVNFSYVMEATFNNTYK	Oxidation/15.9949	hIGHG1_HUMAN Ig gamma-1	M	331			4.64	3.99	4.54	5.79

Normalize Column - (XIC area summed isoX normalized), Level 1  
 Normalize type - Sum  
 Hidden values in: Mod. Names.

Figure 47: Hide Configuration mode

## Pivot Tab Current Tab Settings: Common

To edit the Pivot Tab itself, select **Edit > Current tab settings**:

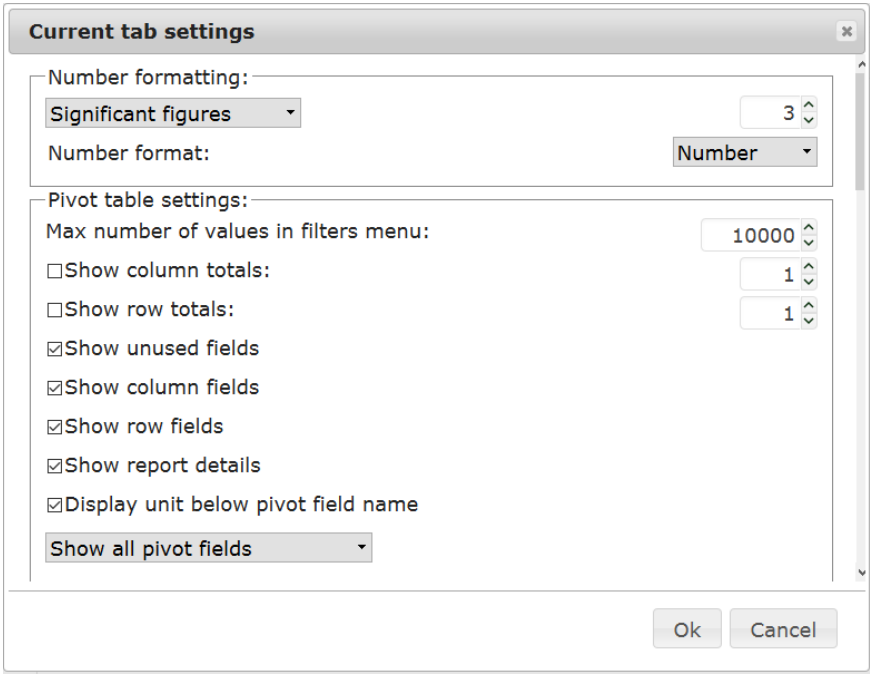


Figure 48: Pivot options in Current tab settings

Setting	Description
Number formatting	Options are Significant figures and Decimal places.
Significant figures	Significant figures range is 1 to 10.
Decimal place	Decimal place range is 0 to 10.
Number format	Options are Numeric, Scientific, Percent, or ppm.
Pivot table settings	
Max number of values in filters menu	Used to limit the number of pivot field values. If there are n values, and n-m is set as max, the last/maximum m values are not displayed.
Show column totals	Displays the totals of all the column values within rows at different levels of pivoting in a column to the right of the table. Level 0 displays a single total for all rows. The highest level displays a total for each table row. The allowed range is 1 to the number of pivot column (or row) fields + 1.
Show row totals	Displays the totals of all the row values within columns at different levels of pivoting in a row at the bottom of the table. Level 0 displays a single total for all columns. The highest level displays a total for each table column. The allowed range is 1 to the number of pivot column (or row) fields + 1.
Show unused fields	Turns off display of the first column containing the unassigned row fields.
Show column fields	Turns off display of the pivot fields above the table.
Show row fields	Turns off display of the second column containing the assigned row fields.
Show report details	When “Show configuration” is unpressed, (set to “Hide configuration mode”), pivot table aggregation and filtering information are displayed at the bottom of the report. See <a href="#">Figure 48</a> and <a href="#">Figure 49</a> .

Show all pivot fields or  
Show all common pivot  
fields

Show all pivot fields – show all fields which comes from the input flat table.  
Show all common pivot fields – show fields which are listed in  
commonly\_used\_column\_names.ccnsn (which is in the application specific  
presets folder, for example, Program Files > ProteinMetrics > PMI-Suite >  
Base > presets > Byologic) as well as all pre pivot dynamic columns.

Protein Metrics

Table: [Apex Time (Posit) AcrossAvg] [Obs. m/z AcrossAvg] [Obs. M AcrossAvg] [ppm AcrossAvg] [SummaryOfChargeStates] [XIC End AcrossAvg] [XIC Start AcrossAvg] [grp mm] [mod ids] [prot\_id] [Apex Int. (Posit)] [Apex Time (Posit)] [Byonic Comment] [Calc. m/z] [Calc. time Var (min)] [Calc. time Wild (min)] [Calc. M] [Center of m/z] [Comment] [Delta (Dalton)] [Delta Score] [Delta Mod. Score] [Delta R.T. Obs-Delta R.T. Ptd.]

Sequence (unformatted)

Mod. Names - [P] [Mod. AAs] [Var. Pos. Proteins] [Labels]

Sequence (unformatted)	Mod. Name	Protein name	Mod. AA	Var. Pos. Proteins	Labels	MSM - MS Alias name	1 Obs 0 (%)	2 Obs 1 (%)	3 Obs 2 (%)	4 Obs 3 (%)
Sequence (unformatted)	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	M	125			5.41	7.54	6.9	10.9
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	100			0.0731	0.121	0.182	0.065
EGREGI	Modification: 1076.4017	EGREGI_BUMAN'lg gamma-1	N	100			1.74	0.754	1.48	1.44
EGREGI	Modification: 1216.4229	EGREGI_BUMAN'lg gamma-1	N	100			1.46	0.933	1.78	1.44
EGREGI	Modification: 1241.4545	EGREGI_BUMAN'lg gamma-1	N	100			0.40	6.4	10.9	10.9
EGREGI	Modification: 1378.4757	EGREGI_BUMAN'lg gamma-1	N	100			0.0841	0	0.0812	0.0843
EGREGI	Modification: 1403.5073	EGREGI_BUMAN'lg gamma-1	N	100			3.18	2.57	3.86	2.56
EGREGI	Modification: 1444.5339	EGREGI_BUMAN'lg gamma-1	N	100			22.2	42.8	22.1	22.7
EGREGI	Modification: 1466.5607	EGREGI_BUMAN'lg gamma-1	N	100			22.9	22	22.2	22.6
EGREGI	Modification: 1768.6395	EGREGI_BUMAN'lg gamma-1	N	100			3.7	2.6	3.63	3.46
EGREGI	Modification: 1809.6661	EGREGI_BUMAN'lg gamma-1	N	100			0.689	0.208	0.717	0.662
EGREGI	Modification: 1807.6821	EGREGI_BUMAN'lg gamma-1	N	100			0.16	0.6438	0.366	0.181
EGREGI	Modification: 2059.7349	EGREGI_BUMAN'lg gamma-1	N	100			0.713	0.6404	0.755	0.7
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	169			0.187	0.7	0.718	0.187
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	159			0.06402	0.06439	0.0076	0.0098
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	169			0.006659	0.675	1.22	2.56
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	267			1.86	1.86	1.49	1.06
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	267		N=D	0.262	1.11	2.25	2.59
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	272		N=mod	1.82	3.93	11.8	18.4
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	272			1.28	1.82	17.3	29
EGREGI	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	W	264			0.0276	0.0034	0.0253	0.0228
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	241			0.0572	0.178	0.455	1.07
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	29			0.108	0.417	0.186	0.449
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	86			0.0585	0.611	1.39	1.18
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	158			3.36	3.55	3.59	3.58
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	158		N=D	0.486	0.611	0.839	1.28
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	158		N=mod	0.486	0.731	0.878	1.08
EGREGI	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	W	156			0.127	0.26	0.229	0.291
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	Q	91			0.00804	0.00991	0.0263	0.0463
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	317			0.433	0.462	0.165	0.223
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	317			0.358	0.473	0.524	0.648
EGREGI	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	M	311			4.04	3.99	4.54	5.76

Figure 49: Show configuration with Show report details unchecked

Protein Metrics

Table: [Apex Time (Posit) AcrossAvg] [Obs. m/z AcrossAvg] [Obs. M AcrossAvg] [ppm AcrossAvg] [SummaryOfChargeStates] [XIC End AcrossAvg] [XIC Start AcrossAvg] [grp mm] [mod ids] [prot\_id] [Apex Int. (Posit)] [Apex Time (Posit)] [Byonic Comment] [Calc. m/z] [Calc. time Var (min)] [Calc. time Wild (min)] [Calc. M] [Center of m/z] [Comment] [Delta (Dalton)] [Delta Score] [Delta Mod. Score] [Delta R.T. Obs-Delta R.T. Ptd.]

Sequence (unformatted)

Mod. Names - [P] [Mod. AAs] [Var. Pos. Proteins] [Labels]

Sequence (unformatted)	Mod. Name	Protein name	Mod. AA	Var. Pos. Proteins	Labels	MSM - MS Alias name	1 Obs 0 (%)	2 Obs 1 (%)	3 Obs 2 (%)	4 Obs 3 (%)
Sequence (unformatted)	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	M	125			5.41	7.54	6.9	10.9
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	100			0.0731	0.121	0.182	0.065
EGREGI	Modification: 1076.4017	EGREGI_BUMAN'lg gamma-1	N	100			1.74	0.754	1.48	1.44
EGREGI	Modification: 1216.4229	EGREGI_BUMAN'lg gamma-1	N	100			1.46	0.933	1.78	1.44
EGREGI	Modification: 1241.4545	EGREGI_BUMAN'lg gamma-1	N	100			0.40	6.4	10.9	10.9
EGREGI	Modification: 1378.4757	EGREGI_BUMAN'lg gamma-1	N	100			0.0841	0	0.0812	0.0843
EGREGI	Modification: 1403.5073	EGREGI_BUMAN'lg gamma-1	N	100			3.18	2.57	3.86	2.56
EGREGI	Modification: 1444.5339	EGREGI_BUMAN'lg gamma-1	N	100			22.2	42.8	22.1	22.7
EGREGI	Modification: 1466.5607	EGREGI_BUMAN'lg gamma-1	N	100			22.9	22	22.2	22.6
EGREGI	Modification: 1768.6395	EGREGI_BUMAN'lg gamma-1	N	100			3.7	2.6	3.63	3.46
EGREGI	Modification: 1809.6661	EGREGI_BUMAN'lg gamma-1	N	100			0.689	0.208	0.717	0.662
EGREGI	Modification: 1807.6821	EGREGI_BUMAN'lg gamma-1	N	100			0.16	0.6438	0.366	0.181
EGREGI	Modification: 2059.7349	EGREGI_BUMAN'lg gamma-1	N	100			0.713	0.6404	0.755	0.7
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	169			0.187	0.7	0.718	0.187
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	159			0.06402	0.06439	0.0076	0.0098
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	169			0.006659	0.675	1.22	2.56
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	267			1.86	1.86	1.49	1.06
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	267		N=D	0.262	1.11	2.25	2.59
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	272		N=mod	1.82	3.93	11.8	18.4
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	272			1.28	1.82	17.3	29
EGREGI	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	W	264			0.0276	0.0034	0.0253	0.0228
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	241			0.0572	0.178	0.455	1.07
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	29			0.108	0.417	0.186	0.449
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	86			0.0585	0.611	1.39	1.18
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	158			3.36	3.55	3.59	3.58
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	158		N=D	0.486	0.611	0.839	1.28
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	158		N=mod	0.486	0.731	0.878	1.08
EGREGI	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	W	156			0.127	0.26	0.229	0.291
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	Q	91			0.00804	0.00991	0.0263	0.0463
EGREGI	Modification: 17.0265	EGREGI_BUMAN'lg gamma-1	N	317			0.433	0.462	0.165	0.223
EGREGI	Modification: 0.9840	EGREGI_BUMAN'lg gamma-1	N	317			0.358	0.473	0.524	0.648
EGREGI	Modification: 15.9949	EGREGI_BUMAN'lg gamma-1	M	311			4.04	3.99	4.54	5.76

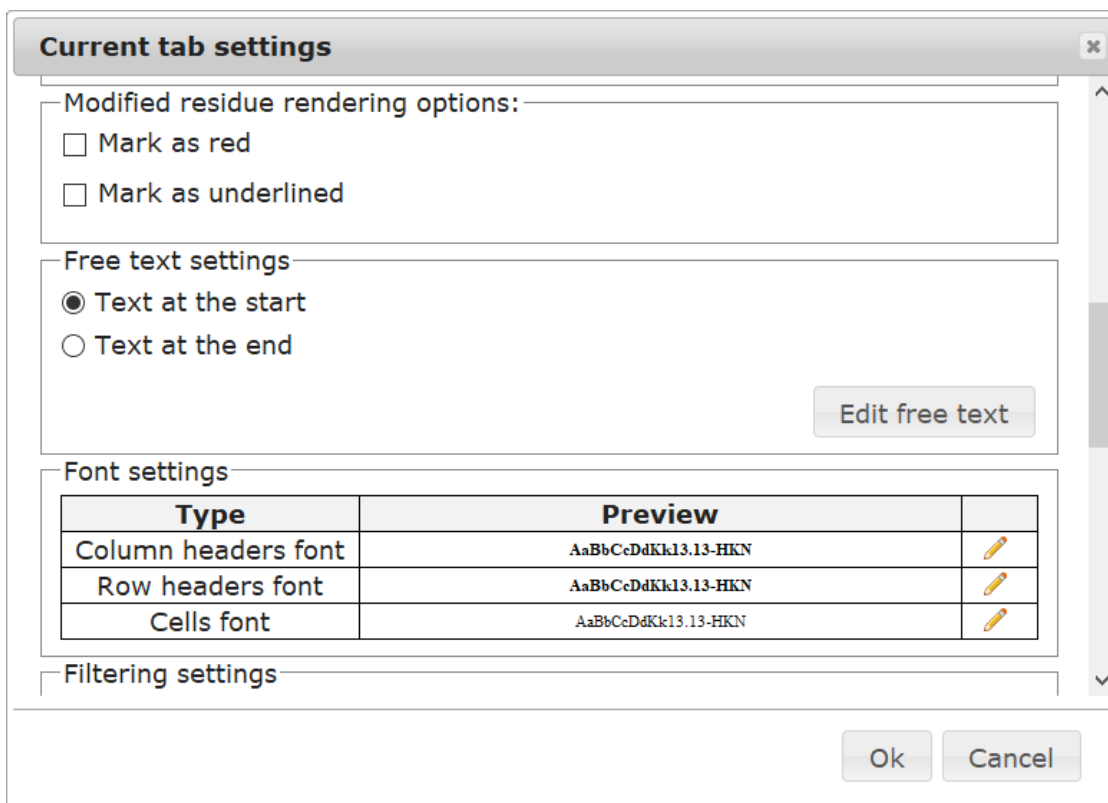
Normalize Column - [XIC area summed is] [Level 1]

Normalize type - Sum

Hidden values in .XIC file

Figure 50: Same pivot table with Show configuration turned off and with Show report details checked.

Text can be added to the top or bottom of the Pivot tab, and text font in the tables can be formatted:



**Current tab settings**

Modified residue rendering options:




- ☐ Mark as red
- ☐ Mark as underlined

Free text settings

- ☒ Text at the start
- ☐ Text at the end

[Edit free text](#)

Font settings

Type	Preview	
Column headers font	AaBbCcDdKk13.13-HKN	
Row headers font	AaBbCcDdKk13.13-HKN	
Cells font	AaBbCcDdKk13.13-HKN	

Filtering settings


[Ok](#) [Cancel](#)

Figure 51: Modified residue rendering and Free text settings in Current tab settings





To mark modified residues as red and/or underlined in the report, the user must check **Mark as red** and/or **Mark as underlined** in the **Modified residue rendering options** settings (figure above).



To add free text to the pivot tab, select whether to add the text at the start of end of the tab, then click **Edit free text**. Enter the free text and click **OK**.


A pop-up window appears with options to change the font, justify text, and add bullets to the text.




**Edit Text at the start**





Crosslink reporter peaks:

Figure 52: Edit Text at the end settings

Adjust the size, weight (Normal or Bold), style (Normal or Italic), name and color of the font and click **OK**. In the figure above, the text “Crosslink reporter peaks:” is added. In addition to the free text, images can be added in the window as well. Users can drag-and-drop an image into the free text in a report.

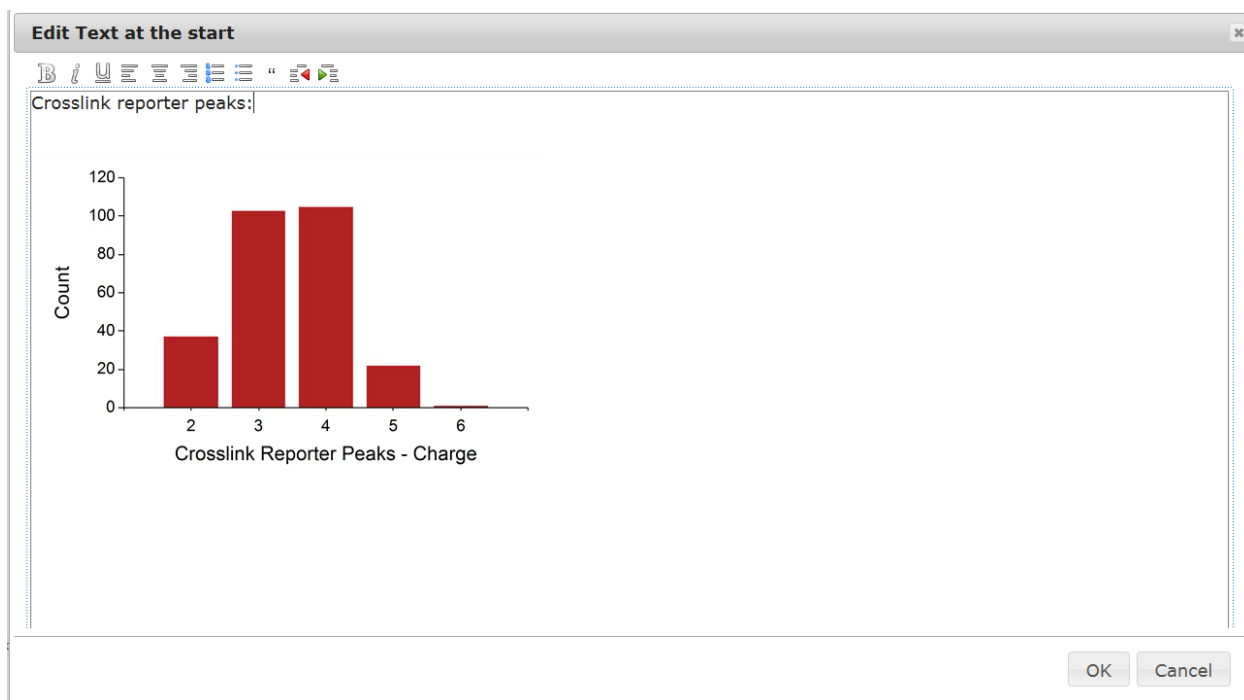
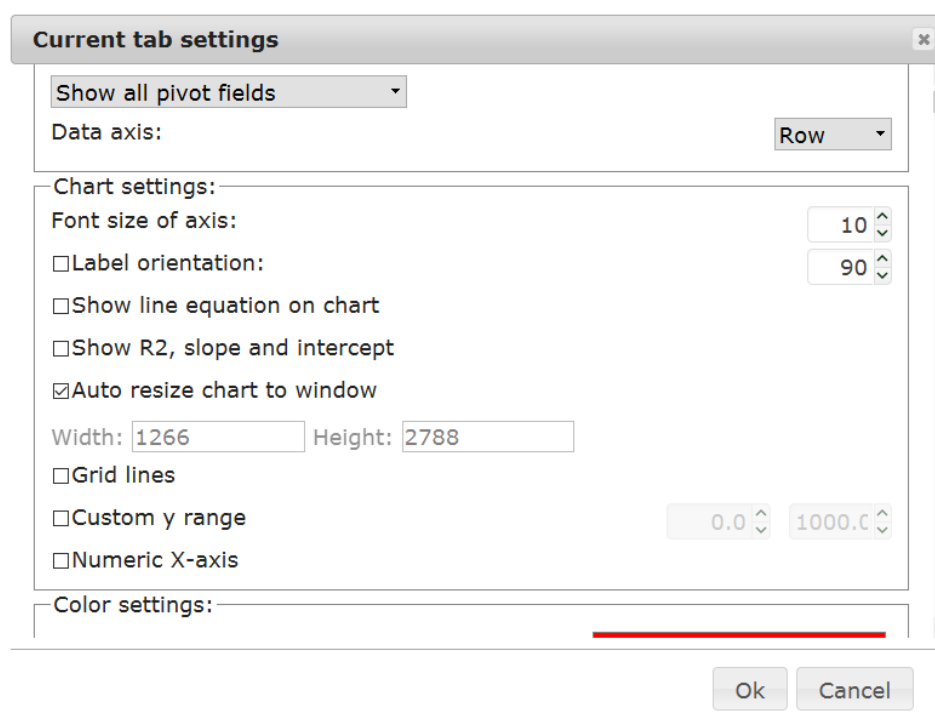


Figure 53: A sample histogram image and free text added to the text box

### Pivot Tab Current Tab Settings: Chart specific



**Current tab settings**

Show all pivot fields

Data axis: Row

Chart settings:

Font size of axis: 10

Label orientation: 90

☐ Show line equation on chart

☐ Show R2, slope and intercept

☒ Auto resize chart to window

Width: 1266 Height: 2788

☐ Grid lines


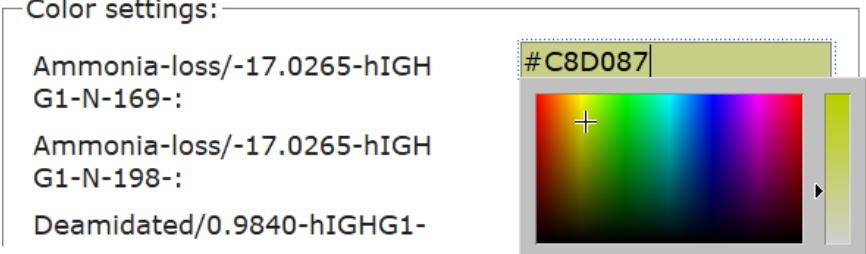
☐ Custom y range: 0.0 to 1000.0

☐ Numeric X-axis

Color settings:

Ok Cancel

Figure 54: Pivot chart options in Current tab settings

Setting	Description
Pivot table settings	
Data axis	By default, the row is the X-axis. Sometimes the user wants to switch row and column. If column is selected, column values will be used on the X-axis and row values on Y-axis.
Chart settings	
Font size of axis	Font size between 1 and 20.
Label orientation	To avoid label collision or for better readability, the user can place the label at an angle. The angle range is -90 to 90 degrees.
Show R <sup>2</sup> , slope and intercept (Line Chart only)	<p>When checked, R<sup>2</sup> values, slopes and intercepts are displayed on the top right of the chart in the format <math>y = mx + b</math>:</p> 
Auto resize chart to window	When checked, the chart will fit within the display screen adjusting for Show configuration (Show unused fields or Show row fields). When unchecked, the chart will fit within the specified width and height pixel settings.
Grid lines	When checked, the chart will display grid lines at the axis values.
Custom y range	When checked, the chart will be plotted on the specified minimum and maximum Y axis range.
Numeric X-axis	(Except Pie chart and Table Barchart) - When checked, displays numeric labels on the X-axis
Color settings	
Color	<p>Colors are assigned to the column field values. Colors in charts default to a pastel palette. To change a color, enter a new RGB value or click the value to display a color chooser. Please note values can be copied and pasted to apply the same color to multiple components, if desired.</p> <p><b>Color settings:</b></p> <p>Ammonia-loss/-17.0265-hIGH G1-N-169-:</p> <p>Ammonia-loss/-17.0265-hIGH G1-N-198-:</p> <p>Deamidated/0.9840-hIGHG1-</p> 
Connect the dots	(Scatter charts only) - When checked, connects the plotted points with line segments



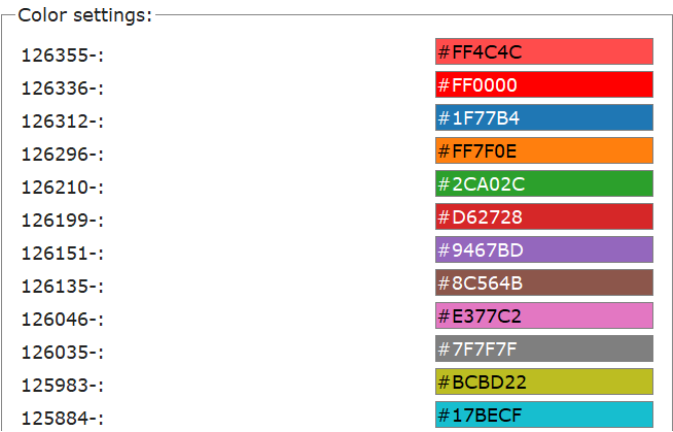
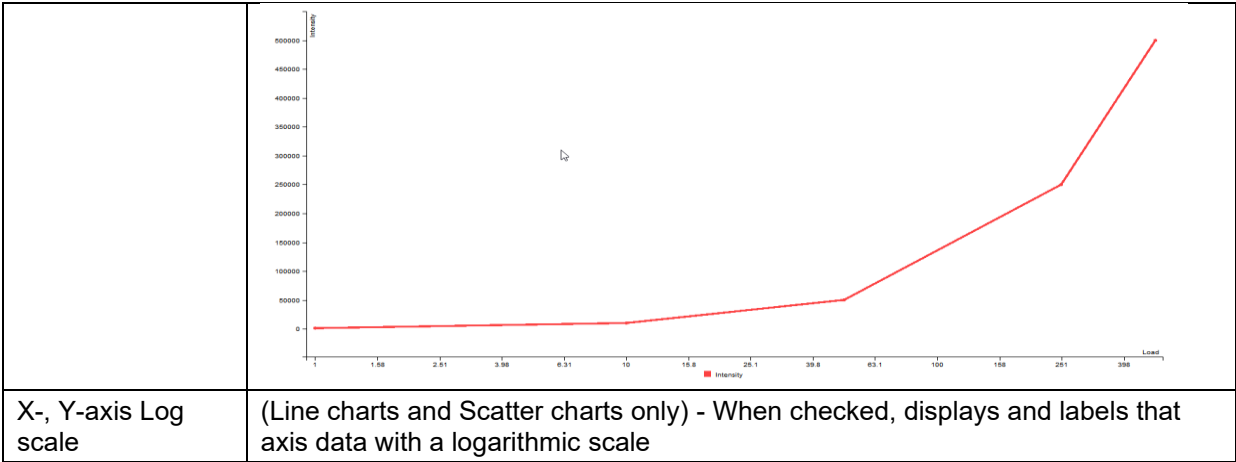


Figure 55: Default colors from a high-contrast palette

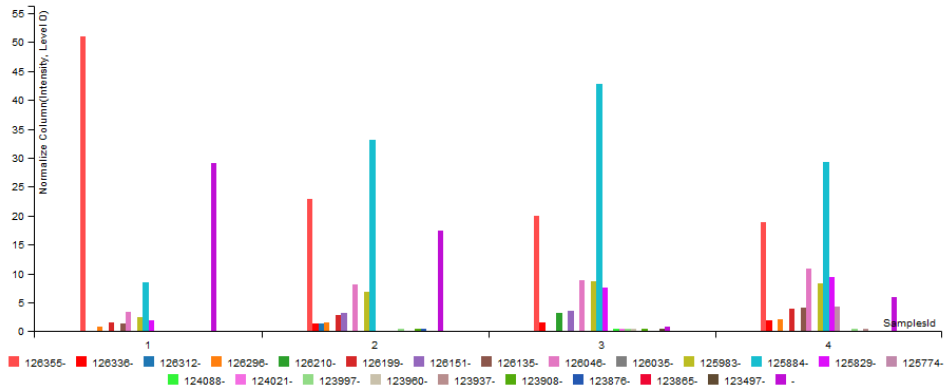
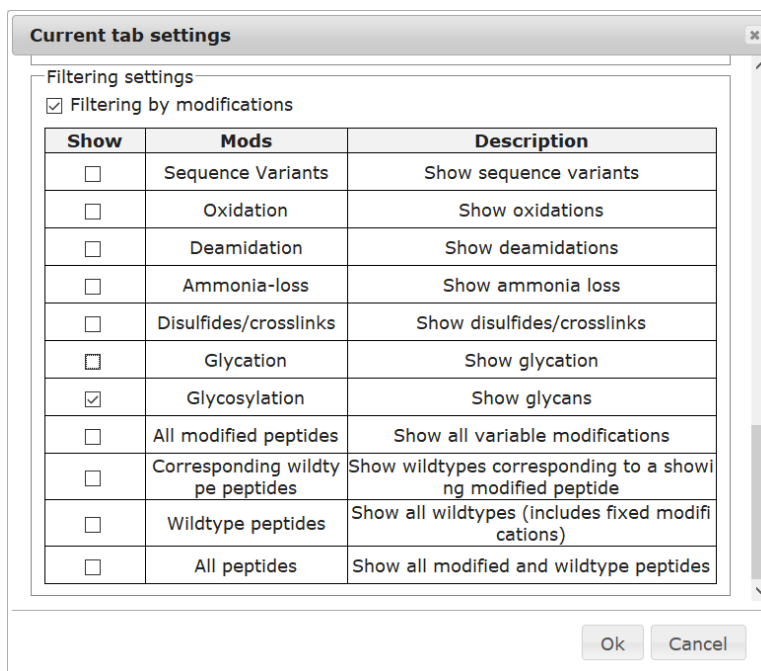


Figure 56: Horizontal bar chart with high-contrast color palette

## Pivot Tab Current Tab Settings: Modification specific



**Current tab settings**

Filtering settings

☒ Filtering by modifications

Show	Mods	Description
<input type="checkbox"/>	Sequence Variants	Show sequence variants
<input type="checkbox"/>	Oxidation	Show oxidations
<input type="checkbox"/>	Deamidation	Show deamidations
<input type="checkbox"/>	Ammonia-loss	Show ammonia loss
<input type="checkbox"/>	Disulfides/crosslinks	Show disulfides/crosslinks
<input type="checkbox"/>	Glycation	Show glycation
<input checked="" type="checkbox"/>	Glycosylation	Show glycans
<input type="checkbox"/>	All modified peptides	Show all variable modifications
<input type="checkbox"/>	Corresponding wildtype peptides	Show wildtypes corresponding to a showing modified peptide
<input type="checkbox"/>	Wildtype peptides	Show all wildtypes (includes fixed modifications)
<input type="checkbox"/>	All peptides	Show all modified and wildtype peptides

Ok Cancel

Figure 57: Filtering Pivot tables by modifications

Pivot tables can be filtered by individual modifications (e.g., oxidation, deamidation), or combinations of modifications. Modification filters include the corresponding wildtypes. **All peptides** is checked by default. To filter by one or more modification, check **Filtering by modifications**, uncheck **All peptides**, and check the modifications to include. For example, the settings above produce a table like this:

Sum ▾

XIC Ratio% ▾

*Mod. Names<sup>F</sup>* ▾

Protein name ▾

Mod. AAs ▾

Var. Pos. Protein ▾

Labels ▾

					MS Id ←	1	2
					MS Alias name ←	NISTmAb_Control_MS2	NISTmAb_Stressed_MS2
Mod. Names ↑	Protein name ↑	Mod. AAs ↑	Var. Pos. Protein ↑	Labels ↑			
NGlycan/1241.4545	gi 002 NISTHC NIST_REFSTD_HC	N	300			65.5	66.1
NGlycan/1444.5339	gi 002 NISTHC NIST_REFSTD_HC	N	300			90.5	91
NGlycan/1606.5867	gi 002 NISTHC NIST_REFSTD_HC	N	300			87.7	88.4
NGlycan/1768.6395	gi 002 NISTHC NIST_REFSTD_HC	N	300			0	0

Figure 58: A pivot table filtered by glycosylation-only

## Pivot Tab Heatmap

Heatmaps are colored according to the values of the field set by the **Color by** option:



Figure 59: Color by settings for heatmap views

The Current tab settings dialog for heatmaps contains color settings:

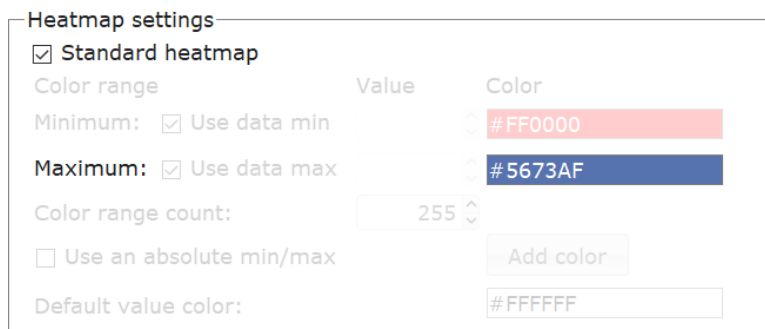


Figure 60: Standard color setting for heatmaps

The **Standard heatmap** is checked by default. This heatmap setting colors table cells from light gray for the minimum values to dark blue for the maximum values. To change the color, enter a new RGB value or click the value to display a color chooser. Values can be copied and pasted to apply the same color to multiple components, if desired.

The user has more color options when Standard heatmap is unchecked:

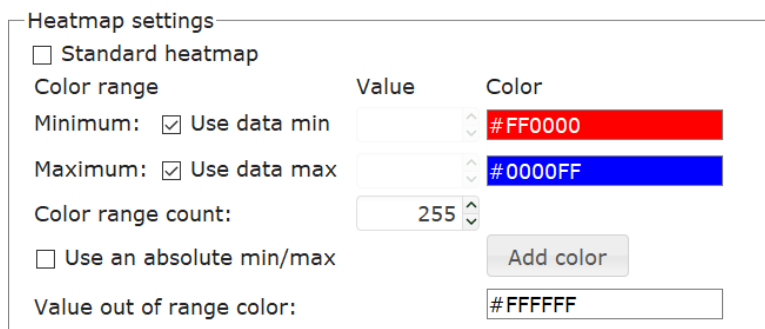


Figure 61: Advanced heatmap color settings

The minimum value color changes to red, and it is editable. Specific minimum or maximum values can be assigned by unchecking **Use data min** or **max** and entering those values.

The **Color range count** represents the number of color gradations between the two color ranges. To create a gradual shift in color across values, use the maximum value, 255. To create distinct colors for a set of like ranges of values, use a much smaller count. The total range will be divided into bins by the color count and values in those bins will be given those distinct colors.

**Use an absolute min/max** applies the larger of the maximum and the absolute value of the negative minimum value as the range, thereby maintaining zero at its center.


The color by feature allows intermediate colors. To add an intermediate color range, click **Add color**. The dialog updates to show an added intermediate color:

Heatmap settings

☐ Standard heatmap

Color range	Value	Color
Minimum: <input checked="" type="checkbox"/> Use data min		#FF0000
Intermediate:	17.20	#EBEBEB
Maximum: <input checked="" type="checkbox"/> Use data max		#0000FF
Color range count:	255	
<input type="checkbox"/> Use an absolute min/max		Add color
Value out of range color:		#FFFFFF

Figure 62: Heatmap color settings with an intermediate color

Two different color ranges are defined with an intermediate color value. This value is midway between the minimum and maximum values. This value and the default color can be edited, as above. Additional intermediate colors can be inserted with the Add color button. Click  after an intermediate color to delete it. The same intermediate color can be used to create a range of values with the same color, to deemphasize some of the data. For example, consider the setting:

Heatmap settings

☐ Standard heatmap

Color range	Value	Color
Minimum: <input checked="" type="checkbox"/> Use data min		#FF0000
Intermediate:	10.00	#FFFFFF
Intermediate:	40.00	#FFFFFF
Maximum: <input checked="" type="checkbox"/> Use data max		#0000FF
Color range count:	15	
<input type="checkbox"/> Use an absolute min/max		Add color
Value out of range color:		#000000

Figure 63: Heatmap with a range of data marked in white

This setting results in following heatmap:

End AA ↑	Sequence ↑	ExchangeTime ←	60			
		Condition ←	Apo	Avg (H3 - Apo)	H3	H3 - Apo
8	-.GHMSKPNL.S		67.9	-4.13	63.8	-4.13
12	-.GHMSKPNLSAKD.L		74.1	-13	61.1	-13
14	-.GHMSKPNLSAKDLA.L		66.5	-34.8	45.3	-21.3
	L.SAKDLA.L		71.8	-34.8	23.4	-48.4
15	-.GHMSKPNLSAKDLAL.L		57.8	-28	37.3	-20.6
	L.SAKDLAL.L		49.7	-28	14.3	-35.4
16	-.GHMSKPNLSAKDLALL.L		50.9	-21.8	30.8	-20.1
	D.LALL.L		11.7	-21.8	-3.51	-15.3
	L.SAKDLALL.L		40.6	-21.8	10.6	-30
	-.GHMSKPNLSAKDLALLL.F		47.4	-18.2	27.8	-19.5

Figure 64: The heatmap resulting from the settings in the Figure above.

**Default value color** is assigned to values that are beyond the range of set minimum and maximum values, or to cells without values.

A new Value out of range Label is introduced to label the feature values that fall out of a customized range. The standard heatmap settings can be customized for a certain range. To change the settings, choose **Edit > Current tab settings** and uncheck **Standard heatmap**. The user has an option to enter a custom value for threshold i.e., uncheck **Use data min** and enter a cut-off to highlight values below the cut-off. Similarly, to highlight values above a defined value, uncheck **Use data max** and enter a cut-off to highlight values above the cut-off. The user can annotate using custom color and text fields. In the below Figure, values < 5 % are highlighted using the Use data min with a setting of 4.99. This results in all intensities less than 5 % to have “<5%” in table/heatmap view (highlighted in cyan boxes). “<5%” is just an example text, any custom text can be used for this label.

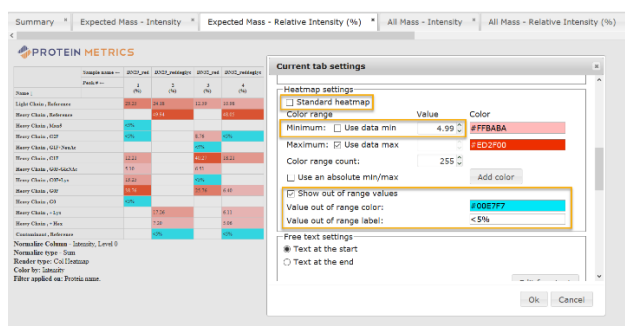


Figure 65: Labels to denote out of range values

## Pivot Tab Error Charts

To create an error chart, add error columns to the pivot table. To add error columns, do the following:

1. Select Presets > Post pivot columns > AllErrorColumns.postpvtjs, RSDErrorColumns.postpvtjs, or StdDevErrorColumns.postpvtjs:

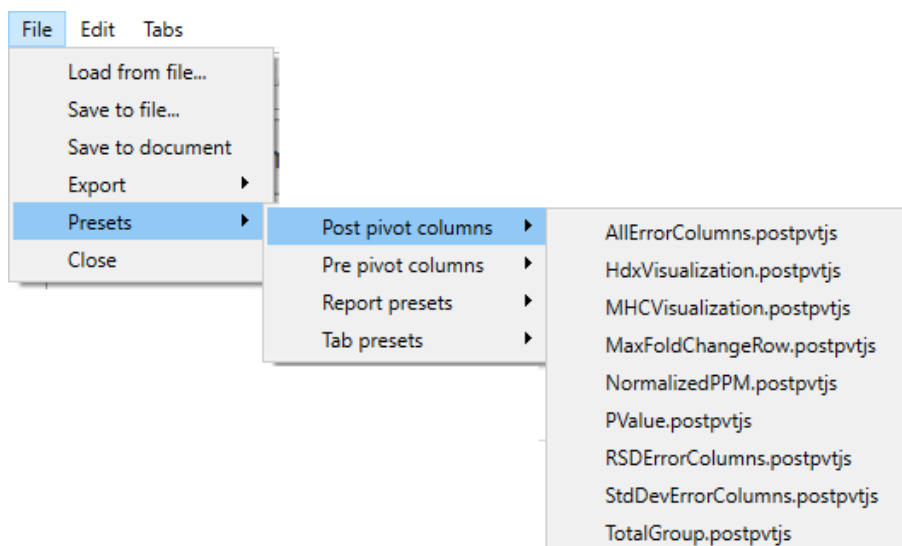


Figure 66: Creating columns for error charts

2. Enter a name for the error column and click **OK**.

The Render options **Error Bar Chart** and **Error Line Chart** are now enabled. When either of these is selected, error bars are displayed on the charts:

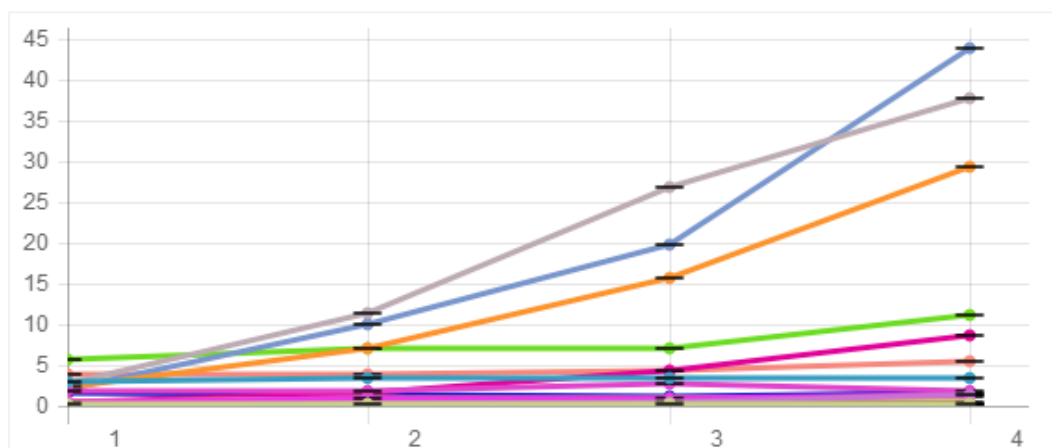
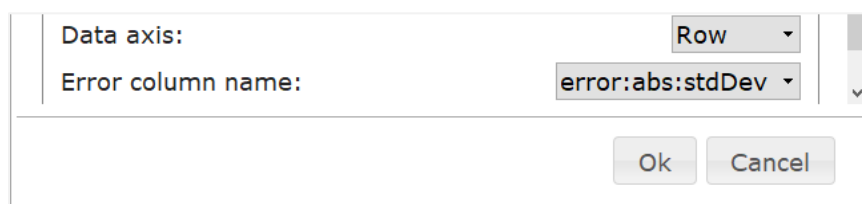


Figure 67: Formatted error line chart

The Current tab settings dialog for error charts contains the Error column name option:



The dialog box contains the following settings:

- Data axis: Row
- Error column name: error:abs:stdDev

Buttons: Ok, Cancel

Figure 68: Error column name setting

- **StdDevErrorColumns** - the error values are based on standard deviation. The Error column name is assigned to error:abs:stdDev
- **AllErrorColumns** - the error values are based on the minimum or maximum value. Choose Error column name: error:abs:lower or error:abs:upper.

Note that the column name such as errors:abs:stdDev is defined in the pivot JavaScript, which can be customized.

## Pivot Tab Principal Component Analysis (PCA) Plots

A PCA view plots across a biosimilar experiment.

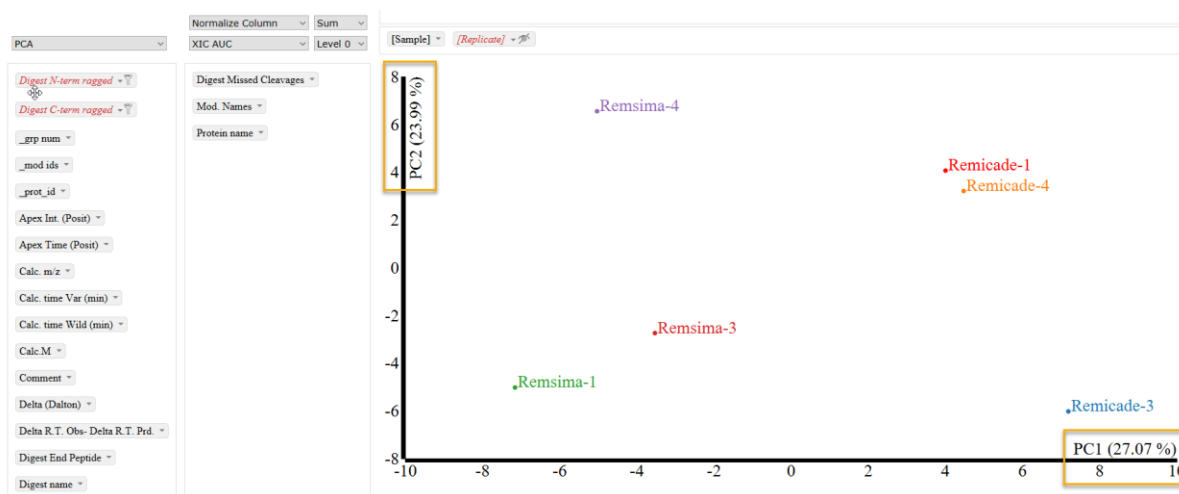
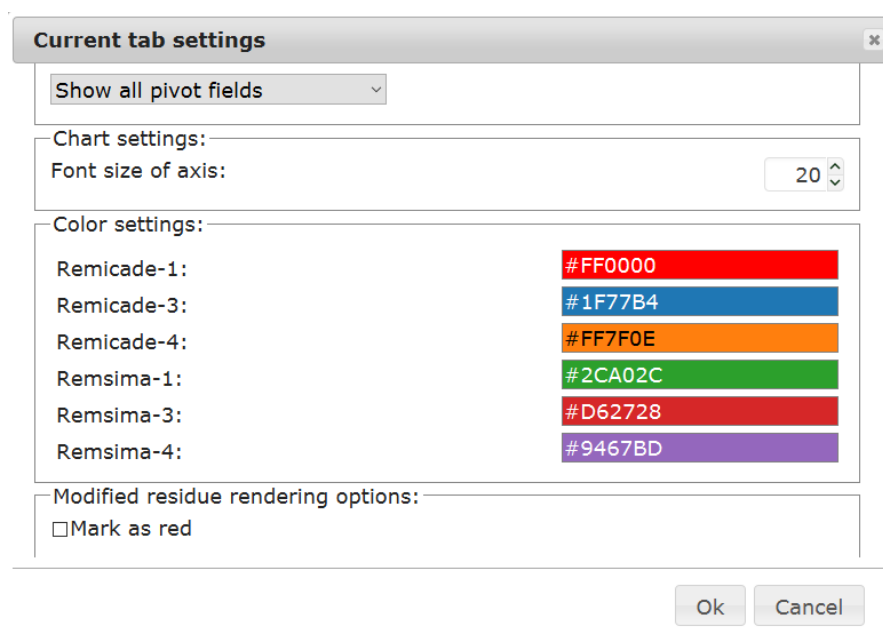


Figure 69: PCA plot

The Current tab settings dialog for PCA plots contains the following options:



The 'Current tab settings' dialog for PCA plots contains the following options:

- Show all pivot fields** (dropdown menu)
- Chart settings:**
  - Font size of axis: 20 (spin box)
- Color settings:**
  - Remicade-1: #FF0000 (red)
  - Remicade-3: #1F77B4 (blue)
  - Remicade-4: #FF7F0E (orange)
  - Remsima-1: #2CA02C (green)
  - Remsima-3: #D62728 (red)
  - Remsima-4: #9467BD (purple)
- Modified residue rendering options:**
  - ☐ Mark as red

Buttons: Ok, Cancel

Figure 70: PCA options in Current tab settings

Setting	Description
Color settings	
Color	Colors are assigned to Sample Name values. To change a color, enter a new RGB value or click the value to display a color chooser.
PCA settings	
Data entries	By default, the row is X-axis/loading plot, and the column is Y-axis/data. Sometimes the user wants to switch the row and column. If column is selected, column values will be used on the X-axis and row values on the Y-axis.
Select component	Specify eigenvalues used to show in the plot. These are sorted from highest to lowest rank. By default, component 1 (the highest) and component 2 (the second highest) are selected.
Show axis	Turns on or off the display of the X and Y axis.
Auto detect range	When checked, the X and Y range is defined by the data set. When unchecked, the X and Y range is set to the specified values.
Show data labels	Turns on or off the display of the data point labels.
Label offset	<p>Label offset can be used to avoid label collision.</p> <p>Syntax: <code>{"data label": [x-offset, y-offset]}</code></p> <p>For example:</p> <pre><code>{"labelsOffset": [ {"-Trioxidation/47.9847": [-150, 0]}, {"-Dioxidation/31.9898": [0, 15]} ]}</code></pre> <p>Note that the X and Y offset are from the label's original location of [0, 0]. Exact label name needs to be used.</p>

## Pivot Tab Pie Chart

Pie charts are now supported in Reports, with an option to create a single or multiple pie charts. To create a **Pie Chart**:

1. Select **File > Export > Report** to open a report.
2. In the Report window, select **Tabs > Add pivot table**. A new tab is created but not selected.
3. In the **Pivot Table** tab, choose **Pie Chart** as the rendering option. The window updates with new report options and a default **Pie Chart** pops up.

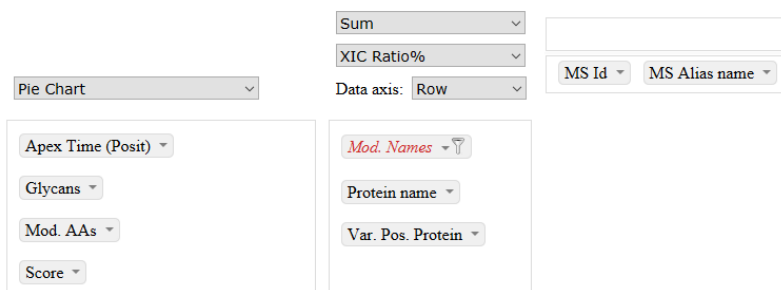


Figure 71: Pie chart settings



- The pivots can be used to filter the data. To simplify the **Pie Chart**, few combinations of **Mod. Names** are selected. This results in a **Pie Chart** which is basically slices of a circle, the area of which explains the numeric proportion of the post-translational and other modifications present in a sample of interest:

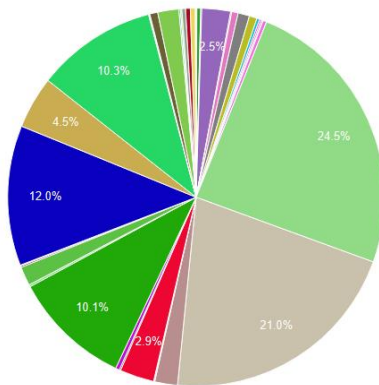


Figure 72: Pie Chart of different modifications present in the sample

- To generate multiple pie charts, click **Edit > Current tab settings**. Under the Chart Settings, enable the checkbox **Display a separate pie chart for each field value** and select the **Field value** of interest to generate multiple pie charts (**Digest End Peptide** is the field selected in below image).

Chart settings:

Font size of axis:
10

☒Auto resize chart to window

Width: 640
Height: 611

☐Grid lines
☐Custom y range
0.0
1000.0
☒Display a separate pie chart for each field value

Field value:
Digest End Peptide

Figure 73: Chart settings within Current tab settings

- The above setting will result in many pie charts, and a snippet of which is shown in the figure below:

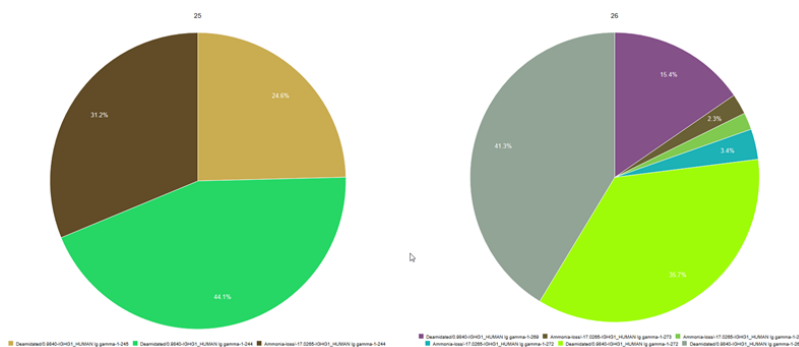


Figure 74: Pie Chart showing proportion of modifications for different Digest End options

## Pivot Tab Protein 3D Plots

Protein 3D Visualization is now supported in Reports, using the three-dimensional structure of the Protein Data Bank (PDB). To create a protein 3D visualization:

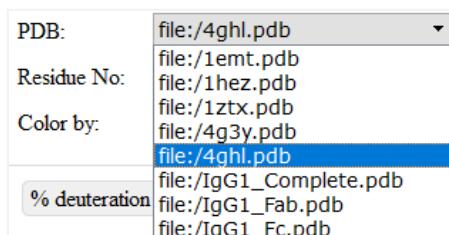
1. Select **File > Export > Report** to open a report.
2. In the Report window, select **Tabs > Add pivot table**. A new tab is created but not selected.
3. In the **Pivot Table** tab, choose **Protein 3D** as the rendering option (the top left drop-down arrow). The window updates with new report options:



The screenshot shows a settings window for Protein 3D visualization. It includes a dropdown menu at the top set to 'Protein 3D'. Below it are four rows of controls: 'PDB:' with a dropdown showing 'file:/4ghl.pdb'; 'Residue No:' with a dropdown showing 'Start AA' and a secondary dropdown showing 'Average'; 'Color by:' with a dropdown showing 'Avg (H3 - Apo)' and a secondary dropdown showing '% deuteration'.

Figure 75: Protein 3D settings

4. For **PDB**, select the desired protein database \*.pdb file:



The screenshot shows a dropdown menu for selecting a PDB file. The 'PDB:' label is on the left. The dropdown list contains several file paths, with 'file:/4ghl.pdb' highlighted in blue. Other visible options include 'file:/1emt.pdb', 'file:/1hez.pdb', 'file:/1ztx.pdb', 'file:/4g3y.pdb', 'file:/IgG1\_Complete.pdb', 'file:/IgG1\_Fab.pdb', and 'file:/IgG1\_Fc.pdb'.

Figure 76: Setting the PDB file

The \*.pdb files are found in [Program Files\ProteinMetrics\PMI-Suite\Base\html\protein3DCoreFiles\protein\\_3d\\_files](#). To include a custom protein database file, in this drop-down list, copy the file to the above directory.

5. For **Color by**, select the desired sample name (each replicate of each sample are options). The pivot column fields will be mapped to the Color by field options. Each column can map to a chain in the PDB.
6. For **Index**, select the pivot row field. The pivot row fields will be mapped to the Index field options. The PDB file can contain multiple chains and amino acids in the sequence of each chain can be accessed through the residue number.
7. Choose the desired statistical method (the default is **Sum**) and the desired pivot field (the default is **XIC Ratio%**). The 3D version of the structure is displayed:

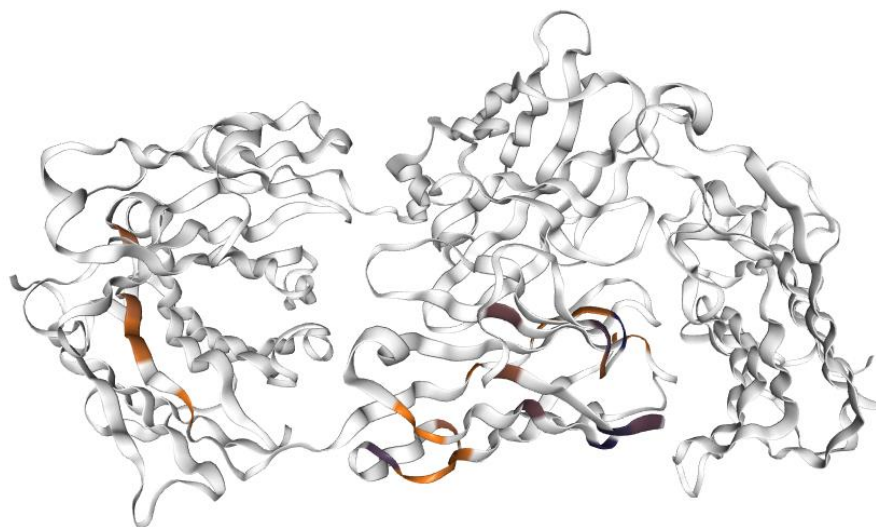


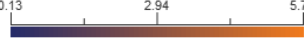


Figure 77: 3D depiction of a protein

To rotate the 3D structure around the horizontal axis, depress the left-click button and move the cursor up and down. To rotate the 3D structure around the vertical axis, depress the left-click button and move the cursor right and left.

By default, only one chain is color mapped. To configure color mapping of additional PDB chains:

1. In the Report, select Edit > Current tab settings.

Protein 3D settings:

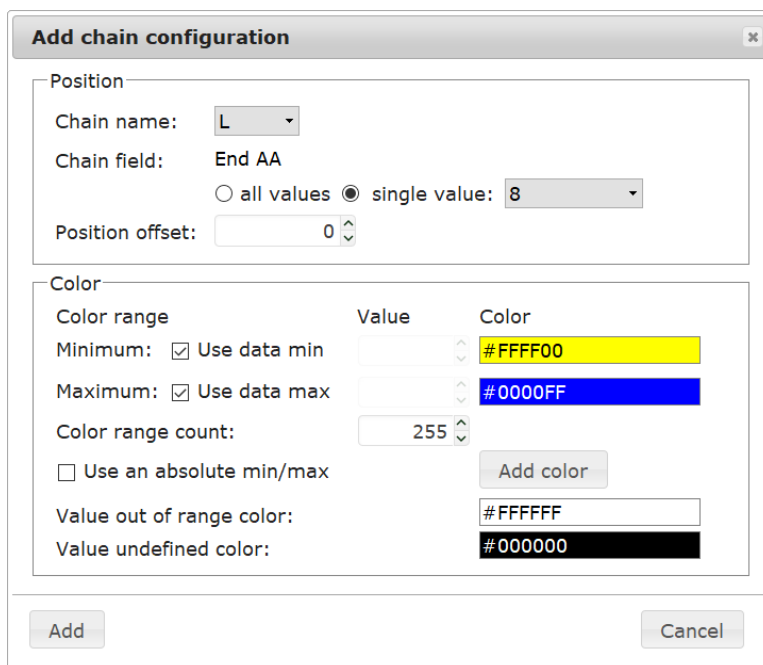
Chain	Protein	Color bar	
L	hIGHG1		 

Add chain configuration

Ok Cancel

Figure 78: Protein 3D chain configuration

- At the bottom, click **Add chain configuration**:



The dialog box is titled "Add chain configuration" and contains two main sections: "Position" and "Color".

**Position section:**

- Chain name: L (dropdown)
- Chain field: End AA
- Radio buttons: ☐ all values, ☒ single value: 8 (dropdown)
- Position offset: 0 (spin box)

**Color section:**

Color range	Value	Color
Minimum: <input checked="" type="checkbox"/> Use data min		#FFFF00
Maximum: <input checked="" type="checkbox"/> Use data max		#0000FF
Color range count:	255	
<input type="checkbox"/> Use an absolute min/max		
Value out of range color:		#FFFFFF
Value undefined color:		#000000

Buttons: Add, Cancel

Figure 79: Add chain configuration dialog

- Use the drop-down arrow to select the **Chain name**.
- For the **Chain field**, select **all values** or select **single value** and choose a value from the drop-down. Optionally, set a **Position offset** value for the chain.
- By default, the first color applies to the dataset minimum. To set a specific minimum value, uncheck **Use data min** and enter the number under **Value**. To change the color for the minimum value, click the **Color** cell and select a new color as the low end of the color range. The color in the cell will update. Repeat as needed for the **Maximum** row.
- The **Color range count** represents the number of color gradations between the two color ranges. To create a gradual shift in color across values, use the maximum value, 255. To create distinct colors for a set of like ranges of values, use a much smaller value. The total range will be divided into bins by the color count and values in those bins will be given those distinct colors.
- An absolute range uses the larger of the absolute value of a negative minimum and the maximum value as the negative minimum value and the positive maximum value. To apply this absolute range, check **Use an absolute min/max**.
- The color by feature allows intermediate colors. To add an intermediate color range, click **Add color**. The dialog updates to show an added intermediate color:

Color		
Color range	Value	Color
Minimum: <input checked="" type="checkbox"/> Use data min		#FFFF00
Intermediate:	-3.10	#EBEBEB ✖
Maximum: <input checked="" type="checkbox"/> Use data max		#0000FF
Color range count:	255	
<input type="checkbox"/> Use an absolute min/max		Add color
Value out of range color:		#FFFFFF
Value undefined color:		#000000

Figure 80: An intermediate color added to the color range

Two different color ranges are defined with intermediate value. This value is midway between the minimum and maximum. This value and the default color can be edited, as above. Additional intermediate colors can be inserted with the Add color button. Click ✖ after an intermediate color to delete it.

9. **Value out of range color** is assigned to values that are beyond the range of set minimum and maximum values. By default, this is white. The **Value undefined color** is assigned to locations without values. By default, this is black. These colors can also be edited. Use this color assignment to give the protein a backbone color.
10. Click the **OK** button. The structure in the report updates with the color-by chain settings:

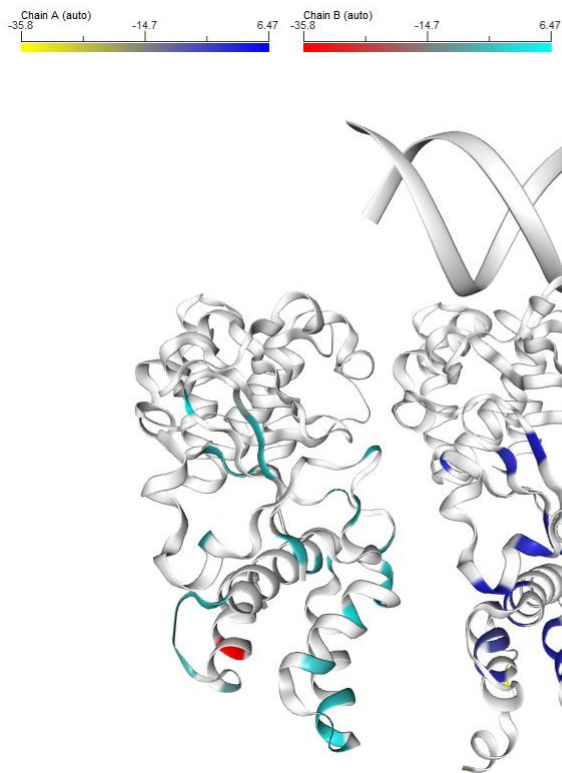



Figure 81: 3D Protein colored by chain

- To edit the color range for a chain in the **Current tab settings** dialog, click the  icon in the corresponding row and repeat the steps listed above. The dialog updates with the new minimum and maximum colors:

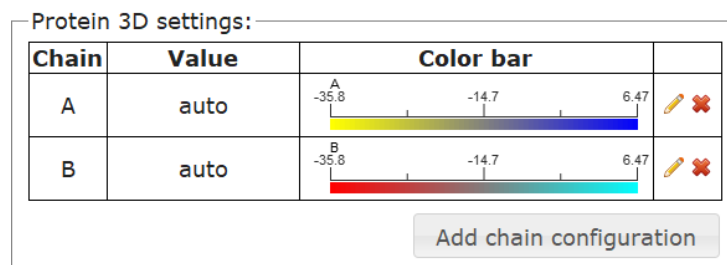


Figure 82: Chain color bar settings

## Pivot Tab Treemap Diagram

According to Wikipedia:

Treemaps display hierarchical (tree-structured) data as a set of nested rectangles. Each branch of the tree is given a rectangle, which is then tiled with smaller rectangles representing sub-branches.

- Select **File > Export > Report** to open a report (if the Report tab is not open).
- In the Report window, select **Tabs > Add pivot table**. A new tab is created but not selected.
- In the **Pivot Table** tab, choose **Treemap** as the rendering option. The window updates with new report options and a default **Treemap** pops up. The pivots used can be filtered accordingly on the sample name and/or the feature name. Below is an example of **Treemap** showing the post-translational and other modifications present in a sample of interest:

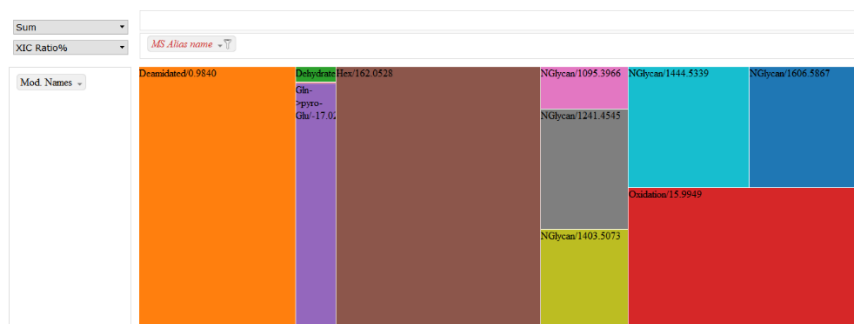


Figure 83: Treemap view of modifications present in a sample

## Pivot Tab Venn Diagram

- Select **File > Export > Report** to open a report (if the Report tab is not open).
- In the Report window, select **Tabs > Add pivot table**. A new tab is created but not selected.
- In the **Pivot Table** tab, choose **Venn Diagram** as the rendering option. The window updates with new report options and a default Venn diagram pops up.
- It is critical to set the fields in pivots appropriately and to limit the number of comparisons made i.e., Compare across sets of samples, charge states. In the below figure, **MS Id** - **MS Alias name** are used to denote the sets:

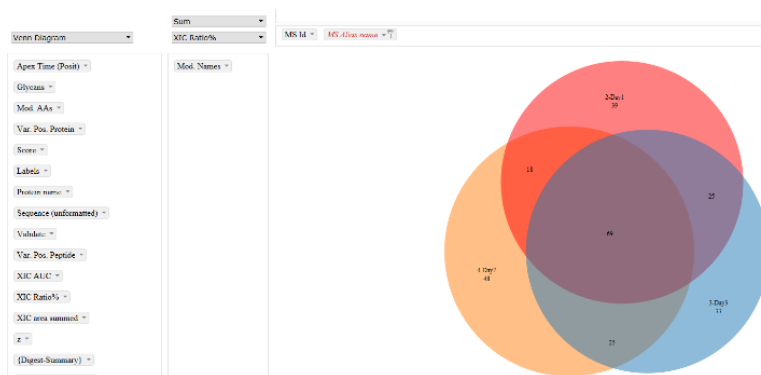


Figure 84: Venn diagram of 3 sets comparing the overlap of modification types

- The number of sets used can be filtered out by using Include/Exclude and Show/Hide option. In the below figure, **MS Alias name** is filtered out to exclude out "WT" from the Venn Diagram visualization:



Figure 85: Filtering sets to be seen in the Venn diagram

- The names of the sets in this Venn diagram are 1-Day1, 2-Day3 and 3-Day7, representing **MS Id** and **MS Alias name**. To rename the sets to Day1, Day3 and Day7 (i.e., **MS Alias name**), remove the **MS Id** pivot and the Venn Diagrams updates as shown below:

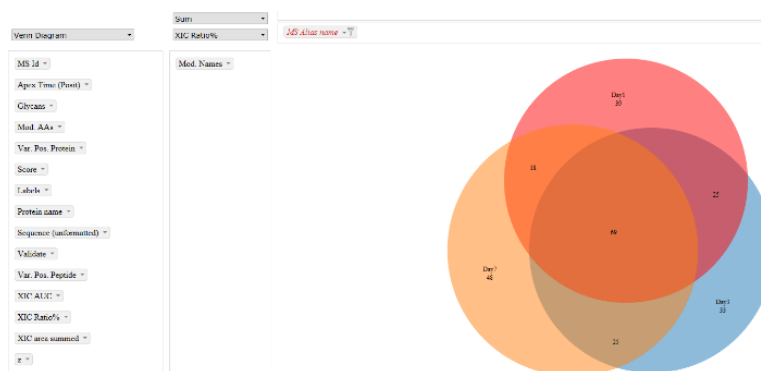


Figure 86: Updated Venn diagram with adjusted sample names (i.e., Day1, Day3, Day7)

- To increase the font size and to change the colors of the sets, click **Edit > Current tab settings**, edit **Font size of axis** (under **Chart settings**) and edit colors (under **Color settings**) as shown in the figure below resulting in the Venn Diagram with an improved font size and different colors for the 3 sets.

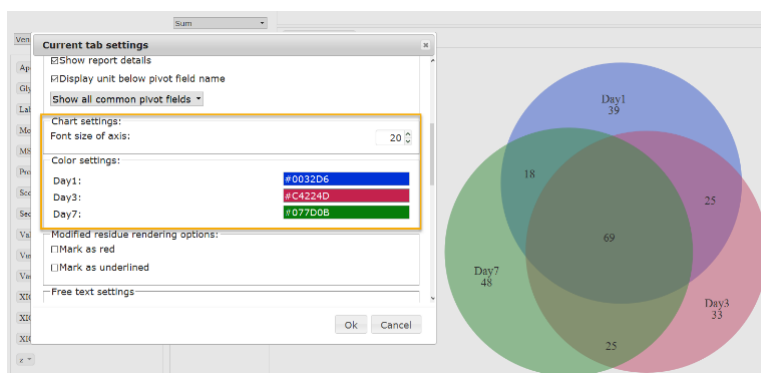


Figure 87: Improved label names and updated colors

## Pivot Tab Volcano Plot

1. Select **File > Export > Report** to open a report (if the Report tab is not open).
2. In the Report window, select **Tabs > Add pivot table**. A new tab is created but not selected.
3. In the **Pivot Table** tab, choose **Volcano Plot** as the rendering option. The window updates with new report options and a default Volcano plot pops up.
4. It is critical to set the fields in pivots appropriately to get a meaningful volcano plot:

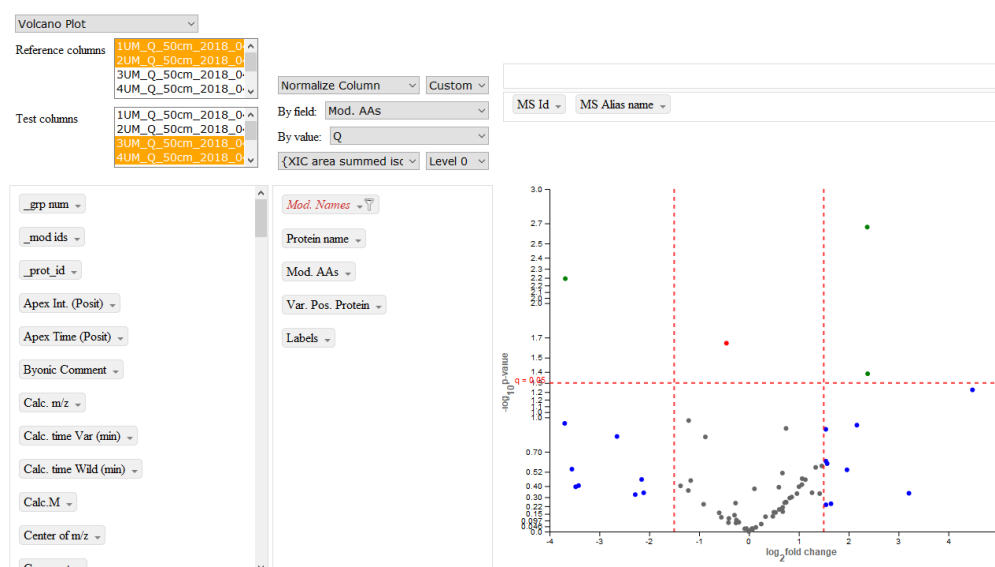


Figure 88: Volcano plot

5. To change the threshold limits of fold change and p-value, select **Edit > Current tab settings** and update the **Significance threshold** and **log2 fold change threshold** values. The **Reference columns** and **Test columns** for generating the volcano plot can be either selected directly inside pivot tab (shown in above figure) or the user has an option to update these columns within the **Edit > Current tab settings** dialog (shown in below figure).



**Current tab settings**

☒ Show report details

☒ Display unit below pivot field name

Show all common pivot fields ▾

Modified residue rendering options:

☐ Mark as red

☐ Mark as underlined

**Volcano plot settings**

Reference columns: 1WT, 2Day1, 3Day3, 4Day7

Test columns: 1WT, 2Day1, 3Day3, 4Day7

Significance threshold: 0.05

log2 fold change threshold: 1.00

Free text settings

Edit sort within level...

Ok Cancel

Figure 89: Filtering settings of volcano plot

## Pivot Tab Protein Map

Protein Maps are found in the [Blgc\\_HDX.rptc](#) report template used by the **HDX** workflow:

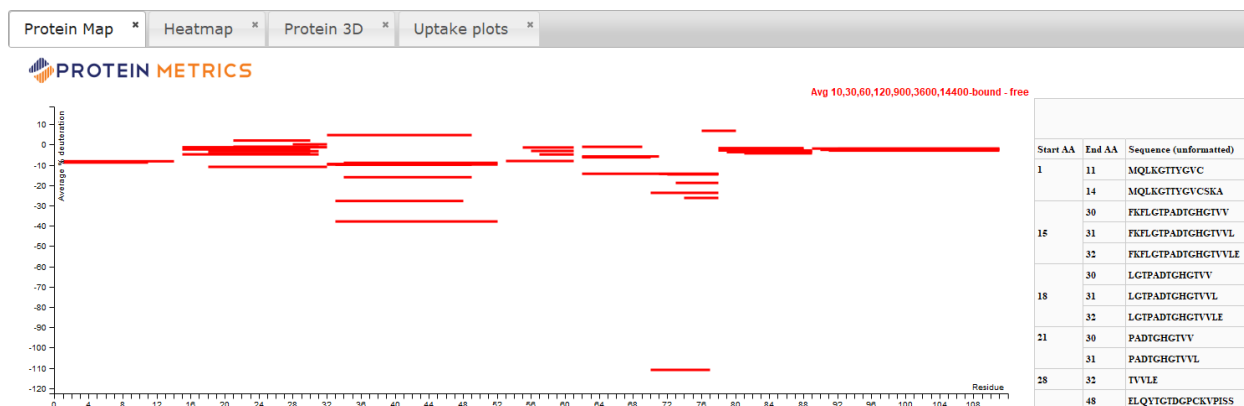


Figure 90: Protein map

The Protein Map creates a visualization of individual segments based on the Y-axis setting for the Uptake plot (percent deuteration, center of  $m/z$  shift, or center of mass shift). Note that the pivot tabs included in the [Blgc\\_HDX.rptc](#) allow for the display of sequence letters instead of, or in addition to residue positions. The Current tab settings dialog for these tabs includes the **Residue option** setting:

Specialized settings

Residue option:

Position and sequence

Position

Sequence

Position and sequence

OK Cancel

Figure 91: Residue option for Position or Sequence letter

The Residue option is also available for pivot tables that have applied the **MHCVisualization.postpvtjs** post-pivot processing.

## Plots Tab

To create a Plots tab, select **Tabs > Add plots**. Each of the plots in the report will be assembled into a single tab, prefaced with identifying and quantifying data:

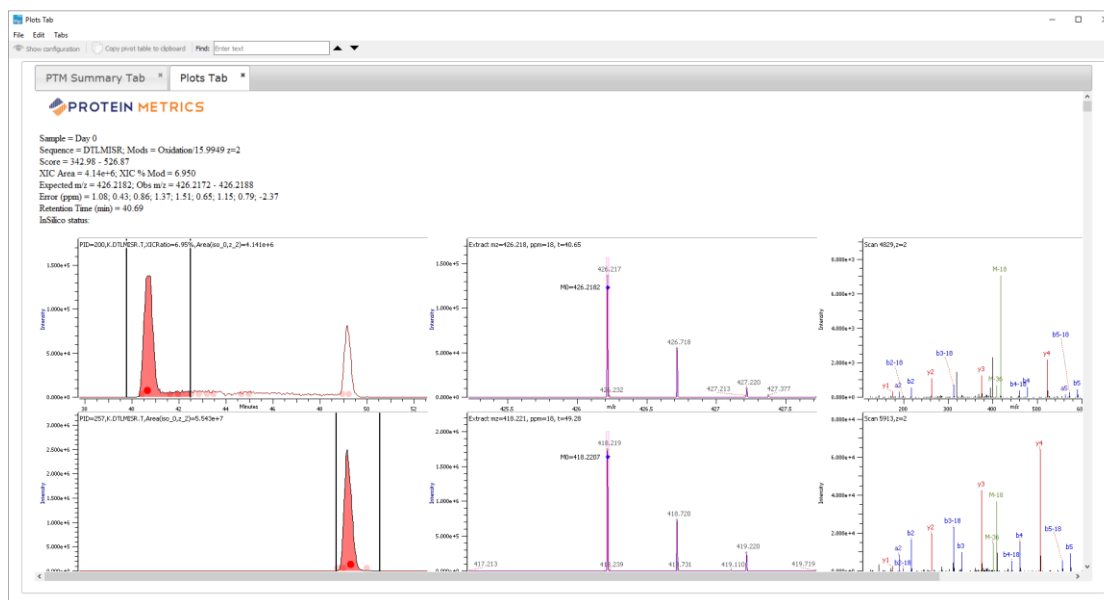


Figure 92: Example Plots tab

## Plots Tab Current Tab Settings

To configure the Plots tab, choose **Edit > Current tab settings**:

Current tab settings

Plots visibility:

☒ Show Whole trace plot  
☒ Show Divided trace plot  
☒ Show Stacked Plots

Font options

Font size:

16

Font weight:

Normal

Font style:

Normal

Font name:

Times New Roman

Font color:

#000000

AaBbCcDdKk13.13-HKN

Free text settings

☒ Text at the start  
☐ Text at the end

Edit free text

Export to PDF:

☐ Page break after each row

Plot options:

☐ Resize plots

Plot scaling:

100.0 %

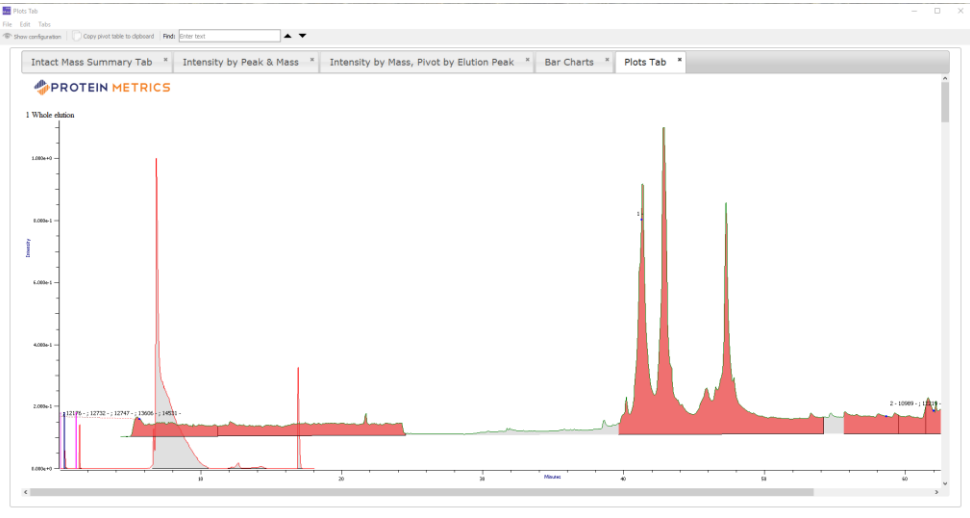

☐ Display only zoomed-in segments

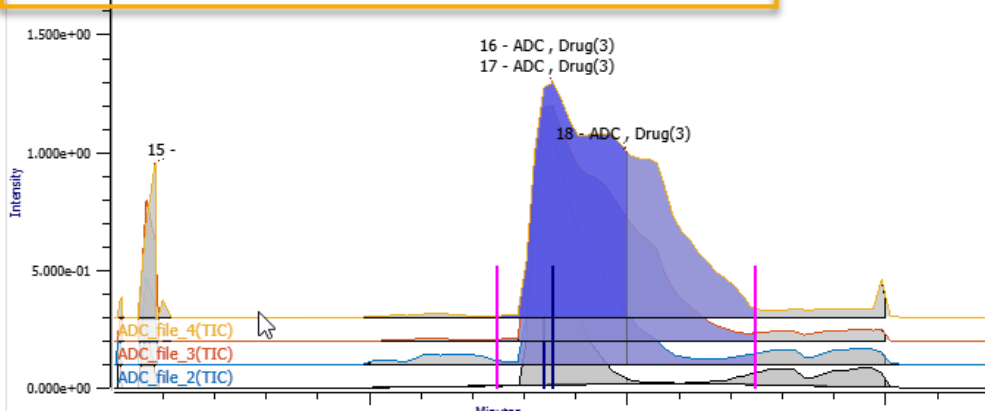
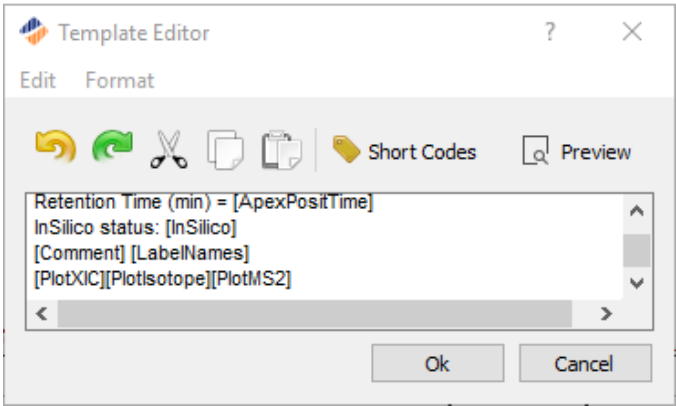
Edit plot sort...

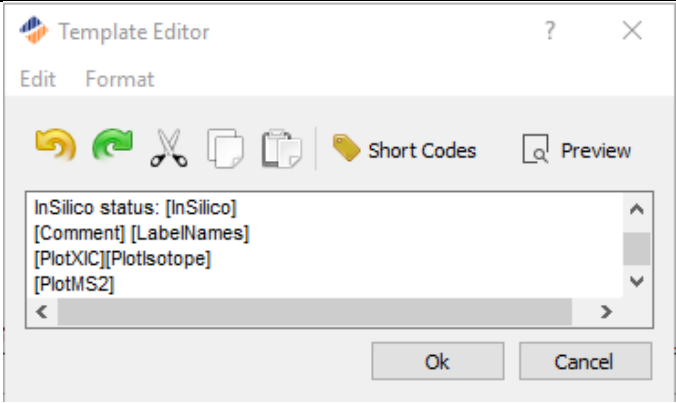
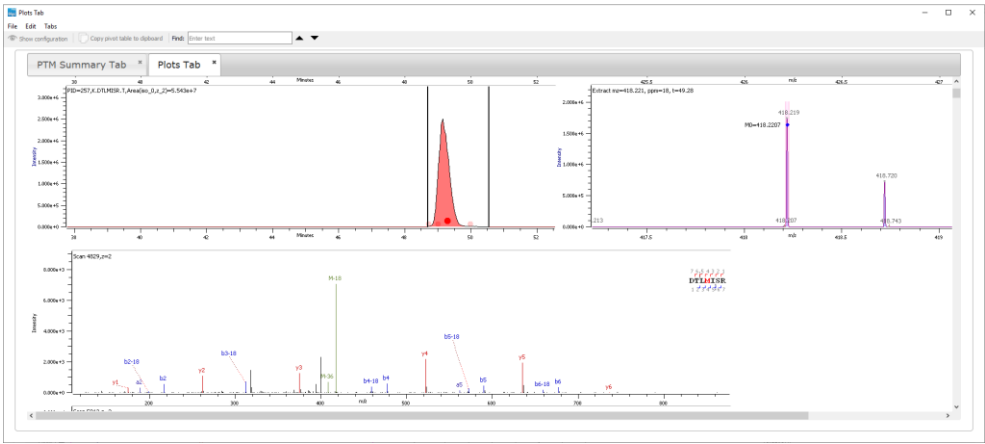
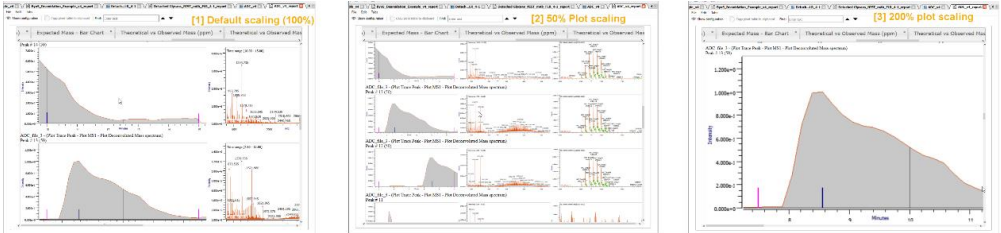
Edit plot template...

OK

Figure 93: Plots tab Current tab settings

Setting	Description
Plots visibility	
Show Whole trace plot	Displays the entire elution as the first plot: 
Show Divided trace plot	Displays the elution into a series of relevant sections. These additional sections are set in the elution plots, using the Add plot segment  icon.
Show Stacked Plots	Displays the selected traces as stacked plots (for Intact, the user should select multiple traces in Trace Peaks table):

	<div data-bbox="451 205 1222 247" style="border: 1px solid orange; padding: 2px;">(Stacked Plots - Plot Trace Peak - Plot MS1 - Plot Deconvoluted Mass spectrum)</div> 
Font options	Adjust the size, weight (Normal or Bold), style (Normal or Italic), name and color of the font. An example of the formatted text is displayed in the dialog.
Export to PDF	
Page break after each row	When checked, this inserts a page break after each row in exports to PDF.
Plot options	
Resize plots	<p>When unchecked, the image will be cached by size, by default to a size that accommodates three plots per row. When checked, the image resolution is adjusted when the user designates counts of one or two images per row. To edit the images counts per row, click the Edit plot template button. Example plot assignments are shown below:</p> <div data-bbox="430 1050 1101 1453">  </div> <p>The string [PlotXIC][PlotIsotope][PlotMS2] designates those plots in that order, three to a row. To separate these into two plots on one row, and third plot on the next row, move the third plot to the following line:</p>

	 <p>This produces the layout:</p>  <p>One plot per row provides the best plot resolution with a tradeoff of largest plot file size and longer retrieval times. Three plots per row provides the most economic resolution and retrieval time. Two plots per row is in between.</p>
Plot scaling	<p>The default value for Plot scaling is 100%, but the user has an option to decrease this value (for example, 50%) to see more smaller sized plots in the same page area, or increase this value (for example, 200%) to see enlarged plots (see figure below). Left figure is the original size, middle figure is with Plot scaling set to 50% and right figure is the Plot scaling set to 200%. This can be used in combination with Resize plots for improving the display of multiple graphs.</p> 
Display only zoomed-in segments	<p>Displays zoomed-in segments of the project. When unchecked, entire plots are displayed.</p>

For IntaBio plots (created from the **IntaBio icIEF-MS** workflow), the Plots tab in the report template **Intact\_IntaBio.rptc** can be displayed or turned off using units of isoelectric point (pI) or minutes, and for whole or divided trace plots:

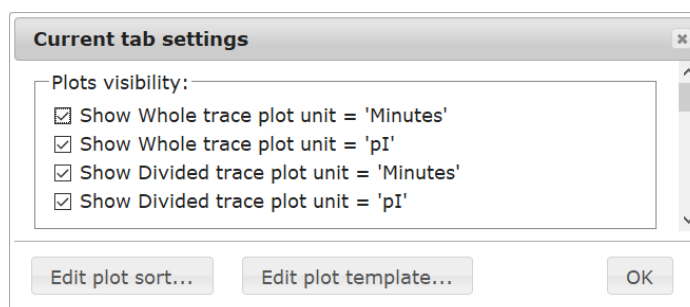


Figure 94: Setting units of pI or Minutes for whole or divided IntaBio plots

Note: Plots are cached during an application session. If plot loading is cancelled, only the retrieved plots will be displayed. Loading of un-cached plots will continue when the Plot tab is refreshed either when the Plot tab becomes the current tab or Update tab is selected from the content menu. If all three plot sizes are cached, changing the plot layout will not cause a re-fetching of plots.

## Plots Tab Sorting

To change the sort order of the plots, click the **Edit plot sort** button:

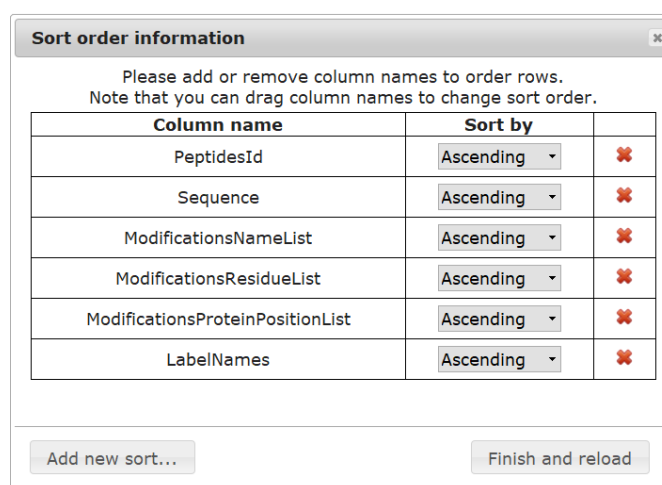


Figure 95: Plot sorting

The table displays the order of sorting by field value and direction. The sorting proceeds by the first field, followed by subsequent fields, as applicable. To change the **Sort by** direction, click the arrow beside the value and select the new direction. To delete a field for sorting, click the ✖ icon. To rearrange the field sorting order, drag the field to the new order:

Column name	Sort by	
PeptidesId	Ascending	✖
Sequence	Ascending	✖
ModificationsNameList	Ascending	✖

Figure 96: Adjust sorting by drag-and-drop

To add a new field to sort by, click the **Add new sort** button:

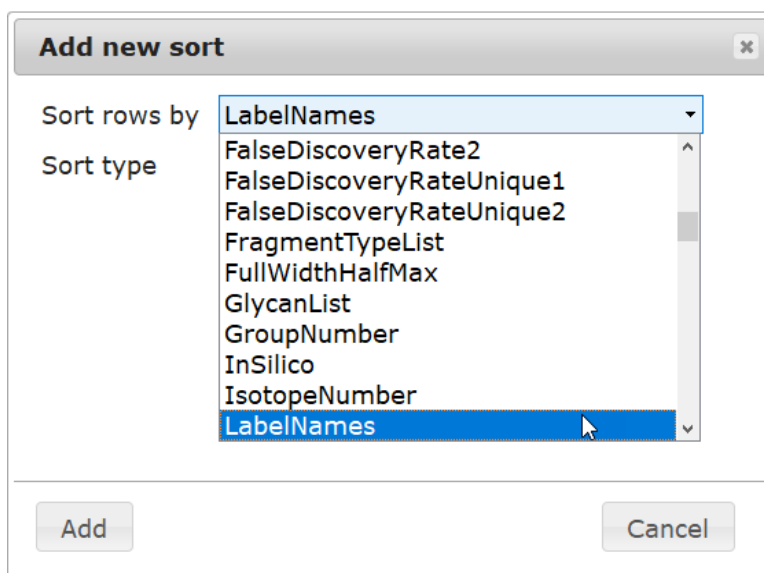


Figure 97: Add new sort type

Select the **Sort rows by** field, select the **Sort type** direction, and then click **OK**. The new field is appended to the end of the sort list.

When all sort edits are completed in the **Sort order information** dialog, click the **Finish and reload** button.

## Plots Tab Filtering

The **Show/Hide configuration** mode is enabled for Plot tabs. This allows filtering of plots by the exposed fields, much the way Pivot tables are filtered:

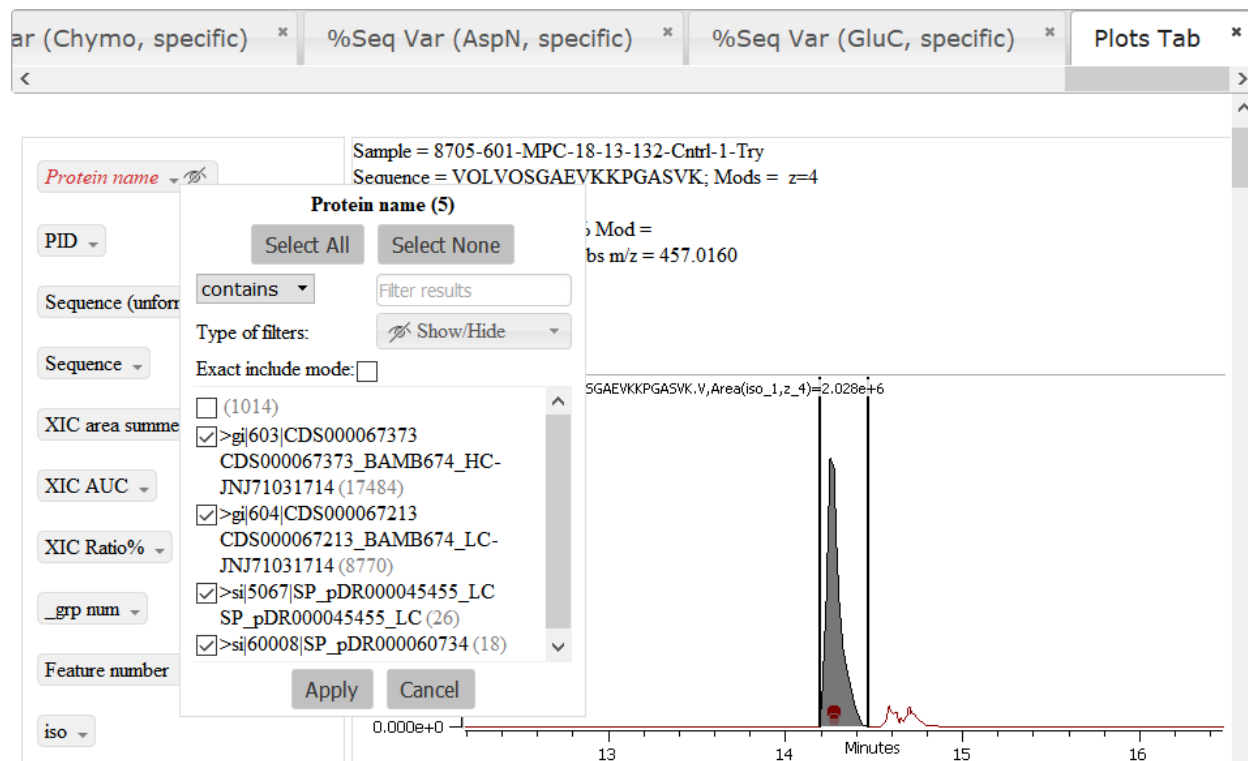


Figure 98: Show configuration for Plots tab to filter the plots by field values

## Plots Tab Template Editor

The headers and values displayed with the plots can be customized. To edit the headers in the Plots Tab, choose **Edit > Current tab settings** and click the **Edit plot template** button to open the **Template Editor** dialog:

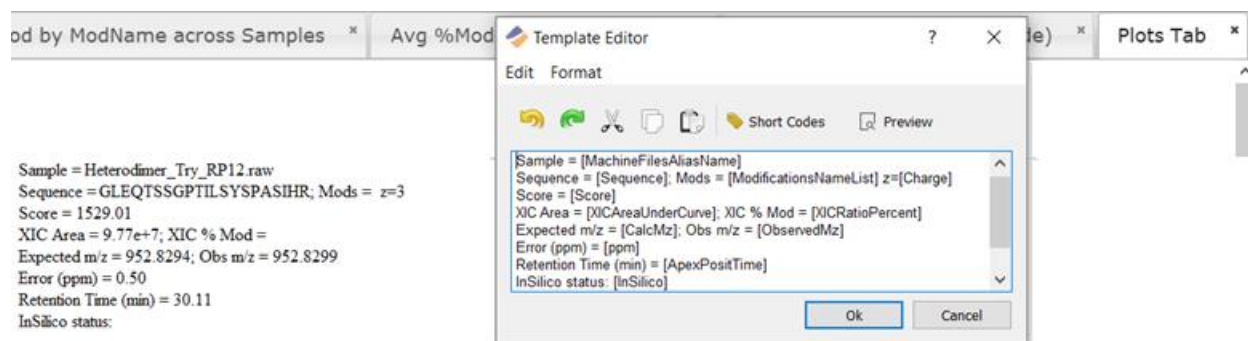


Figure 99: Plot data labels for Peptide Analysis projects

For Peptide Analysis projects ( \*.blgc ), the plots are prefaced with primary data. The data labels correspond to the following **Peptides** table field names:

Label	Field Name
Sample	MS alias name
Sequence	Sequence (unformatted)
Mods	Mod. Names
z	z
Score	Score
XIC Area	XIC AUC
XIC % Mod	XIC Ratio%
Expected m/z	Calc. m/z
Obs m/z	Obs. m/z
Error (ppm)	ppm
Retention Time (min)	Apex Time (Posit)
InSilico status	In silico

For more information about this dialog, see the **Template Editor and Short Codes** section below.

## Template Editor and Short Codes

The Template Editor allows a user to customize a tab using HTML tags and predefined Short Codes.

The following section uses the Summary Tab as an example. Even though Short Code content might differ between applications or tabs, Preview and Short Code usages are the same among the Report tabs.



## Summary Tab Template Editor

To open the Template Editor from the Summary Tab, select **Edit > Current tab settings**, and click the **Edit summary template** button:

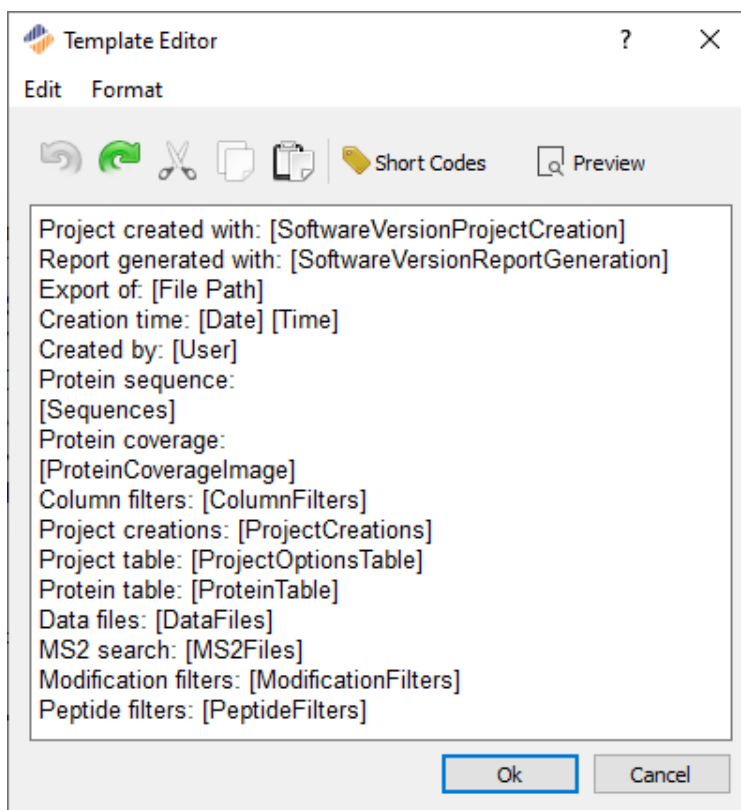


Figure 100: Summary tab Template Editor

The **Edit** menu contains the functions Undo, Redo, Cut, Copy, Paste. These same functions are also available as the first five toolbar buttons.

Format menu contains the function Short Codes. This function is also available as a toolbar button by that name.

The **Preview** toolbar button displays the label text (without HTML tags) as it would appear in the report tab.


In the editor itself, terms in square brackets are reserved Short Codes. Text in angle brackets (<>) are standard HTML tags. All other text is displayed either in line or above Short Codes, as formatted.

## Summary Tab Short Code Reference

Short Code	Description
All Applications	
[ByosProjectCreationOptions]	Byonic search parameters used to create projects in Byos
[PublicByosProjectCreationOptions]	Byos Project Creation content excluding sample file names and sequences (often confidential)
[File Path]	Project document file path.
[Date]	Project document file creation date.

[Time]	Project document file creation time.
[User]	Project creator.
[Sequences]	Sequence text.
[ColumnFilters]	Applied Peptide column filter.
[MS file paths]	Original and edited MS file paths (changed by Edit > Adjust MS paths)
[ProjectCreations]	Project Creation settings. The values are preset to display 6 significant figures: (Note that the types of values vary by application.) Peak smoothing width (TIC) Baseline smoothing width (TIC) Peak tolerance max (TIC) Peak tolerance min (TIC) Baseline minimum angle (TIC) Baseline maximum angle (TIC) Baseline push tolerance (TIC) Blur Skewness
[ProjectOptionsTable]	Summary Project Table.
[ProteinTable]	Summary Protein Table.
[LoginUserName]	Current windows login user.
[ProteinCoverageImage filter = "filtername"]	Protein Coverage summary and percent values for the proteins filtered by a saved table (Peptides, Peaks, Trace Peaks) filter
[ProteinCoverageImage]	Protein Coverage image from the application. Fragment coverage is based on application settings.
[FragmentProteinCoverageImage]	Display protein and fragmentation coverage simultaneously.
[SoftwareVersionProjectCreation]	Version of the Protein Metrics Inc. application when project is created
[SoftwareVersionReportGeneration]	Version of the Protein Metrics Inc. application when report is generated
Peptide Analysis Only	
[MS2Files]	Imported MS2 ( *.byrsIt ) files.
[DataFiles]	Raw source data files.
[PeptideFilters]	Applied Peptide filters.
[ModificationFilters]	Applied Modification filters.
[ByonicSearchParameters]	All parameters saved within the *.byparms file (including Fixed and variable modifications, Glycan modifications, Byonic parameters, etc.
Chromatogram Analysis and Intact Analysis Only	
[ProjectFiles]	Raw source files.
[FilterOptions]	Peak filtering settings. The following values are preset to display 6 significant figures: Lock Mass (m/z) Interest time end Interest time start

[DeltaMass]	Delta Mass values for named masses.
[ProjectOptions]	Project Settings.

Note: Protein Coverage can be filtered and saved, and then the filtered view can be displayed in the Summary tab. To save a Protein Coverage filter, click the  icon above the **Peptides** table, add the filter rows, choose **Presets > Save to document > Save with new name**, add a name, and click **OK** twice:

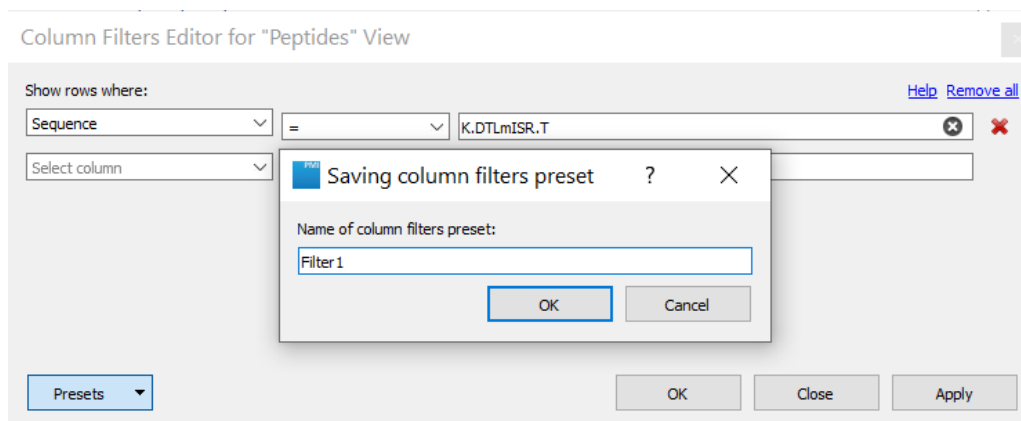


Figure 101: Saving a Protein Coverage filter in the Peptides table

To load the filter into the report **Summary** tab, choose **Edit > Current tab settings**, click **Edit summary template**, add a line to place the filtered Protein Coverage image, and click **Short codes**. An additional item named for the saved filter appears for **ProteinCoveragelImage**. Click **Insert** and click **OK** to add the filtered Protein Coverage:

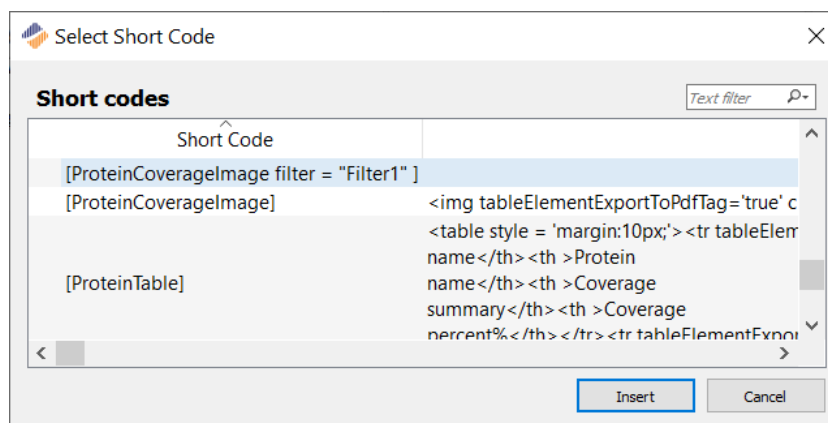


Figure 102: The Short Code generated for the saved Protein Coverage filter

## Summary Tab and Plot Tab Short Codes

The Summary tab Short Codes for Peptide Analysis, Chromatogram Analysis, and Intact Analysis are as follows:

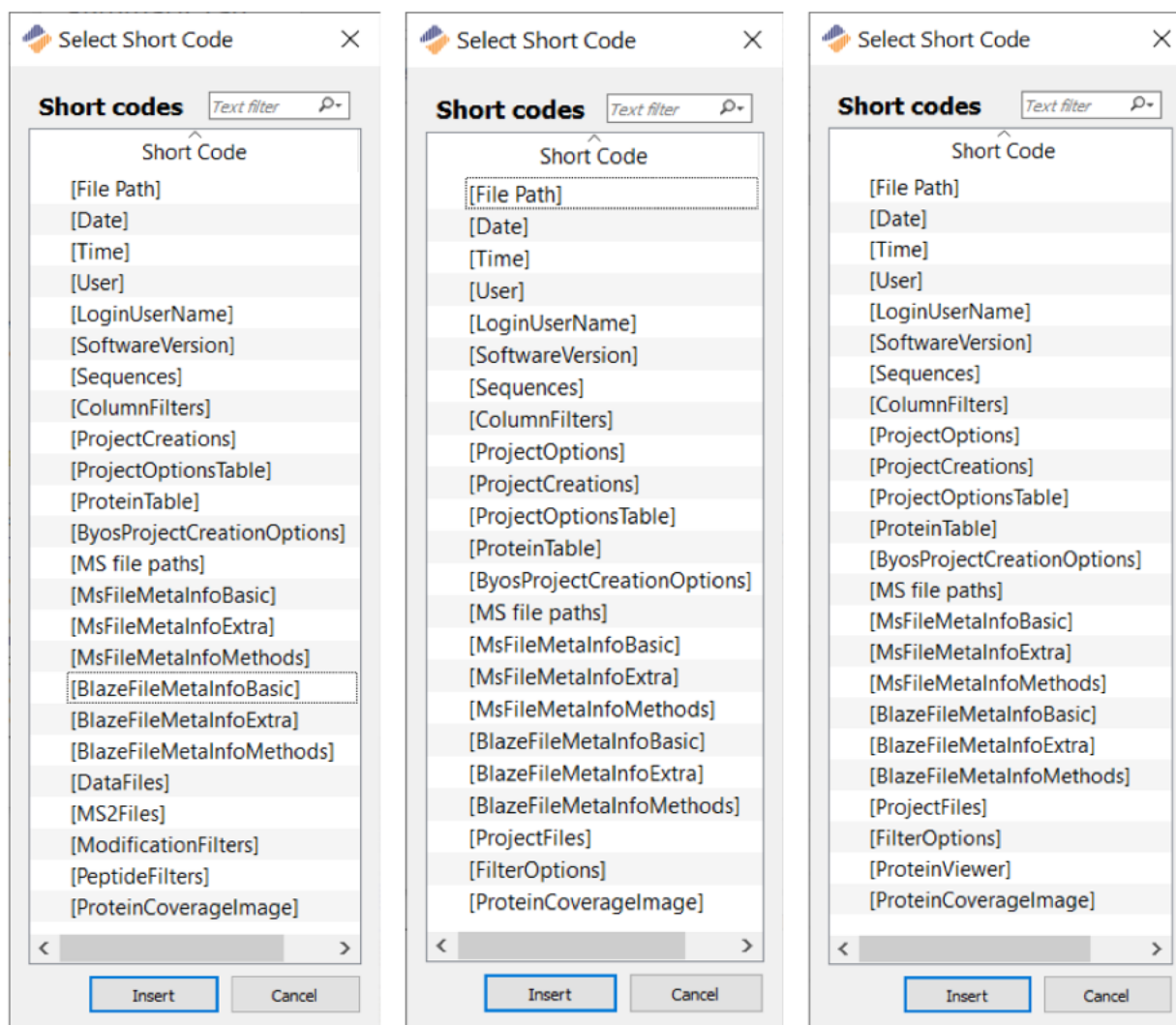


Figure 103: Short Codes for Peptide Analysis, Chromatogram Analysis & Intact Analysis.

Note: Short Codes can be searched by entering a string in the **Text filter** box.

The Plot tab Short Codes for Peptide Analysis are as follows:

Short Code	Short Code Name	Short Code Description
[ApexPositIntensity]	Apex Int. (Posit)	Apex Posit Intensity
[ApexPositTime]	Apex Time (Posit)	Apex Posit Time
[ByonicComment]	Byonic Comment	Comment Field From Byonic
[CalcMr]	Calc.M	Calculated neutral mass
[CalcMz]	Calc. m/z	Calculated m/z
[CenterOfMz]	Center of m/z	Center of m/z
[Charge]	z	Charge
[Comment]	Comment	Comments
[Delta]	Delta Score	Delta Score
[DeltaDalton]	Delta (Dalton)	Observed M. - Calculated M.
[DeltaMod]	Delta Mod. Score	Delta Modification Score
[DeltaObservedMinusDeltaPredicted]	Delta R.T. Obs- Delta R.T. Prd.	Time differences of (minutes): (Obs.Variant - Obs.Wildtype) - (Prd.Var...
[DigestCTermOffset]	Digest C-term ragged	Digest c-terminus ragged number. Zero means digest is specific and ...
[DigestEndPeptide]	Digest End Peptide	Digest end peptide.
[DigestMissedCleavages]	Digest Missed Cleavages	Number of missed cleavages.
[DigestNTermOffset]	Digest N-term ragged	Digest n-terminus ragged number. Zero means digest is specific and...
[DigestStartPeptide]	Digest Start Peptide	Digest start peptide.
[EndPosition]	End AA	End amino acid position with respect to the protein sequence
[FalseDiscoveryRate1]	FDR 1D	(# Decoy PSMs) / (# Target PSMs) in full PSM list ranked by PEP 1D
[FalseDiscoveryRate2]	FDR 2D	(# Decoy PSMs) / (# Target PSMs) in full PSM list ranked by PEP 2D
[FalseDiscoveryRateUnique1]	FDR uniq. 1D	(# Decoy Peptides) / (# Target Peptides) in full unique peptide list ran...
[FalseDiscoveryRateUnique2]	FDR uniq. 2D	(# Decoy Peptides) / (# Target Peptides) in full unique peptide list ran...
[FixedModificationsSummaryList]	Fixed Mod. Summary	Fixed modifications formatted to show both positions and modificati...
[FragmentTypeList]	Fragment type(s)	MS/MS fragment type information
[FullWidthHalfMax]	FWHM	FWHM (Full-Width-Half-Maximum) measures the width of the most ...
[GlycanList]	Glycans	Glycan composition. If in numeric form(e.g. 0 1 2 0 0 0): HexNAc Hex ...
[GroupNumber]	_grp num	Primary peptide group number. This is the same number as the Feat...
[InSilico]	In silico	"Yes" if in silico addition
[IsotopeNumber]	iso	Isotope number used for XIC quantification. Zero means the monois...
[LabelNames]	Labels	Label Names
[MachineFilesAliasName]	MS Alias name	Alias name of the mass spectrometry file (defined during the project ...
[MachineFilesDigestionType]	Digest name	Digest name.
[MachineFilesFilename]	MS Filename	Path of the mass spectrometry file
[MachineFilesId]	MS Id	MS file identifier number
[MassSequenceTable]	Mass sequence table	Mass sequence table
[MobilityValueList]	Mobility value(s)	Ion mobility value(s)
[ModificationsIdList]	_mod ids	Modification Id List (internal ids for modifications)

Figure 104: Peptide Analysis Plots tab Short Codes, part 1

Select Short Code ×


**Short codes** Text filter 🔍

Short Code	Short Code Name	Short Code Description
[ModificationsIdList]	_mod ids	Modification Id List (internal ids for modifications)
[ModificationsNameList]	Mod. Names	Modification Names
[ModificationsPositionList]	Var. Pos. Peptide	Variant location within Peptide
[ModificationsProteinPositionList]	Var. Pos. Protein	Variant location within protein sequence
[ModificationsResidueList]	Mod. AAs	Amino acid residues with modifications
[ModificationsSummaryList]	Mod. Summary	Modifications formatted to show both positions and modifications
[MS1Correlation]	MS1 correlation	MS1 correlation score measures how closely the measured MS1 isot...
[ObservedFragmentSumIntensity]	Obs. Frag. Sum	Fragment Intensity Sum Value from Mascot results
[ObservedMr]	Obs.M	Observed neutral mass
[ObservedMz]	Obs. m/z	Observed m/z
[ObservedTimeVariant]	Obs. time Var (min)	Observed time of Variant (min). Note: The time is from scan time (no...
[ObservedTimeWildtype]	Obs. time Wild (min)	Observed time of Wildtype (min). Note: The time is from scan time (n...
[OffByX]	Off- By-X	Precursor monoisotope error, 1=iso1, 2=iso2, ...
[PEP1]	PEP 1D	Protein-oblivious posterior error probability
[PEP]	PEP 2D	Protein-aware posterior error probability
[PeptidesId]	PID	Peptide Identifier A unique ID across all MS and MS2 search results.
[PivotTable]	<pivottable data-skipzoomedsegment='...	Content of pivot table can be customized by settings field
[PlotChromatogramXIC]	Chromatogram XIC plot	Chromatogram XIC plot
[PlotIsotope]	Isotope plot	Isotope plot
[PlotMS2]	MS2 plot	MS2 plot
[PlotXIC]	XIC plot	XIC plot
[PlotXY]	XY plot	XY plot
[ppm]	ppm	Mass error (calculated - observed) in parts of million
[PredictedTimeVariant]	Calc. time Var (min)	Calculated time of Variant (min). Note: When the variant has no corre...
[PredictedTimeWildtype]	Calc. time Wild (min)	Calculated time of Wildtype (min). Note: When the variant has no cor...
[PrimaryPeptidesId]	Sample-charge ID	A sample-charge Id defines a unique peptide for a specific sample a...
[ProteinAccessionName]	Protein name	The name for the given protein.
[ProteinAliasName]	Protein alias name	Alias name
[ProteinAnnotation]	Protein annotation	Describes regions of interest in the protein sequence
[ProteinIsoelectricPoint]	Protein isoelectric point	Protein isoelectric point
[ProteinMolecularWeight]	Protein molecular weight	Protein molecular weight
[ProteinOccurrences]	Protein occurrence(s)	Total number of occurrences of the peptide within and across protei...
[ProteinsId]	_prot_id	ProteinsId, an internal id for proteins
[ProxyGroupNumber]	Feature number	A feature number contains a unique peptide across all charges and s...
[QueryNumber]	Qry.#	Mascot Query Number
[RankNumber]	Score Rank	Peptide Rank Number
[RowTypeName]	Row type	Row type (e.g. Peptide level information, MS2 level information)

Insert Cancel

Figure 105: Peptide Analysis Plots tab Short Codes, part 2

Select Short Code ✕

**Short codes** Text filter 

Short Code	Short Code Name	Short Code Description
[QueryNumber]	Qry.#	Mascot Query Number
[RankNumber]	Score Rank	Peptide Rank Number
[RowTypeName]	Row type	Row type (e.g. Peptide level information, MS2 level information)
[SampleType]	Sample type	Sample type
[ScanNumberList]	Scan Number(s) (Posit)	Scan number list Note: Scan numbers maybe reconstructed by this a...
[ScanTimeList]	Scan Time(s) (Posit)	Scan time list Note: Scan numbers (hence scan times) maybe reconst...
[Score]	Score	MS2 Search Score
[ScoreDelta]	Score Delta	(Top Score) - Score
[ScoreRatio]	Score Ratio	Score / (Top Score)
[SearchResultAliasName]	MS2 Search Alias name	Alias name of the MS2 search (defined during project creation)
[SearchResultFilename]	MS2 Search Filename	Path of the MS2 search file
[SearchResultsId]	MS2 Search Id	MS2 Search Identifier Number
[Sequence]	Sequence (unformatted)	Peptide sequence without additional information
[SequenceDot]	Sequence	Peptide sequence with before and after amino acid letters (E.g. K.PEP...
[StartPosition]	Start AA	Starting amino acid position with respect to the protein sequence
[ValidateType]	Validate	Assign validate type. You may use the following shortcuts: Empty fiel...
[VendorScanMeta]	Scan info	For example, Thermo scan filter
[XICAreaEnd]	XIC End	XIC end time (minutes).
[XICAreaStart]	XIC Start	XIC start time (minutes).
[XICAreaUnderCurve]	XIC AUC	XIC area under curve (intensity x seconds)
[XICAreaUnderCurveAllIsotopeProxy]	Total XIC AUC Averagine	Theoretical total XIC area based on current XIC AUC value scaled by t...
[XICAreaUnderCurveSummed]	XIC area summed	XIC area under curve (intensity x seconds) summed over its valid chil...
[XICCorrelation]	XIC correlation	XIC correlation score measures how closely the variant's XIC plot mat...
[XICQuantLevel]	Quant level	This column provides information about how to use quantification v...
[XICRatioPercent]	XIC Ratio%	XIC area ratio with respect to wildtype (in percent). If no wildtype, thi...
[XICTimeIntervalProposals]	XIC proposals	XIC start time and end time proposals. These can be used for splittin...
[{Digest-Summary}]	Dynamic columns	Dynamic columns which will be mapped to {Digest-Summary} dyna...
[{Missed Cleavage?}]	Dynamic columns	Dynamic columns which will be mapped to {Missed Cleavage?} dyna...
[{Peptide-Label}]	Dynamic columns	Dynamic columns which will be mapped to {Peptide-Label} dynamic ...
[{XIC area summed isoX normalized}]	Dynamic columns	Dynamic columns which will be mapped to {XIC area summed isoX n...

Insert
Cancel

Figure 106: Peptide Analysis Plots tab Short Codes, part 3


The Plot tab Short Codes for Chromatogram Analysis are as follows:

Short codes		
Short Code	Short Code Name	Short Code Description
[[Glycan Name]]	Dynamic columns	Dynamic columns which will be mapped to [Glycan Name] dynamic colu...
[[ppm]]	Dynamic columns	Dynamic columns which will be mapped to [ppm] dynamic column values
[ApexPositTime]	XIC Apex Time (Posit)	XIC Apex Posit Time
[ApexTime]	Apex time	Apex time associated with the peak
[ApexTimeOriginal]	Apex time original	Original apex time (i.e. without any virtual time shift)
[CalcMr]	Calc.M	Calculated neutral mass
[CalcMz]	Calc. m/z	Calculated m/z
[CandidatesId]	Cand. Id	Candidates Id, a unique and persistent identifier for the given candidate
[Charge]	z	Charge
[ComputedArea]	Area	The area of the peak less the baseline
[DigestCTermOffset]	Digest C-term ragged	Digest c-terminus ragged number. Zero means digest is specific and non...
[DigestEndPeptide]	Digest End Peptide	Digest end peptide.
[DigestMissedCleavages]	Digest Missed Cleavages	Number of missed cleavages.
[DigestNTermOffset]	Digest N-term ragged	Digest n-terminus ragged number. Zero means digest is specific and non...
[DigestStartPeptide]	Digest Start Peptide	Digest start peptide.
[EndTime]	End time	End time
[EndTimeOriginal]	End time Original	Original end time (without any shift)
[GlycanList]	Glycans	Glycan composition. If in numeric form(e.g. 0 1 2 0 0 0): HexNAc Hex Fuc ...
[ISSAComment]	Imported comment	Imported user created comment for this comment.
[ModificationsNameList]	Mod. Names	Modification name(s) for the given peptide.
[ModificationsPositionList]	Var. Pos. Peptide	Variant location within peptide
[ObservedMr]	Obs.M	Observed neutral mass
[ObservedMz]	Obs. m/z	Observed m/z
[PeakAreaNormed]	Normed area %	The peak area divided by total trace area, where the total trace area is sig...
[PeaksCandidatesId]	_pks _c_id	PeaksCandidatesId: a unique SQL identifier.
[PeaksComment]	Peak Comment	Peak comment
[PeaksDynamicNumber]	Peak #	Ordered peak number based on the peak apex. This number will change i...
[PeaksId]	_pks _id	A unique and persistent identifier number for a given peak (internal SQL i...
[PivotTable]	<pivottable data-skipzoomedsegment='tru...	Content of pivot table can be customized by settings field
[PlotFilteredTrace]	Filtered Plot Trace Peak	Filtered Plot Trace Peak

Figure 107: Chromatogram Analysis Plots tab Short Codes, part 1



Select Short Code ×

**Short codes** Text filter 

Short Code	Short Code Name	Short Code Description
[PlotFilteredTrace]	Filtered Plot Trace Peak	Filtered Plot Trace Peak
[PlotMS1]	Plot MS1	Plot MS1
[PlotName]	Plot name	Plot name (Deconvoluted Mass spectrum, MS1, Trace Peak)
[PlotsId]	_plt_id	PlotsId: a unique SQL identifier.
[PlotTracePeak]	Plot Trace Peak	Plot Trace Peak
[ProteinAccessionName]	Protein name	The name for the given protein.
[ProteinAliasName]	Protein alias name	Alias name
[ProteinEndPosition]	End AA	End amino acid position
[ProteinId]	_prot_id	ProteinId, an internal id for proteins
[ProteinStartPosition]	Start AA	Start amino acid position
[SampleName]	Sample name	Sample name
[SamplesId]	Samples Id	A unique identifier for each sample.
[SamplesRunsId]	_sr_idx	SamplesRunsId: Items within a given sample; a unique SQL identifier.
[SamplesType]	Samples type	Type of sample. Either reference or non-reference.
[Score]	MS2 Score	MS2 database search score
[ScoreRatio]	Score Ratio	Score / (Top Score)
[Sequence]	Sequence	Peptide sequence
[SourceType]	_cand_src_t	Candidate source type (e.g. from MS2 search, import list, or from user)
[StartTime]	Start time	Start time
[StartTimeOriginal]	Start time Original	Original start time (without any shift)
[TotalTraceAreaWithinInterest]	Total area within interest	The total trace area within the range of interest above the baseline
[UserComment]	Candidate Comment	Users created comment
[Visible]	Visible	Visible
[XICAreaUnderCurve]	XIC AUC	XIC area under curve (intensity x seconds)

Insert Cancel

Figure 108: Chromatogram Analysis Plots tab Short Codes, part 2

The Plot tab Short Codes for Intact Analysis are as follows:

Select Short Code ✕

Short codes Text filter

Short Code	Short Code Name	Short Code Description
[[protein name]]	Dynamic columns	Dynamic columns which will be mapped to [pro...
[ApexPositIntensity]	Intensity	Intensity at mass
[ApexPositTime]	XIC Apex Time (Posit)	XIC Apex Posit Time
[ApexTime]	Apex time	Apex time associated with the peak
[ApexTimeOriginal]	Apex time original	Original apex time (i.e. without any virtual time s...
[CalcMr]	Mass	Neutral mass found
[CandidatesId]	Mass Id	Mass Id, a unique and persistent identifier for th...
[ComputedArea]	Trace peak Area	The area of the peak less the baseline
[DAR Fraction]	Dynamic columns	Dynamic columns which will be mapped to DAR...
[Delta Mass ppm]	Dynamic columns	Dynamic columns which will be mapped to Delt...
[DeltaMassFromCalculated]	Delta mass from calc.	Mass difference of observed less calculated
[DeltaMassName]	Delta name	The name of the delta mass
[DeltaMassToMostIntenseAssigned]	Delta mass from most intense assigned	Mass difference from the most intense assigned...
[DeltaMonoisotopicMass]	Delta mono mass	Delta monoisotopic mass - the difference betwe...
[DeltaMonoisotopicMassPPM]	Delta mono mass (ppm)	Delta monoisotopic mass (ppm) - the ppm diffe...
[DeltaMonoisotopicMassToMostIntenseAssigned]	Delta mono mass from most intense as...	Mass difference from the most intense assigned...
[Drug Count]	Dynamic columns	Dynamic columns which will be mapped to Dru...
[EndTime]	End time	End time
[EndTimeOriginal]	End time Original	Original end time (without any shift)
[ExpectedMass]	Expected mass	The calculated mass of the protein and any delt...
[ExpectedMonoisotopicMass]	Expected mono mass	Expected monoisotopic mass calculated from us...
[ExpectedType]	Expected type	Expected mass type, such as expected and unde...
[GlycanList]	Glycans	Glycan composition. If in numeric form(e.g. 0 1 ...
[Injection]	Injection	Injection
[IntactLocalRelativeIntensity]	Local Rel. Int.	Local relative intensity (e.g. by 20%)
[MassArea]	Mass Area	Mass area
[MassEnd]	Mass End	Mass end
[MassMonoisotope]	Mono mass	Monoisotopic mass based on averagine model
[MassStart]	Mass Start	Mass start
[MatchesAcrossSampleCount]	Match across count	Matches to reference masses across all samples
[MatchesAcrossSampleDetails]	Match across details	Matches to reference masses across all samples
[MatchesWithinSampleCount]	Match within count	Matches to reference masses within the given sa...

Insert Cancel

Figure 109: Intact Analysis Plots tab Short Codes, part 1

Select Short Code

Short codes Text filter

Short Code	Short Code Name	Short Code Description
[MatchesWithinSampleCount]	Match within count	Matches to reference masses within the given sa...
[MatchesWithinSampleDetails]	Match within details	Matches to reference masses within the given sa...
[PeakAreaNormed]	Normed area %	The peak area divided by total trace area, where...
[PeaksCandidatesId]	_pks _c_id	PeaksCandidatesId: a unique SQL identifier.
[PeaksComment]	Peak Comment	Peak comment
[PeaksDynamicNumber]	Peak #	Ordered peak number based on the peak apex. ...
[PeaksId]	_pks _id	A unique and persistent identifier number for a ...
[PivotTable]	<pivottable data-skipzoomedsegment=...	Content of pivot table can be customized by set...
[PlotDeconvolution]	Plot Deconvoluted Mass spectrum	Plot Deconvoluted Mass spectrum
[PlotFilteredTrace]	Filtered Plot Trace Peak	Filtered Plot Trace Peak
[PlotMS1]	Plot MS1	Plot MS1
[PlotName]	Plot name	Plot name (Deconvoluted Mass spectrum, MS1, ...
[PlotsId]	_plt _id	PlotsId: a unique SQL identifier.
[PlotTracePeak]	Plot Trace Peak	Plot Trace Peak
[ProteinAccessionName]	Protein name	The name for the given protein.
[ProteinAliasName]	Protein alias name	Alias name
[SampleName]	Sample name	Sample name
[SamplesId]	Samples Id	A unique identifier for each sample.
[SamplesRunsId]	_sr _idx	SamplesRunsId: Items within a given sample; a u...
[SamplesType]	Samples type	Type of sample. Either reference or non-reference.
[Sequence]	Name	Intact mass name
[SourceType]	_cand _src_t	Candidate source type (e.g. from MS2 search, i...
[StartTime]	Start time	Start time
[StartTimeOriginal]	Start time Original	Original start time (without any shift)
[TotalTraceAreaWithinInterest]	Total area within interest	The total trace area within the range of interest ...
[UserComment]	Mass Comment	Users created comment
[Visible]	Visible	Visible
[XICAreaUnderCurve]	XIC AUC	XIC area under curve (intensity x seconds)

Insert Cancel

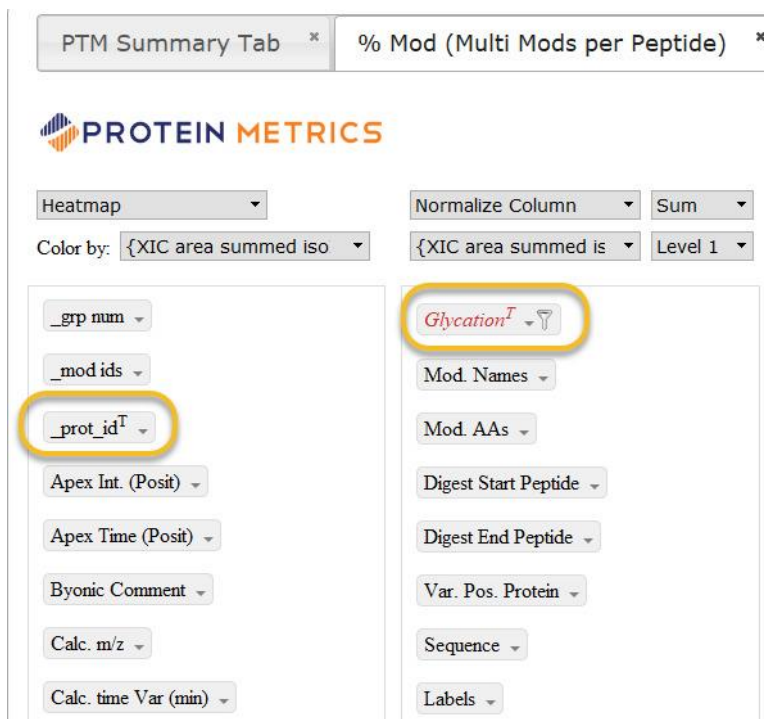
Figure 110: Intact Analysis Plots tab Short Codes, part 2

## Dynamic Columns: Pre-Pivot and Post-Pivot JavaScript

The user can use JavaScript to add Dynamic Columns to the input file that is used to create a pivot table.

Pre Pivot JavaScript ([.prepvajs](#)) can be added to all tabs or just the current tab.

Per Tab Pre Pivot JavaScript ([.prepvajs](#)) applies to the current tab only, and is identified with a superscript T following the field name.



PTM Summary Tab x % Mod (Multi Mods per Peptide) x

**PROTEIN METRICS**

Heatmap  Normalize Column  Sum

Color by: {XIC area summed iso  {XIC area summed is  Level 1

\_grp num

\_mod ids

\_prot\_id<sup>T</sup>

Apex Int. (Posit)

Apex Time (Posit)

Byonic Comment

Calc. m/z

Calc. time Var (min)

**Glycation<sup>T</sup>**

Mod. Names

Mod. AAs

Digest Start Peptide

Digest End Peptide

Var. Pos. Protein

Sequence

Labels

Figure 111: Per tab Pre Pivot fields identified with “T”

Post Pivot JavaScript ([.postpvtjs](#)) applies to the current tab only.

To add Pre Pivot JavaScript, choose **File > Presets > Pre pivot columns** and select the column name to add.

To add Post Pivot JavaScript, select **Presets > Post pivot columns** and select the column name to add.

## Pre Pivot JavaScript Reference

Pre Pivot JavaScript	Description
All Applications	
DAR	Calculates drug-to-antibody ratio by using the formula: intensity * DrugCount / (sum of intensities).
DigestEnzymeSummary	Summarize the enzyme digestion to fit known nomenclature.
DisulfideLinkedPeptides	Report the Base protein (Start AA – End AA) and Partner protein (Start AA – End AA) in disulfide linkage reporting
DrugCount_Intensity	Creates a column of drug value multiplied by intensity, where drug value comes from the string in the parenthesis in "Drug()" from the "Delta name" column.
DrugsCount	Creates a column with the drug count value, which comes from the string in the parenthesis in "Drug()" in the "Delta name" column.
GlycanFamily	Returns "1" if the peptide has a glycan or if the peptide sequence matches a peptide with a glycan. For example, both EEQYN[+1444.5]STYR and EEQYNSTYR (wildtype) return 1.
GlycanShortname	Creates a column of glycan short names (such as G0F, etc), determined by the glycan mass.

IsCTerm	Creates a Yes/No column which identifies if the peptide contains the protein c-terminus residue.
IsDeamOrOxOrPyro	Creates a column which identifies if the peptide contains deamidation, pyrolization or oxidation; otherwise displays "No".
IsSVmod	Creates a column of SV values if the peptide has a sequence variant modification (if Mod. Names contains the -> indicator); otherwise, it is blank.
ModType	Creates a column identifying the row as "Modified" or "Wildtype"
ProteinNameStartEndPeptideLabel	Creates a column which prefixes AA as a heavy chain or light chain, or if neither, the first letter of the protein name.
RenameCols	Provides the means to easily rename a column header in the report
SeparateReplicates	Searches for a substring of the form "r()" in the column MS Alias name and creates a column with the string inside the parenthesis.
SeparateSamples	Searches for a substring of the form "s()" in column MS Alias name and creates a column with the string inside the parenthesis.
XlinkType	Creates a column identifying the modification as "Disulfide" or "Trisulfide".
UpdateXlinkPartnerPeptideProteinName	Replaces <b>Xlink Partner Peptide Protein Name</b> with <b>Protein name</b> if <b>Xlink Partner Peptide Protein Name</b> is <b>(self)</b> .
Peptide Analysis and Chromatogram Analysis	
ProteinCols	Parses the Protein Summary content into separate columns.
Peptide Analysis Only	
ADCQuant	Uses cleaved wildtype peptides for ADC quantification of lysine-conjugated linker drugs.
AvgValues	Creates four columns: [Avg Obs M], [Avg Obs m/z], [Avg ppm], and [Avg RT], which average the range or list of values in the respective columns.
CDRLocationInfo	Reports the modification status within complementarity determining regions (CDRs) of the antibody.
ChargeRankGlyco	Creates a column to display the most abundant charge state for each glycopeptide.
ChargeRankWildType	Creates a column to display the order of charge state abundance of the peptide. If the peptide is modified, returns the order of charge state abundance of the corresponding wildtype. This column can be filtered to easily set up a single-charge state peptide/PTM quantification.
ChargeStatesCalculation	Like AvgValues, except it also averages the values across different charge states.
DigestSummary	Creates a summary of protein digestion based on start/end peptide, n-term/c-term offsets, and accession name.
DisulfideLocationMult	Creates a dynamic column to allow the grouping of disulfide containing peptides by Cys location.
GlycanGroupings.prepvtjs	Creates a column including glycan group identities
GlycanCartoon.prepvtjs	Displays the glycans on glycopeptides.

IsoDmodname	Overrides the Mod Names column if Label contains “iso”.
LessThanThreePeptides	Determines if a peptide belongs to a protein that has less than three peptides identified. This is useful for proteomics or host cell protein analysis.
MinError	Enables the user to report their best ppm (closest to zero) to assess instrument accuracy and aid in validation strategy.
NGlycanFamily	Detects if the specified row has an N-glycan or the peptide sequence matches a peptide with N-glycan, and returns the N-glycan location
NumberOfPeptides	Determines the number of peptides that belong to a protein.
PeakEval	Warns if a modification is a possible artifact, i.e., in source oxidation, off-by-x, poor recovery, or low scoring. This filter looks at metrics gathered from the flat table. For poor recovery, a distribution of XICs is calculated and all wildtype peptides in the bottom two percentile are listed as poor recovery. If a modification shares similar retention time to its wildtype, it is flagged as an ESI artifact.
PeptideLength	Creates a column to display the number of amino acids in the peptide. Useful for filtering out small peptides.
PeptideRanking	Creates a column to display the rank of peptides based on their XIC AUC across charge states and per each protein. The user can filter peptide ranks of 1, 2, and 3 for “Top-3 quant”.
PrefixSum	Creates prefix sum of XIC ratio values
ProteinAccession	Parses Uniprot formatted protein headers and creates three columns with this information.
QuantifyingGlycation	Creates a column that groups wildtype peptides to quantify glycations by tryptic digests.
SPQuantifier	Creates a column to display if a peptide contains part of the n-terminus for signal peptide quantification.
SVA	Creates a column to classify sequence variants into possible “true/false positive” and “check manually” categories. This filter first checks retention time differences and whether the sequence variant makes sense relative to the digestion, and then looks for low scores, high AUC, and whether the sequence variant can be explained by a more common adjacent modification like oxidation. The peptide will be labeled “check manually” if it fails one of these checks. All others are labeled as “true positive”.
SeparateReplicates	Creates different columns or rows based on different replicates
SeparateSamples	Creates different columns or rows based on different samples
ScoresThresholding	Filters out peptide identifications with a score below 100 and a Delta Mod score below 10.
UniprotProteinName	[deprecated] Creates an accession name column based on uniprotformatted protein name.
WildcardCluster	Clusters wildcard identification by their fractional mass, i.e. 10.23 and 10.24 will be clustered into 10.2.
XicAreaSummedIsoXNormalized	Creates a column for formalized XIC area summed for peptides that contain deamidation alongside other modifications. The XIC area summed may be calculated using different isotopes for the

	deamidated peptide (monoisotope) and the other modifications (determined by MS extract options table). The new column normalizes XICs by using the formula: $\text{XIC area summed} * \text{XIC ratio} / (1 - \text{XIC Ratio})$ .
Chromatogram Analysis Only	
PPMMassError	Computes ppm error, as a function of Observed m/z and Calculated m/z.
PrefixSum	Displays a running total of Start times (?)
Intact Analysis Only	
GenericTokenExtract	Creates new columns for each label found in a specified column (default "SamplesName"). A label is in the form "label(value)", an alphanumeric name, followed by a value within parentheses. The new column header is assigned the name and the value of the string within the parentheses. In the example above, the "label" header would contain "value" in its cell.
PPMMassError	Converts "Delta Mass from Calculated" values from Da to ppm units.
ThresholdedDeltaMassDa	Creates a column that displays 1 if the "Delta Mass from Calculated" value in Daltons is above a pre-defined threshold, and 0 if it does not. This can be used as a heatmap to highlight out of range masses.

## Post Pivot JavaScript Reference

Post Pivot JavaScript	Description
All Applications	
AllErrorColumns	Creates all error columns and enables error bar charts and error line charts
RegressionLinear	Add the linear regression analysis data to show <b>intercept</b> , <b>r2</b> (indicating R <sup>2</sup> ) and <b>slope</b> columns
RSDErrorColumns	Creates relative standard deviation column and enables error bar charts and error line charts
StdDevErrorColumns	Creates standard deviation column and enables error bar charts and error line charts
TotalGroup	Supports subtotal columns based on a pivot table row field
Peptide Analysis Only	
HdxVisualization	Supports the HDX Visualization view for HDX projects
MHCVisualization	Supports MHC reports
MaxFoldChangeRow	Finds the maximum fold change between a reference file and each of the non-reference files. The calculation applies to normalized columns
NormalizedPPM	Calculates "normalized ppm", using the formula: $\text{value} / \text{max} * 1,000,000$
PvalueBetweenEachSampleAndControlSample	Calculates p-value and all other helper values from t-test between control and each sample
PValueFpopExperimentFocused	Calculates p-value and all other helper values from t-test between two groups of values

Intact Analysis Only	
BranchDifference	Creates a column to display the difference of two of the first columns
ExtendPivotTable	Extends pivot data cells by creating new Mass columns

## Editing Pre or Post Pivot JavaScript

To edit Pre or Post Pivot JavaScript, select **Edit > Edit dynamic columns** followed by the JavaScript type:

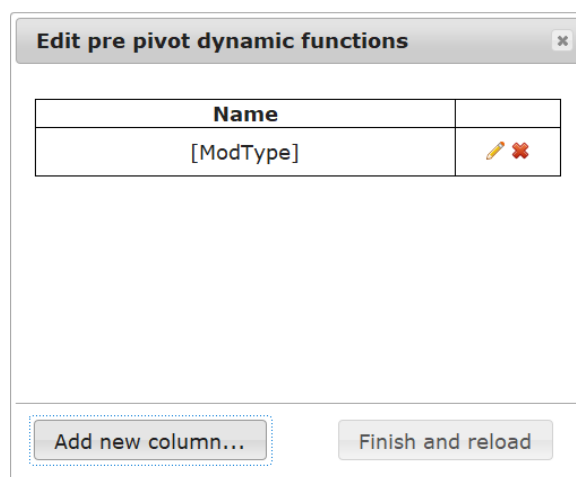




Figure 112: Editing pre pivot dynamic functions

To edit the JavaScript for a dynamic column, click the  icon. To delete a dynamic column, click the  icon. To add a new dynamic column, click the **Add new column** button, click the gray drop-down box at the lower left, and select the column field file to add:

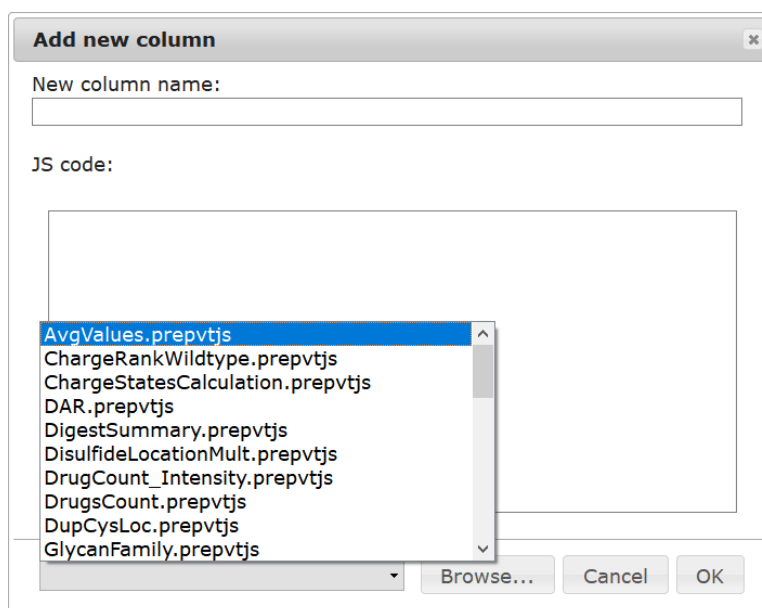
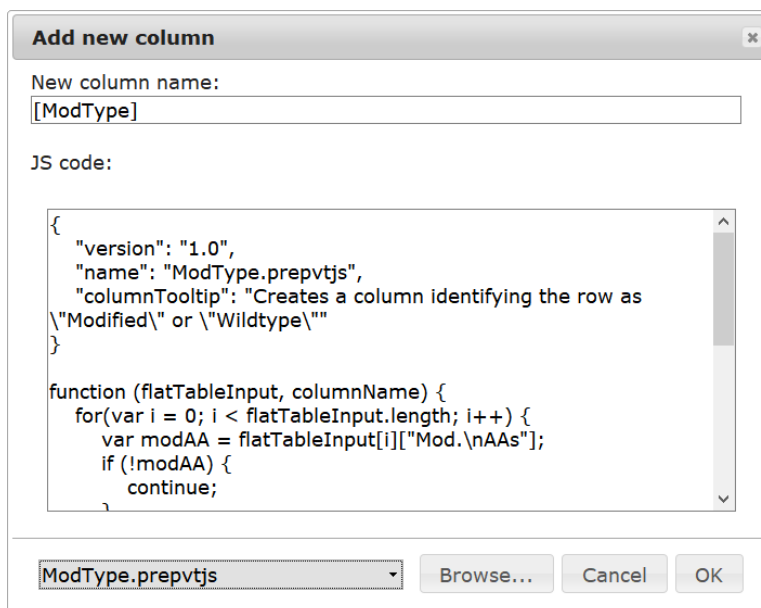


Figure 113: Adding a column as a pre pivot function



The drop-down at bottom left selects from the standard JavaScript functions. The **Browse** button allows the user to load a custom JavaScript function. The dialog loads the JavaScript written for that dynamic column:



**Add new column**

New column name:  
[ModType]

JS code:

```
{
  "version": "1.0",
  "name": "ModType.prepvtjs",
  "columnTooltip": "Creates a column identifying the row as
  \"Modified\" or \"Wildtype\""
}
```

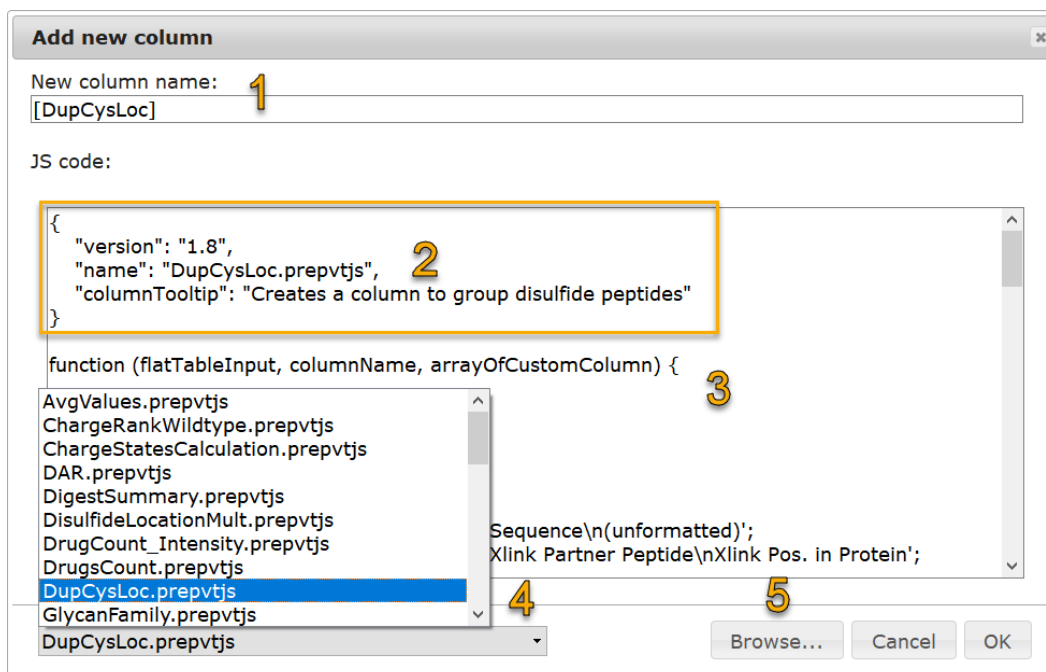
function (flatTableInput, columnName) {  
 for(var i = 0; i < flatTableInput.length; i++) {  
 var modAA = flatTableInput[i]["Mod.\nAAs"];  
 if (!modAA) {  
 continue;  
 }  
 }  
}

ModType.prepvtjs

Browse... Cancel OK

Figure 114: Pre pivot JavaScript

## Tour of JavaScript Add New Column Dialog



**Add new column**

New column name: 1  
[DupCysLoc]

JS code:

2

```
{
  "version": "1.8",
  "name": "DupCysLoc.prepvtjs",
  "columnTooltip": "Creates a column to group disulfide peptides"
}
```

3

function (flatTableInput, columnName, arrayOfCustomColumn) {  
 AvgValues.prepvtjs  
 ChargeRankWildtype.prepvtjs  
 ChargeStatesCalculation.prepvtjs  
 DAR.prepvtjs  
 DigestSummary.prepvtjs  
 DisulfideLocationMult.prepvtjs  
 DrugCount\_Intensity.prepvtjs  
 DrugsCount.prepvtjs  
 DupCysLoc.prepvtjs  
 GlycanFamily.prepvtjs  
 DupCysLoc.prepvtjs

4

Sequence\n(unformatted);  
Xlink Partner Peptide\nXlink Pos. in Protein';

5

Browse... Cancel OK

Figure 115: JavaScript areas in the Add new column dialog

No	Item	Description
----	------	-------------

1	New column name	Dynamic column name to be used in the Report.
2	Metadata	Optional. <pre>{   "version": "1.2",   "name": "AvgValues.prepvtjs",   "columnTooltip": "Create column of averages for Obs M value(s), Obs m/z value(s), and ppm value(s)" }</pre>
3	JavaScript code	Contents of JavaScript.
4	Available JavaScript	Drop down at the bottom right contains all available JavaScript in the application preset directory which is typically Program Files > Protein Metrics > PMI Suite > Base > presets > [application] > [pre or post] pivot_script. Byos preset applies to all applications. For example, the drop down for Peptide Analysis Pre Pivot JavaScript including all *.prepvtjs files in the following directories: <a href="#">PMI-SuiteBasepresetsByologicprepivot_script</a> <a href="#">PMI-SuiteBasepresetsByosprepivot_script</a>
5	Browse button	Opens file browser to open custom JavaScript files

Pre-Pivot JavaScript is formatted as:

```
function (flatTableInput, columnName, arrayOfCustomColumn)
```

Parameter	Description
flatTableInput	Current input flat table. Contains all previously created pre pivot columns.
columnName	New column name.
arrayOfCustomColumn	Optional custom output column name if not using the new column name input field as the column name. An example that uses column name: <pre>function (flatTableInput, columnName) {   for (var i = 0; i &lt; flatTableInput.length; ++i) {     flatTableInput[i][columnName] = i;   }   return flatTableInput; }</pre> An example that uses custom names: <pre>function (   flatTableInput,   columnName,   arrayOfCustomColumn) {   /** Column names that will be added to Flat Input Table */   var avgObsM = '[Avg Obs. M]';   var avgObsMZ = '[Avg Obs. m/z]';   var avgPPM = '[Avg ppm]';   arrayOfCustomColumn.push(avgObsM);   arrayOfCustomColumn.push(avgObsMZ);   arrayOfCustomColumn.push(avgPPM); }</pre>

	<pre>return flatTableInput; }</pre>
--	-------------------------------------

Post Pivot JavaScript is formatted as:

```
function (postPivotTableInput, columnName, arrayOfCustomColumn,
mapOfErrorColumnNameAndColumnName)
```

Parameter	Description
postPivotTableInput	Current pivot table. Contains all previously created post pivot columns.
columnName	New column name.
arrayOfCustomColumn	Custom column names that will be in the Report.
mapOfErrorColumnNameAndColumnName	<p>Optional parameter.</p> <p>Maps arrayOfCustomColumn to error column type name.</p> <p>For example, in AllErrorColumns.postpvtjs, AbsMax is mapped to error type error:abs:upper, and AbsMin to error:abs:lower:</p> <pre>var arrayOfColumnNames = ["[Avg]", "[AbsMax]", "[AbsMin]"]; var arrayOfErrorType = ["error:abs:upper", "error:abs:lower"]; mapOfErrorColumnNameAndColumnName[   arrayOfColumnNames[1]] = arrayOfErrorType[0]; mapOfErrorColumnNameAndColumnName[   arrayOfColumnNames[2]] = arrayOfErrorType[1];</pre>

## Multi-Document Report

Multi-document reports display the results of multiple projects within a single tabbed document. All reports must come from the same application type (for example, Peptide Analysis). To create a multi-document report, select **File > Export > Generate Multi-document Report**, then drag in the project files to include in the report:

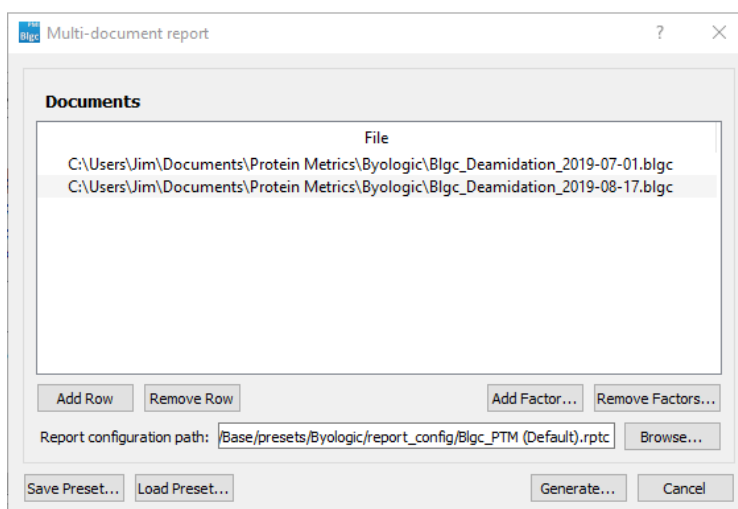



Figure 116: Multi-document report input dialog

Alternatively, click **Add Row**, double-click **<Enter path to document>**, click the  icon, then navigate to the directory and filename of the project to add. To remove a project from the list, select that project and click **Remove Row**. The **Add Factor** button creates custom factors and default values that can be added as fields associated with all projects:

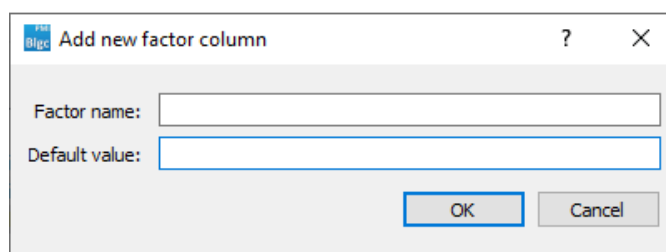


Figure 117: Add new factor column

A factor represents an additional field that can be included to customize reports. For example, a factor can be run order, date, personnel, etc.

The **Report configuration path** shows the file used as the default report template used. To use a different report template, click the **Browse** button, then navigate to the directory and filename of the report template to add. For details about the report template, see the **Report Template and Default Report Template** section.

Existing report presets can be loaded for the multi-document report or saved for future reports. For more details about presets, see the **Report File Menu** section.

Click **Generate** to create the merged report.

## Customize Report

Contact [support@proteinmetrics.com](mailto:support@proteinmetrics.com) for information on a variety of existing and new report templates and dynamic columns.

Up-to-date release and product information are listed on our website. Please visit: [www.proteinmetrics.com](http://www.proteinmetrics.com) and [www.proteinmetrics.com/announcement/version-release-updates/](http://www.proteinmetrics.com/announcement/version-release-updates/).