

PMI Reporting

User's Manual

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Contents

Introduction 2
Data Flow 2
Creating Reports 3
Report Menu Overview 4
Report File Menu 5
Report Edit Menu 7
Report Tabs Menu 8
Report Toolbar 8
Report and Tab Templates 9
Report Tab Management 11
Summary Tab 11
Pivot Tab 15
Tour of Pivot Table Areas 17
Rendering Options 17
Aggregator Options 18
Field Management 19
Filters 20
Sorting 24
Show/Hide Configuration 24
Pivot Tab Current Tab Settings: Common 25
Pivot Tab Current Tab Settings: Chart specific 29
Pivot Tab Heatmap 31
Pivot Tab Error Charts 33
Pivot Tab Principal Component Analysis (PCA) Plots 35
Pivot Tab Protein 3D Plots 37
Pivot Tab Protein Map 41
Plots Tab 41
Template Editor and Short Codes 47
Summary Tab Template Editor 47
Summary Tab Short Code Reference 47
Dynamic Columns: Pre-Pivot and Post-Pivot JavaScript 57
Pre Pivot JavaScript Reference 58
Post Pivot JavaScript Reference 61
Editing Pre or Post Pivot JavaScript 61
Tour of JavaScript Add New Column Dialog 63
Multi-Document Report 65
Customize Report 66

Introduction

Protein Metrics applications have common Reporting features:

- **R** eview all plots on the same page through the Plot Tab.
- **E** xport the report into PDF, Microsoft Excel workbook, or CSV (common separated values) format.
- **P** erform further data analysis through the Pivot Table.
- **O** rganize project information into a Summary.
- **R** euse the report design saved as a template on future data sets.
- **T** ime saving – Reports are automatically generated through Byos workflows.

This manual will focus on the Byos suite of applications (Peptide Mapping, Intact, and Chromatogram Analyses).

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:

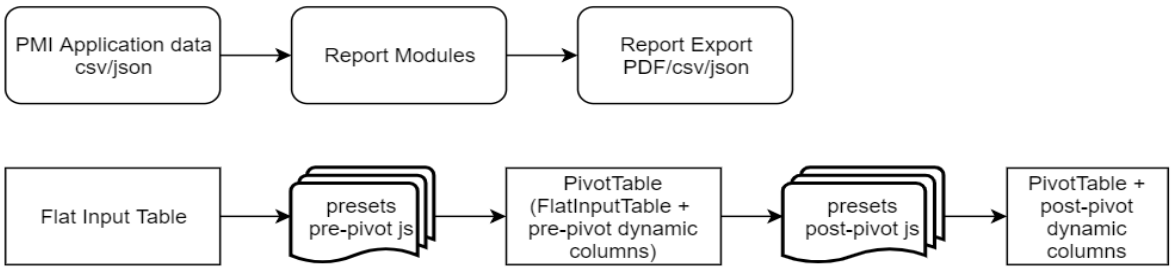


Figure 1: Data flow module for report generation

Creating Reports

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

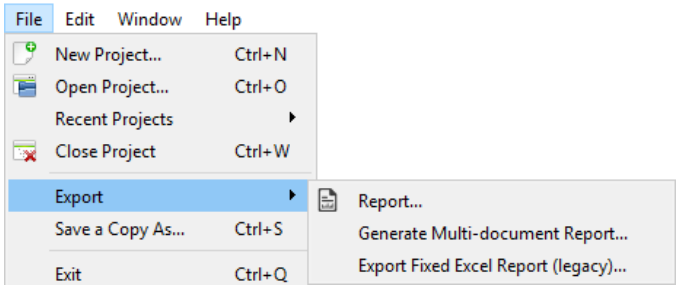


Figure 2: Generating a report from the project File menu

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

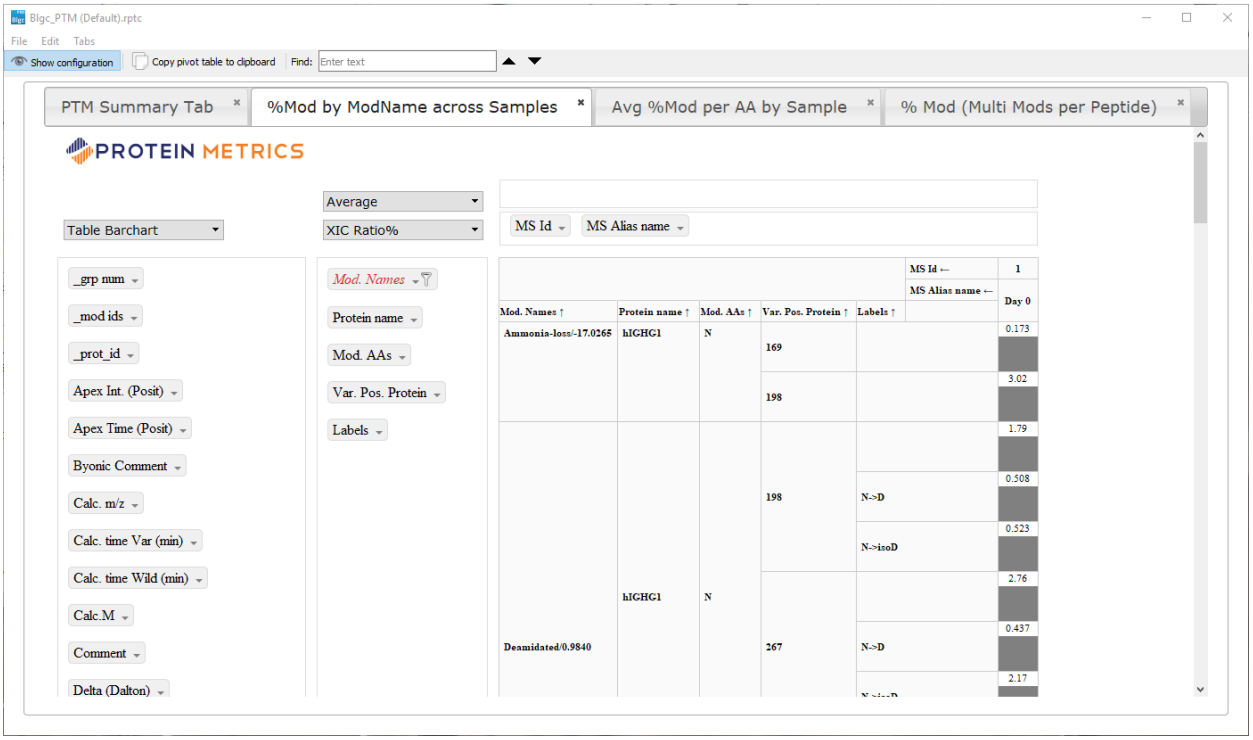


Figure 3: A default report.

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.

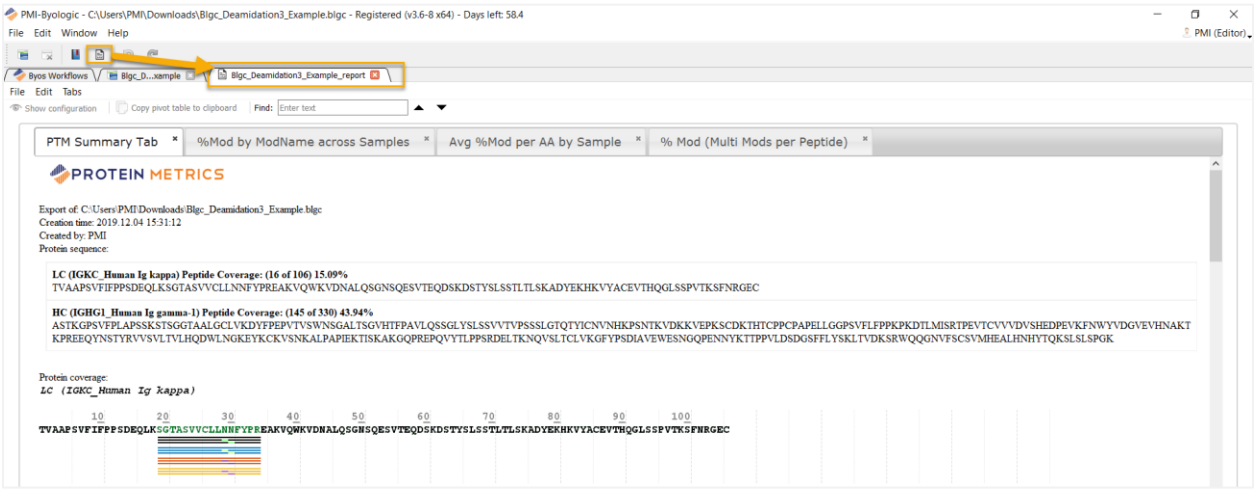


Figure 4: A default report template from Byos

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.

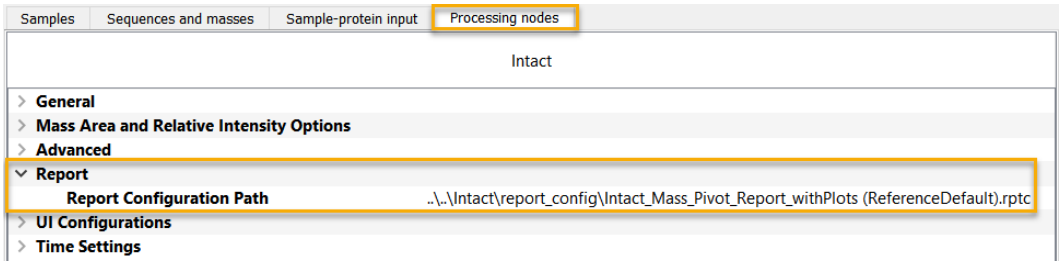


Figure 5: Set the report configuration in the Processing nodes tab during project creation

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

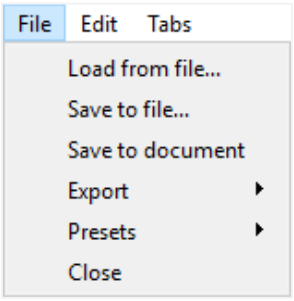


Figure 6: File Menus

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:

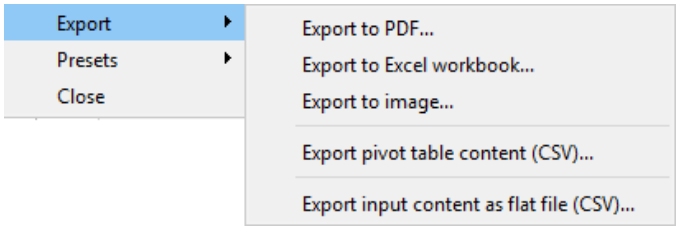


Figure 7: File > Export menus

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

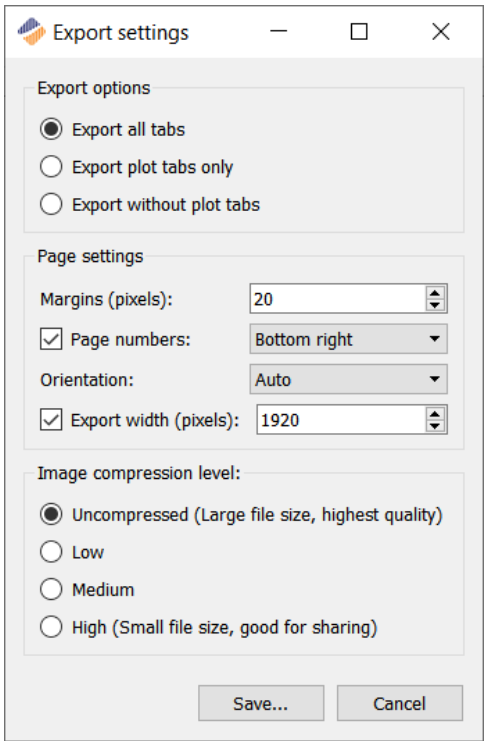


Figure 8: Export to PDF settings

The Export to PDF settings includes:

- **Export options** to choose to export all tabs, only plots or all tabs except plots.
- **Page settings** 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** sets 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. **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).

File > Presets refer to files that configure report formats:

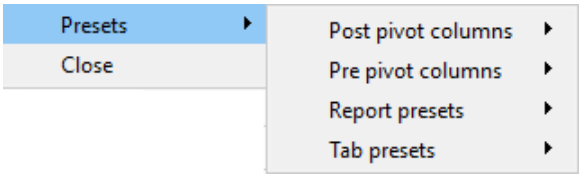


Figure 9: File > Presets menus

Post pivot columns and Prep 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:

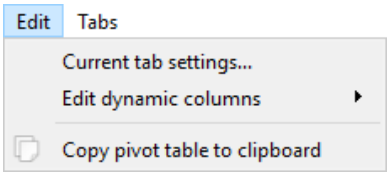


Figure 10: Edit menus

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:

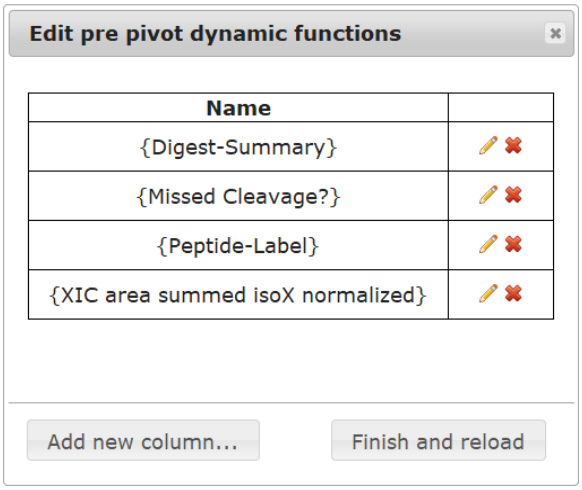


Figure 11: Edit dynamic columns

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 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:

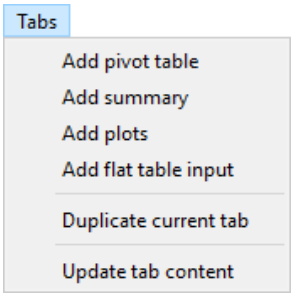


Figure 12: Tabs menus

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 of 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

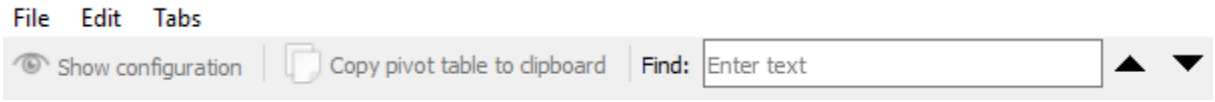


Figure 13: Report toolbar

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:

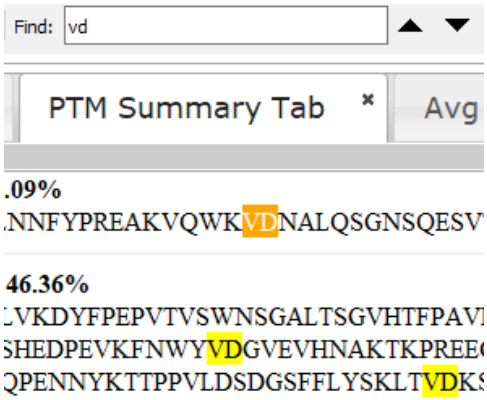


Figure 14: Find function

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:

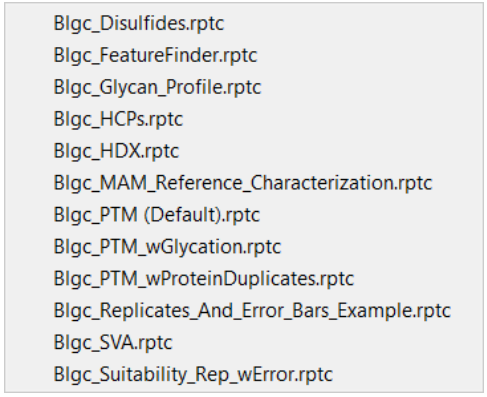


Figure 15: Peptide Analysis report templates

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

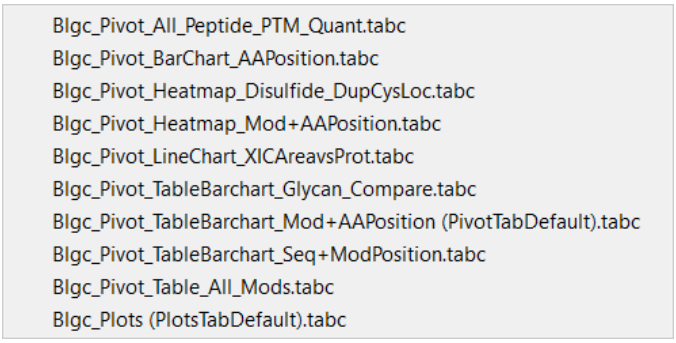


Figure 16: Peptide Analysis tab templates

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

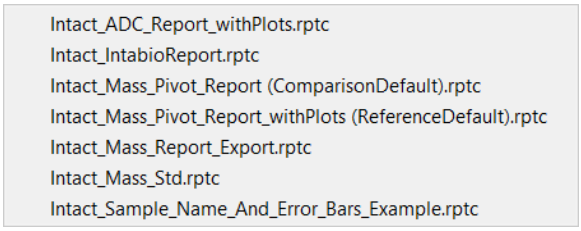


Figure 17: Intact Analysis report templates

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

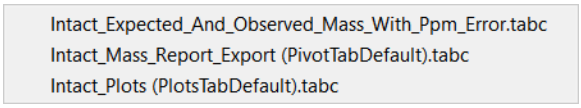


Figure 18: Intact Analysis tab templates

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

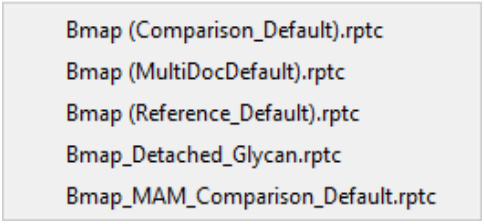


Figure 19: Chromatogram Analysis report templates

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

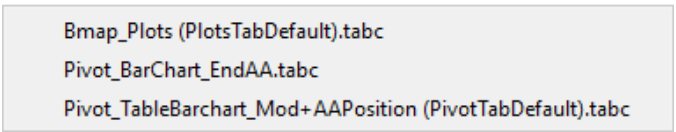


Figure 20: Chromatogram Analysis tab templates

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 must 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 21: 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:

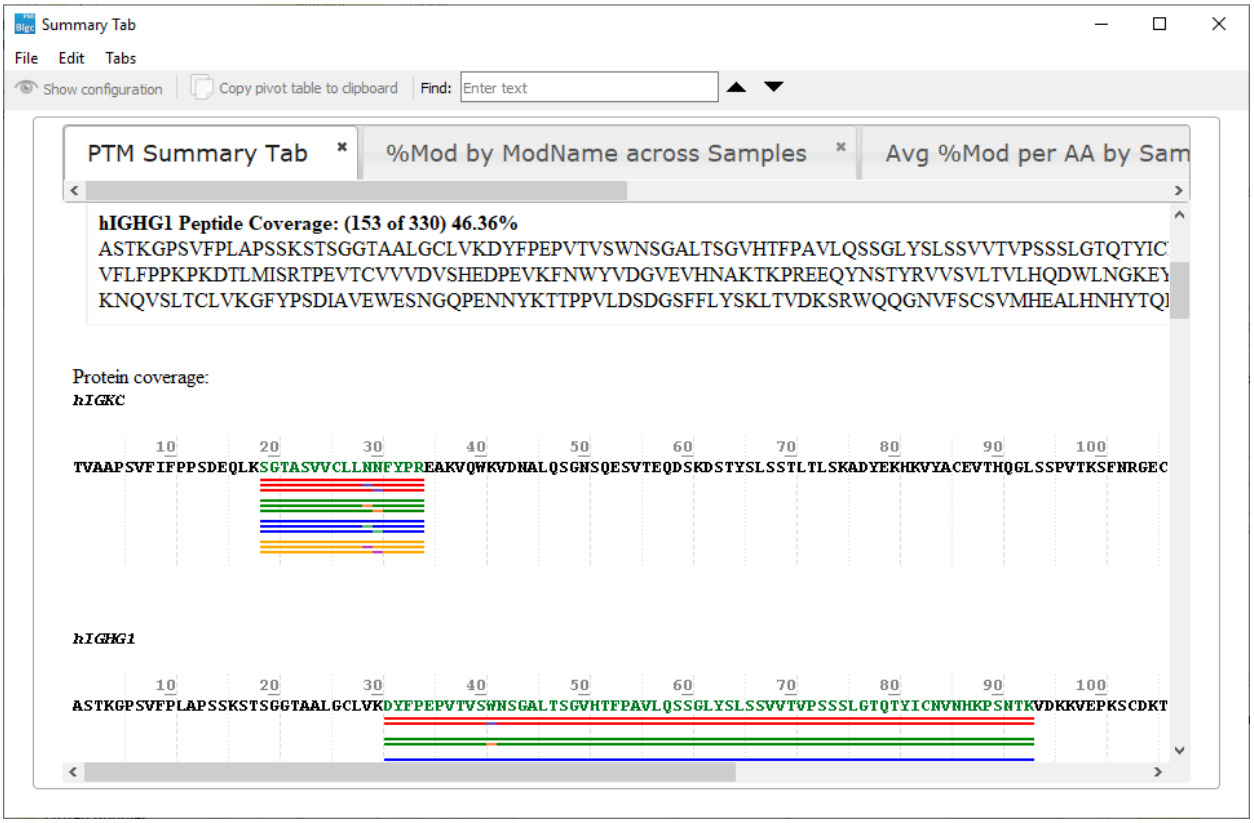


Figure 22: Summary tab

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

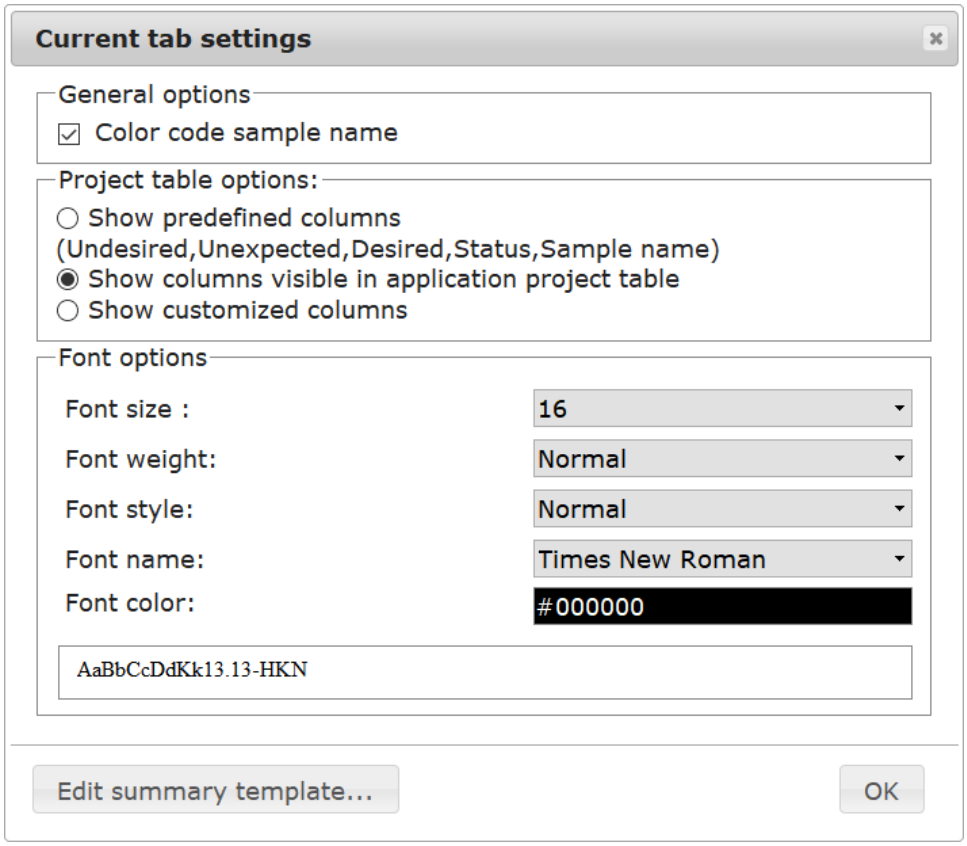
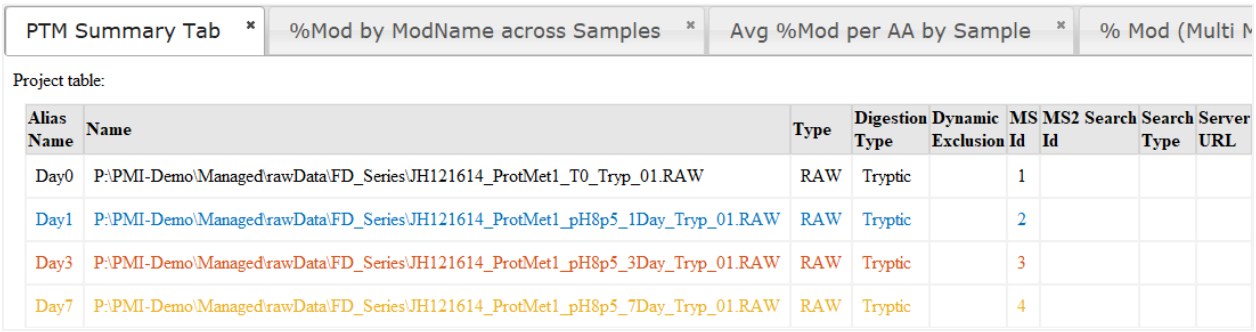


Figure 23: Editing the Summary tab in Current tab settings

Current tab settings for the Summary tab has three sections:

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



Alias Name	Name	Type	Digestion Type	Dynamic Exclusion	MS Id	MS2 Search Id	Search Type	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 24: Project table in Summary tab color-coded by sample name

- **Project table options** determine 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.

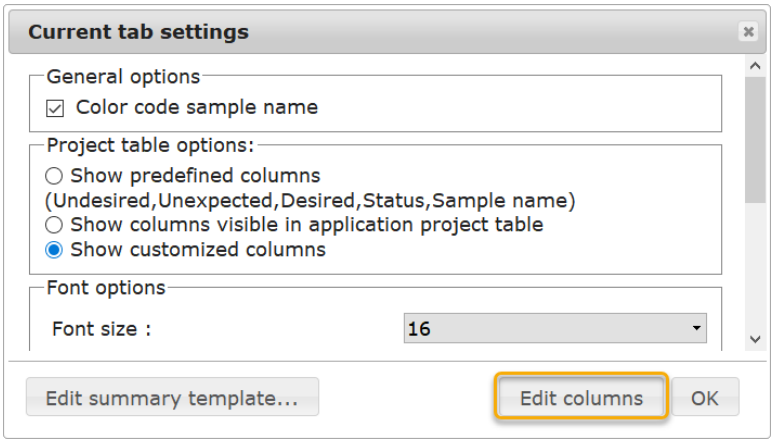


Figure 25: Current tab settings with **Show customized columns** selected

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

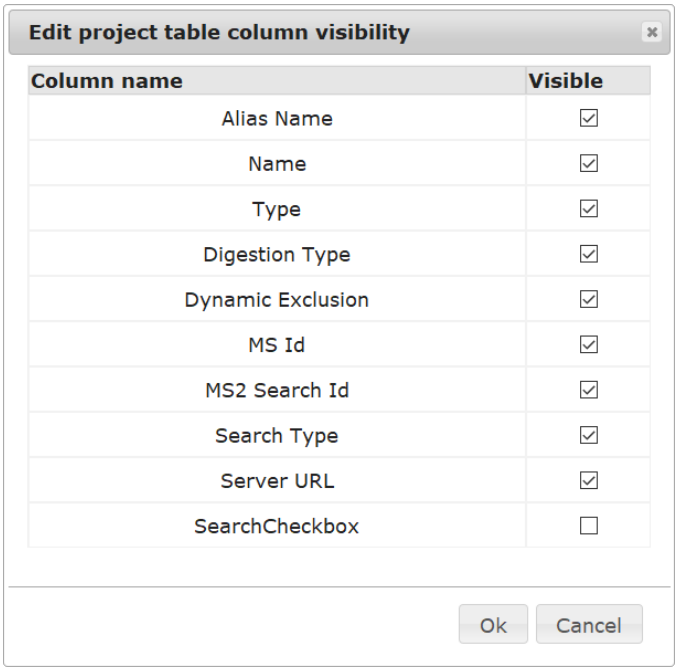


Figure 26: Setting Project table column visibility and order in the Summary tab

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** allow 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:

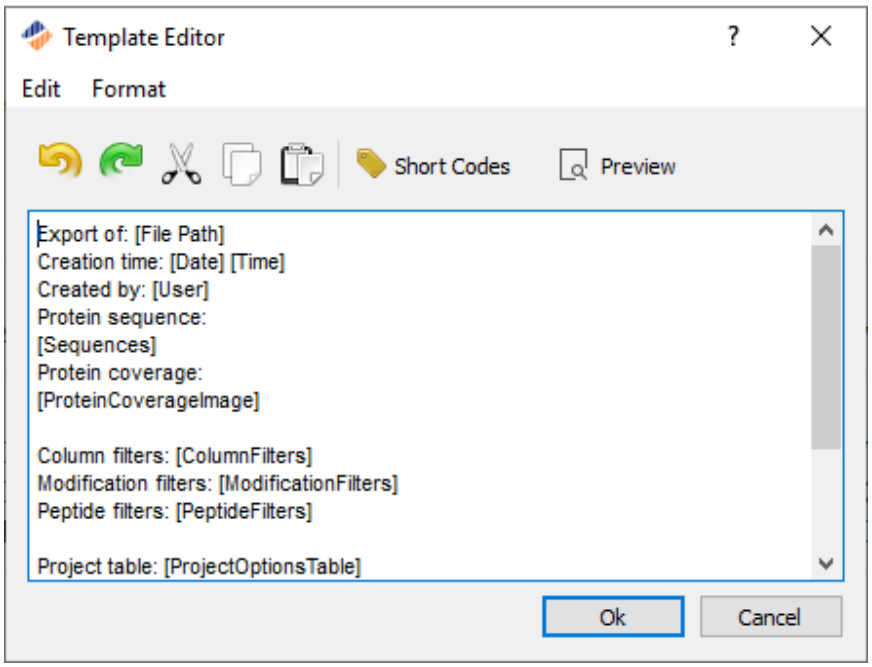


Figure 27: Summary tab template editor

See the Summary Tab Template Editor section for additional details.

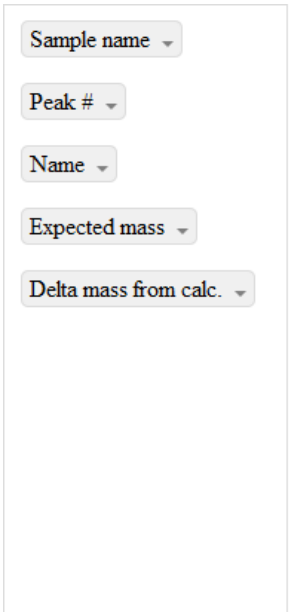
Pivot Tab

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.

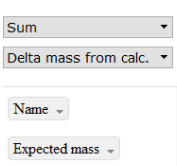
For example, the data in the flat table in Figure 28 displays across 64 rows:



Sample name ↓	Peak # ↑	Name ↓	Expected mass ↑	Delta mass from calc. ↑
ADC 1000ug-ml_2-D,2_01_1185.d	4	ADC_linker , Drug(6)	151150	-3.85755
		ADC_linker , Drug(5)	150191	-3.16754
		ADC_linker , Drug(4)	149227	2.85268
		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 28: Flattened table data

The same data can be reorganized in a much more intelligible structure using a pivot table with just 16 rows, as show in Figure 29:



		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 # ←	1	2	3	4
Name ↓	Expected mass ↑					
ADC_linker , Drug(6)	151150		-5.656011	-3.029556	-2.168420	-3.857550
ADC_linker , Drug(5)	150191		-1.071813	-1.647766	-1.129801	-3.167542
ADC_linker , Drug(4)	149227		6.420644	4.485616	4.504757	2.852682
ADC_linker , Drug(3)	148274		-0.600375	-0.012828	1.830595	-0.653685
ADC_linker , Drug(2)	147316		2.353646	1.420844	1.655275	0.814321
ADC_linker , Drug(1)	146357		2.775643	3.045493	3.821059	0.876487
ADC_linker , Drug(0)	145399		1.843527	4.306960	8.389733	2.683840
ADC , Drug(8)	152835		-2.388330	2.832138	1.282910	-2.575723
ADC , Drug(7)	151877		-3.638739	-2.834629	-2.215001	-3.168253
ADC , Drug(6)	150918		1.376561	-0.239236	0.395879	-1.790259
ADC , Drug(5)	149960		0.335146	0.753834	-0.627207	-1.579847
ADC , Drug(4)	148996		7.586617	6.335042	7.026441	4.496590
ADC , Drug(3)	148043		1.324480	1.237413	1.530265	0.235289
ADC , Drug(2)	147084		2.879652	2.299738	2.770845	0.938870
ADC , Drug(1)	146126		3.820522	3.596316	3.437995	2.876987
ADC , Drug(0)	145167		5.236307	4.782913	4.458601	2.848939

Figure 29: 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

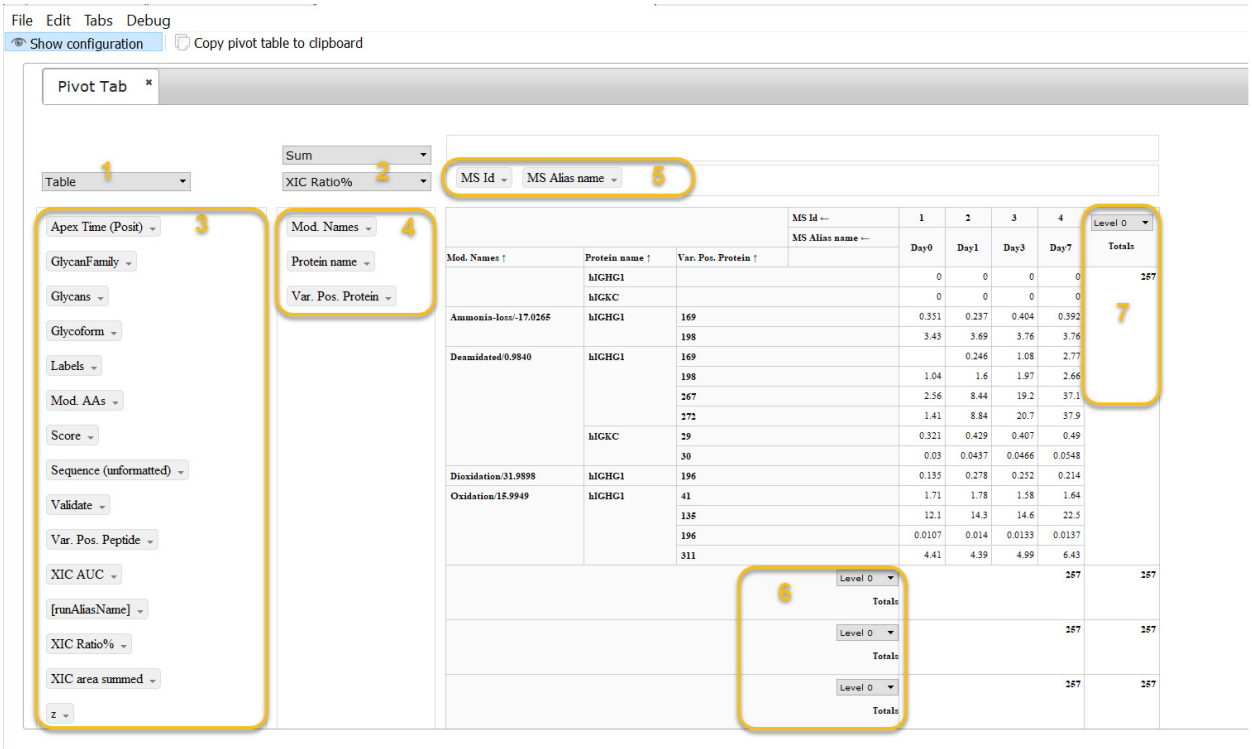


Figure 30: The regions in a Pivot Table

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:

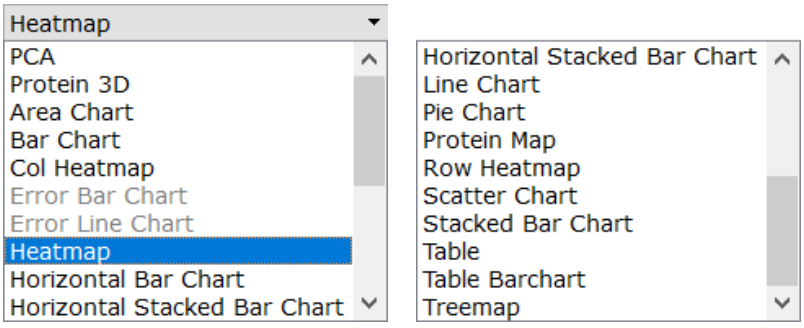


Figure 31: Pivot tab rendering options

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 R squared 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 is 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.

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:

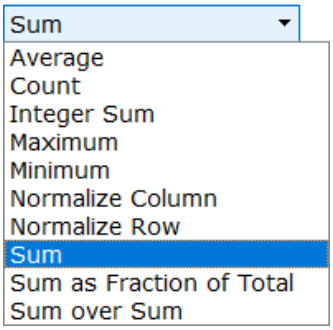
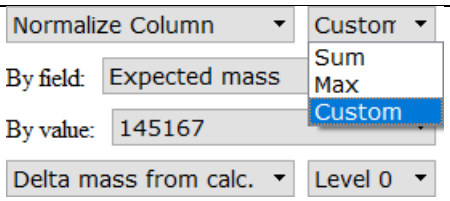
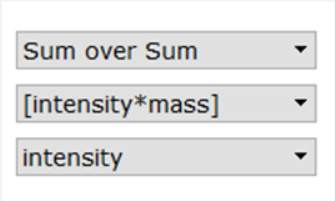


Figure 32: Pivot tab Aggregator options

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	Displays normalized values by column or row.

	 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.
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	For example: Mn = Sum(intensity*mass)/Sum(intensity). 

Field Management

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

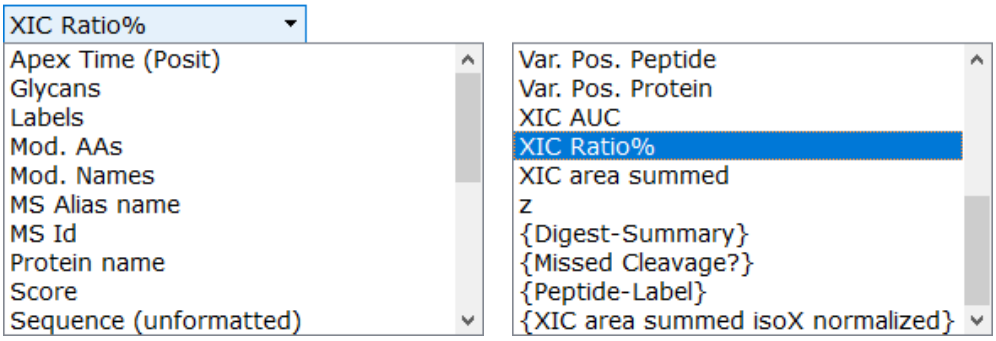


Figure 33: Data field to select for the pivoting

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:

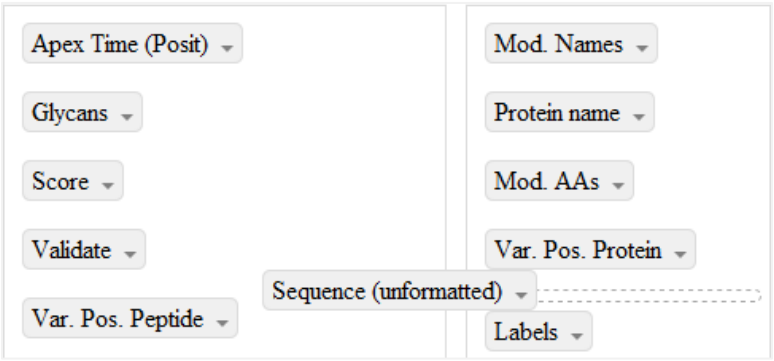


Figure 34: Drag-and-drop new fields into the table

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:

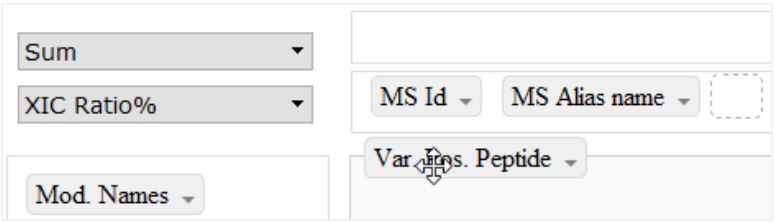


Figure 35: Drag-and-drop new fields into the pivoting

The pivot table editing as in Figure 35 updates to reflect the new layer of pivoting shown in Figure 36:

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 36: Pivoted results after the table edit

Filters

To include or exclude specific data from the report, click the dropdown to the right of the display field name in the second column or in the pivot field name above the table:

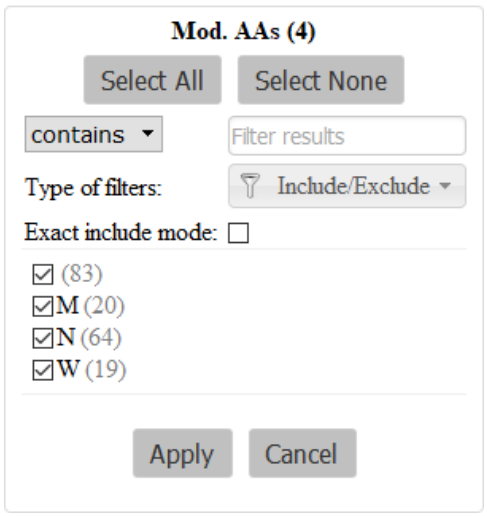


Figure 37: Table Data filters

If the **Type of filters** option is set to **Include/Exclude**, all checked items will be included in the report. All unchecked items will be excluded from the report. Click **Select All** to check all unique values and **Select None** to uncheck all values. If any values are unchecked, the pivot field name will be marked in red with a filter funnel to indicate it has been filtered, as shown in Figure 38 below.

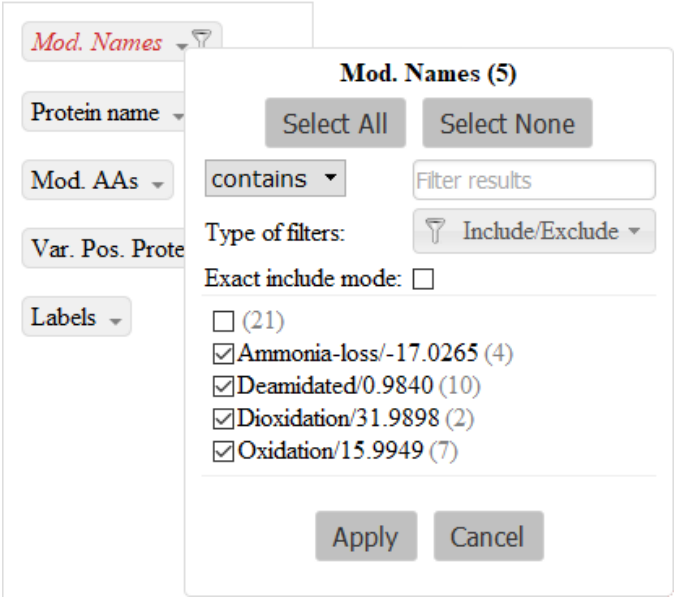


Figure 38: Filtered data is marked in red

For numeric data, the filter applies to the aggregator calculation. Checked items are included in the calculation and unchecked items are excluded from the calculation:

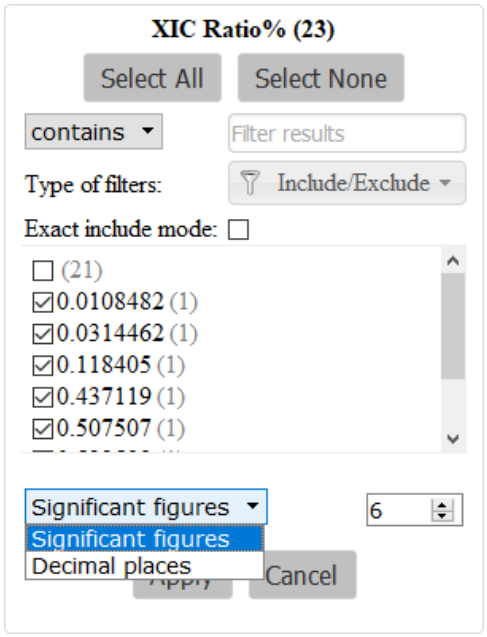


Figure 39: Filtering data from the aggregator calculation

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:

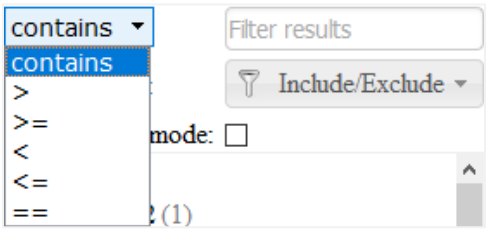


Figure 40: Text filters using operators

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

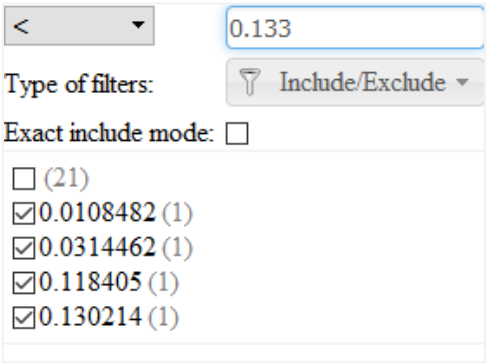


Figure 41: Numeric filters using operators

The user can choose to display or not display a numeric value in the report without changing the aggregator calculation. Set the Type of filters to **Show/Hide**. Checked items will be displayed and unchecked items will be hidden. All values including those unchecked will be used in the aggregator calculation:

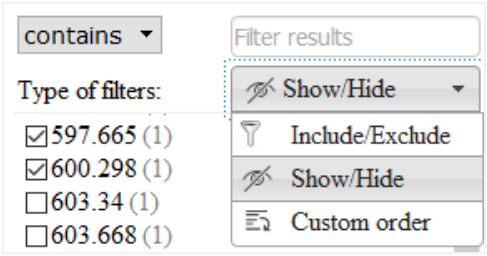


Figure 42: Show and Hide data

If the Show/Hide setting includes unchecked items, the pivot field name will be marked in red with a filter eye icon to indicate it has been filtered:



The user can only Show or Hide values that are included in the pivot tab. A value that is excluded from the report will be disabled from selection

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:

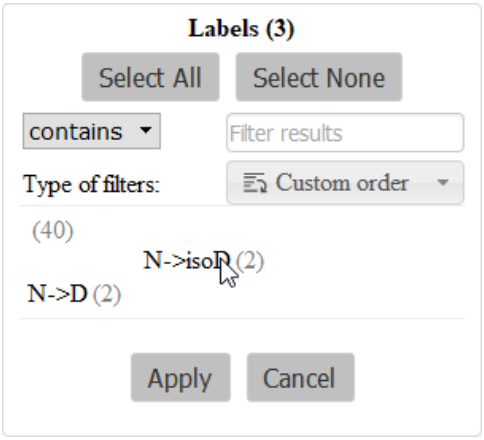
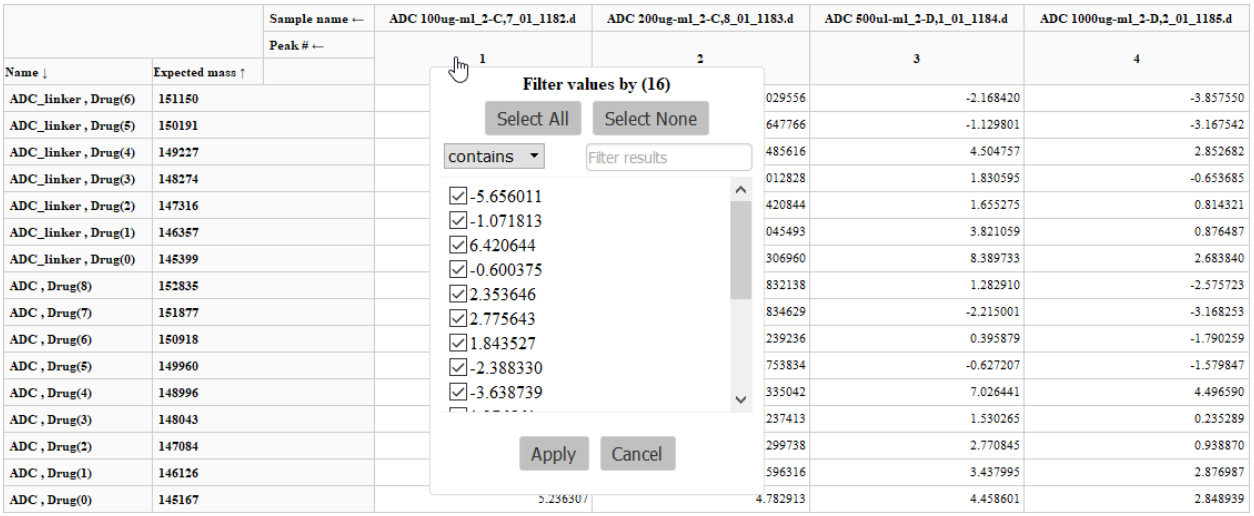


Figure 43: Reordering labels by drag-and-drop

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 # ←	1	2	3	4
Name ↓	Expected mass ↑					
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 44: 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 ↑		
Oxidation/15.9949	hIGHG1	M	135		98.3
			311		262
		W	41		135
			196		117
Dioxidation/31.9898	hIGHG1	W	196		234
Deamidated/0.9840	hIGHG1	N	198		351
			267		270
			272		180
	hIGKC	N	29		115
			30		115
Ammonia-loss/-17.0265	hIGHG1	N	169		160
			198		234

Figure 45: 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:

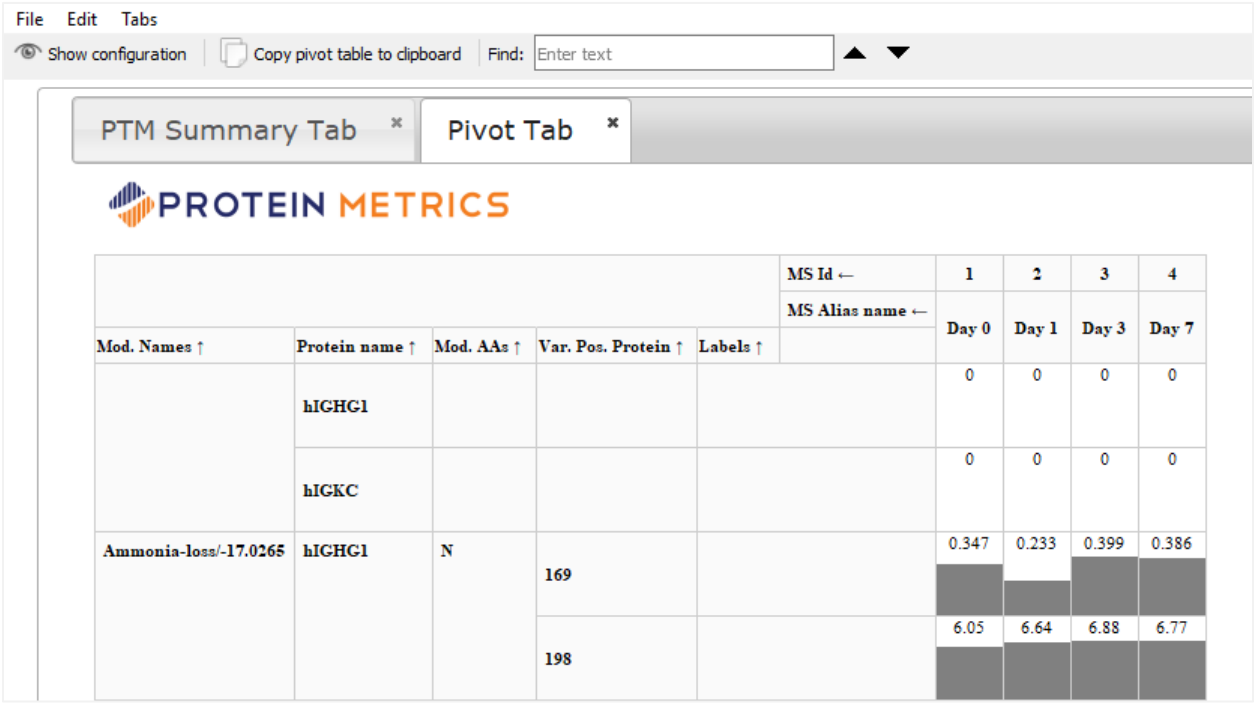


Figure 46: Hide Configuration mode

Pivot Tab Current Tab Settings: Common

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

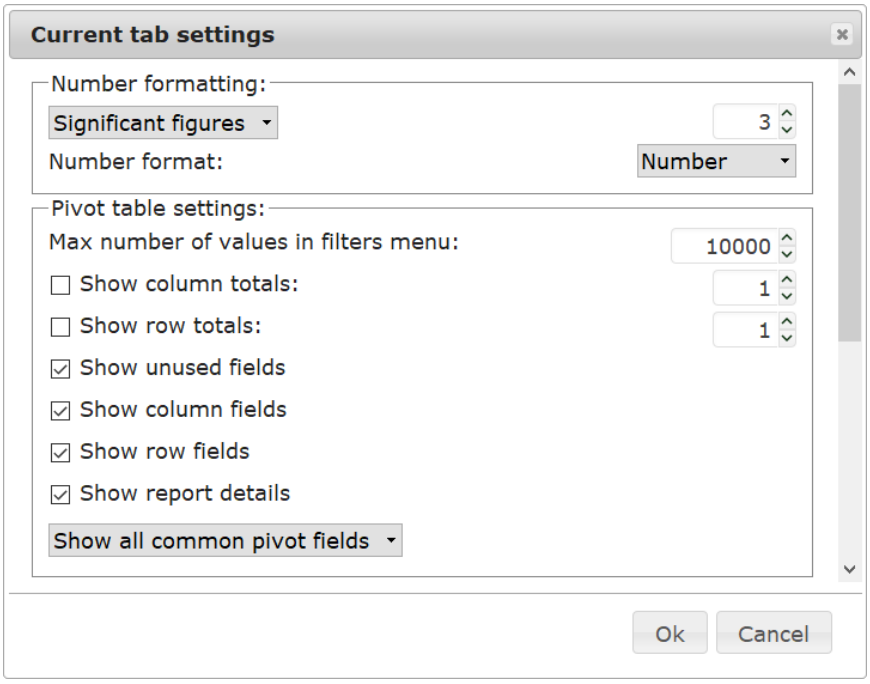


Figure 47: Pivot options in Current tab settings

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 Figure 48 and Figure 49.
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.ccnson (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.
Show report details	Displays a legend under the pivot table with configuration settings when Show configuration is turned off.

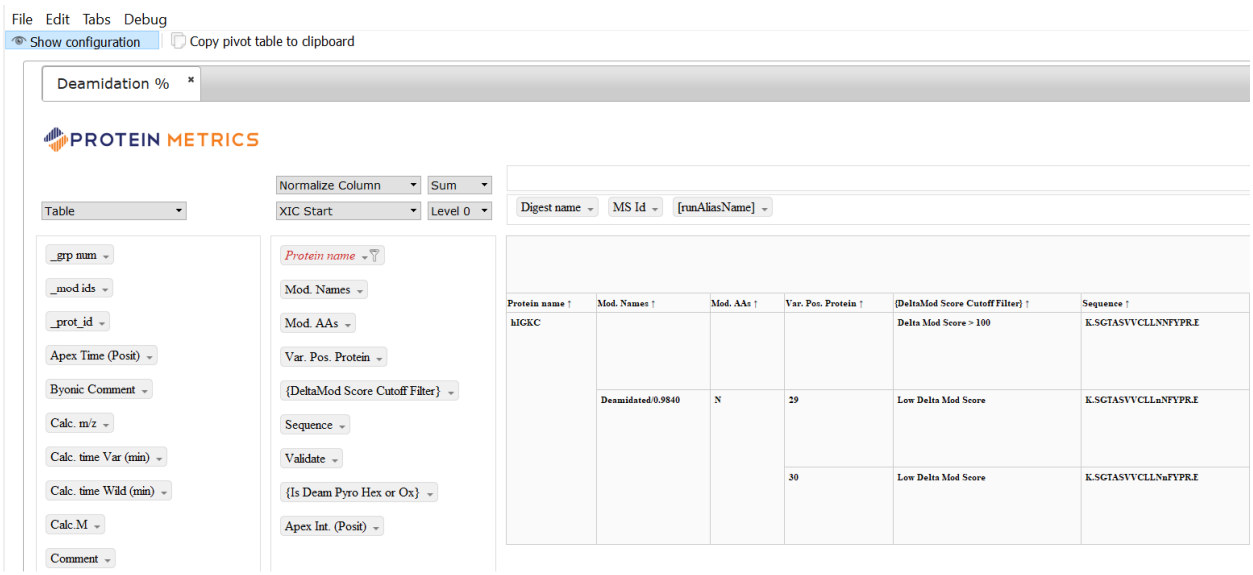


Figure 48: Hide configuration with Show report details unchecked

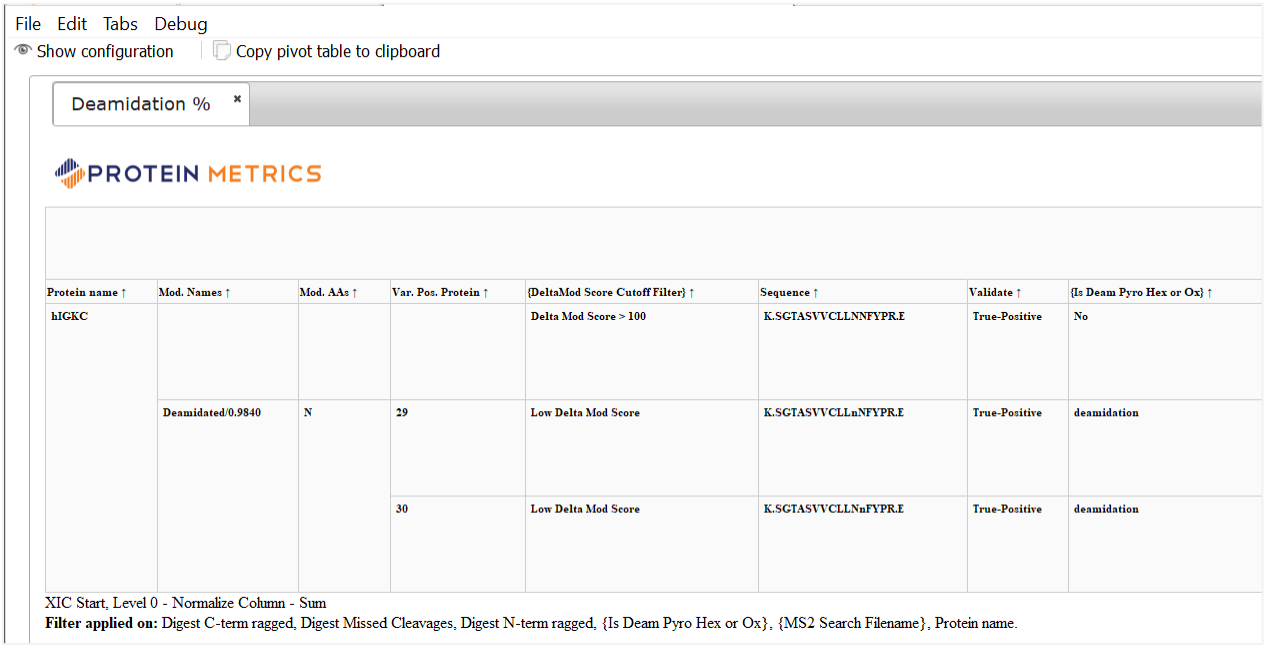


Figure 49: Same pivot table with Show configuration turned off and with Show report details checked.

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

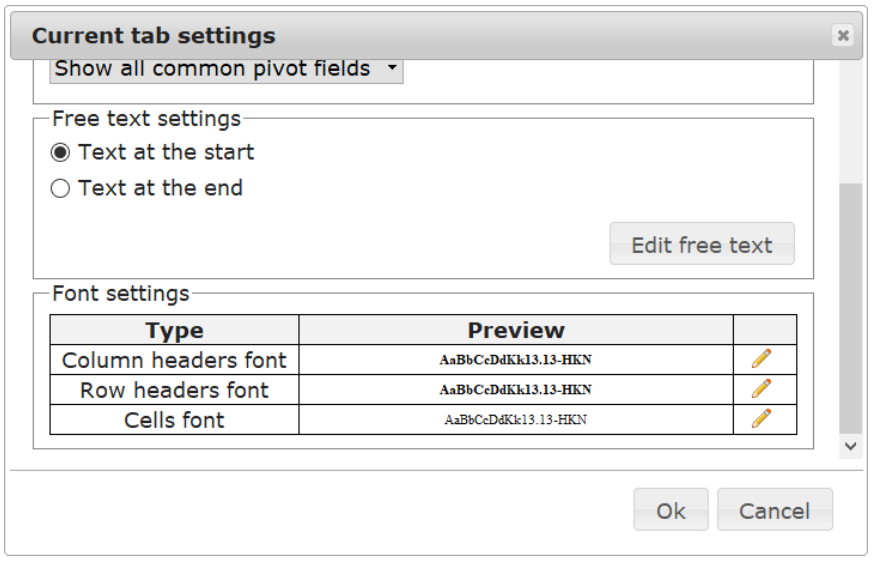


Figure 50: Text editing in Current tab settings

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**.

To edit the fonts of the column or row headers, or the entries in the tables, click after the usage type. The **Edit <type> font** dialog opens:

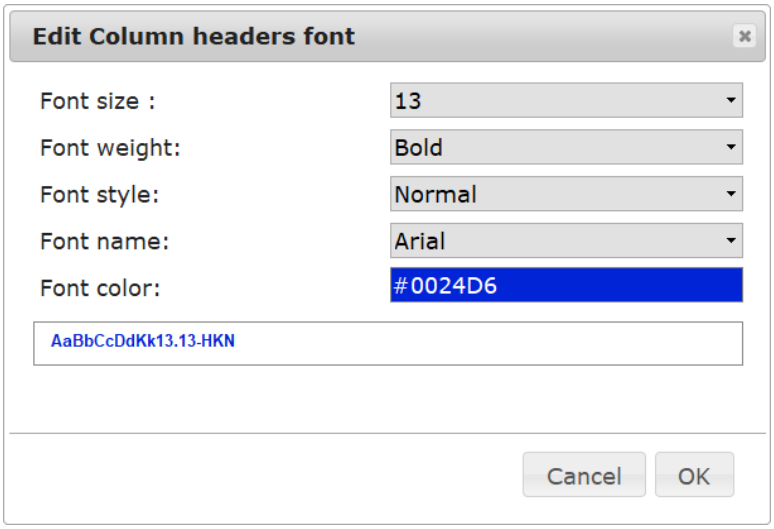


Figure 51: Edit Pivot tab fonts

Adjust the size, weight (Normal or Bold), style (Normal or Italic), name and color of the font and click **OK**.

Pivot Tab Current Tab Settings: Chart specific

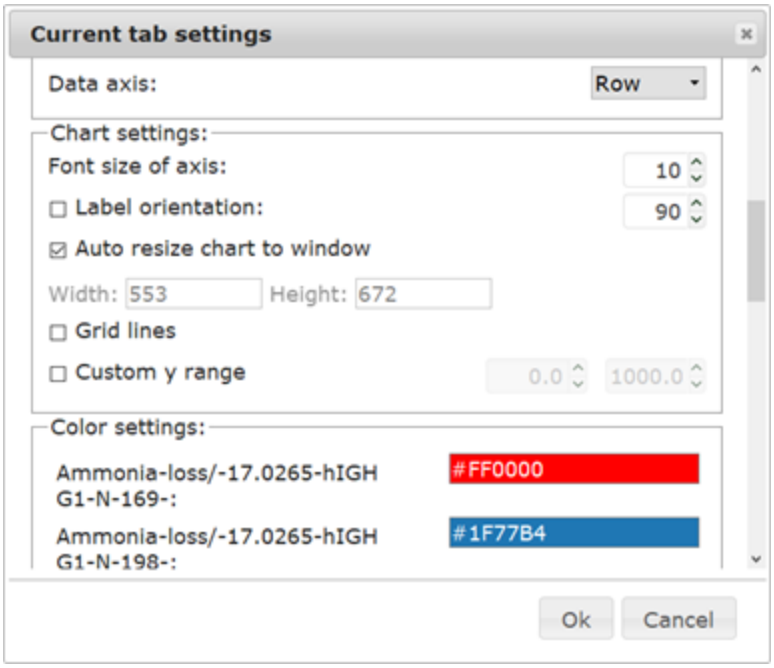
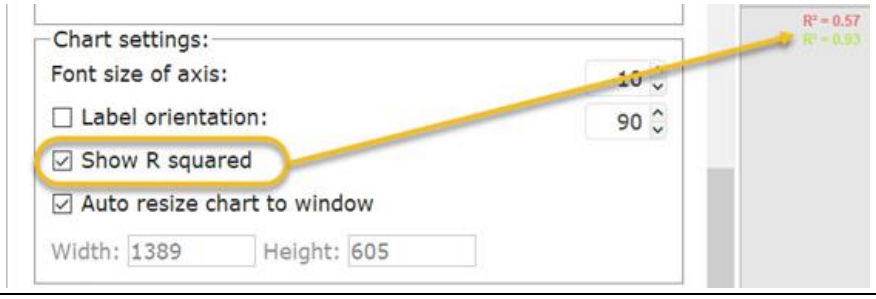
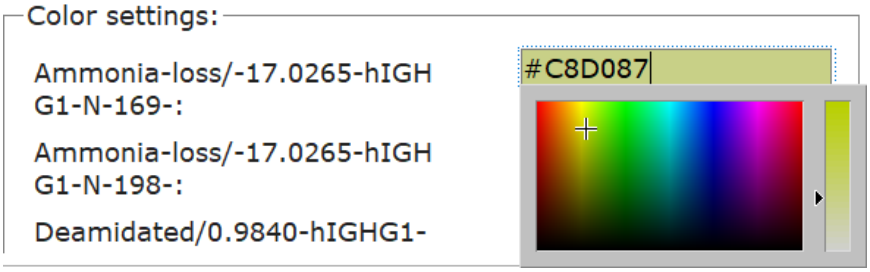
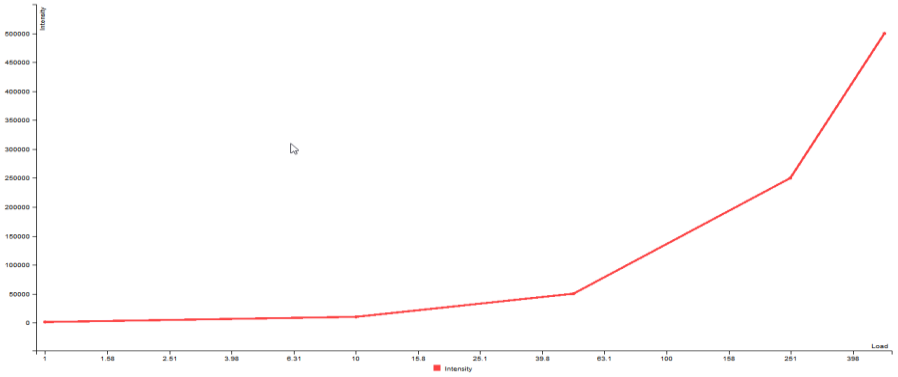


Figure 52: Pivot chart options in Current tab settings

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 squared (Line Chart only)	When checked, R^2 value is displayed on the top right of the chart. 
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.

Color settings	
Color	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. 
Axis settings	
Numeric X-axis	(Except Pie chart and Table Barchart) - When checked, displays numeric labels on the X-axis
Connect the dots	(Scatter charts only) - When checked, connects the plotted points with line segments 
X-, Y-axis Log scale	(Line charts and Scatter charts only) - When checked, displays and labels that axis data with a logarithmic scale

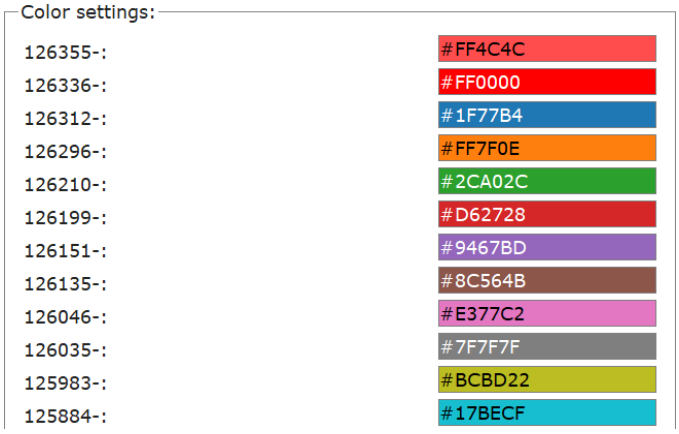


Figure 53: Default colors from a high-contrast palette

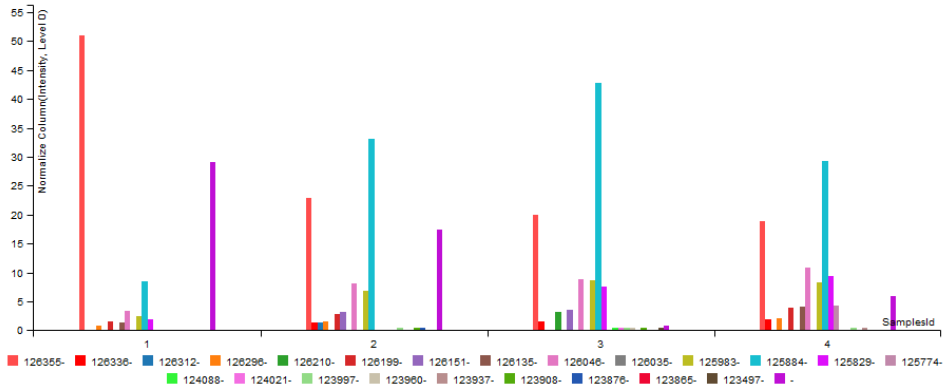


Figure 54: Horizontal bar chart with high-contrast color palette

Pivot Tab Heatmap

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



Figure 55: Color by settings for heatmap views

The Current tab settings dialog for heatmaps contains color settings:

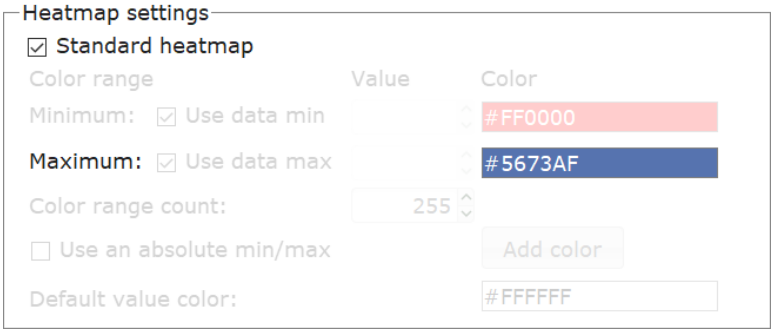


Figure 56: Standard color setting for heatmaps

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:

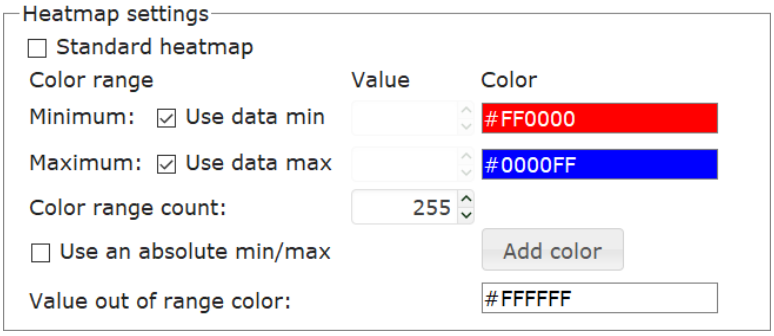


Figure 57: Advanced heatmap color settings

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:

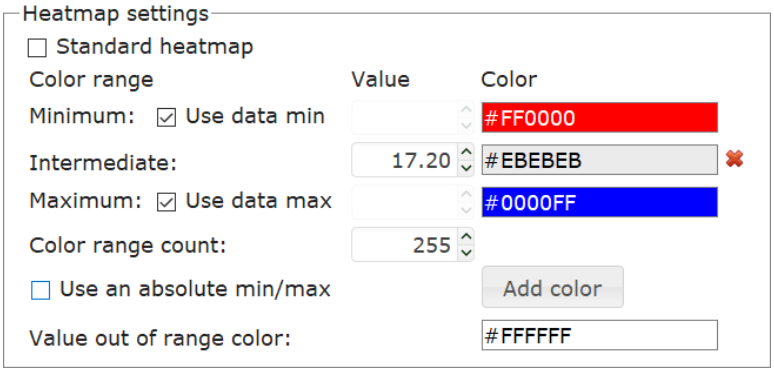


Figure 58: Heatmap color settings with an intermediate color

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:

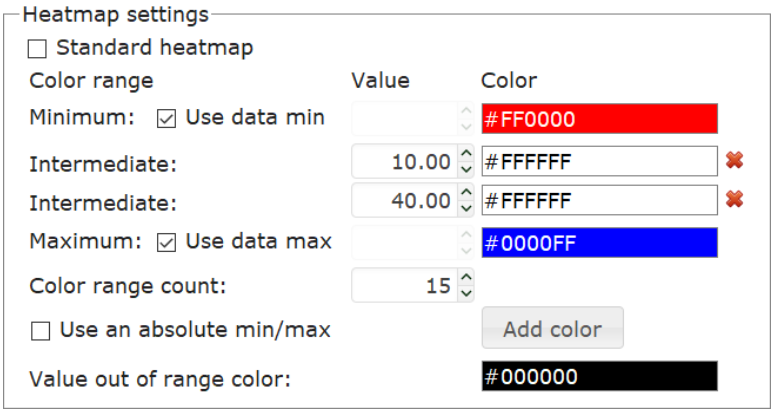


Figure 59: Heatmap with a range of data marked in white

This setting results in following heatmap:

		ExchangeTime ←	60			
		Condition ←	Apo	Avg (H3 - Apo)	H3	H3 - Apo
End AA ↑	Sequence ↑					
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 60: The heatmap resulting from the settings in Figure 59

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

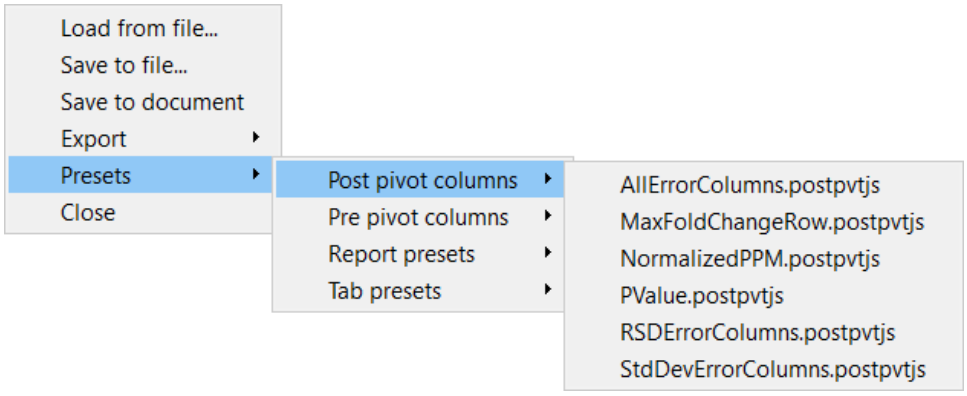


Figure 61: Creating columns for error charts

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:

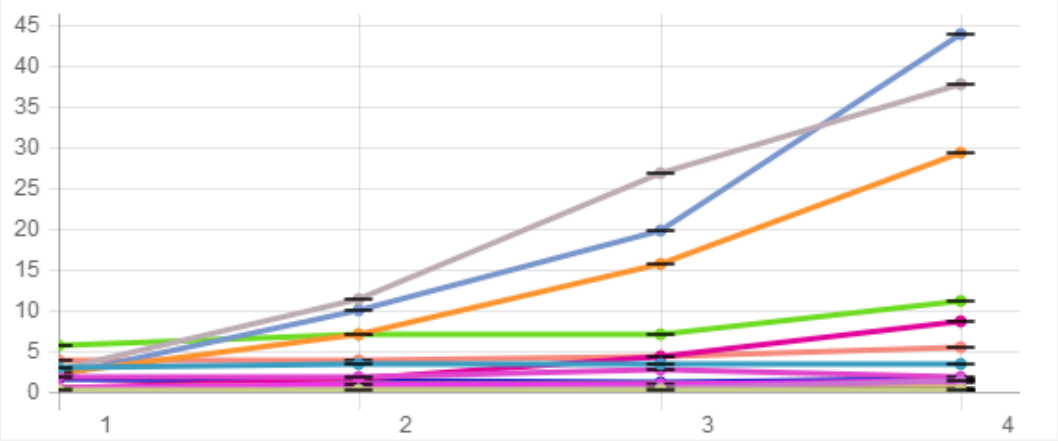


Figure 62: Formatted error line chart

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



Figure 63: 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.

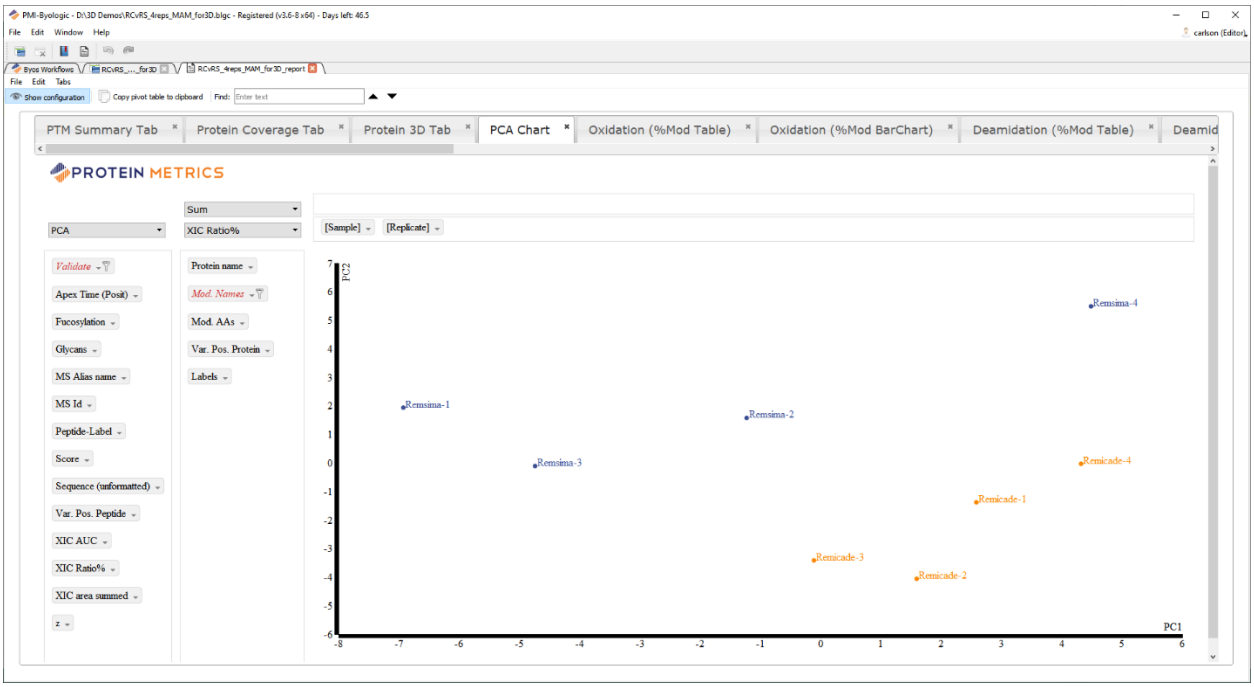


Figure 64: PCA plot

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

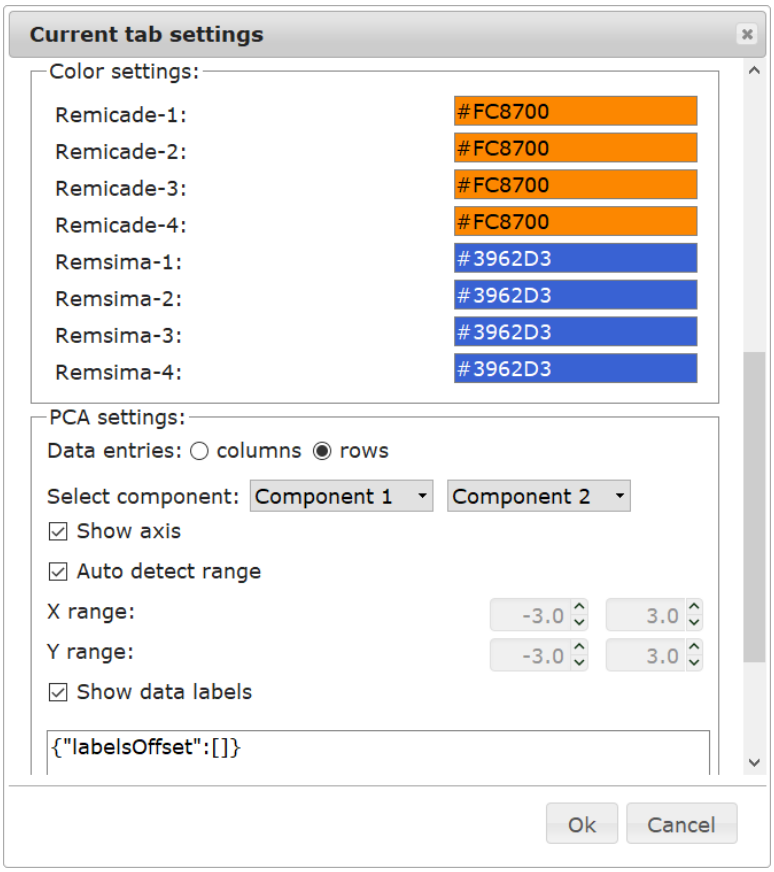


Figure 65: PCA options in Current tab settings

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	Label offset can be used to avoid label collision. Syntax: {“data label”:[x-offset, y-offset]} For example: {“labelsOffset”:[{“-Trioxidation/47.9847”:[-150,0]},

	{“-Dioxidation/31.9898”:[0,15]}]} Note that the X and Y offset are from the label’s original location of [0, 0]. Exact label name needs to be used.

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:

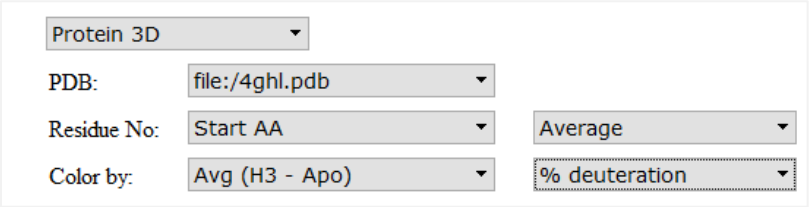


Figure 66: Protein 3D settings

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

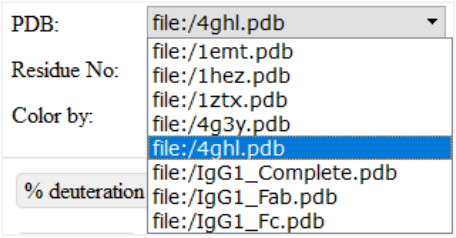


Figure 67: Setting the PDB file

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:

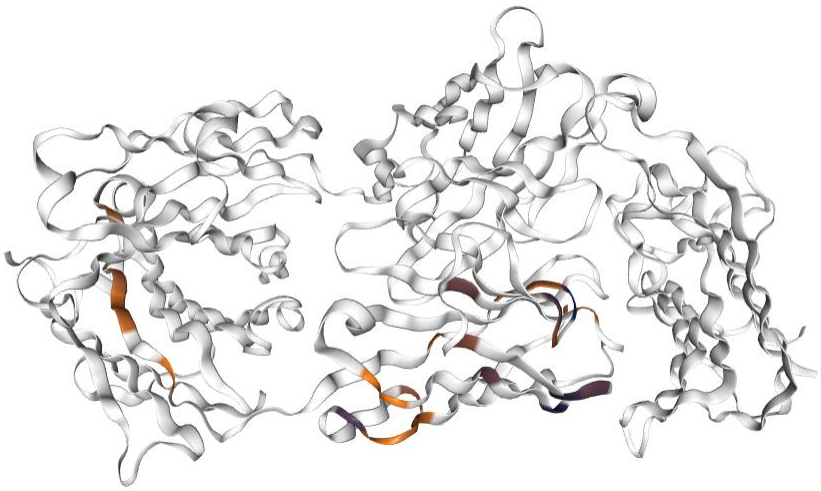


Figure 68: 3D depiction of a protein

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.

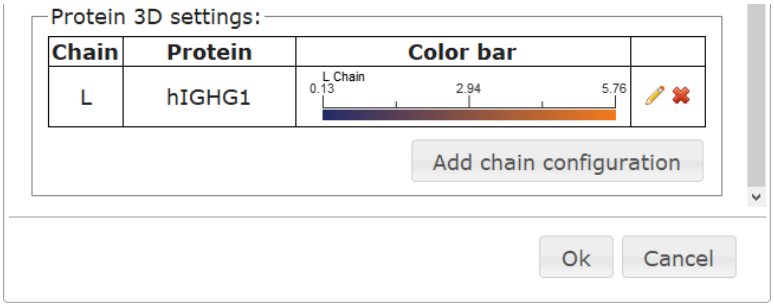


Figure 69: Protein 3D chain configuration

2. At the bottom, click **Add chain configuration**:

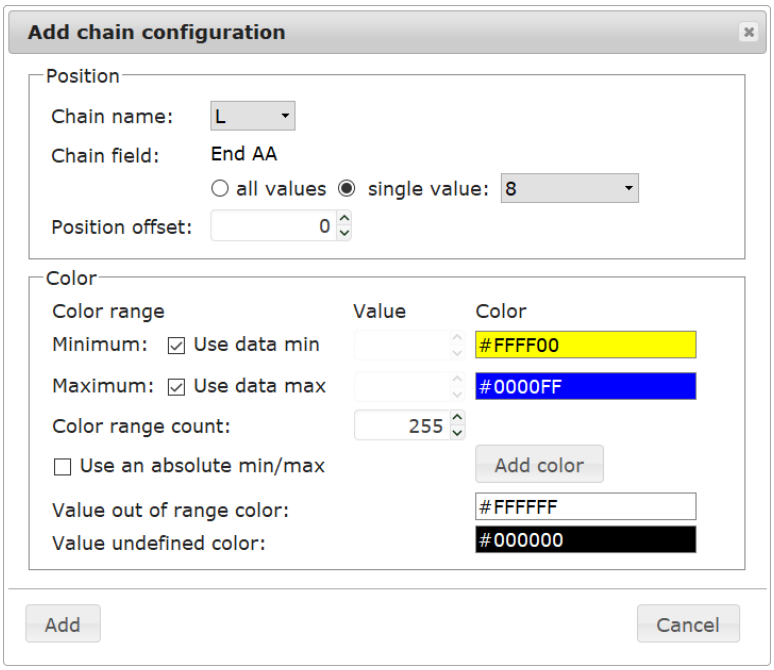


Figure 70: Add chain configuration dialog

3. Use the drop-down arrow to select the **Chain name**.
4. 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.
5. 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.
6. 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.
7. 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**.
8. 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:

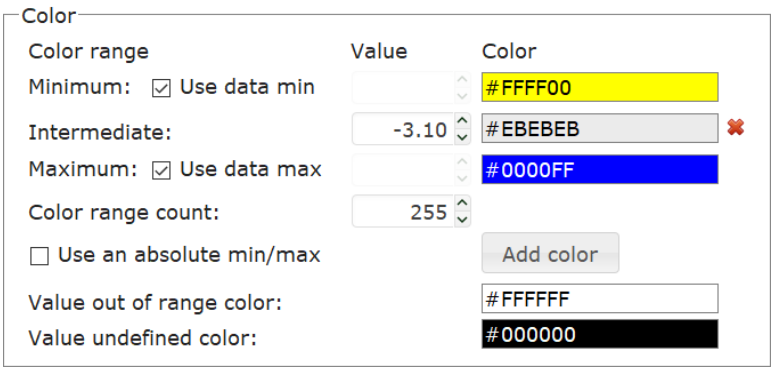


Figure 71: An intermediate color added to the color range

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:

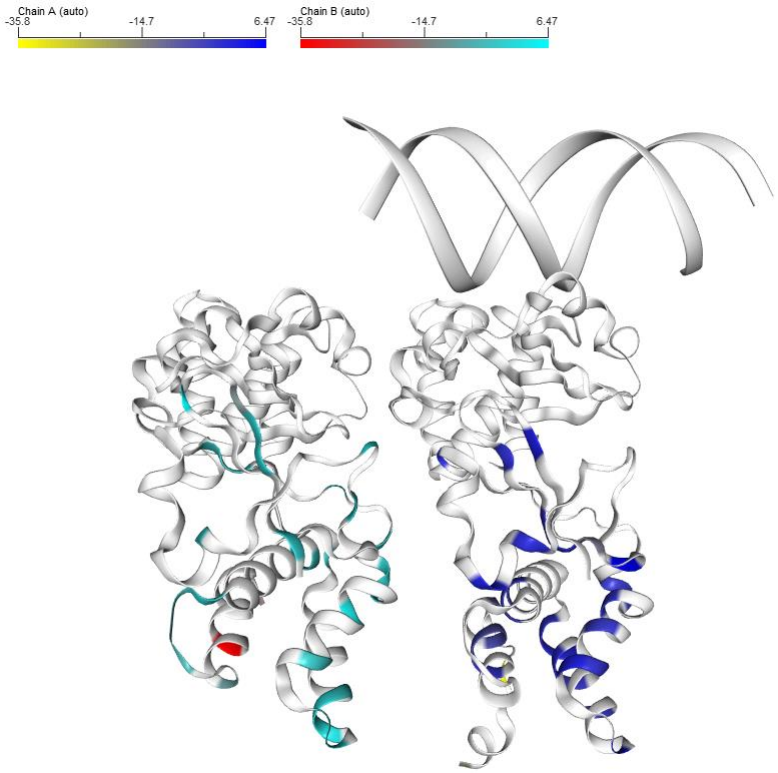


Figure 72: 3D Protein colored by chain

11. 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:

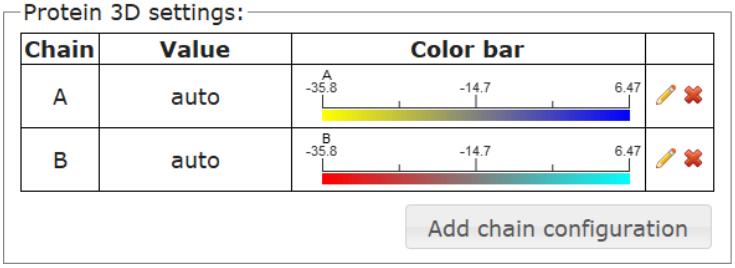


Figure 73: Chain color bar settings

Pivot Tab Protein Map

Protein Maps are found in the Blgc_HDX.rptc report template used by the **HDX** workflow:

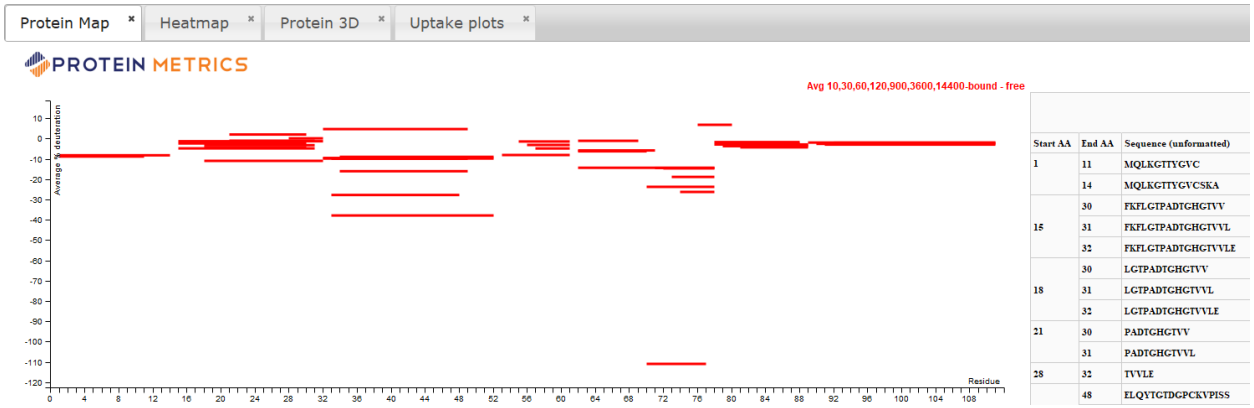


Figure 74: Protein map

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).

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:

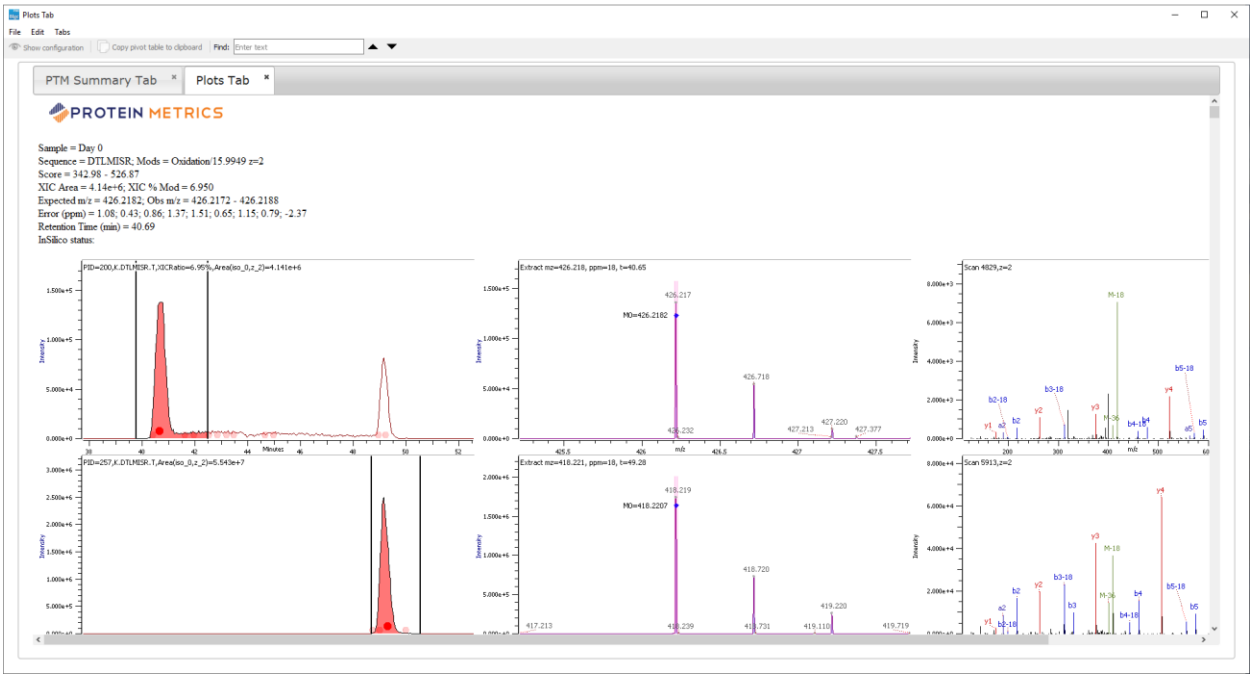


Figure 75: Example Plots tab

Note that the **Show Configuration** button is disabled. To configure the tab, select **Edit > Current tab settings**:

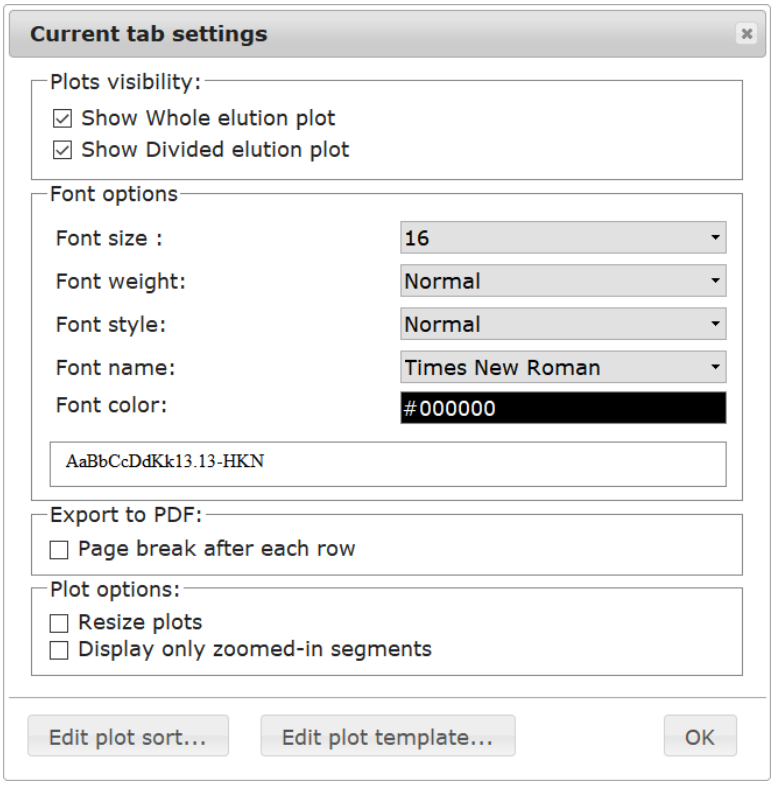
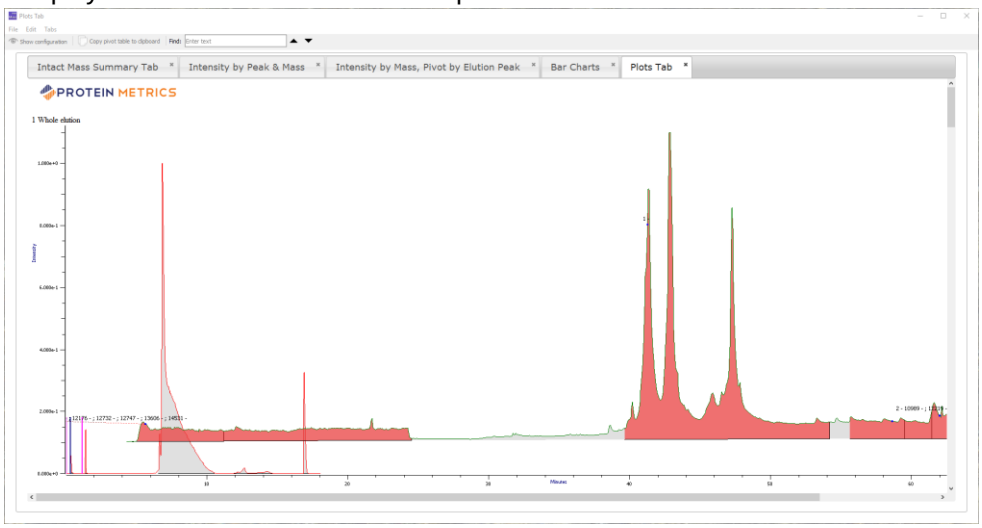
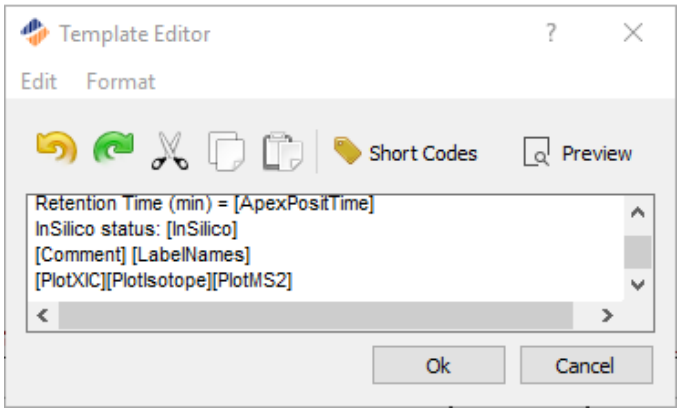
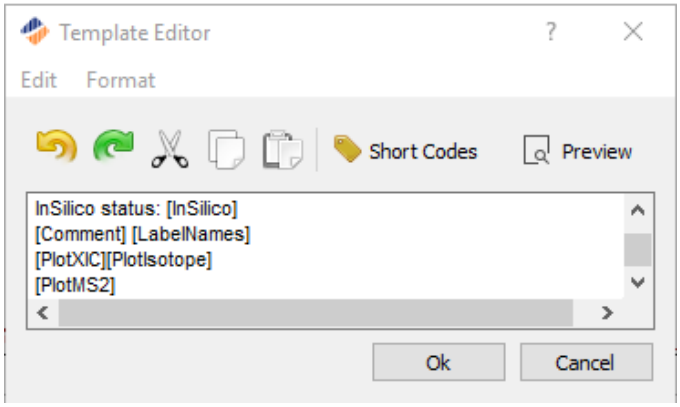
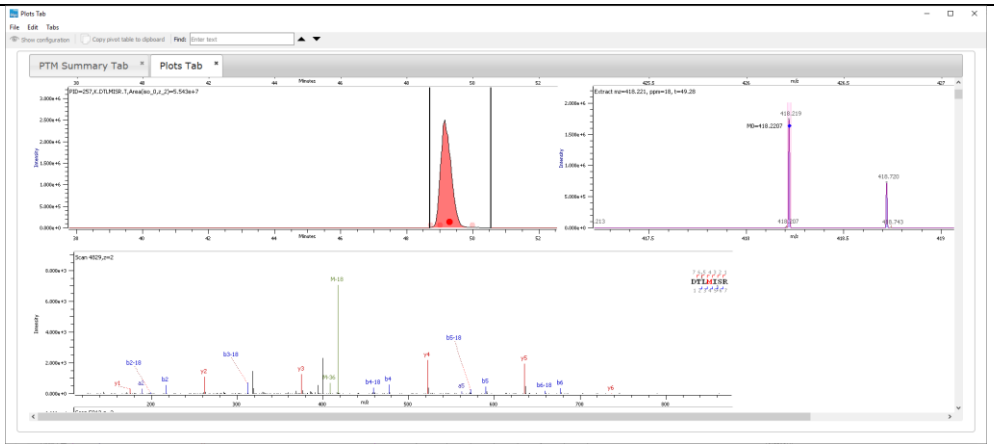


Figure 76: Plots tab Current tab settings

Setting	Description
Plots visibility	
Show Whole elution plot	Displays the entire elution as the first plot: 
Show Divided elution 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.

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	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:  The string [PlotXIC][PlotIsopte][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:  This produces the layout:

	 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.
Display only zoomed-in segments	Displays zoomed-in segments of the project. When unchecked, entire plots are displayed.

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.

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

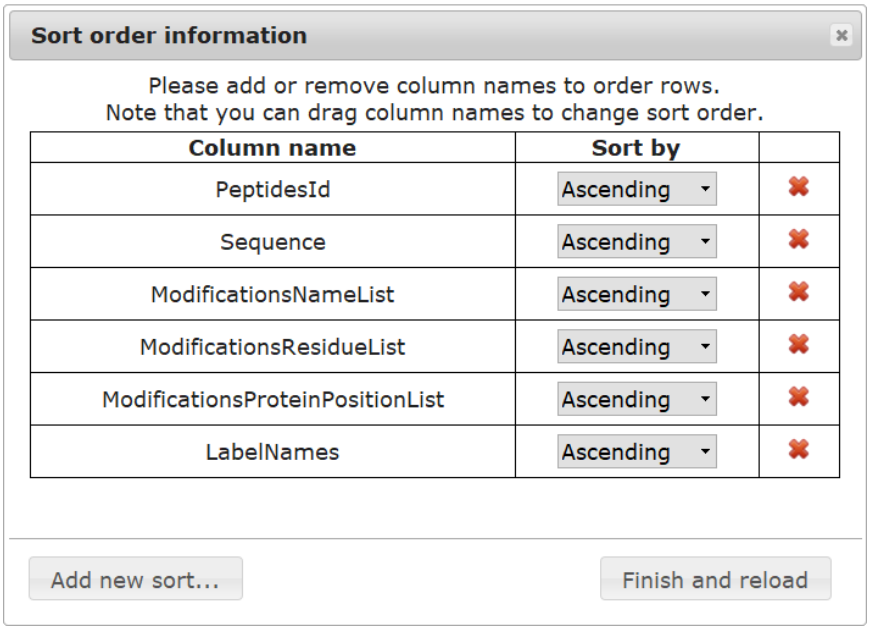


Figure 77: Plot sorting

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:

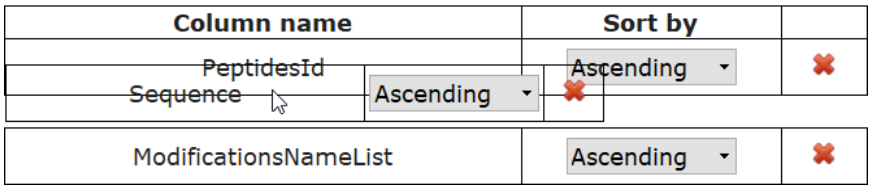


Figure 78: Adjust sorting by drag-and-drop

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

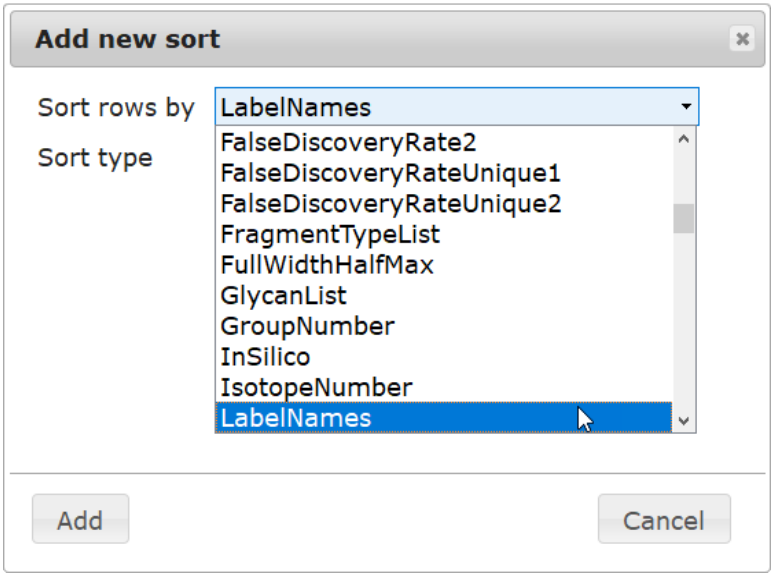


Figure 79: Add new sort type

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.

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:

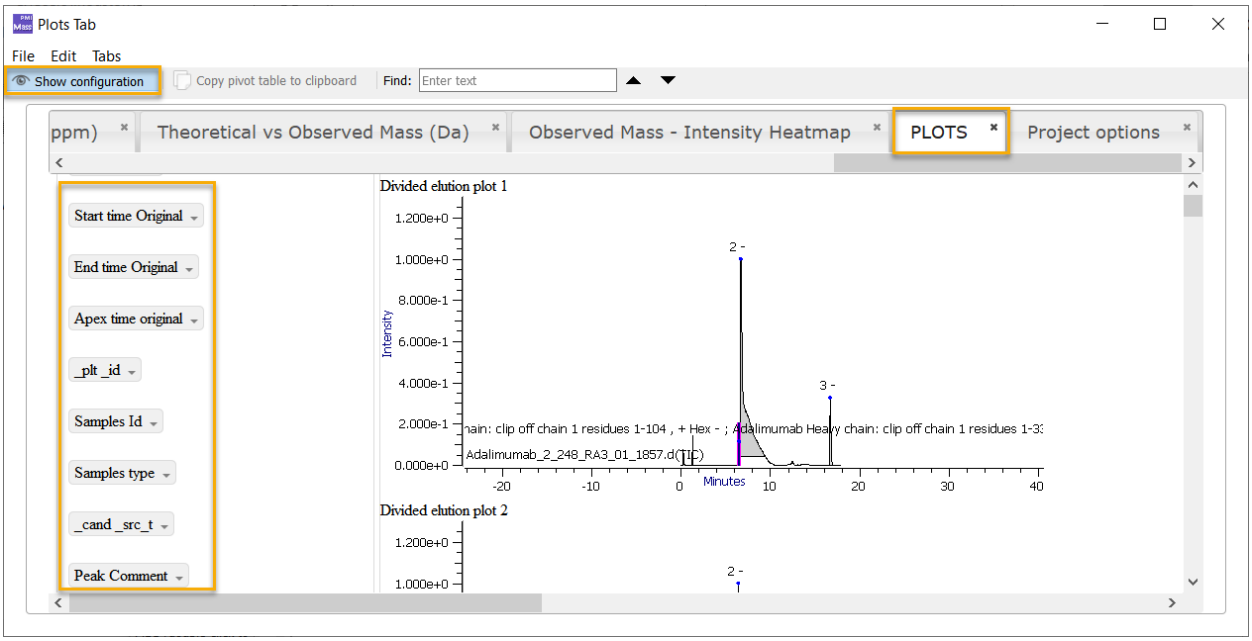


Figure 80: Show configuration for Plots tab to filter the plots by field values

In the Plots Tab **Current tab settings** dialog, the **Edit plot template** button opens the **Template Editor Dialog**:

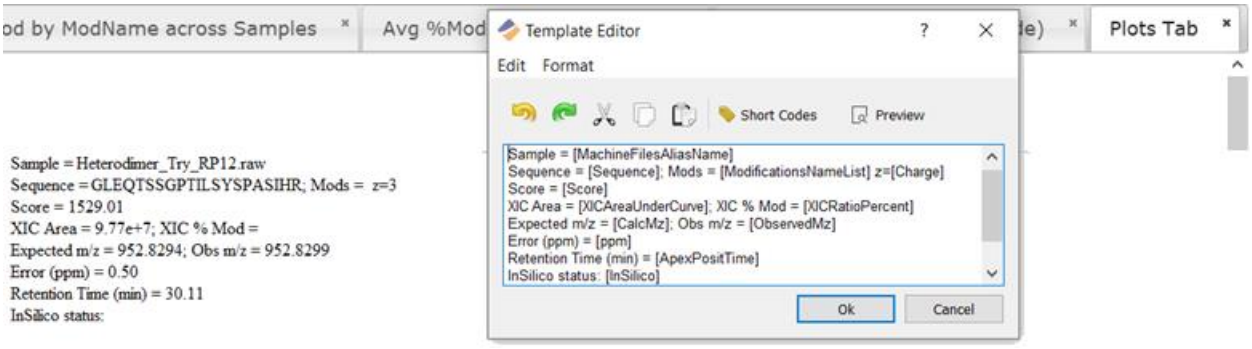


Figure 81: Plot data labels for Peptide Analysis projects

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:

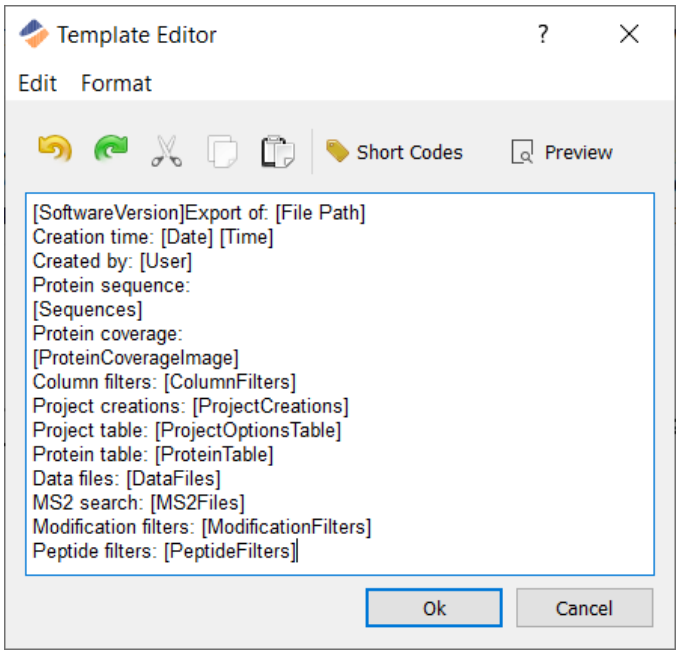


Figure 82: Summary tab Template Editor

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
[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]	Protein Coverage image from the application. Fragment coverage is based on application settings.
[SoftwareVersion]	Version of the Protein Metrics Inc. application
Peptide Analysis Only	
[MS2Files]	Imported MS2 (*.byrslt) 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:

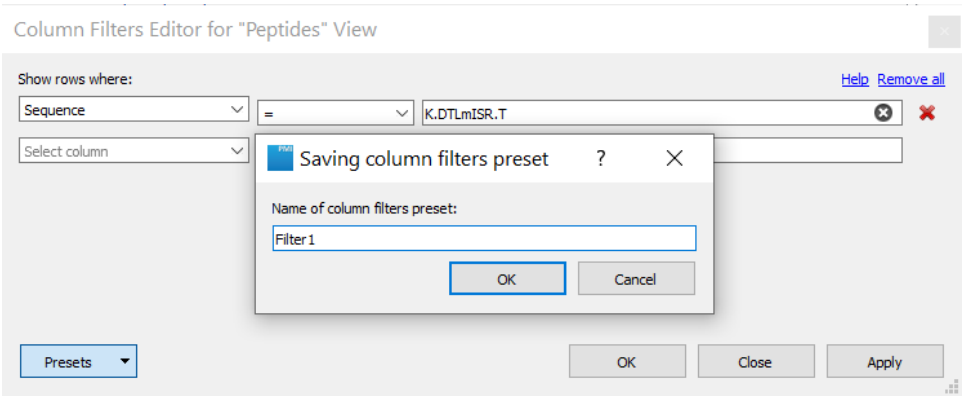


Figure 83: Saving a Protein Coverage filter in the Peptides table

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 **ProteinCoverageImage**. Click **Insert** and click **OK** to add the filtered Protein Coverage:

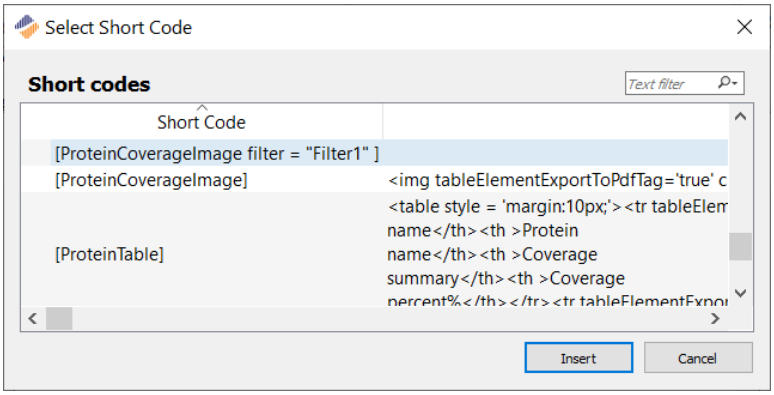


Figure 84: The Short Code generated for the saved Protein Coverage filter

Summary Tab and Plot Tab Short Codes

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

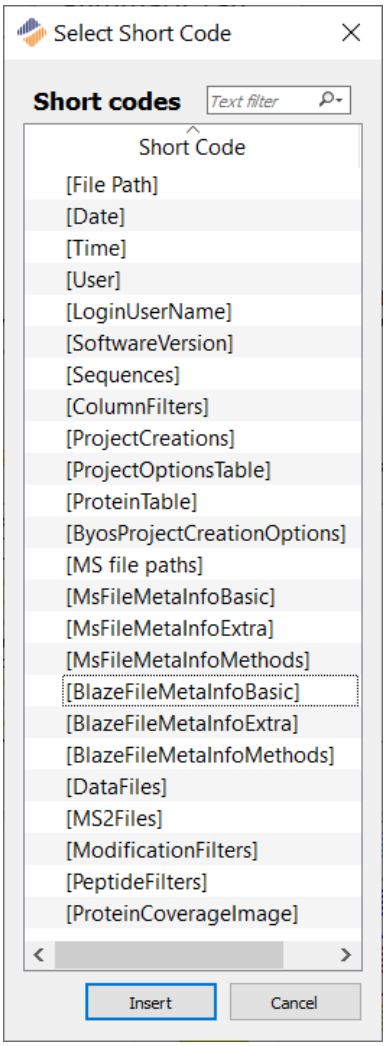


Figure 85: Peptide Analysis Short Codes

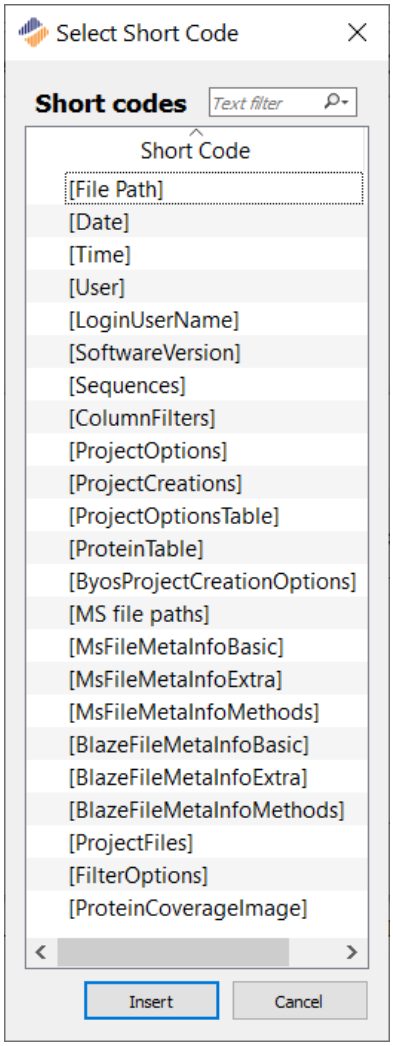


Figure 86: Chromatogram Analysis Short Codes

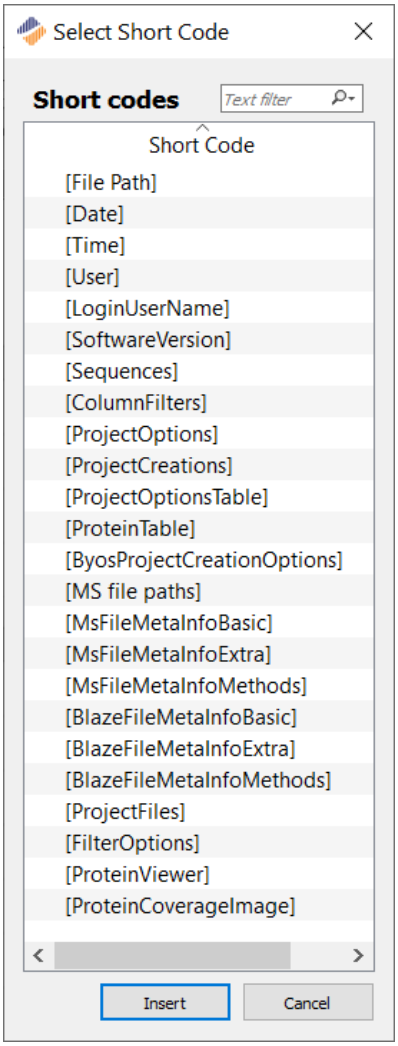


Figure 87: Intact Analysis Short Codes

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:

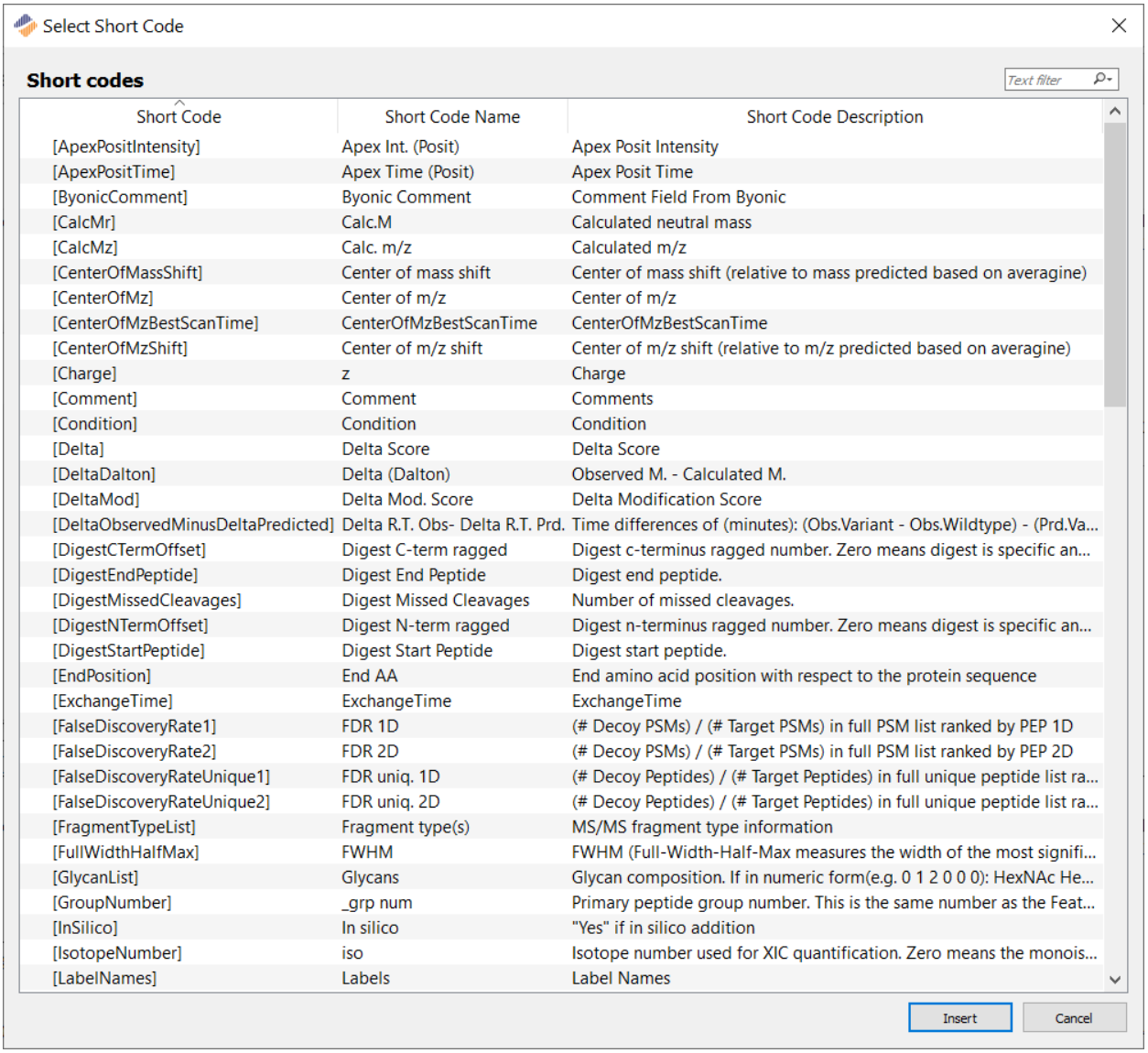


Figure 88: Peptide Analysis Plots tab Short Codes, part 1

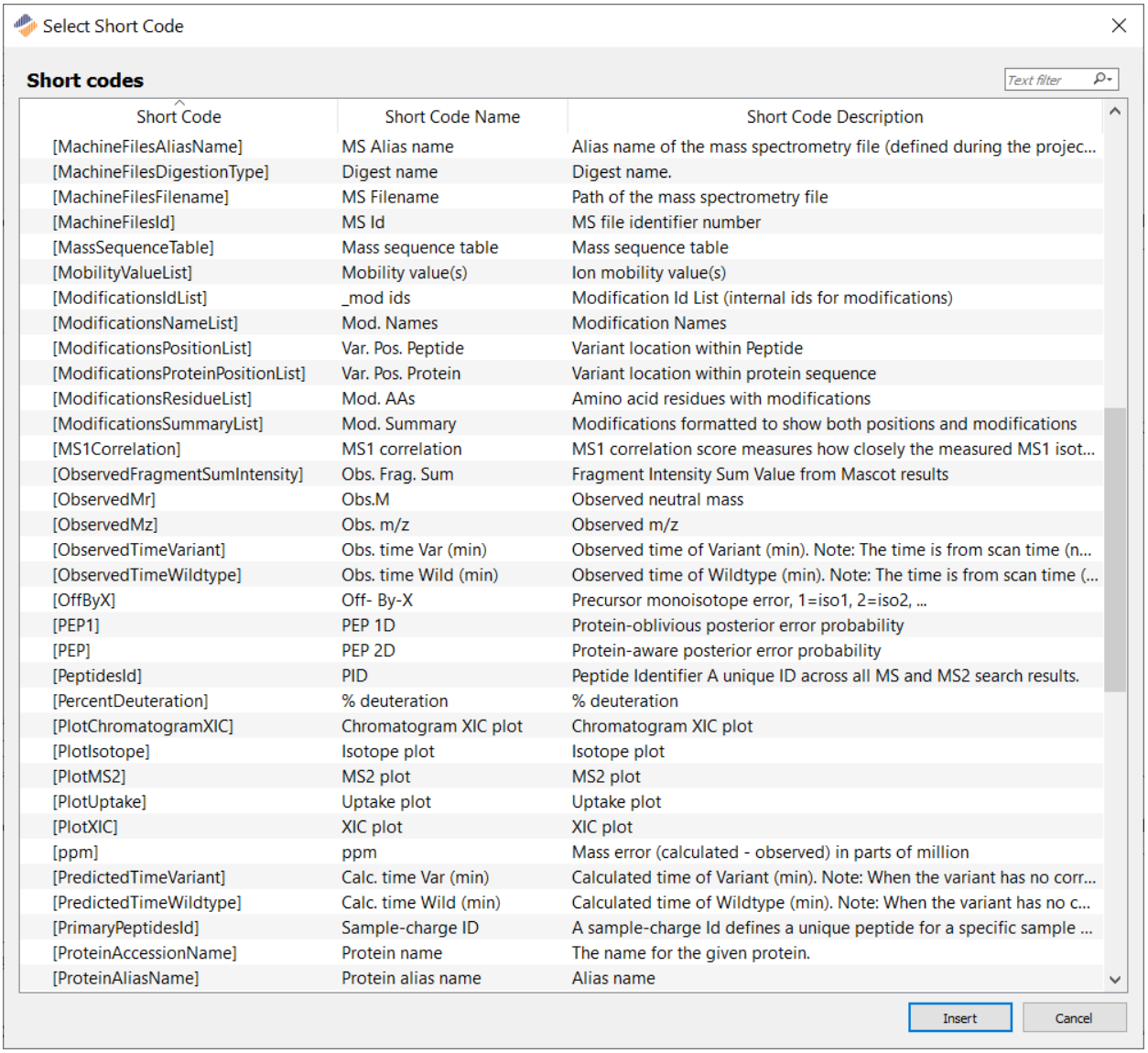


Figure 89: Peptide Analysis Plots tab Short Codes, part 2

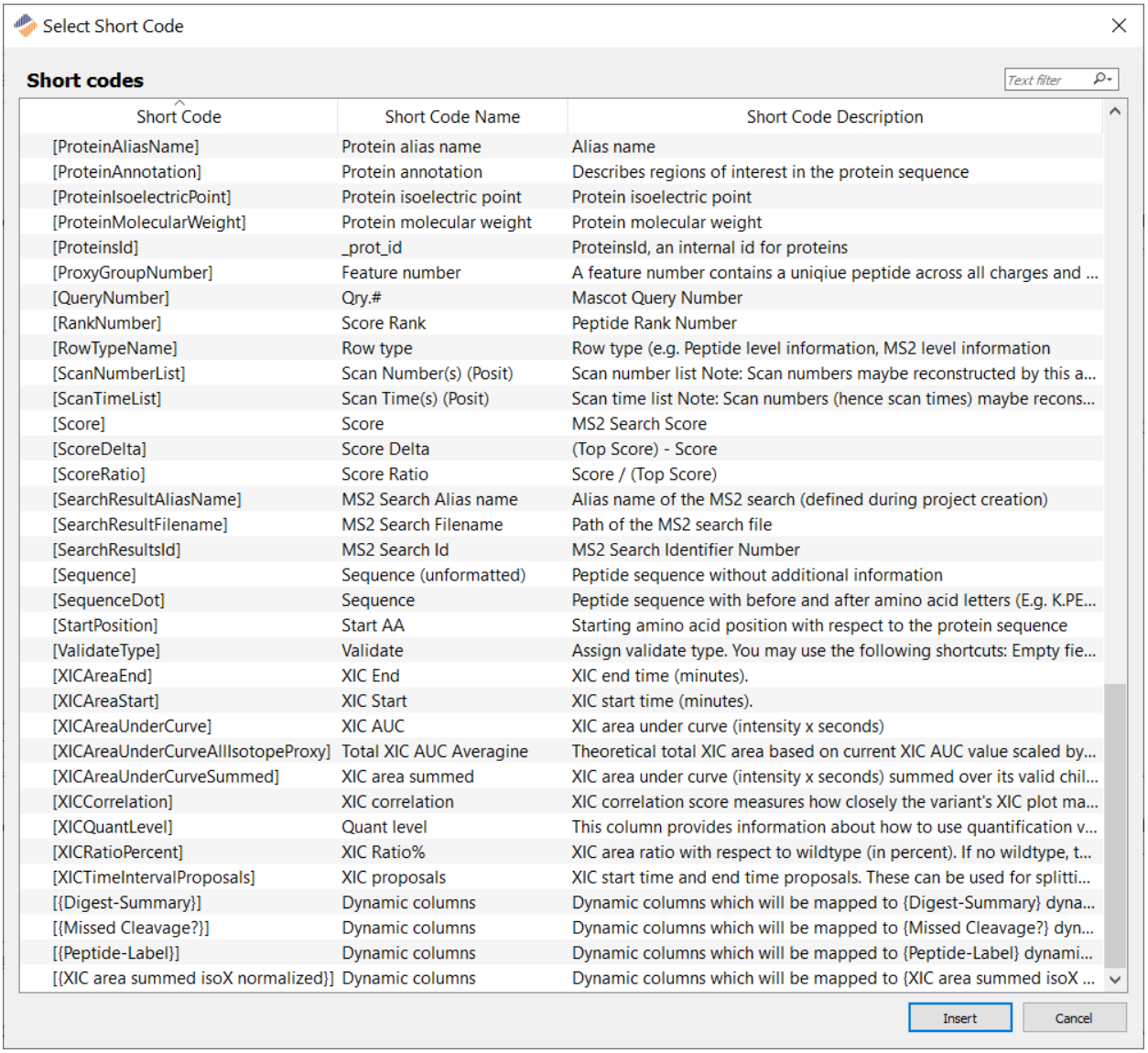


Figure 90: Peptide Analysis Plots tab Short Codes, part 3

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

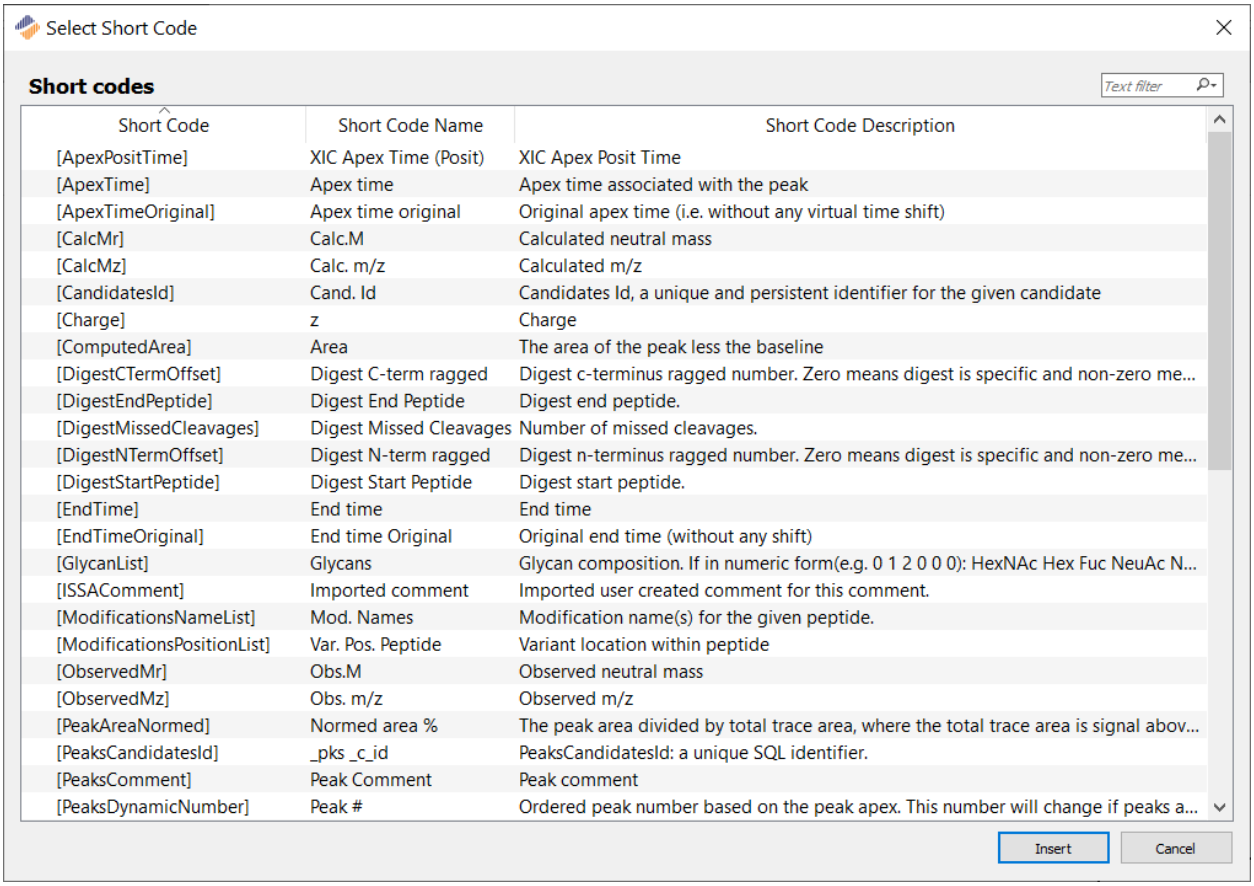


Figure 91: Chromatogram Analysis Plots tab Short Codes, part 1

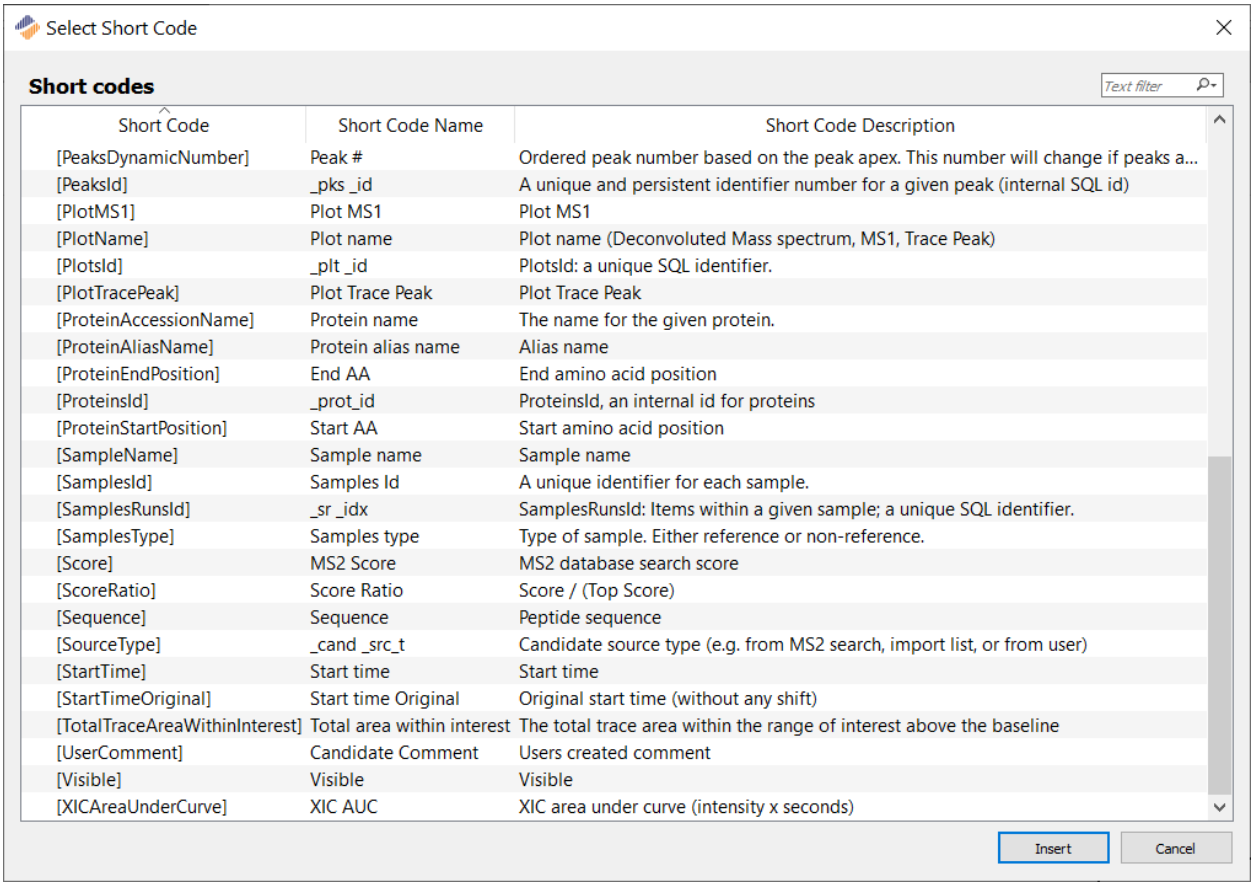


Figure 92: Chromatogram Analysis Plots tab Short Codes, part 2

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

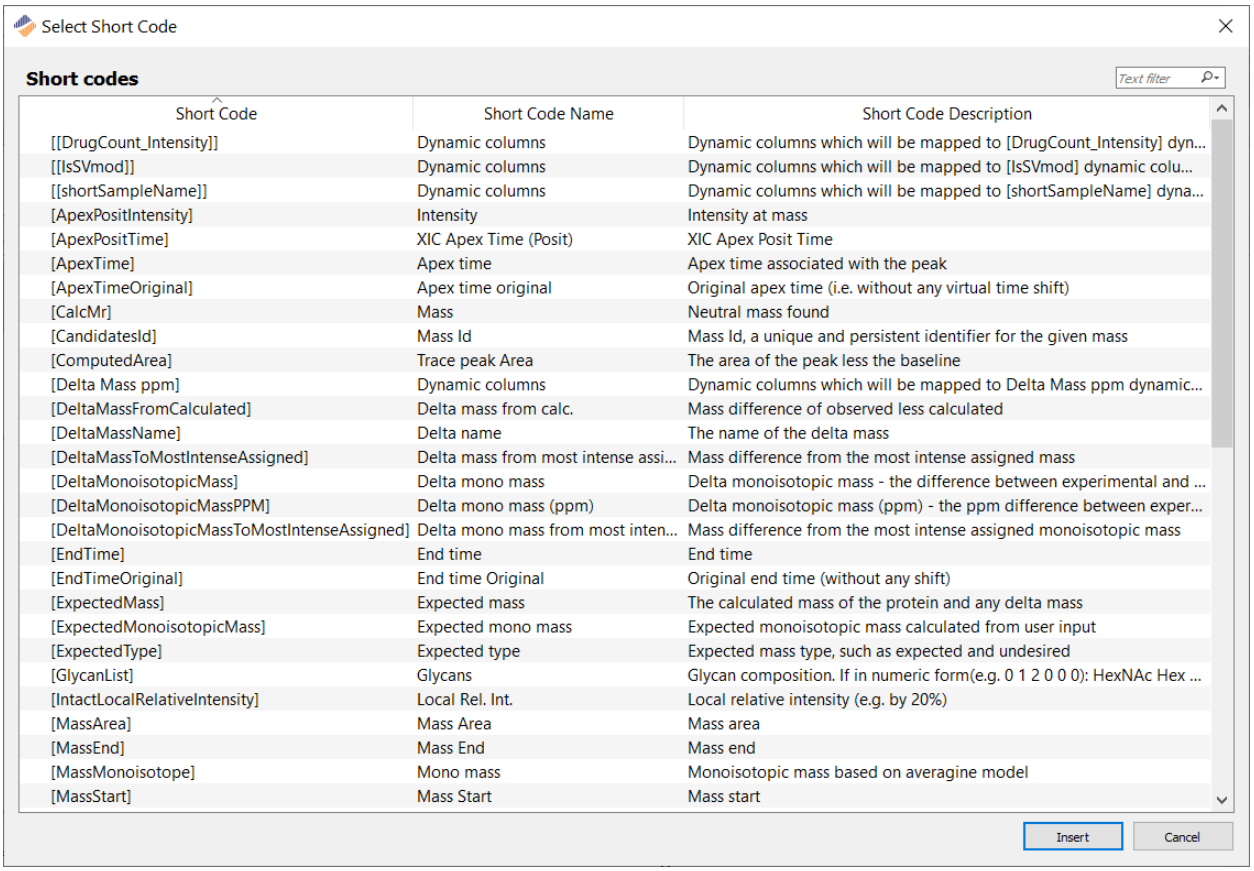
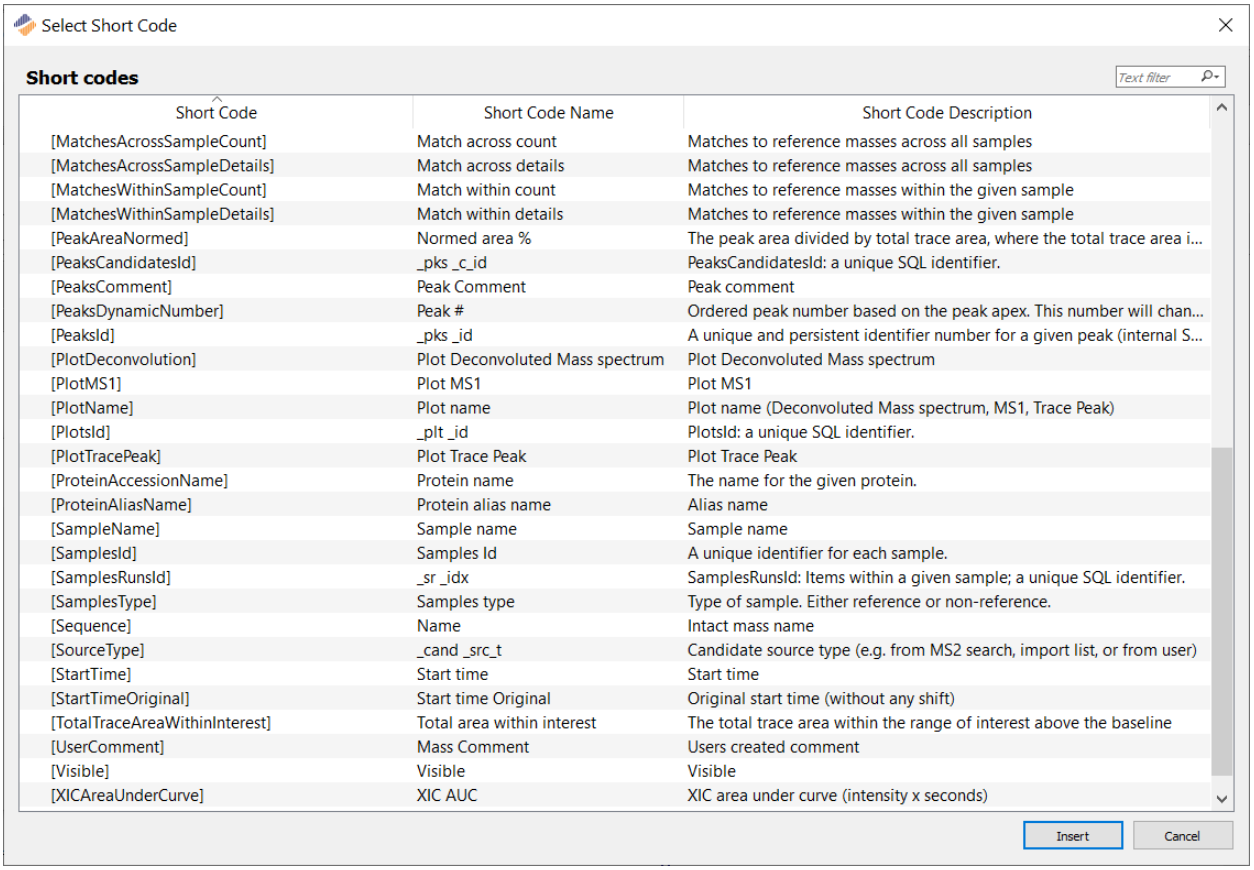


Figure 93: Intact Analysis Plots tab Short Codes, part 1



Short Code	Short Code Name	Short Code Description
[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 sample
[MatchesWithinSampleDetails]	Match within details	Matches to reference masses within the given sample
[PeakAreaNormed]	Normed area %	The peak area divided by total trace area, where the total trace area i...
[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 chan...
[PeaksId]	_pks _id	A unique and persistent identifier number for a given peak (internal S...
[PlotDeconvolution]	Plot Deconvoluted Mass spectrum	Plot Deconvoluted Mass spectrum
[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
[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.
[Sequence]	Name	Intact mass name
[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]	Mass Comment	Users created comment
[Visible]	Visible	Visible
[XICAreaUnderCurve]	XIC AUC	XIC area under curve (intensity x seconds)

Figure 94: 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 (.prepvtjs) can be added to all tabs or just the current tab.

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

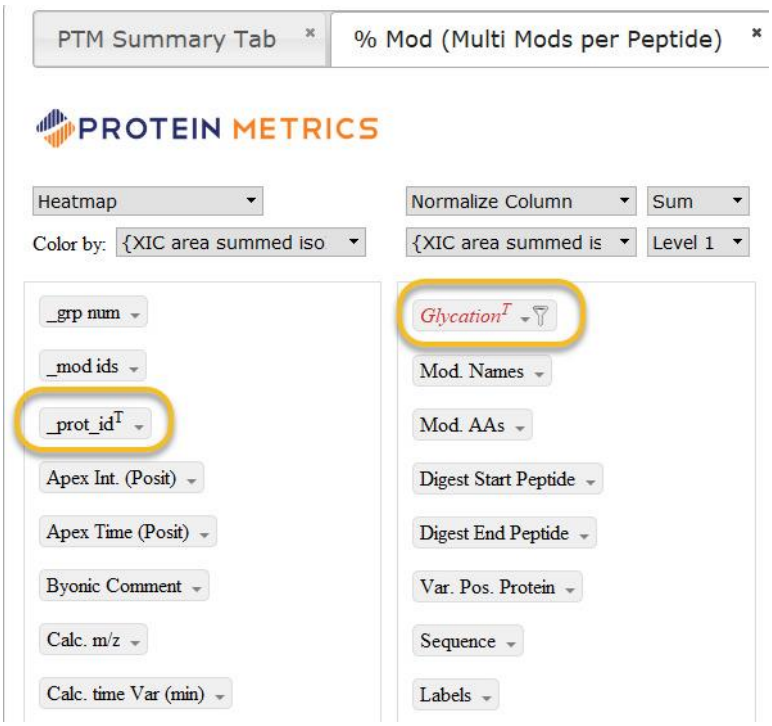


Figure 95: Per tab Pre Pivot fields identified with “T”

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

To add Pre Pivot JavaScript, choose **File > Presets > Post 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).
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"
ProteinDigestNumbering	Creates a summary of protein digestion based on start/end peptide, n-term/c-term offsets, and accession name.
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”.
Peptide Analysis Only	
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.
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.
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.
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: XIC area summed * XIC ratio / (1 - 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
StdDevErrorColumns	Creates standard deviation column and enables error bar charts and error line charts
RSDErrorColumns	Creates relative 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	
MaxFoldChangeRow	Finds the maximum fold change between a reference file and each of the non-reference files
NormalizedPPM	Calculates "normalized ppm", using the formula: value / max * 1,000,000
Pvalue	Calculates p-value and all other helper values which are used to calculate t-test value for two group of values.
Intact Analysis Only	
BranchDiffrence	Creates a column to display the difference of two of the first columns
ReNormedArea	Normalizes the area % for the filtered peaks instead of all peaks so that the displayed percentages add to 100%

Editing Pre or Post Pivot JavaScript

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

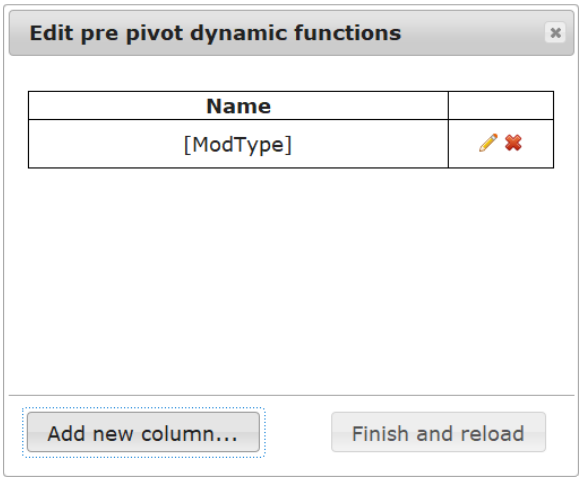


Figure 96: Editing pre pivot dynamic functions

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:

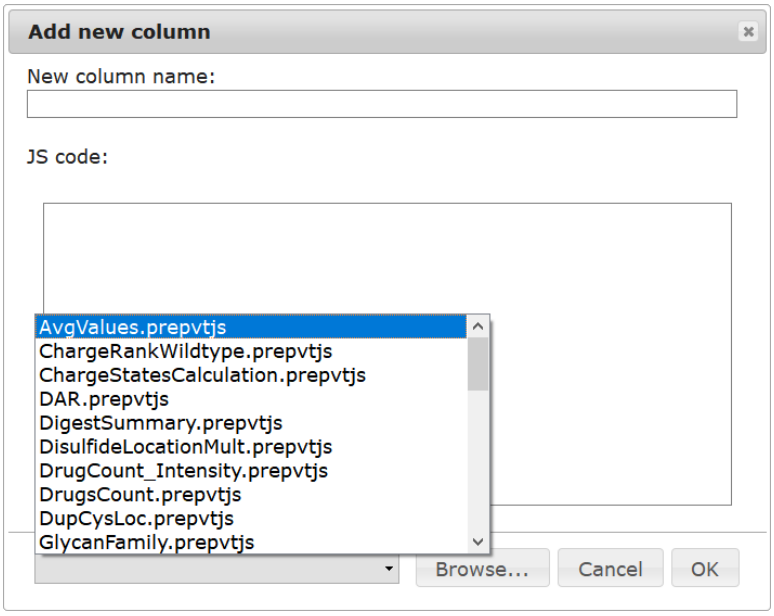


Figure 97: Adding a column as a pre pivot function

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:

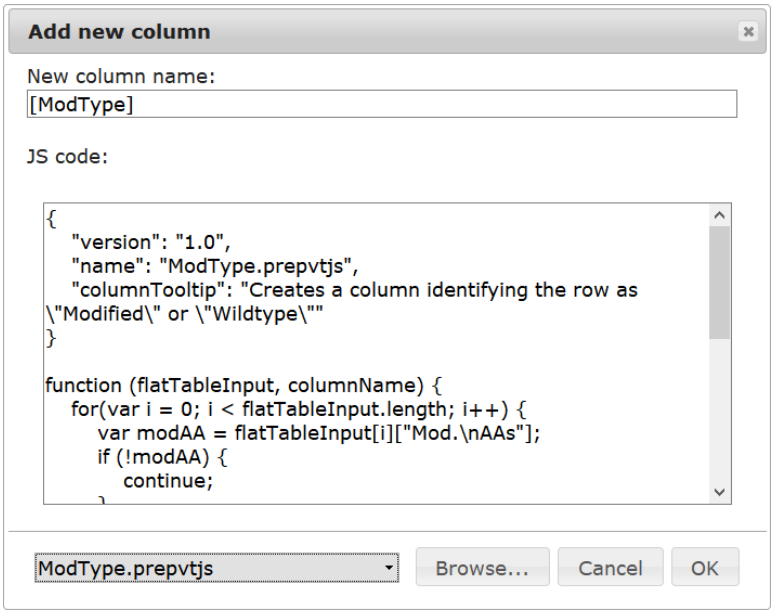


Figure 98: Pre pivot JavaScript

Tour of JavaScript Add New Column Dialog

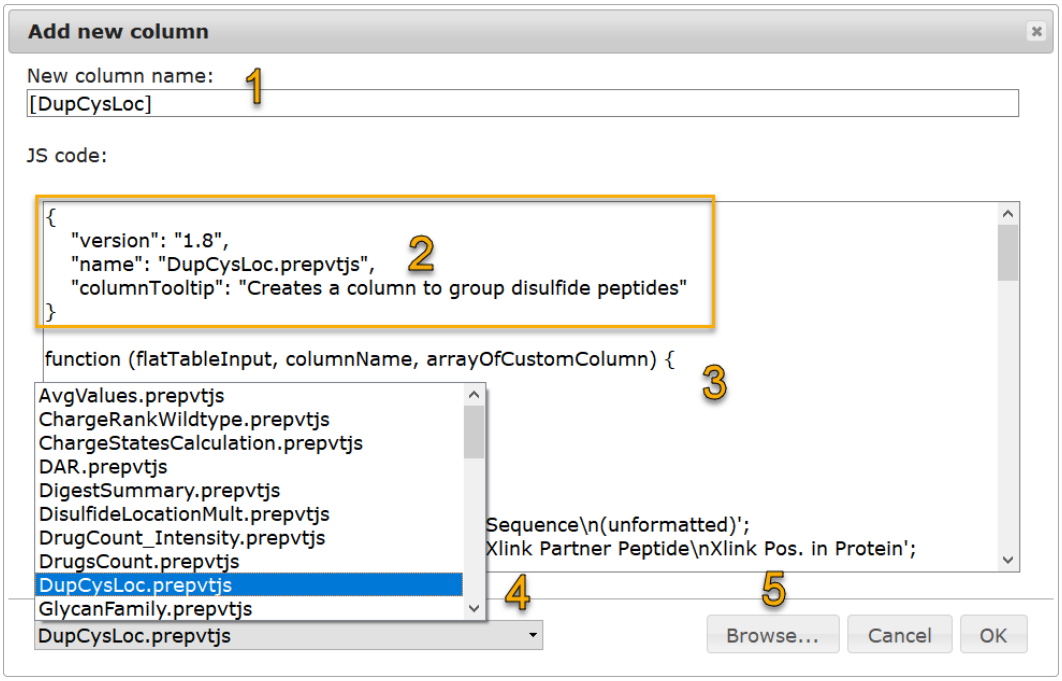


Figure 99: JavaScript areas in the Add new column dialog

No	Item	Description
1	New column name	Dynamic column name to be used in the Report.

2	Metadata	Optional.
		{
		“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)”
		}

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: PMI-SuiteBasepresetsByologicprepivot_script PMI-SuiteBasepresetsByosprepivot_script
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:
	function (flatTableInput, columnName) {
	for (var i = 0; i < flatTableInput.length; ++i) {
	flatTableInput[i][columnName] = i;
	}
	return flatTableInput;
	}
	An example that uses custom names:
	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);
	return flatTableInput;
	}

Post Pivot JavaScript is formatted as:

function (postPivotTableInput, columnName, arrayOfCustomColumn,

mapOfErrorColumnTypeNameAndColumnName)

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.

mapOfErrorColumnTypeNameAndColumnName	Optional parameter.
	Maps arrayOfCustomColumn to error column type name.
	For example, in AllErrorColumns.postpvtjs, AbsMax is mapped to error type error:abs:upper, and AbsMin to error:abs:lower:
	var arrayOfColumnNames = ["[Avg]", "[AbsMax]", "[AbsMin]"];
	var arrayOfErrorType = ["error:abs:upper", "error:abs:lower"];
	mapOfErrorColumnTypeNameAndColumnName[arrayOfColumnNames[1]] = arrayOfErrorType[0];
	mapOfErrorColumnTypeNameAndColumnName[arrayOfColumnNames[2]] = arrayOfErrorType[1];

Multi-Document Report

Multi-document reports display the results of multiple projects within a single tabbed document. All of the 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:

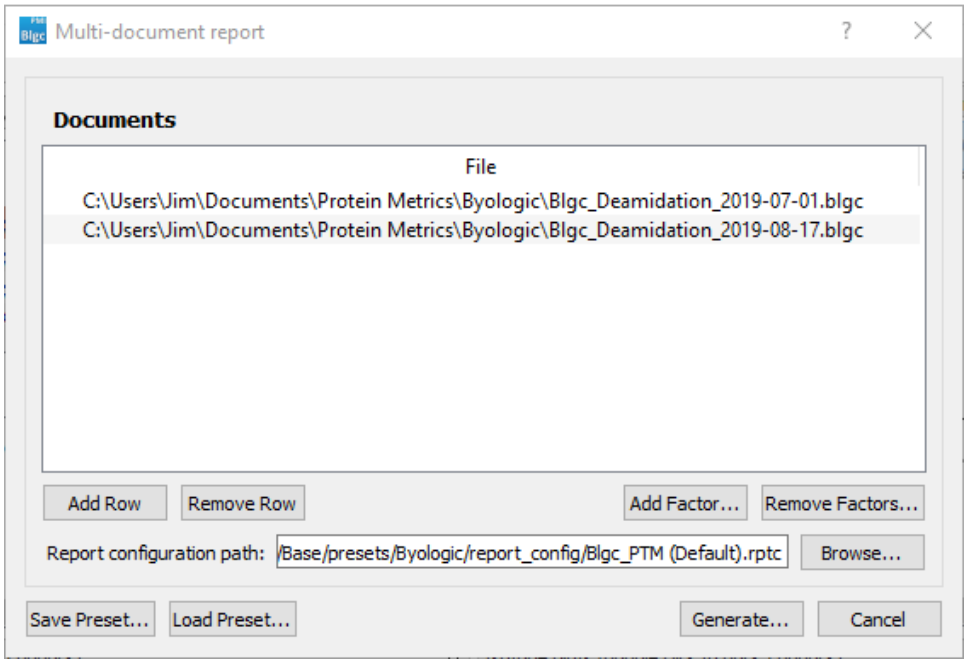


Figure 100: Multi-document report input dialog

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 of the projects:

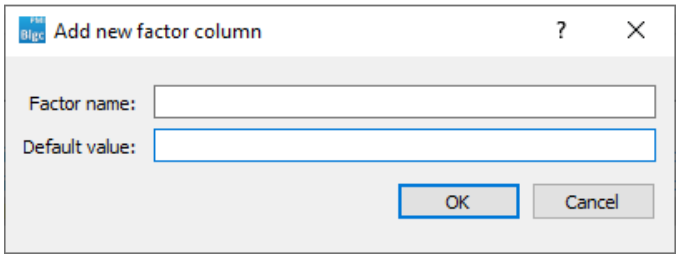


Figure 101: Add new factor column

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 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 and www.proteinmetrics.com/announcement/version-release-updates/.