



Byosphere[®] Dashboards (Powered by Deep Query)

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Overview

Byosphere® Deep Query allows a user to collate data to build Visualizations. Features include:

1. Multiple customizable Visualization types that can be used to represent data
2. Query all PMI analyzed data and upload data and projects into Byosphere to use with Deep Query in real-time
3. Access to building and viewing Dashboards within the Byosphere Web Client—no additional software required
4. Leverage the use of Metadata within Visualizations
5. Add user-defined Derived Fields to a Visualization
6. Build different data value transformations and calculated fields to apply to data
7. Background Alerts to notify the user when certain conditions have been met for data within a Dashboard

User Privileges


To use **Deep Query**, users must have at least the **Advanced Viewer** or **Contributor** Role. **Basic Viewers** do not have access to Deep Query.

Introduction

Byosphere® Deep Query Dashboards allow a user to interrogate data from multiple projects within a Data Source to provide detailed information. **Dashboards** are a collection of **Visualizations** that support viewing data across multiple projects. They provide a dynamic view of data that can be used to monitor processes, assess changes over time, or to create descriptive models of data for business intelligence purposes. A **Visualization** is a chart, table, or other kind of visual component that renders data.

Load a Dashboard

To load a Dashboard that has already been created, the user must select a Dashboard from the list of all Dashboards the user has been given Viewer privileges to. If a user wishes to Edit or Publish a Dashboard, they must have Viewer *and* File Editor privileges. The file name extension for Dashboards is **.bdash**.









				5913	Report test
				1569	ptm 1
				2115	verify: 10000

Figure 1: View Dashboard button in the Actions column

Actions available for the files listed under the Dashboards tab differ from options available for other files by the presence of the **View Dashboard** icon . Clicking on **View Dashboard** will launch the selected Dashboard. For more information on additional Action icons available in the Web Client, see the **Byosphere Web Client Manual**.

Once a Dashboard is loaded, the user can freely move between tabs of Byosphere within the same browser and any edits made to the Dashboard and associated Visualizations will be retained.


File History

Users can view all published versions of a Dashboard by clicking the **File History** icon  within the File Browser page.

File History for Dashboard documents performs similarly to any other document within the Byosphere Web Client, with the following exceptions for the **Change** column:

- The Change column will read **Create Content** when the Dashboard file is first created from the Dashboard Editor

File History: PTM Project.bdash

Download File History Report for version 





Action	Version	Folder Name	File Alias	File Name	Changed By	Changed On	Change
 	1	Morgan V	PTM Project	PTM Project.bdash	Morgan Vasas	2025-06-02 15:23:51	Create Content
 	2	Morgan V	PTM Project	PTM Project.bdash	Morgan Vasas	2025-06-02 15:23:52	Edit Content

Figure 2: Change Column for new Dashboards

- The Change column will read **Edit Content** when the Dashboard is edited and Published

File History: PTM Project.bdash

Download File History Report for version 





Action	Version	Folder Name	File Alias	File Name	Changed By	Changed On	Change
 	1	Morgan V	PTM Project	PTM Project.bdash	Morgan Vasas	2025-06-02 15:23:51	Create Content
 	2	Morgan V	PTM Project	PTM Project.bdash	Morgan Vasas	2025-06-02 15:23:52	Edit Content

Figure 3: The Change column for the same Dashboard after being published

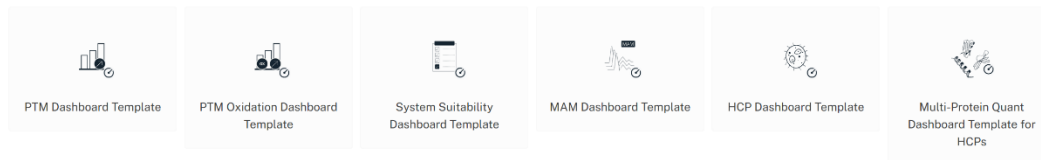
Create a Dashboard

Using a Template

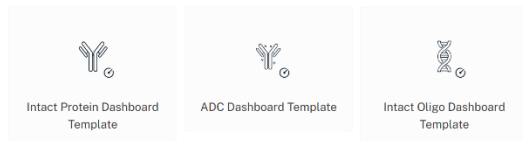
Users will be provided with different types of example/template dashboards under **System Dashboards**, which can be found on the Deep Query Dashboards page.

System Dashboards

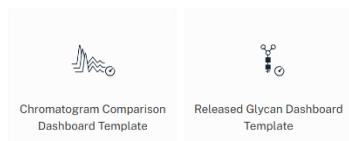
Peptide



Intact



Chromatogram



Combined

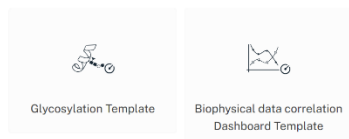


Figure 6: System Dashboards from the Home page

Peptide templates

The **PTM Dashboard Template** can be used to deep query across different analyses for post translational modifications (PTMs). The PTM Dashboard Template contains the following visualizations:

- **Pivot table for Relative Glycosylation Short Name:** This converts the glycan subunit name from the glycopeptide identification to short name nomenclature. For example: HexNAc(4)Hex(3)Fuc(1) to G0F. This will then calculate the relative % of each Glycan that is identified.
- **Stacked bar chart for Stacked Bar Chart Glycan Distribution:** This is the same as the pivot table described above but presented in a stacked bar chart.
- **Pivot table for Relative Fucosylation %:** This will categorize glycopeptides into a-Fucose (where the Glycan does not contain a Fucose) and Fucose (where the identified Glycan does contain a Fucose). The relative % between these two categories is then calculated.
- **Bar chart for Relative Fucosylation %:** This is the same as the pivot table described above but presented in a bar chart.
- **Pivot table for % Modification (Multiple Mods per Peptide):** This table is the same as the pivot table used in Byos reports to quantitate the relative levels of modified and unmodified peptides. Normalization occurs at the peptide level. By default, the unmodified (or Wild Type) peptides are hidden using a filter. This filter may be removed by editing the visualization and going to the Filter and Sort tab. The filter is applied as a Show/Hide filter and can be removed simply by deleting the filter.
- **Line chart for % Modification (Multiple Mods per Peptide) Trend for Indicator Peptides:** This allows the user to monitor a trend of defined peptides and is useful for monitoring trends over time of a modification; for example, % oxidation between samples. This uses the same normalization calculation as the previous pivot table. A user may define their own peptides and modifications by using the filters. An Include/Exclude filter may be used for the peptide sequence, as normalization

occurs at the peptide level. However, it is important to remember to define specific modification information using a Show/Hide filter, so it will not affect the normalization calculation.

- **Pivot Table for Average XIC Ratio Percent of Modifications per Peptide:** This will show the XIC ratio percent of modified peptides per sample.

The **PTM Oxidation Dashboard Template** can be used to deep query across different analyses for oxidation as a post translational modification (PTM).

This template contains the following Visualizations:

- **Line chart for % Oxidation Modification (Multiple Mods per Peptide) Trend for Indicator Peptides:** This allows the user to monitor a trend of defined peptides and is useful for monitoring oxidation trends over time. This uses the same normalization calculation as the pivot tables in the Dashboard. A user may define their own peptides and modifications by using the filters, and the template is filtered for a specific peptide as an example, which may be changed after Dashboard creation. An Include/Exclude filter may be used for the peptide sequence, as normalization occurs at the peptide level. However, it is important to remember to define specific modification information using a Show/Hide filter, so it will not affect the normalization calculation.
- **Pivot table for % Oxidation Modification (Multiple Mods per Peptide):** This table is similar to the pivot table used in Byos reports and is used to quantitate the relative levels of modified and unmodified peptides. Normalization occurs at the peptide level. By default, the unmodified (or Wild Type) peptides are hidden using a filter. This filter may be removed by editing the visualization and going to the Filter and Sort tab. The filter is applied as a Show/Hide filter and can be removed simply by deleting the filter.
- **Pivot table for Average XIC Ratio Percentage of Oxidations per Peptide:** This pivot table is used to calculate the average XIC ratio across all charge states for a modified peptide for each sample.

The **System Suitability Dashboard Template** can be used for the suitability assessment of LC-MS/MS systems or sample preparation. The following visualizations can be useful for monitoring LC-MS/MS system performance:

- **Most Recent ppm:** This visualization is presented as a gauge on the Dashboard, where a user can define the range in which a ppm is acceptable (by default this is green) and red where the value falls outside of the defined range. Settings for the gauge visualization may be configured under the Visualization Settings tab when editing the visualization. By default, this visualization is monitoring the most recent project file or a specific peptide, defined by its sequence. The peptide sequence to be monitored and the number of n most recent project to be queried may be defined in the Filter and Sort tab when editing the visualization.
- **Line Chart for Average ppm trend:** This chart will display the average ppm of all peptides within a given sample file over time (average ppm vs Created On Date).
- **Line Chart for Retention Time Trend:** This shows the average intensity of an XIC peak apex vs Created On Date for a single peptide. A user may define a custom peptide and/or instrument in the Include/Exclude filters when editing the visualization.

There are also visualizations within the System Suitability Template that will allow a user to monitor parameters related to sample preparation, such as:

- **Pivot Table to monitor over and under alkylation of peptides:** Peptides are categorized into those that have been under alkylated, those that have been over alkylated, and all other peptides. The filters applied only include those peptides that are under- or over-alkylated. Categorization is dependent upon the modification names provided in the Byos project. Over alkylated peptides must contain the name "overalkylation" and under alkylated peptides must contain the name "(de) carboxymethyl" in their modification names. Here, the values are determined by averaging the XIC Ratio Percent.

- **Bar chart to monitor alkylation levels:** This is the same as the pivot table described above but presented in a bar chart.
- **Pivot Table to calculate the relative % of missed cleavages:** This will calculate the relative levels of miss cleaved peptides. This visualization will only populate for those analyses that have their enzyme defined.
- **Bar chart displaying the relative % of miss cleaved peptides:** This is the same as the pivot table described above but presented in a bar chart.
- **Data Grid for Digestion Specificity :** This will calculate the average level of non-specific cleavages.
- **Bar Chart for Digestion Specificity:** This is the same as the pivot table described above but presented in a bar chart.

The **MAM Dashboard Template** can be used to deep query results across different peptide analysis projects for MAM studies. The MAM Dashboard Template contains the following Visualizations:

- **Line chart – Monitoring of CQA Peptide Levels** This displays the relative % modification of peptides that have the label CQA (Critical Quality Attributes) and is useful for monitoring trends over time of those peptides. For example, a user would be able to monitor the relative % oxidated peptides across samples. This uses a similar Normalization calculation as used in the default Byos PTM Report to calculate relative % of different peptide species (% Mod (Multi Mods per Peptide)). There is a Show/Hide filter applied to only display those peptides which were set to have the label CQA within the BYOS project. An Include/Exclude filter may be used for the peptide sequence, as Normalization occurs at the peptide level. However, it is important to remember to only use a Show/Hide filter on the following data fields: Modifications Summary List, and Label Names, so it will not affect the normalization calculation.
- **Data Grid – Fold Change from Reference for All Peptides XIC AUCs (Filtered ≥ 4 Fold Change from Reference):** This data grid will display the XIC AUC of peptides and the fold change of that XIC AUC in samples that have been classified as Non-Reference Sample Type vs a sample that has been given the Sample Type Reference within a Byos project. There is a default Show/Hide filter applied to only display those peptides that have a fold change of ≥ 4 in Non-Reference data type samples compared to a Reference data type sample. This value can be changed by a user in the Filter & Sort tab when editing the visualization. All Non-Reference samples are compared to a single Reference, which is important to keep in mind when querying multiple projects. At this time, the Visualization will only support one sample defined with the Sample Type Reference from a Byos Project.
- **Pivot Table – Fold Change from Unknown XIC AUCs (Filtered ≥ 4 Fold Change from Reference):** This data grid will display the XIC AUC of unknown but detected peaks and fold change of that XIC AUC in samples that have been classified as a Non-Reference Sample Type vs a sample that has been given the Sample Type Reference within a Byos project. This is calculated for unknown XICs that were found as a result of running the feature finder algorithm in Byos. These unknown XICs are not linked with any peptide identification, so this visualization will allow a user to monitor levels of XICs that have not previously been identified. There is a default Show/Hide filter applied to only display those unknown XICs that have a fold change of ≥ 4 in Non-Reference Sample Type samples compared to a Reference Sample Type sample. This value can be changed by a user in the Filter & Sort tab when editing the visualization. All Non-Reference samples are compared to a single Reference. At this time the visualization will only support one sample defined with the Sample Type Reference from a Byos Project. If queried Byos projects do not contain any of these unknown XICs (for example, if feature finder had not been implemented for that project), the visualization will be empty.
- **Pivot table for Relative Glycosylation Short Name:** This converts the glycan subunit name from the glycopeptide identification to a short name nomenclature. For example: HexNAc(4)Hex(3)Fuc(1) to G0F. This will then calculate the relative % of each Glycan that is identified.

- **Stacked bar chart for Stacked Bar Chart Glycan Distribution:** This is the same as the pivot table described above but presented in a stacked bar chart.
- **Bar Chart – Fold Change from Unknown Peaks:** This bar chart displays the fold change of all unknown XIC AUCs for Non-Reference samples vs a Reference sample and is grouped based upon MS Alias Name. There is a visual indicator (dotted constant red line) set to a value of 4, to enable a user to readily view samples that contain unknown peaks where the value of XIC AUC has increased ≥ 4 fold from the reference sample. This setting can be changed in the Constant Lines section of the Visualization Settings tab when customizing the visualization.
- **CQA and Peptide Labels % All Modifications (Multiple Mods per Peptide):** This table is the same as the pivot table used in Byos reports used to quantitate the relative levels of modified and unmodified peptides and also uses the same Normalization calculation as described in the Visualization below. By default, there is a Show/Hide filter to only display the relative % of those peptides which were set to have the label CQA within the BYOS project. In addition, there is a column to display Peptide Label. The Label is concatenated from the Protein Alias Name, and the start/end peptide number.
- **Pivot table for % Modification (Multiple Mods per Peptide):** This table is the same as the pivot table used in Byos reports used to quantitate the relative levels of modified and unmodified peptides. Normalization occurs at the peptide level. By default, the unmodified (or Wild Type) peptides are hidden using a filter. This filter may be removed by editing the Visualization and going to the Filter and Sort tab. The filter is applied as a Show/Hide filter and can be removed simply by deleting the filter.
- **% Deamidation - (Multiple Mods per Peptide):** This table is the same as the pivot table explained above, except there is a Show/Hide filter applied to only display deamidated peptides.
- **% Oxidation - (Multiple Mods per Peptide):** This table is the same as the pivot table explained above, except there is a Show/Hide filter applied to only display oxidated peptides.
- **Line chart Trend of Sum of Deamidation XIC AUC per Residue:** This line chart monitors the trend of XIC levels for residues such as Q and N that have been deamidated. Each data point represents the sum of the XICs for peptides that contain that residue that has been deamidated. This allows the user to monitor a trend of instrument response dependent level of total deamidations on their proteins across different samples (as we are reporting an XIC value not a relative quantitative value).
- **Average XIC Ratio of Modifications per Region:** This pivot table is similar to the pivot table % Mod by ModName across Samples in the default PTM template used in Byos reports, which is used to report the average XIC ratio for different modifications at different protein positions, across samples. In this Visualization, these values are displayed alongside the protein region, as defined via Protein Annotation in Byos (such as CDR regions of mAbs). There is an Include/Exclude filter applied to only display those XIC ratio values that related to parts of the protein sequence that have a designated Protein Annotation.
- **Bar chart of % Oxidation per Sample and Region:** This Bar Chart displays the relative% of oxidated peptides per Sample, per Region (where there may be differing CDR locations such as CDR-L1, CDR-H3 etc). By default, it will only display oxidated peptides that are within a sequence position that is covered by a Protein Annotation within Byos (there is a Show/Hide filter to only display peptides that are oxidated and contain a Protein Annotation). This Bar Chart uses the same Normalization calculation as in the other relative peptide quantitation Visualizations
- in tabular form.

The **HCP Dashboard** template facilitates the querying of projects focused on discovery, analysis, and monitoring of Host Cell Proteins (HCPs) by mass spectrometry and contains the following Visualizations:

- **Relative Protein Abundance - Top 3 Peptides per Protein:** This pivot table shows the relative protein abundance within a sample based on top 3 peptides for each named protein.

- **XIC AUC - Top 3 Peptides per Protein:** This pivot table shows the XIC AUC values of the top 3 peptides for each named protein across samples and replicates.
- **Relative Protein Abundance - All Peptides per Protein:** This pivot table shows the relative protein abundance based on all detected peptides for each named protein across samples and replicates.
- **XIC AUC - All Peptides per Protein:** This pivot table shows the XIC AUC for all detected peptides for each named protein.
- **Bar Chart - HCPs per Sample (All Peptides):** This bar chart shows the relative levels of HCPs per sample based on all peptides detected by protein.
- **Error Bar Chart per Sample - HCPs per Sample (All Peptides):** This bar chart shows the average relative levels of HCPs per sample for all peptides with error bars conveying variation amongst replicates.

The **Multi-Protein Quant Dashboard template for HCPs**. The Multi-Protein Quant Dashboard template for HCPs contains the following Visualizations:

- **Pivot Table - XIC AUC Protein Abundance - With Peptides:** This pivot table provides a tabular representation of the XIC AUC levels of the top 3 peptides per protein.
- **Pivot Table - Total XIC Area Summed per Protein:** This pivot table provides a tabular representation of the summed XIC AUC levels per protein.
- **Bar Chart - Total XIC Area Summed per Protein with Standard Deviation Error Bars:** This bar chart is to visualize proteins based on the summed XIC AUC levels using Protein Accession Numbers as X-axis value, hiding the most abundant protein to better visualize the lower level host cell contaminants.
- **Pivot Table - Relative Protein Abundance - With Peptides:** This pivot table provides a tabular representation of the relative levels of top 3 peptide per protein displayed relative to the most abundant peptide.
- **Pivot Table - Relative Protein Abundance:** This pivot table provides a tabular representation of the relative protein levels based on summed XIC area and relative to the most abundant protein.
- **Bar Chart - Relative Protein Abundance:** This bar chart is to visualize the relative protein levels based on XIC quantitation and relative to the most abundant protein
- **Stacked Bar Chart - Relative Protein Abundance:** This bar chart is to visualize the relative protein levels based on XIC quantitation and normalized to total protein abundance.
- **Pivot Table - Protein ppm Concentration – Relative to mAb:** This Pivot Table provides the average protein ppm concentration based upon the mAb across different replicates and conditions.
- **Stacked Bar Chart – Protein ppm Concentration:** This bar chart is used to visualize the relation outlined above.

Intact templates

The **Intact Protein Dashboard Template** facilitates queries across different analyses for Intact Proteoform analysis. The Intact template contains the following Visualizations:

- **Pivot Table for All Mass Intensity:** This pivot table is used to display the mass intensity for each mass peak. This includes all mass peaks, both identified and non-identified. Grouping is by sample and peak number.
- **Pivot Table for Expected Mass Intensity:** This pivot table is used to display the mass intensity for identified mass peaks only. Grouping is by sample and peak number.

- **Pivot Table for Expected Mass Relative % Modification:** Normalization occurs at the protein level and is grouped by sample and peak number.
- **Bar Chart – Relative % Modification grouped by Sample Name/Peak Number/Protein (Expected Mass):** This is the same as the pivot table described above but presented in a bar chart.
- **Pivot Table for Expected mass – mass accuracy (ppm):** This pivot table is used to display the mass accuracy in ppm for identified mass peaks. Grouping is by sample and peak number.
- **Line Chart Expected mass – mass accuracy (ppm):** A line chart displaying the same information as described in the pivot table above.

The **ADC Dashboard Template** facilitates queries across different analyses for Antibody Drug Conjugate (ADC) and Drug to Antibody Ratio (DAR) analysis. The ADC template contains the following Visualizations:

- **Bar Chart – DAR per Sample:** This bar chart is used to display the calculated DAR per sample (and is grouped by sample name).
- **Bar Chart – Relative % Drug Count per Sample:** This bar chart is used to display the relative % of conjugated mAb/ADC species distinguished by the number of drugs conjugated to the antibody. Normalization occurs at the protein level and calculates the relative % based on mass intensities per different delta mass species for the same protein (in this case, n-drug). Bars are grouped by sample and peak number.
- **Pivot Table for Expected Mass Intensity:** This pivot table is used to display the mass intensity for identified mass peaks only. Grouping is by sample and peak number.
- **Pivot Table for Relative % Drug Count and DAR:** This pivot table is used to display the relative % of ADC species (specified in the Visualization as modifications determined by delta mass) and calculated DAR value. Normalization occurs at the protein level and is grouped by sample and peak number.
- **Pivot Table for Expected mass – mass accuracy (ppm):** This pivot table is used to display the mass accuracy in ppm for identified mass peaks. Grouping is by sample and peak number.
- **Line Chart Expected mass – mass accuracy (ppm):** A line chart displaying the same information as described in the pivot table above.
- **Pivot Table for Expected Mass Relative Intensity:** This pivot table is used to display the relative % of matched masses per delta masses. Normalization occurs at the protein level and is grouped by sample and peak number.
- **Pivot Table for All Mass Intensity:** This pivot table is used to display the mass intensity for each deconvoluted mass peak. This includes all mass peaks, both identified and unidentified. Grouping is by sample and peak number.

The **Intact Oligonucleotide template** facilitates the querying of results across different analyses for Intact Oligonucleotide analysis and contains the following Visualizations:

- **All Oligo Mass Intensity:** This pivot table displays the mass intensity for all deconvoluted masses per sample.
- **Expected Oligo Mass Intensity:** This pivot table displays the mass intensity for all expected and identified oligonucleotide species per sample.
- **Expected Oligo Mass – Relative Intensity %:** This pivot table displays the relative intensity% for all identified expected oligonucleotide species per sample.
- **Expected Oligo Mass – Mass Accuracy (ppm):** This pivot table displays the mass accuracy in ppm of all identified expected oligonucleotides per samples.

- **Bar Chart - Expected Mass Relative Intensity % Across Sample:** This bar chart displays the mass accuracy in ppm of all identified expected oligonucleotides per sample.
- **Bar Chart - Expected Mass Relative Intensity % per Oligo Candidate:** This bar chart displays the mass accuracy in ppm of all identified expected masses per sample.
- **Line Chart Expected Oligo - Mono Mass Accuracy (ppm):** This line chart displays the monoisotopic mass accuracy per sample.

Chromatogram templates

The **Chromatogram Comparison** template contains the following Visualizations:

- **Line Chart Displaying Norm Peak Area for each Peak across Multiple Samples:** This line chart is to visualize the normed peak area trends for the same peak across different samples for monitoring purposes
- **Bar Chart - Relative Trace Peak Area Grouped by Peaks Comment:** This bar chart is to visualize the relative normalized trace peak area values within a group of peaks of interest when identified to belong to a group by a Peak Comment.
- **Pivot Table - Trace Peak Area Grouped by Peaks Comment:** This Pivot table is a tabular representation of trace peak area values for peaks of interest when identified to belong to a group by a Peak Comment.
- **Bar Chart Average Apex Time (minutes) per Peak across Samples (Error bar +/- 3 Std. Dev):** This line chart is to visualize apex time consistency and standard deviations across samples within a comparison study.
- **Scatter Plot Average Apex time per peak across samples (Error bar +/- 2 Std. Dev) for monitored peaks:** This scatter plot is to visualize the same apex time monitoring for a selected few peaks of interest with 2*standard deviation as error bar.
- **Bar Chart - Normalized Peak Area % All Peaks:** This bar chart is to visualize the normed area values for peaks across samples to allow observation of obvious deviations.
- **Bar Chart Average Normed Area% per Peak across Samples (Error bar +/- 1 Std. Dev):** This bar chart is to visualize average normed area with standard deviation for peaks across samples.
- **Line Chart Average Normed Area% per Peak per Sample filtered for monitored peaks:** This line chart is to visualize average normed area for peaks across samples to present visual differences between samples.
- **Pivot Table – Normed Area% - All Peaks:** This pivot table is a tabular representation of normed area% values of all peaks across samples.

The **Released Glycan** template can facilitate the querying of projects focused on the characterization of glycans and contains the following Visualizations:

- **Annotations by Peak# - Normed Area % - based Relative Glycan Quantitation:** This pivot table displays relative glycan levels per sample glycans shown by chromatographic peak within the table.
- **Annotations by Glycan - Normed Area % - based Relative Glycan Quantitation** This pivot table displays relative glycan levels by glycan short name.
- **Glycan Area Bar Chart - Normed Area % Grouped Across Samples:** This bar chart shows normed area% for glycans grouped across samples.
- **Peak Area Bar Chart - Normed Area % Across Samples:** This bar chart shows normed area% for glycans grouped across peaks and samples.

- **Bar Chart - Normed Area % for Each Glycan:** This bar chart shows normed area% per glycan as resulted in the released glycan analysis.
- **Line Chart - Normed Area % for Each Glycan Peak across Samples:** This line chart shows normed area% for each glycan peak across samples.

Combined templates

The **Multi-level Glycosylation Dashboard Template** uses the **Combined Analysis** data source, which ingests data from both **Intact** and **Peptide** projects. This template can be used for mapping glycosylation levels and distribution using both Intact and Peptide assay results within one Dashboard.

- **Pivot Table for Expected Mass Relative % Glycosylation (Intact Protein Analysis):** This pivot table is used to quantitate the relative levels of Glycans on proteins from intact analysis.
- **Stacked Bar Chart showing the Relative Levels of Glycans per Sample and Protein:** This is the same as the pivot table described above but presented in a stacked bar chart.
- **Pivot Table for Relative Glycosylation Distribution of Glycopeptides:** This converts the glycan subunit name from the glycopeptide identification to short name nomenclature. For example: HexNAc(4)Hex(3)Fuc(1) to G0F. This will then calculate the relative % of each Glycan that is identified.
- **Stacked Bar Chart Glycan Distribution (Glycopeptide Quantitation):** This is the same as the pivot table described above but presented in a bar chart.
- **Stacked Bar Chart - Glycan Distribution (Released Glycan Analysis):** This bar chart shows the relative% of different glycans for samples processed in Released Glycan analysis projects.
- **Glycan Distribution (Released Glycan Analysis):** This pivot table shows the same information

The **Biophysical data correlation template** uses the **Biophysical Analysis** data source, which ingests data from both **Intact** and **Peptide** projects that are correlated with **Biophysical data**. This template can be used for comparing results from Biophysical analyses such as ICIEF, CE-SDS, and SEC to Byos Intact and Byos Peptide results, respectively.

- **Pivot Table - icIEF - Comparing Relative % of Trace Peak Area across Biophysical Data Samples:** This pivot table provides a tabular representation of relative % trace peak area across samples (using icIEF Biophysical data).
- **Pivot Table - SEC - Comparing Relative % of Trace Peak Area across Biophysical Data Samples:** This pivot table provides a tabular representation of relative % trace peak area across samples (using SEC Biophysical data).
- **Pivot Table (icIEF vs Peptide MS) - Comparing % Deamidation of a Specific Peptide at Different Residue Positions vs % Acidic Peak Area:** This pivot table is used to visualize % deamidation for the same peptide at different residue positions and their relationship with % acidic peak area coming from an icIEF analysis of the same sample.
- **Pivot Table (Peptide MS) - Relative % Modification at Protein Position across Samples:** This pivot table provides a tabular representation of relative % modifications at specific positions across different samples (using Peptide data).
- **Line Chart (icIEF vs Peptide MS)- Comparing % Deamidation of a Specific Peptide at Different Residue Positions vs % Acidic Peak Area:** This line chart is used to visualize % deamidation for the same peptide at different residue positions and their relationship with % acidic peak area coming from an icIEF analysis of the same sample.
- **Bar Chart - Comparing % Deamidation of a Specific Peptide at Different Residue Positions vs % Acidic Peak Area:** The same comparison as the above Visualization using a bar chart.

- **Line Chart - Comparing % Modification of All Modified Peptides at Different Residue Positions vs % Acidic Peak Area:** This line chart compares % modification (not limited to deamidation) for the same peptide at different residue positions to the % acidic peak from an icIEF analysis of the same sample.
- **Pivot Table - Intact MS relative Intensity Expected mass:** This pivot table shows the Intact relative intensity for expected masses.
- **Pivot Table - Intact MS relative Intensity - All masses:** This pivot table shows the Intact relative intensity for all masses, including those that are not named.
- **Line Chart (icIEF vs Intact MS)- Comparing Relative Levels of Expected Intact Species vs % Acidic Peak Area:** This line chart compares relative levels of expected species identified using Intact MS with the % acidic peak area obtained when running icIEF analysis on the same sample.
- **Line Chart (icIEF vs Intact MS) - Comparing Relative Levels of Expected Intact Species vs % Basic Peak Area:** This line chart compares relative levels of expected species identified using Intact MS with the % basic peak area obtained when running icIEF analysis on the same sample.
- **Line chart - (SEC vs Intact MS) LMWS 2 peak vs Intact mass relative intensity:** This line chart compares the Intact mass relative intensity obtained using Intact MS to the LMWS peak area obtained when running SEC analysis on the same sample.
- **Line chart - (SEC vs Intact MS) LMWS 2 peak area vs Intact mass relative intensity <5%:** This line chart compares the Intact mass relative intensity with values under 5% obtained using Intact MS to the LMWS peak area obtained when running SEC analysis on the same sample.
- **Bar chart (SEC vs Intact MS) - SEC HMWS 1 peak vs expected Intact mass relative intensity:** This bar chart compares the expected Intact mass relative intensity obtained using Intact MS to the HMWS peak obtained when running SEC analysis on the same sample.
- **Stacked bar chart (SEC vs Intact MS) - SEC Main peak Relative Levels vs relative normalized levels of Intact Expected Species:** This bar chart depicts SEC main peak relative levels vs the normalized levels of Intact Expected Species obtained using Intact MS.

Once the desired template is selected, the **Add Resource** dialog prompts the user to enter a name and file location for the new Dashboard. The new Dashboard will be populated with settings copied from the template, and from there the user can modify their copy of the template as desired.



The 'Add Resource' dialog box is shown with a close button (X) in the top right corner. It contains two input fields: 'File Alias:' with the text 'System Suitability' and 'Folder:' with a dropdown menu showing 'Morgan'. At the bottom right, there are two buttons: 'Add' (blue) and 'Cancel' (white with a grey border).

Figure 4: Add Resource

From Scratch

To create a new Dashboard from scratch, click **New Dashboard** on the Deep Query Dashboards page.

Dashboards

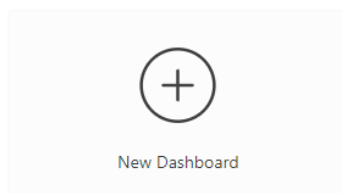
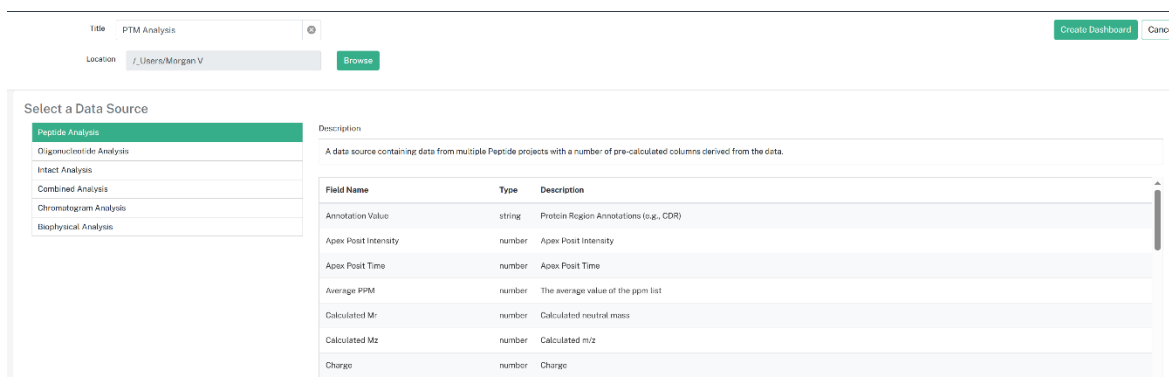


Figure 5: New Dashboard button

On the Dashboard creation screen, the user will be prompted to add a **Title** to the Dashboard and specify a **Location** where the Dashboard should be saved.


 The dashboard creation screen shows a form with a "Title" field (containing "PTM Analysis") and a "Location" field (containing "/Users/Morgan V"). There are "Create Dashboard" and "Cancel" buttons. Below the form is a "Select a Data Source" section with a list of data sources on the left and a table of fields on the right.

Field Name	Type	Description
Annotation Value	string	Protein Region Annotations (e.g., CDR)
Apex Posit Intensity	number	Apex Posit Intensity
Apex Posit Time	number	Apex Posit Time
Average PPM	number	The average value of the ppm list
Calculated Mr	number	Calculated neutral mass
Calculated Mz	number	Calculated m/z
Charge	number	Charge

Figure 6: Dashboard creation screen

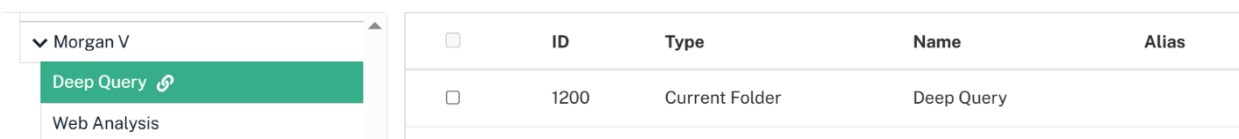
A red exclamation point symbol specifies that an entry by the user is required to proceed with Dashboard creation.


 A form field labeled "Title" with a red border and a red exclamation point icon. The text "Dashboard title" is entered. Below the field is a red error message: "Please add a title".

Figure 7: The Title is a required field, as designated by the exclamation point icon

When creating a Title for the Dashboard, the user will be warned if there is already a Dashboard with the same name within the same Folder. The following special characters are allowed in Dashboard titles: , / , : , * , ? , < , > , | , ' , and " . A Dashboard title can be no longer than 255 characters.

To choose a location to save the Dashboard, click **Browse**, which will launch the **Dashboard Folder Structure** dialog.


 The dialog shows a folder tree on the left with "Morgan V" expanded, showing "Deep Query" (selected) and "Web Analysis". On the right is a table of folders.

<input type="checkbox"/>	ID	Type	Name	Alias
<input type="checkbox"/>	1200	Current Folder	Deep Query	

Figure 8: Dashboard Folder Structure

Select a folder using the checkbox and click **Select Folder**. The location will update to the selected folder and will be viewable on the Dashboard creation page.

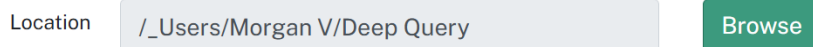


Figure 9: New Dashboard Page with Title and Location

The user must also select a **Data Source** from which data is derived for the Visualizations. A **Data Source** is the database view that all data for a Dashboard is pulled from. The data pulled from this view will be fed to all Visualizations within the Dashboard, although there are options to filter Globally or per Visualization once the Dashboard has been established. The Data Source *cannot* be changed once in the Dashboard Editor.

Select a Data Source

Peptide Analysis
Oligonucleotide Analysis
Intact Analysis
Combined Analysis
Chromatogram Analysis
Biophysical Analysis

Figure 10: Data Source selection

Currently data from the following Project types is supported by Deep Query: **Peptide Analysis**, **Oligonucleotide Analysis**, **Chromatogram Analysis**, and **Intact Analysis**. Project data from Oligo, HRIM, Intabio, Supernovo, or HDX is not yet supported. The **Combined Analysis** data source includes data from both **Intact** and **Peptide** projects. The **Biophysical Analysis** data source includes data from both **Intact** and **Peptide** projects as well as **Biophysical** projects processed through Chromatogram analysis in Byos. Note that queries can only be made in the Biophysical analysis data source *against* Biophysical data and Intact and Peptide projects cannot be queried together. More information about the Biophysical data source can be found in the [Biophysical Data](#) section. Please contact support@proteinmetrics.com for additional help in configuring Dashboards using the Biophysical data source.

Note: Data in Custom columns from Peptide projects have the field name “MS Custom Columns” and data from Intact/Chromatography projects have the field name “Samples Custom Fields”.

Once a data source has been selected, the Dashboard can be created by clicking **Create Dashboard**. The user will be notified that the Dashboard has been saved and the Dashboard will open in **View mode**.

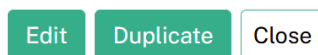
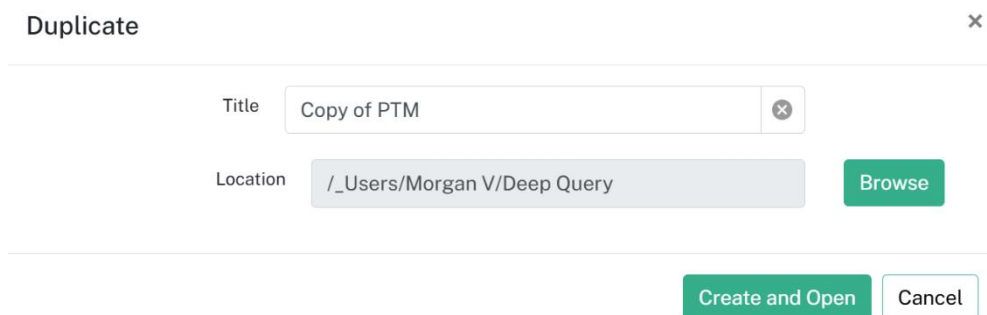


Figure 11: Icons available in View mode.

To enter **Edit** mode, where the user can add and update Visualizations within the Dashboard, the user must click **Edit**.

Duplicate will open a dialog prompting the user to provide a name and location for a copy of the Dashboard to be created. The new Dashboard will be opened upon creation. **Note:** Duplicating a Dashboard will not duplicate any associated Background Alerts of the original Dashboard. For more on Background Alerts, see [Background Alerts](#).



The dialog box is titled "Duplicate" with a close button (X) in the top right corner. It contains two input fields: "Title" with the text "Copy of PTM" and a clear button (X), and "Location" with the text "/_Users/Morgan V/Deep Query" and a "Browse" button. At the bottom, there are two buttons: "Create and Open" and "Cancel".

Figure 12: Duplicate Dashboard

Cancel takes the user away from the Edit mode of the Dashboard. From there, the user can click **Close** to close out the Dashboard currently being viewed. This takes the user back to the page they were on previously before launching the Dashboard creation (e.g., the Home page, Search Result page, File Browser, or File History page).

Once in **Edit Mode**, the user has the following options available:

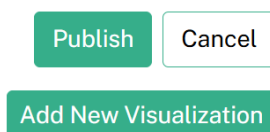


Figure 13: Dashboard options

Publish will save the Dashboard and publish it to the designated Location that the user has provided. **Add New Visualization** populates the Dashboard with a new, empty Visualization. **Cancel** sends the user back to the Dashboard start page, discarding any changes that have been made to the Visualization since it was last published or creation.

Global Filters

Additionally, the user can apply **Global Filters**. **Global Filters** are filters that are applied to *all* data from the Data source present in *all* Visualizations within a Dashboard. Users are *highly encouraged* to use Global Filters, as extra-large data sets can increase processing time and may limit the analysis.

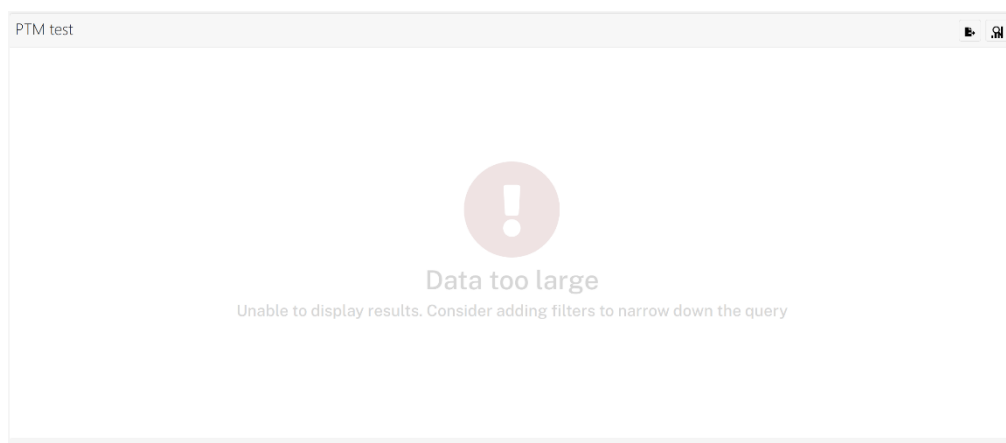



Figure 14: When a query is too large, the user is notified and encouraged to use filters

The Global Filters dialog can be opened by clicking the  icon next to the Data Source.

Data source: **Peptide Analysis**



Figure 15: Open Global Filters

To add a filter within the Global Filters dialog, click **Add condition**.

Apply Global Filters

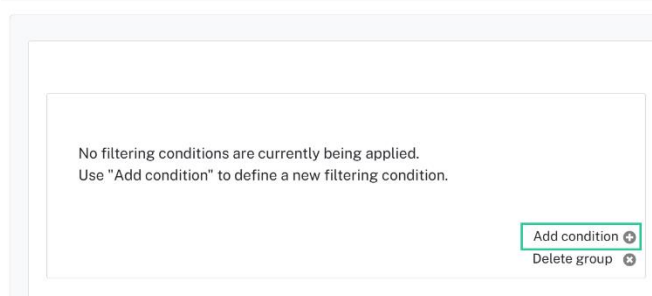


Figure 16: Global Filters dialog

The user can view, add, update, or remove “Include/Exclude” filters that are part of the **Global Filter** when in **Edit** mode. When the user applies changes to the global filter, all Visualizations within the Dashboard are refreshed and correctly adjust their display with the newly filtered data.

Apply Global Filters

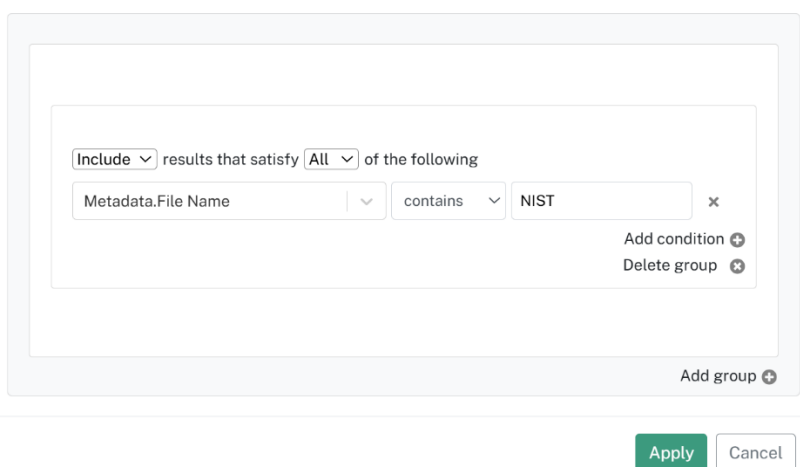


Figure 17: Global Filters dialog with added filter condition

In the above example, the user includes all data that satisfies the condition of containing “NIST” within the value for the Metadata field “File Name”. Only data that meet this condition will be included in the entire Dashboard.

When the user applies changes to a Global Filter, all Visualizations in the Dashboard are refreshed and correctly adjust their display with the newly filtered data.

Filter conditions offer operations specific to the type of value for the selected field:

Value Type	Operations available
String	=, !=, contains, does not contain, begins with, ends with, is null, is not null
Number	>, <, =, !=, between, null, not null
Date	>, <, >=, <=, between, null, not null, is in last, is in previous
All	Null/Not Null

Figure 18: Filter Conditions

Users have the option to define groups of *multiple* conditions. For example:

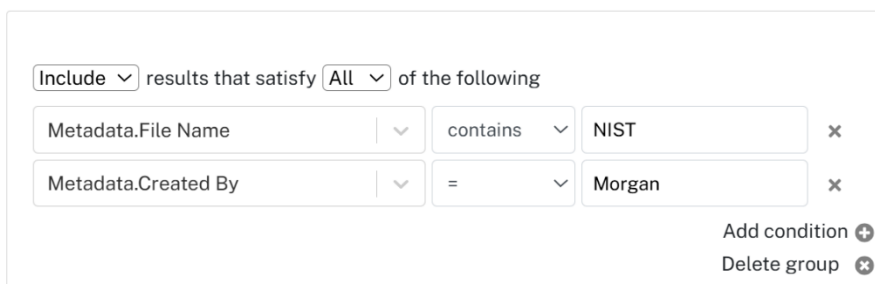


Figure 19: Global Filters use case

In the above use case, the user has chosen to include results that satisfy **both** of the outlined conditions; the File Name **must** contain the string “NIST” and the Created By value must = “Morgan”.

Alternatively, if the user specifies “Any” in their group, only one of the conditions outlined must be met in order for the data to be included in the query

Note: All/Any is equivalent to AND/OR as seen in the filters present in **Byosphere Web Client** search utility.

Add New Visualization

A new Dashboard (not created from a template) will be blank until a Visualization is added. To add a Visualization, click **Add New Visualization**. This will add a generic Visualization pane to the Dashboard.

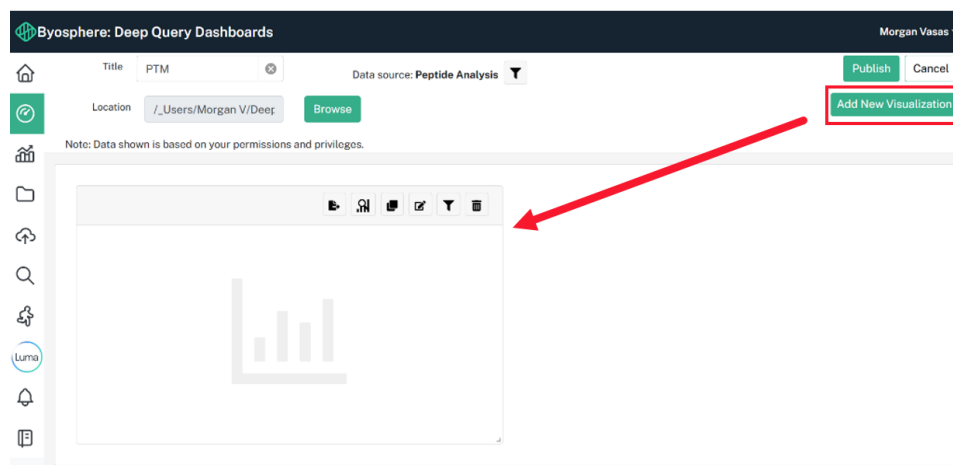


Figure 20: Adding a Visualization

Users are reminded that the data included in a Dashboard is based upon their permissions. Users will only see data from Projects that are in folders they have privileges to view.



To **Duplicate** a Visualization, click  while the Dashboard is in Edit mode. The duplicated Visualization will contain the same content as the original Visualization, including all filter settings, derived fields, and chart/pivot table settings. Note: Background Alerts will be excluded. When the user makes changes to this copy, the original remains unchanged. The duplicate Visualization will only be saved to the Dashboard if the user publishes the Dashboard.



Figure 21: Duplicating a Visualization

To **Edit Visualization**, click the Edit  icon. There are four main panes within a Visualization: the **sidebar**, which contains settings based upon user selection, the **Visualization Builder**, the **Visualization** itself, and **Data Preview**.

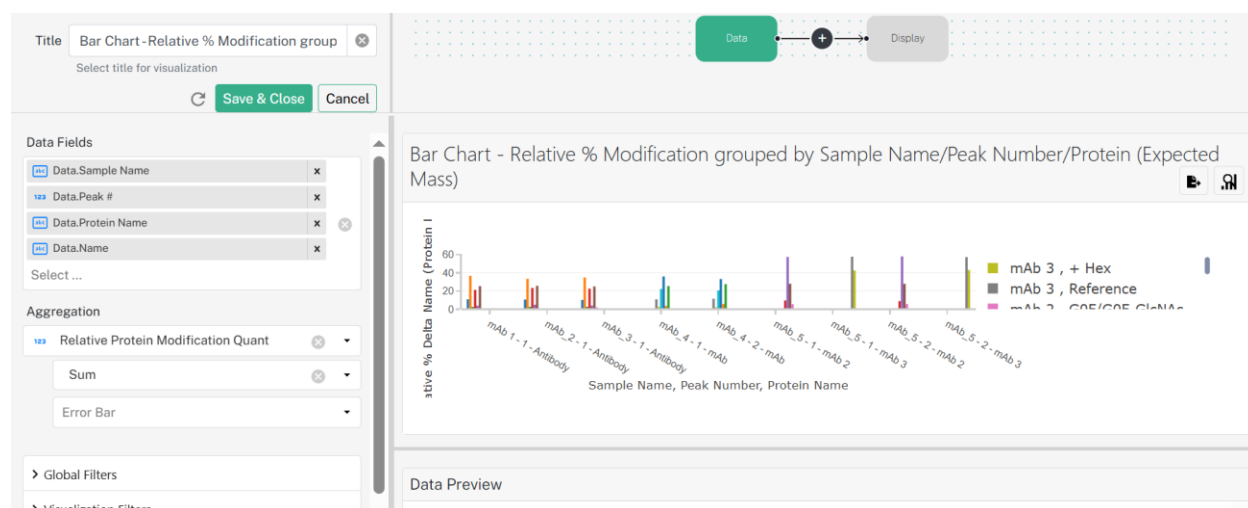


Figure 22: Visualization Editor

Users can drag the separation between the each of these panes to resize each section.

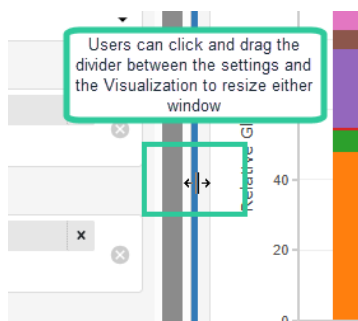


Figure 23: Adjust the size of the Visualization window

The sidebar contains settings that the user can modify and Apply to update the Visualization and Data Preview windows. The settings available in the sidebar for each Visualization type are detailed below. The options available in the sidebar are controlled by the **Visualization Builder** present at the top of the Visualization Editor page. This flowchart contains two blocks by default representing the fundamental settings available in the Visualization: **Data** and **Display** settings. These blocks cannot be removed from the flowchart.



Figure 24: Visualization Builder

Clicking on a block will highlight it in the flowchart and populate the sidebar with relevant controls. Shown below is the Data block highlighted with data settings present in the left sidebar:

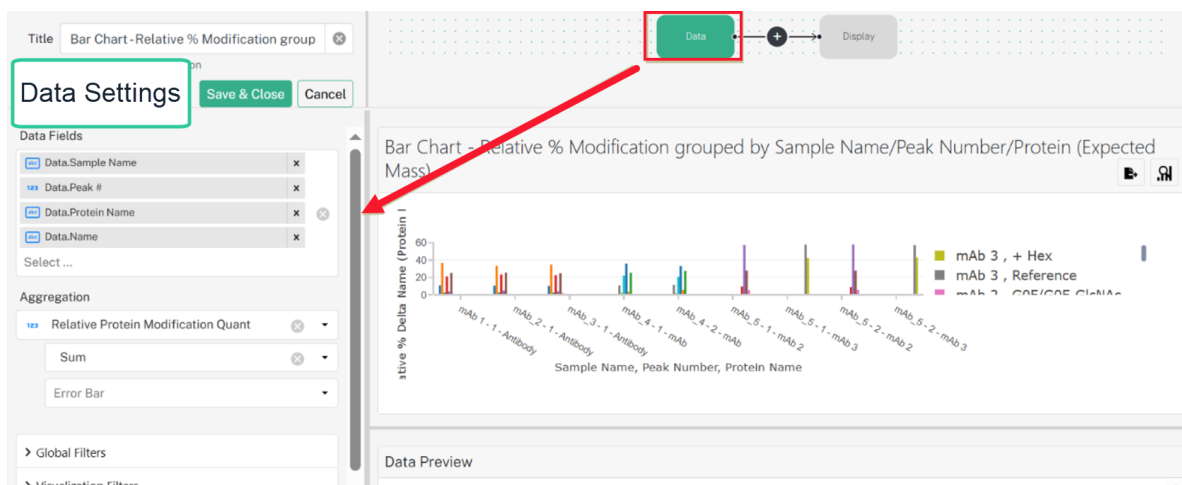


Figure 25: Data settings selected from Visualization Builder




Figure 26: Display settings selected from Visualization Builder

The **Data Preview** pane provides the user with a data grid containing the underlying data being used to generate the Visualization. Updates to the Data Preview occur in sync with any updates made to the Visualization itself, excluding any numerical display changes applied to the Visualization (since these only affect the visualization of the data rather than the underlying values themselves).

Data Preview			
Data.MS Alias Name	Glycan Short Name	SUM(Relative Glycan Quant)	
09315_E_SN_NIST_Guanidine_CTrypsin	G2F NA	0.507553603609197	
09315_E_SN_NIST_Guanidine_CTrypsin	GlcNAc	0.09663941557671231	
09315_E_SN_NIST_Guanidine_CTrypsin	Man3	0.12819015909568296	
09315_E_SN_NIST_Guanidine_CTrypsin	Man3 + GlcNAc	0.17689039263642065	
09315_E_SN_NIST_Guanidine_CTrypsin	Man3F	0.40373345402184335	
09315_E_SN_NIST_Guanidine_CTrypsin	Man4	0.038639133949044516	
09315_E_SN_NIST_Guanidine_CTrypsin	Man5	0.3014283145592117	
09315_E_SN_NIST_Guanidine_CTrypsin	other	0.6898753533623342	
09315_E_SN_NIST_Guanidine_LysC	AGly	0.508788440069641	
09315_E_SN_NIST_Guanidine_LysC	G0F	31.044163819321696	
09315_E_SN_NIST_Guanidine_LysC	G0F - GlcNAc	1.7223853112500473	
09315_E_SN_NIST_Guanidine_LysC	G1 - GlcNAc	0.011072569350648919	
09315_E_SN_NIST_Guanidine_LysC	G1F	52.70200958451611	

Figure 27: Data Preview

A red exclamation point present within the Visualization settings indicate fields that are required to be defined for or removed from the Visualization. To view all issues with the Visualization at once, the user can click the red exclamation point icon  in the corner, which will launch the **Issues** dialog.

Issues

The visualization contains the following issues:

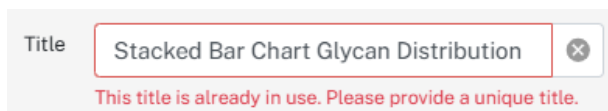
- Missing aggregation field

Ok

Figure 28: Issues dialog

Potential issues that could arise in the Visualization include not adding a title, forgetting an essential field or aggregation, or the presence of an unsupported field in a project uploaded from a Visualization created in a previous release version.

The user must provide a unique title for the Visualization. If the user tries to provide a title that is already in use, they will be notified that the title is already in use and will be unable to save the Visualization until a unique title is provided.

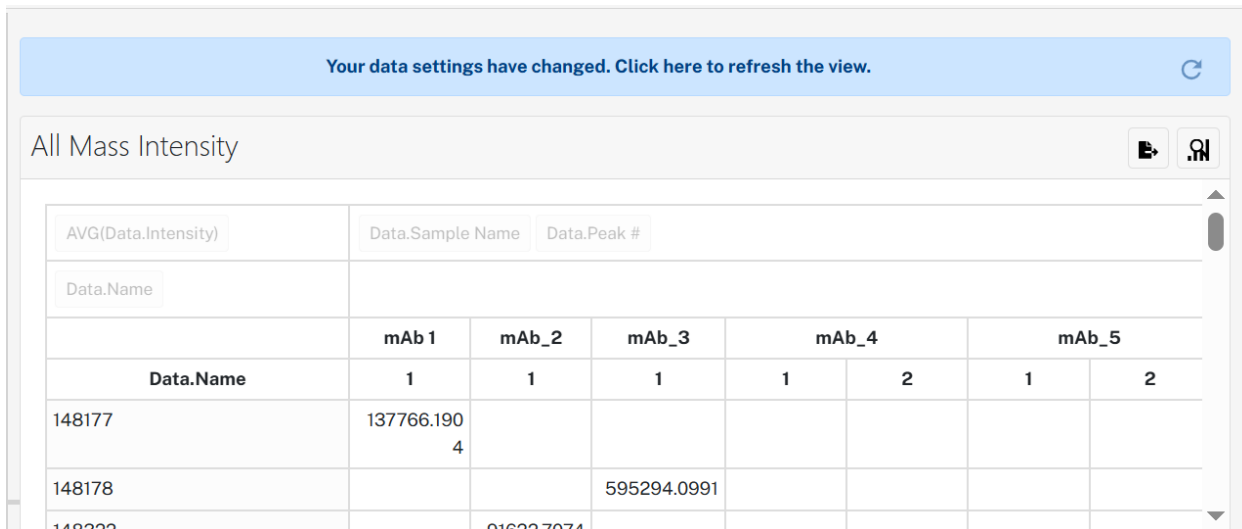


Title

This title is already in use. Please provide a unique title.

Figure 29: Please provide a unique title

Once any changes have been made to the settings, the user will be prompted with a dialog in the Visualization pane which, if clicked, will update the Visualization/Data Preview with any changes made.




Your data settings have changed. Click here to refresh the view.

All Mass Intensity

AVG(Data.Intensity)	Data.Sample Name	Data.Peak #						
Data.Name								
	mAb_1	mAb_2	mAb_3	mAb_4		mAb_5		
Data.Name	1	1	1	1	2	1	2	
148177	137766.1904							
148178			595294.0991					
148222		81622.7074						

Figure 30: User prompt to refresh the Visualization

The **refresh** button  can also be clicked to push a refresh to the Visualization/Data Preview at any time. Clicking **Save and Close** will refresh the Visualization/Data Preview one final time and save all changes before going back to the Dashboard. Clicking **Cancel** when in Edit mode will take the user back to the Dashboard, canceling any changes that were made/applied.

Selecting a Visualization

From **Display Settings**, users can select their Visualization. **Select Visualization Type** allows the user to choose a type of data representation to show in the Visualization. The value can be selected from the dropdown or searched by the user to narrow the displayed options. The selected Visualization Type will determine the modifiable values available in the tabs present under Display settings.

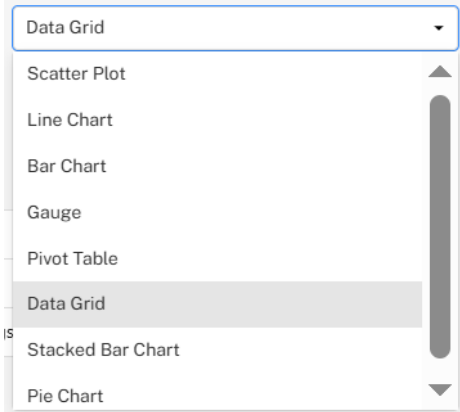
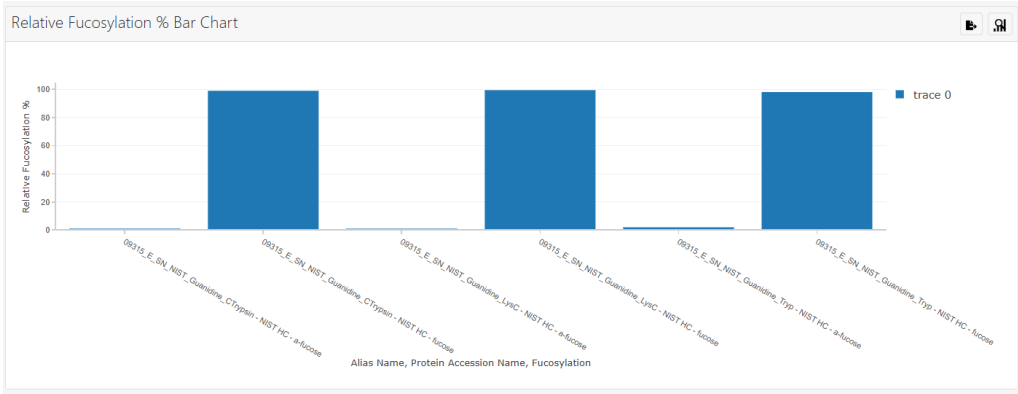


Figure 31: Select Visualization Type dropdown

Types of Visualization:

Visualization																																											
Bar Chart	<div><p>Relative Fucosylation % Bar Chart</p></div>																																										
Data Grid	<div><p>Data Grid</p><table><tr><td colspan="3">Search: 22 records...</td></tr><tr><th>Metadata.Folder</th><th>Metadata.ID</th><th>Metadata.File Alias</th></tr><tr><td>DQ-Dashboard-Data</td><td>1065.0000</td><td>001.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1065.0000</td><td>001.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1065.0000</td><td>001.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1065.0000</td><td>001.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1065.0000</td><td>001.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1065.0000</td><td>001.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1065.0000</td><td>001.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1066.0000</td><td>002.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1066.0000</td><td>002.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1066.0000</td><td>002.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1066.0000</td><td>002.blgc</td></tr><tr><td>DQ-Dashboard-Data</td><td>1066.0000</td><td>002.blgc</td></tr></table></div>	Search: 22 records...			Metadata.Folder	Metadata.ID	Metadata.File Alias	DQ-Dashboard-Data	1065.0000	001.blgc	DQ-Dashboard-Data	1065.0000	001.blgc	DQ-Dashboard-Data	1065.0000	001.blgc	DQ-Dashboard-Data	1065.0000	001.blgc	DQ-Dashboard-Data	1065.0000	001.blgc	DQ-Dashboard-Data	1065.0000	001.blgc	DQ-Dashboard-Data	1065.0000	001.blgc	DQ-Dashboard-Data	1066.0000	002.blgc	DQ-Dashboard-Data	1066.0000	002.blgc	DQ-Dashboard-Data	1066.0000	002.blgc	DQ-Dashboard-Data	1066.0000	002.blgc	DQ-Dashboard-Data	1066.0000	002.blgc
Search: 22 records...																																											
Metadata.Folder	Metadata.ID	Metadata.File Alias																																									
DQ-Dashboard-Data	1065.0000	001.blgc																																									
DQ-Dashboard-Data	1065.0000	001.blgc																																									
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DQ-Dashboard-Data	1066.0000	002.blgc																																									

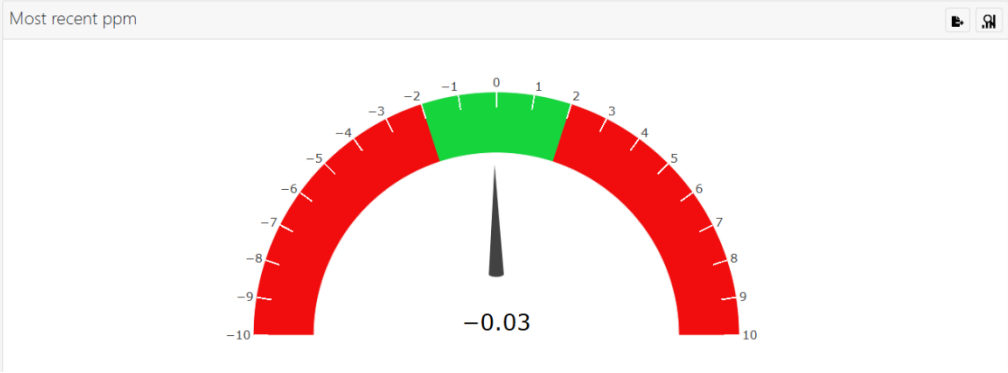
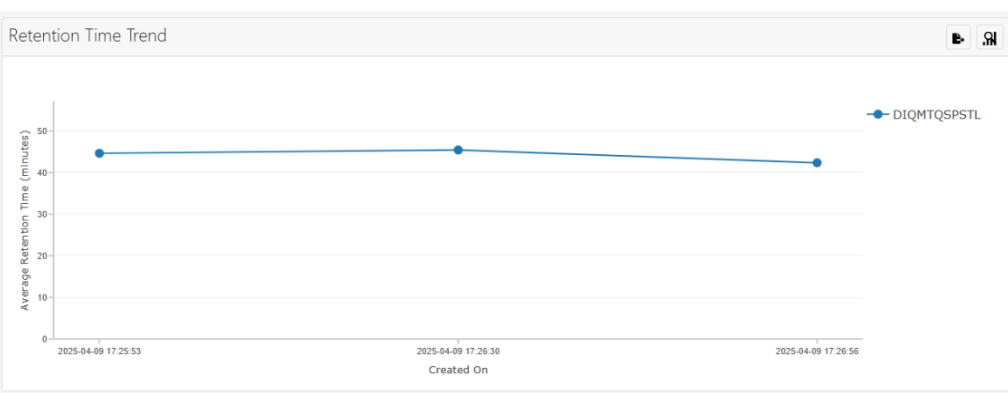

Gauge	<div><div>Most recent ppm</div><div></div></div>
Line Chart	<div><div>Retention Time Trend</div><div></div></div>
Pie Chart	<div><div>Pie Chart with Local Filter</div><div></div></div>



Figure 32: Types of Visualization

Unsupported Fields

If a Visualization created in a previous version of Byosphere and uploaded to the latest release contains any currently unsupported fields, a red box will show up around the box and a warning dialog will indicate that the unsupported data fields need to be removed to proceed with the Visualization to show queried results. Once these are removed, the user can proceed with their Dashboard as normal.

If there is a Global Filter applied that contains an unsupported field, all Visualizations will show the following error card and will not render until the Global Filter has been replaced or removed.

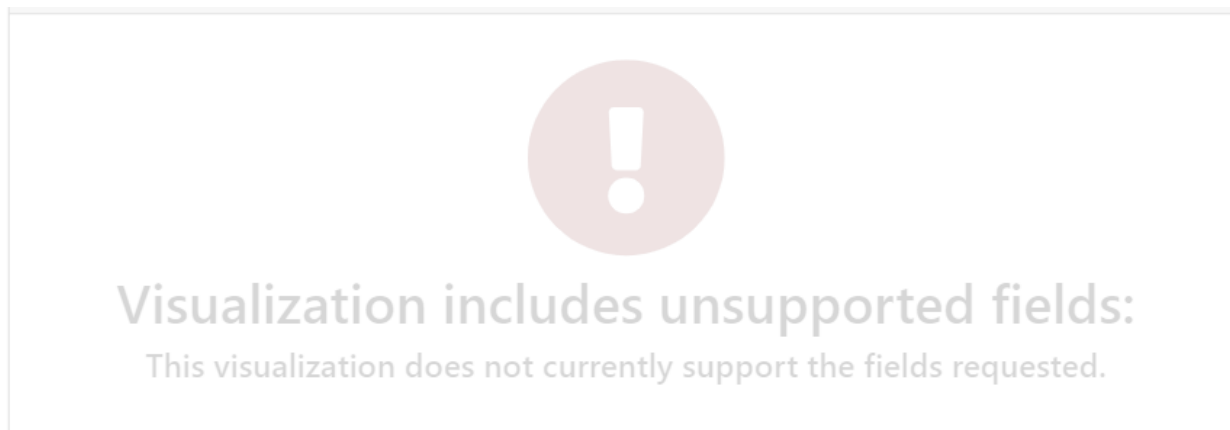


Figure 33: Unsupported fields error card

Once all unsupported fields have been removed, click the **Refresh** button to ensure that changes have been processed.

Note: The majority of these unsupported fields are planned to be reintroduced in later releases.

Line Charts and Scatter Plots

Users can select from either Line Charts or Scatter Plots. The basic Visualization settings for Line Chart and Scatter Plot Visualizations are the same.

Basic Data Settings

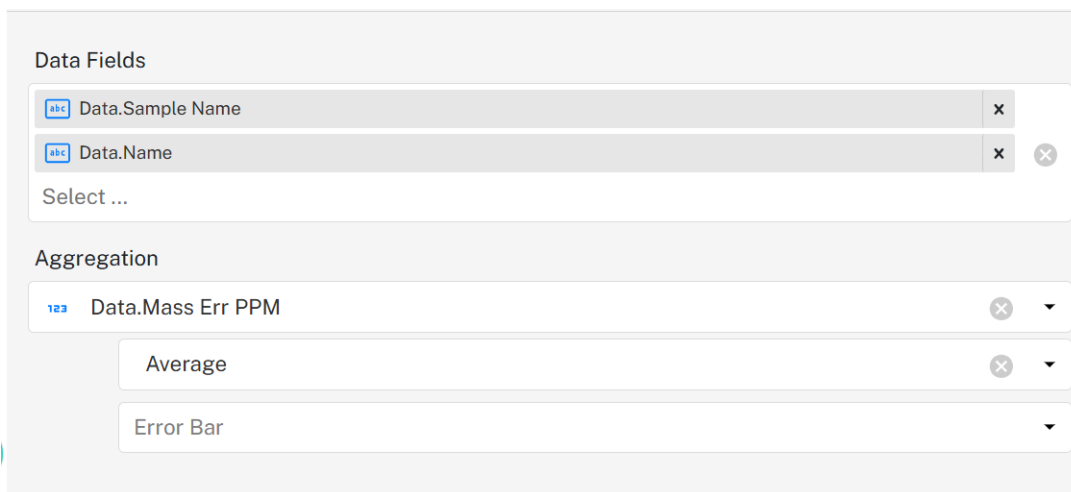
A screenshot of the "Basic Data Settings" interface. It is divided into two main sections: "Data Fields" and "Aggregation". The "Data Fields" section has a search bar with "abc" and a list of selected fields: "Data.Sample Name" and "Data.Name". Each field has a small "x" icon to its right. Below the list is a "Select ..." button. The "Aggregation" section has a search bar with "123" and a list of selected aggregation options: "Data.Mass Err PPM", "Average", and "Error Bar". Each option has a small "x" icon to its right. The interface is light gray with white input fields and buttons.

Figure 34: Example of Basic Settings for Line Charts

- **Group By Fields (X axis):** Field(s) to be represented on the X-axis. The user has the option to select multiple fields. Fields can be selected directly from the dropdown, or the user can type within the box to filter through the available fields to find a specific field. Users can select both Data Source Fields and Metadata fields. In this case, the field **Data.MS Alias Name** has been selected, and the user has the option to search for and add additional fields.

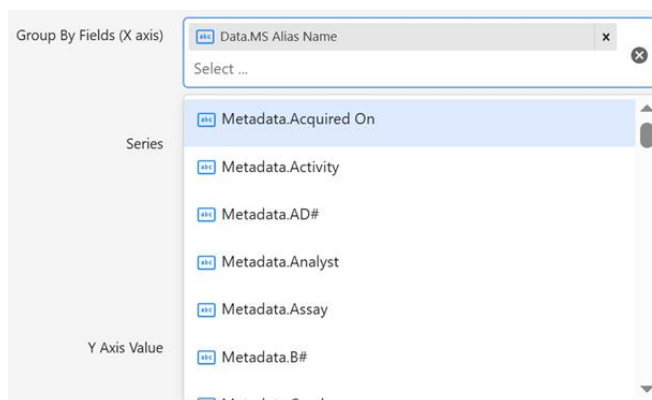


Figure 35: Group by Fields (X axis)

- **Series:** Field to group for separate series in a chart. In the example below, multiple fields have been added to be included in the series grouping.

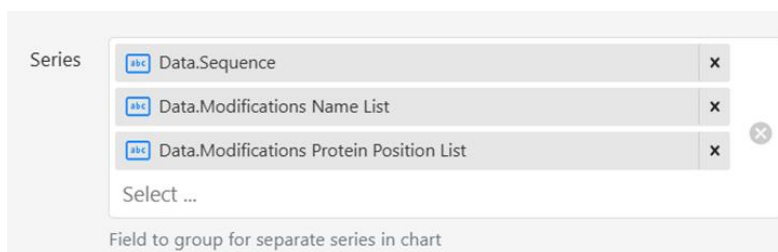


Figure 36: Series field

If multiple fields have been added, they are clustered within the Visualization to represent groups combining values from each field as shown below:

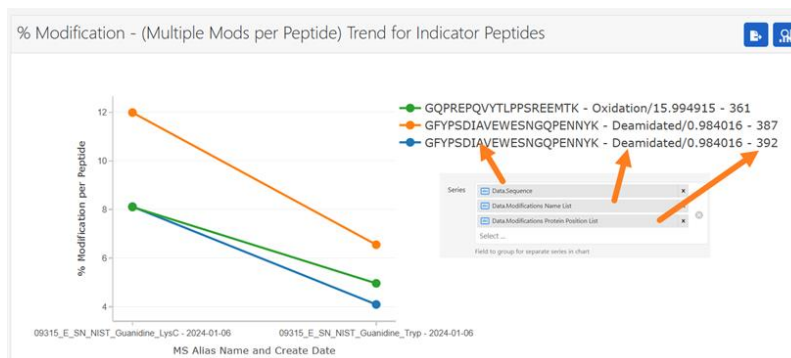


Figure 37: Multiple fields grouped into separate series

- **Y Axis Value:** Field(s) to be represented on the Y-axis. Requires an aggregation function.
 - **Aggregation:** Available aggregation options will depend upon the data type selected e.g., Data.Apex Posit time has all aggregations available, while Data.Modifications Name List is only a string field and only has count available.

Data Type	Available Aggregations
-----------	------------------------

Numeric	Average, count, max, min, standard deviation, standard deviation (Pop), standard deviation(Sample), sum, variance, variance (Pop), variance (Sample)
String	Count
Date	Count, max, min

Figure 38: Aggregation Types

X-axis and Y-axis labels are automatically populated within the Visualization once a field has been selected and applied. If the field(s) is (are) removed and another added, the user will have to manually update the X-axis or Y-axis label values under the Group By Axis and Value Axis tabs.

Note: If you start by selecting an aggregation function, your data fields will be filtered based upon the selected function; for instance, if you select a numeric aggregation e.g., average, text fields such as “Sample name” will not appear.

- **Display as relative to/Groups to normalize on:** These settings support the following normalization calculations:

- Min (where min is 100%)
- Max (where max is 100%)
- Sum (where sum is 100%)

Options for Groups to Normalize By include:

- Series
- Group By

Note that these settings only pertain to Line Charts, Bar Charts, and Scatter Plots (excluding Stacked Bar Charts).

- **Error Bars:** Error bar values can be added for Min/Max, Std. Dev, 2 Std. Dev, and 3 Std. Dev. All values are + or - of the aggregation selected, with the exception of min/max. When a user selects a +/- Min/Max the error bar will function as a range (low value is the min and the highest value is the max). If Variance is used as the aggregation error bars will *not* be present. Note that SDTEV.P and VAR.P are used when determining error values.

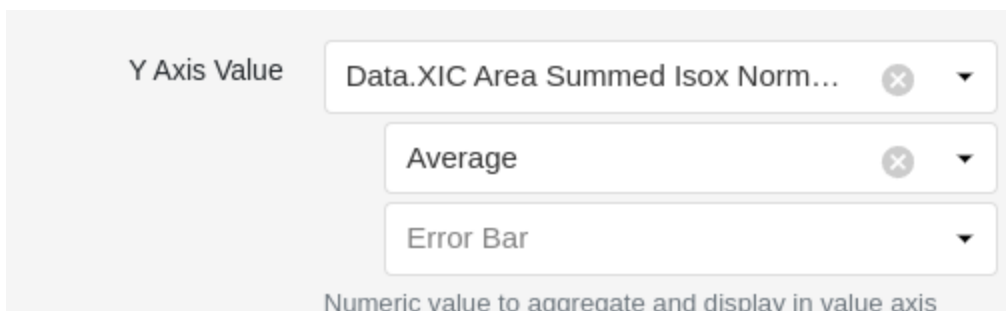


Figure 39: Error bar settings under Y Axis Value

Basic Display Settings

Select Visualization Type: Line Chart

Chart type

Group By Fields (X axis): Data.Sample Name

Select ...

Field to use for the x axis

Series: Data.Name

Select ...

Field to group for separate series in chart

Y Axis Value: AVG(Data.Mass Err PPM)

Numeric value to aggregate and display in value axis

Low Error Bar: Select values

Lower bound for the error bar

High Error Bar: Select values

Higher bound for the error bar

Figure 40: Basic Display Settings for Line and Bar Chart Visualizations

As of release v5.10, users are directed to **Select Visualization Type** within the basic Display settings. In addition, the fields used to build the Visualization itself, including Group By Fields, Series, and Y Axis value, are all specified within the Display settings. Available fields are based upon the fields selected within the Data Settings.

Users can also error bars within the Display settings for Line Charts.

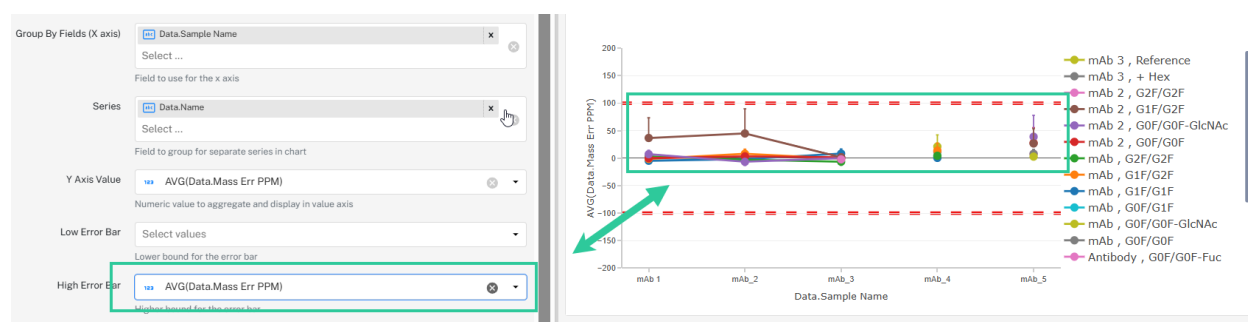
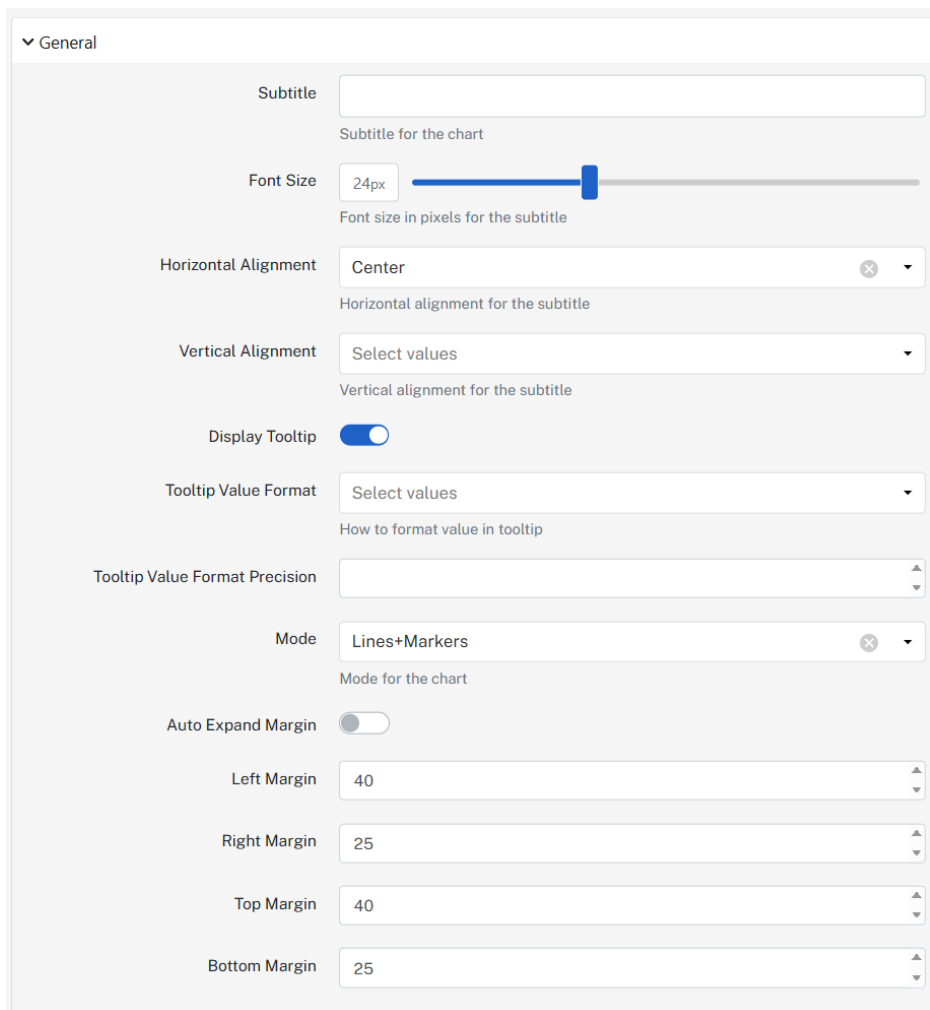


Figure 41: Error bars

Additional Display Settings

General



The screenshot shows the 'General' tab of a settings panel. It contains the following controls:

- Subtitle**: A text input field with a placeholder 'Subtitle for the chart'.
- Font Size**: A slider control set to '24px' with a label 'Font size in pixels for the subtitle'.
- Horizontal Alignment**: A dropdown menu set to 'Center' with a label 'Horizontal alignment for the subtitle'.
- Vertical Alignment**: A dropdown menu set to 'Select values' with a label 'Vertical alignment for the subtitle'.
- Display Tooltip**: A toggle switch that is currently turned on.
- Tooltip Value Format**: A dropdown menu set to 'Select values' with a label 'How to format value in tooltip'.
- Tooltip Value Format Precision**: A numeric input field.
- Mode**: A dropdown menu set to 'Lines+Markers' with a label 'Mode for the chart'.
- Auto Expand Margin**: A toggle switch that is currently turned off.
- Left Margin**: A numeric input field set to 40.
- Right Margin**: A numeric input field set to 25.
- Top Margin**: A numeric input field set to 40.
- Bottom Margin**: A numeric input field set to 25.

Figure 42: General tab

The **General** tab under the **Display Settings** enables the user to make modifications to the chart. The user can add a subtitle to any kind of chart and adjust its size/alignment accordingly. If **Display Tooltip** is enabled, hovering over a data point will show a popup of its value with the format and precision determined by the user (e.g., hundredths place, thousandths place, percentage).

All non-table Visualizations (e.g., Line Charts, Gauges, Scatter Plots) have options under the **General Display** tab to adjust the margins of the Visualization.



This screenshot shows a section of the settings panel for margin adjustments:

- Auto Expand Margin**: A toggle switch that is currently turned off.
- Left Margin**: A numeric input field set to 40.
- Right Margin**: A numeric input field set to 25.
- Top Margin**: A numeric input field set to 40.
- Bottom Margin**: A numeric input field set to 25.

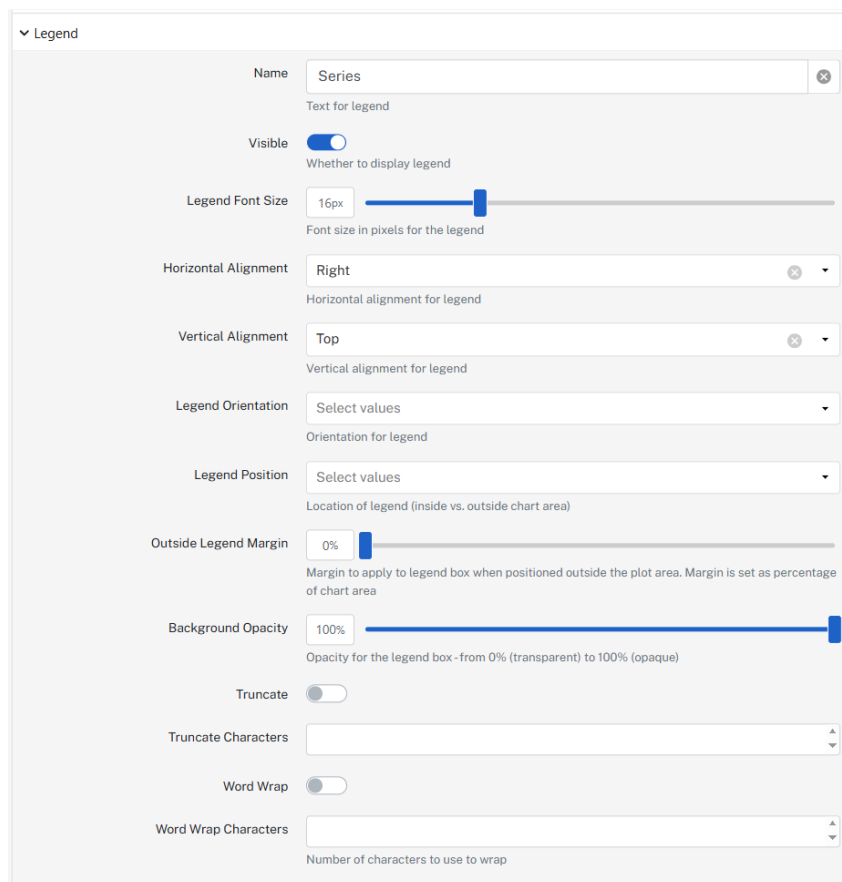
Figure 43: Margin settings

Increasing the value of the Margin for each direction will increase the space on that side (e.g., increasing the **Left Margin** will create more space between the edge of the Visualization itself (for instance, the tick marks) and the Visualization settings panel).

If **Auto Expand Margin** is toggled **on**, the dimensions of the Visualization will automatically adjust so that any tick labels are not cut off.

Legend

The **Legend** tab enables the user to add a Legend to their chart and configure its position and visibility.



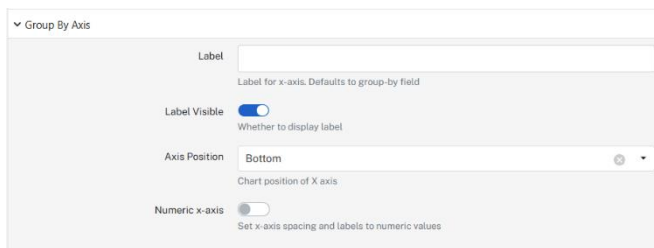
The Legend tab settings panel includes the following controls:

- Name:** A text input field containing "Series" with a clear button (X).
- Text for legend:** A label for the legend text.
- Visible:** A toggle switch that is currently turned on, with the label "Whether to display legend".
- Legend Font Size:** A slider set to "16px" with the label "Font size in pixels for the legend".
- Horizontal Alignment:** A dropdown menu set to "Right" with the label "Horizontal alignment for legend".
- Vertical Alignment:** A dropdown menu set to "Top" with the label "Vertical alignment for legend".
- Legend Orientation:** A dropdown menu set to "Select values" with the label "Orientation for legend".
- Legend Position:** A dropdown menu set to "Select values" with the label "Location of legend (inside vs. outside chart area)".
- Outside Legend Margin:** A slider set to "0%" with the label "Margin to apply to legend box when positioned outside the plot area. Margin is set as percentage of chart area".
- Background Opacity:** A slider set to "100%" with the label "Opacity for the legend box - from 0% (transparent) to 100% (opaque)".
- Truncate:** A toggle switch that is currently turned off.
- Truncate Characters:** A text input field with up and down arrow buttons.
- Word Wrap:** A toggle switch that is currently turned off.
- Word Wrap Characters:** A text input field with up and down arrow buttons and the label "Number of characters to use to wrap".

Figure 44: Legend tab

Group By Axis

The **Group By Axis** tab provides options for modifying the x-axis label and positioning.



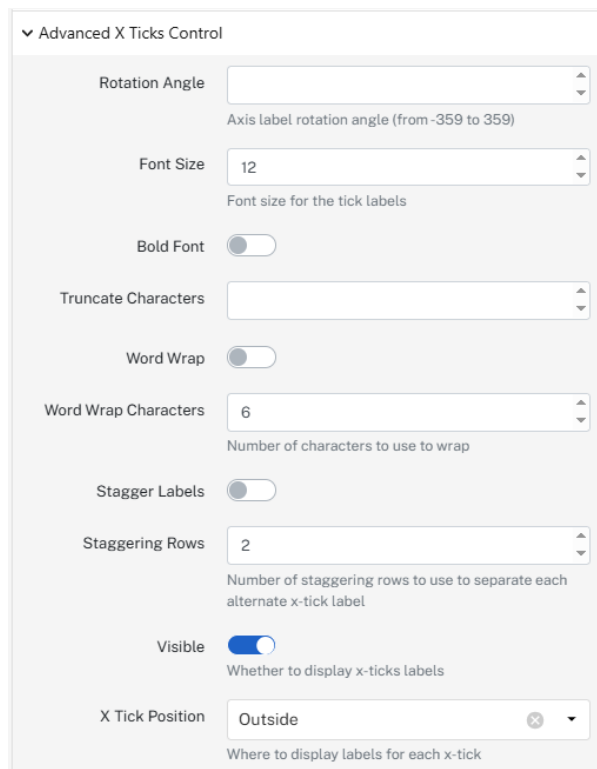
The Group By Axis tab settings panel includes the following controls:

- Label:** A text input field with the label "Label for x-axis. Defaults to group-by field".
- Label Visible:** A toggle switch that is currently turned on, with the label "Whether to display label".
- Axis Position:** A dropdown menu set to "Bottom" with the label "Chart position of X axis".
- Numeric x-axis:** A toggle switch that is currently turned off, with the label "Set x-axis spacing and labels to numeric values".

Figure 45: Group By Axis

Advanced X Tickets Control

The **Advanced X Ticks Control** tab provides several tools that can be used to refine the readability of the labels on the x-axis.



Advanced X Ticks Control

Rotation Angle Axis label rotation angle (from -359 to 359)

Font Size Font size for the tick labels

Bold Font ☐

Truncate Characters

Word Wrap ☐

Word Wrap Characters Number of characters to use to wrap

Stagger Labels ☐

Staggering Rows Number of staggering rows to use to separate each alternate x-tick label

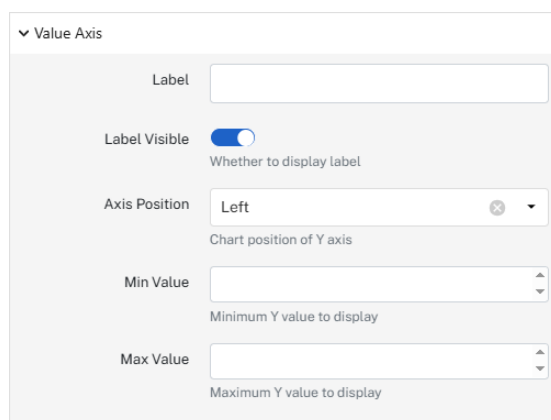
Visible ☒ Whether to display x-ticks labels

X Tick Position Where to display labels for each x-tick

Figure 46: Advanced X Tickess Control

Value Axis

The **Value Axis** tab provides options for modifying the position of and the values and labels shown on the y-axis.



Value Axis

Label

Label Visible ☒ Whether to display label


Axis Position Chart position of Y axis

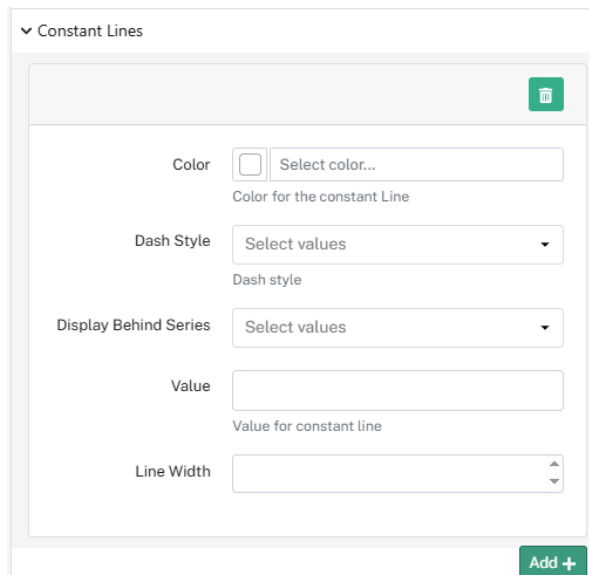
Min Value Minimum Y value to display

Max Value Maximum Y value to display

Figure 47: Value Axis tab

Constant Lines

The **Constant Lines** tab allows the user to modify the color, style, size, and value for any constant lines added to the chart. Constant lines can be added by clicking **Add** and deleted by clicking the blue trash can icon  at the top of the window.

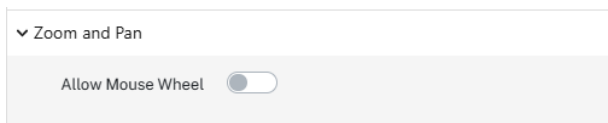


The Constant Lines tab interface includes a title bar with a dropdown arrow and the text "Constant Lines". Below the title bar is a light gray header area containing a blue trash can icon. The main content area contains several settings: a "Color" section with a color picker icon and a "Select color..." text input; a "Dash Style" section with a "Select values" dropdown menu; a "Display Behind Series" section with a "Select values" dropdown menu; a "Value" section with a text input; and a "Line Width" section with a vertical slider. Each setting has a descriptive label below it. At the bottom right of the main content area is a green "Add +" button.

Figure 48: Constant Lines tab

Zoom and Pan

Allow Mouse Wheel, if checked, enables the use of the mouse wheel to zoom in and out when the mouse is hovering over the Visualization.

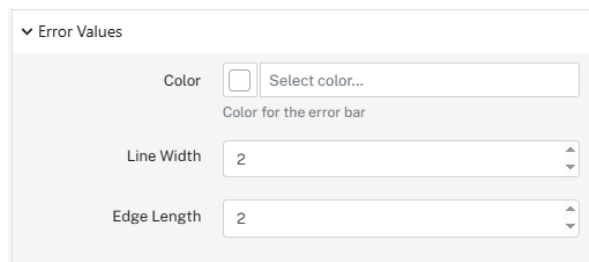


The Zoom and Pan tab interface features a title bar with a dropdown arrow and the text "Zoom and Pan". Below the title bar is a light gray header area. The main content area contains a single setting: a toggle switch labeled "Allow Mouse Wheel".

Figure 49: Zoom and Pan tab

Error Values

The **Error Values** tab provides users with options to modify the characteristics of the error bar, if one is present. Error bars are added within the basic settings. Note: Error Values do not apply to Stacked Bar Charts.



The Error Values tab interface includes a title bar with a dropdown arrow and the text "Error Values". Below the title bar is a light gray header area. The main content area contains three settings: a "Color" section with a color picker icon and a "Select color..." text input; a "Line Width" section with a vertical slider set to 2; and an "Edge Length" section with a vertical slider set to 2. Each setting has a descriptive label below it.

Figure 50: Error Values tab

Annotations

The Annotations tab provides users with the ability to create one or multiple Annotations within their Visualization. Annotations can be added by clicking **Add +** and providing the following information:

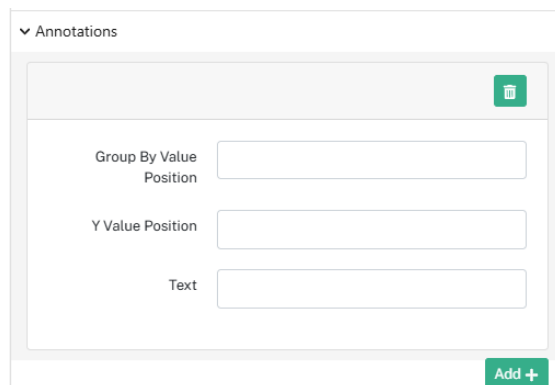


Figure 51: Annotations tab

Bar Charts and Stacked Bar Charts

Users can select from either **Bar Charts** or **Stacked Bar Charts**. The basic Visualization settings for all Bar Chart Visualizations are the same (excluding Error Bars, which are not present for Stacked Bar Charts).

Basic Data and Display Settings

Basic Data and Display Settings are the same for both Line Charts and Bar Charts. See [Basic Data Settings](#) and [Basic Display Settings](#) above for more information. Any exceptions have been outlined below.

Within the General settings, Error Bars do not apply to **Stacked Bar Charts**.

Note that if a Chart-type Visualization is created (including Line Charts and Scatter Plots) and then switched to another Chart-type Visualization, all applicable settings should remain in place.

Display Settings

Refer to [Display Settings](#) for Line Charts and Scatter Plots as the settings for Bar Charts are the same, with two exceptions. Under **Display > General** for Bar Charts, **Bar Normalization** provides the ability to normalize values based upon each group-by value, with the following options: **Fraction**, **Percent**, or **None** (default).

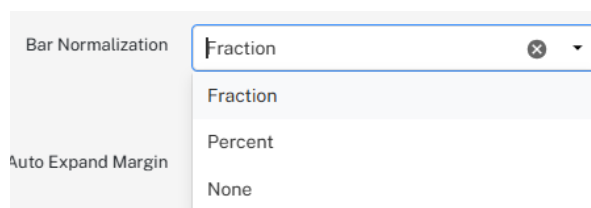
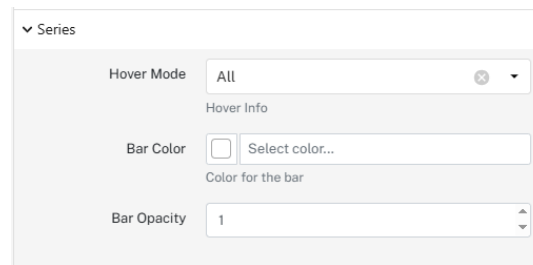


Figure 52: Bar Normalization

There is one additional tab available under Display Settings for Bar Charts called **Series**. The **Series** tab (applicable to the Bar Chart and Stacked Bar Chart only) provides options for highlighting series elements.

Note: Color and opacity options do not apply to Stacked Bar Charts.



Series

Hover Mode: All

Hover Info

Bar Color: ☐ Select color...

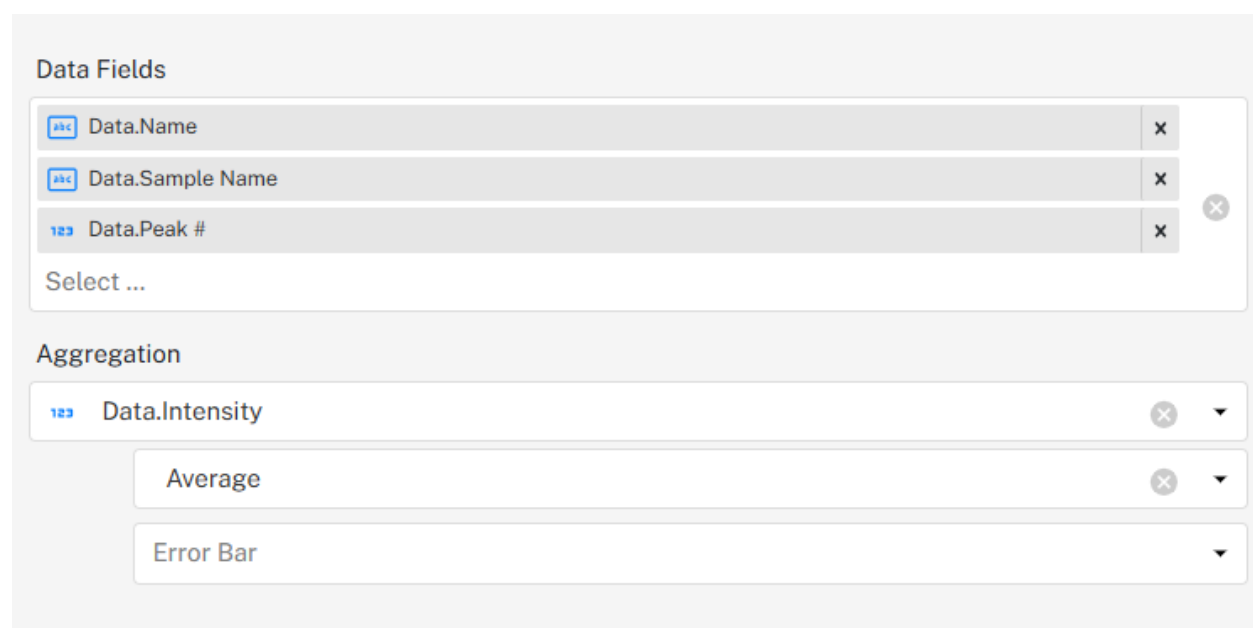
Color for the bar

Bar Opacity: 1

Figure 53: Series tab

Pivot Tables

Basic Data Settings



Data Fields

<input checked="" type="checkbox"/> Data.Name	x
<input checked="" type="checkbox"/> Data.Sample Name	x
<input checked="" type="checkbox"/> Data.Peak #	x
Select ...	

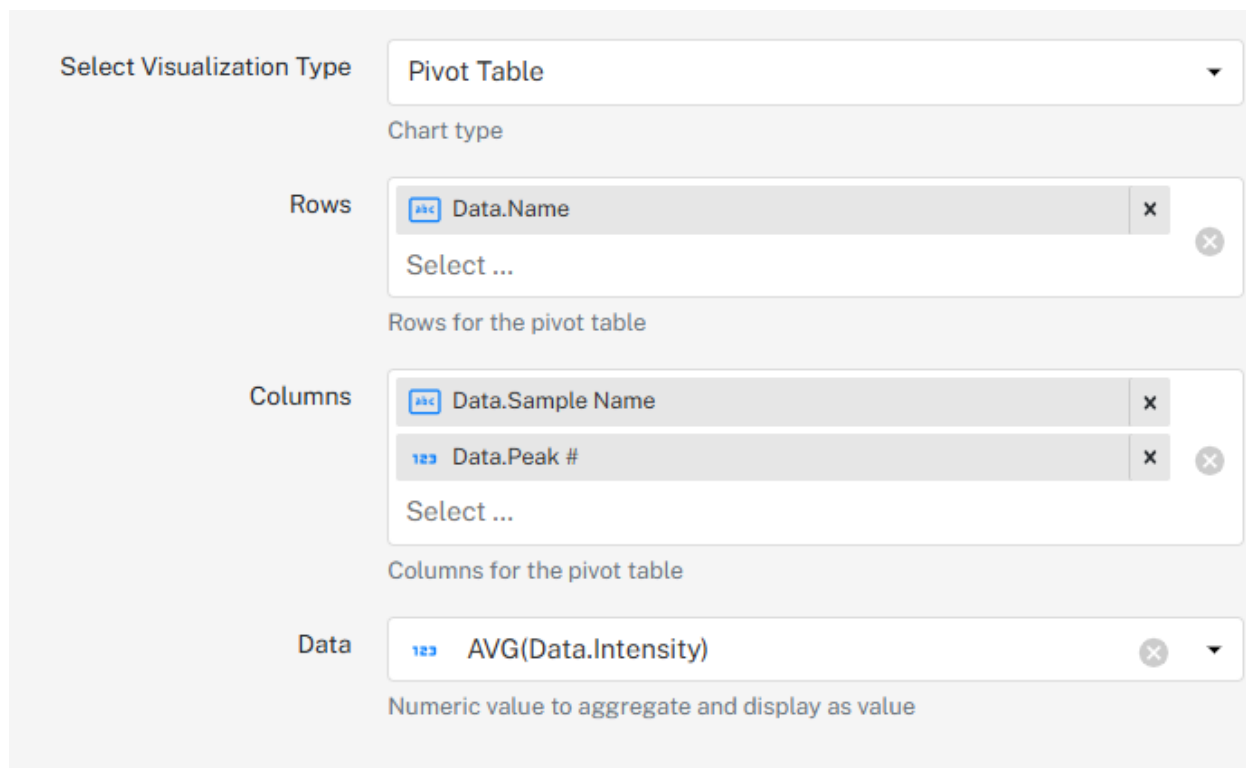
Aggregation

<input checked="" type="checkbox"/> Data.Intensity	x
Average	x
Error Bar	

Figure 54: Basic Data Settings

- **Data Fields:** Select data fields which can be added to the Visualization and configured within the Display settings
- **Aggregation:** Numeric value to aggregate and display as value

Basic Display Settings



Select Visualization Type: Pivot Table

Chart type

Rows: Data.Name

Columns: Data.Sample Name, Data.Peak #

Data: AVG(Data.Intensity)

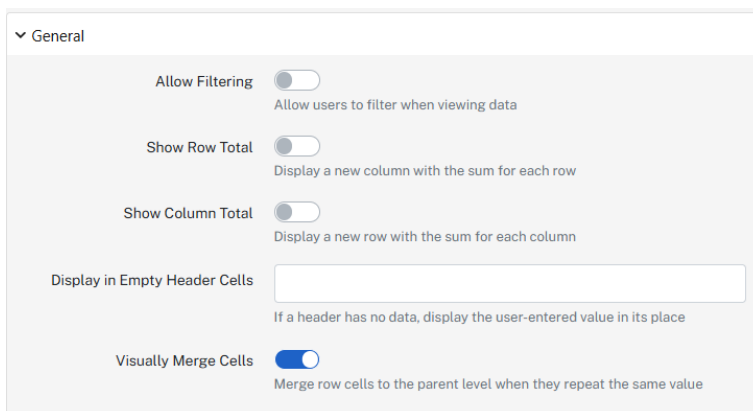
Numeric value to aggregate and display as value

Figure 55: Basic Display Settings for Pivot Table Visualizations

As of release v5.10, users are directed to **Select Visualization Type** within the basic Display settings. In addition, the fields used to build the Visualization itself, including the rows, columns, and data aggregated and displayed within the Pivot Table, are specified within the Basic Display Settings. Available fields are based upon the fields selected within the Data Settings.

Additional Display Settings

General



General

Allow Filtering: ☐ Allow users to filter when viewing data

Show Row Total: ☐ Display a new column with the sum for each row

Show Column Total: ☐ Display a new row with the sum for each column

Display in Empty Header Cells: If a header has no data, display the user-entered value in its place

Visually Merge Cells: ☒ Merge row cells to the parent level when they repeat the same value

Figure 56: General Display Settings for Pivot Table Visualizations

The **General** tab under the Display tab provides the user with the ability to modify their view of the pivot table, including adding row and column totals and designating the value provided when there is a blank cell.

Allow Filtering provides the user with a filter search within each column of the pivot table. Typing in a value will filter the results in that column to include only cells that meet the query.

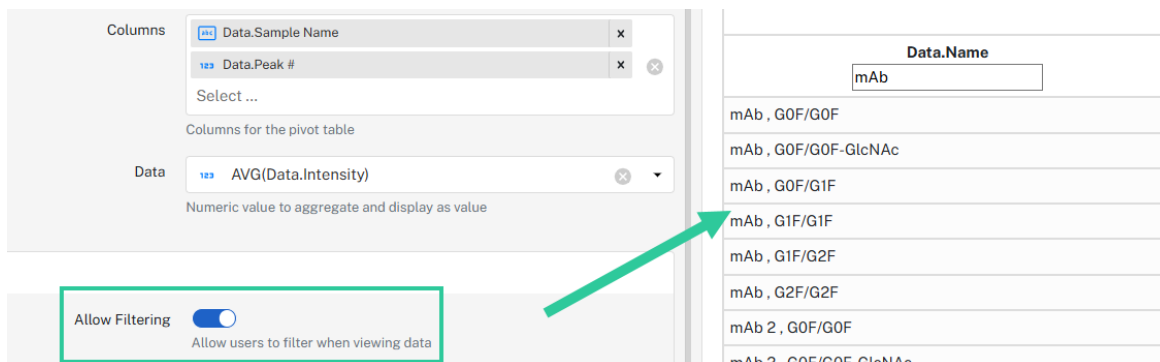


Figure 57: Narrowing results with filtering

Display in Empty Header Cells will provide a user-entered value in the place of a blank cell when there is no data in the cell. The default value is <NO VALUE>.

Field Panel

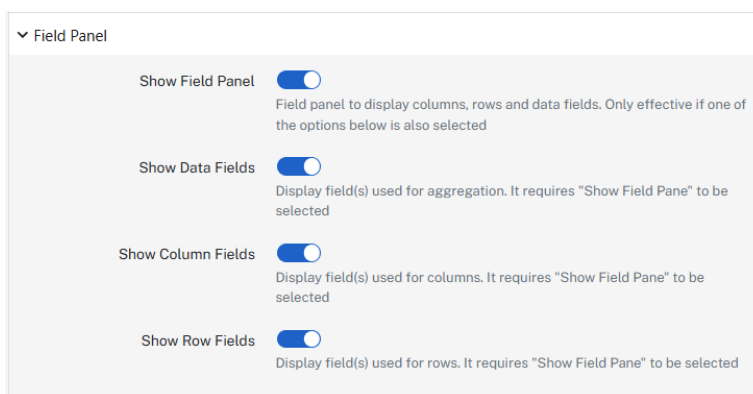


Figure 58: Field Panel Tab in Pivot Table Visualization

The **Field Panel** tab toggles visibility of the **Field Panel** as well as data fields and row/column fields (which appear in the Field Panel). Field panels visibility is enabled by default.

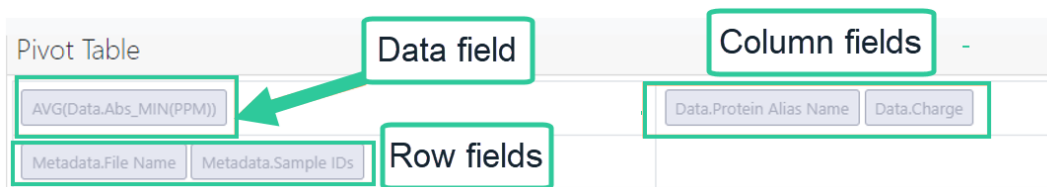
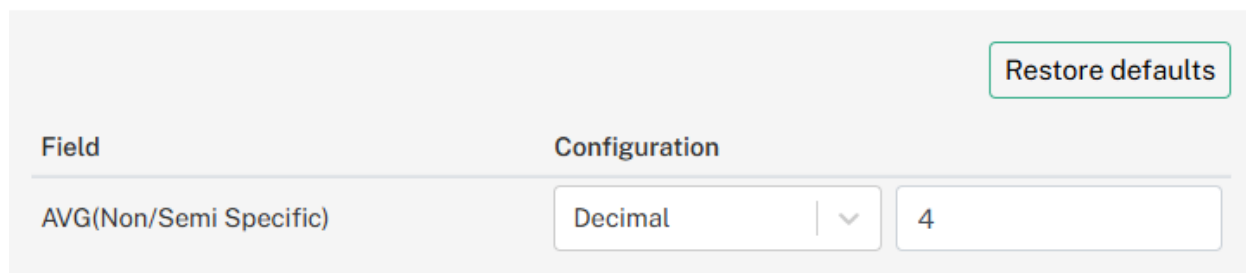


Figure 59: The Field Panel, showing all Fields

Numerical Display Settings

▼ Numerical Display Settings



Field	Configuration
AVG(Non/Semi Specific)	Decimal 4

Figure 60: Numerical Display Settings

The **Numerical Display Settings** tab allows the user to specify the configuration and number of decimal places to include for each numerical field present in the Visualization.

Data Grids

Basic Data Settings


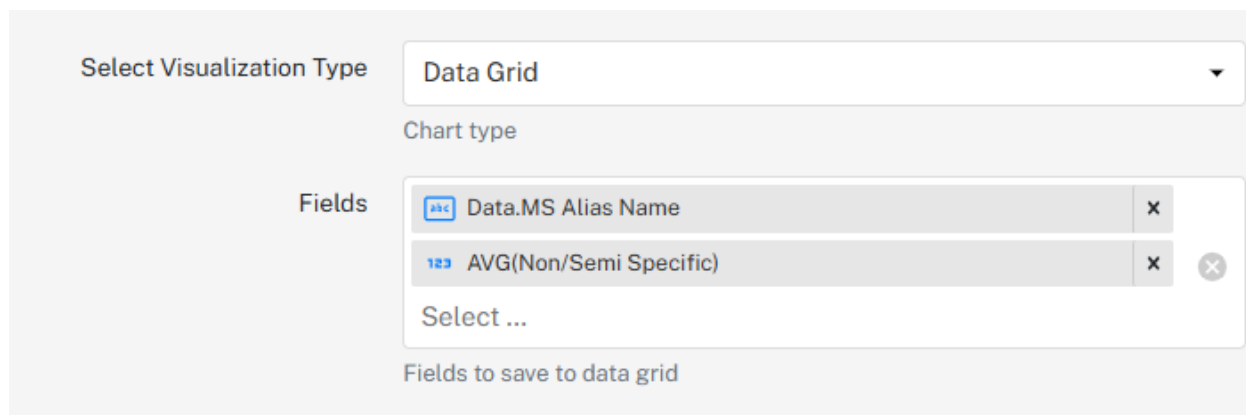


Figure 61: Basic Data Settings for Data Grid Visualizations

- **Data Fields:** Data fields that can be selected in Display Settings to be included in the Data Grid
- **Aggregations:**
 - **Aggregation:** Numeric value to aggregate and display as value
 - **Error bar:** Error bar values can be added for Min/Max, Std. Dev, 2 Std. Dev, and 3 Std. Dev. All values are + or - of the aggregation selected, with the exception of min/max. When a user selects a +/- Min/Max the error bar will function as a range (low value is the min and the highest value is the max). If Variance is used as the aggregation error bars will not be present. Note that SDTEV.P and VAR.P are used when determining error values.

Basic Display Settings



The interface shows the 'Select Visualization Type' dropdown set to 'Data Grid'. Below it, the 'Chart type' label is present. The 'Fields' section contains a list of fields: 'Data.MS Alias Name' (with a blue icon) and 'AVG(Non/Semi Specific)' (with a blue icon). Each field has a close button (X). A 'Select ...' button is at the bottom of the list. Below the fields list, the text 'Fields to save to data grid' is displayed.

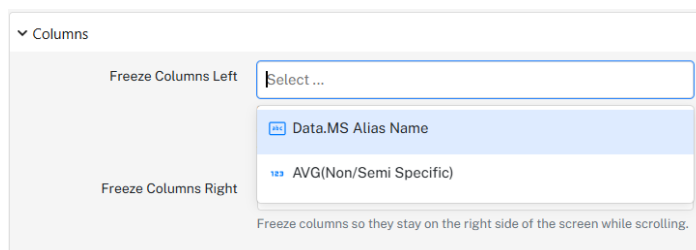
Figure 62: Basic Display Settings for Data Grid Visualizations

As of release v5.10, users are directed to **Select Visualization Type** within the basic Display setting. For Data Grid visualizations, users only need to specify a list of fields to add to the Data Grid. Available fields are based upon the fields selected within the Data Settings.

Additional Display Settings

Columns

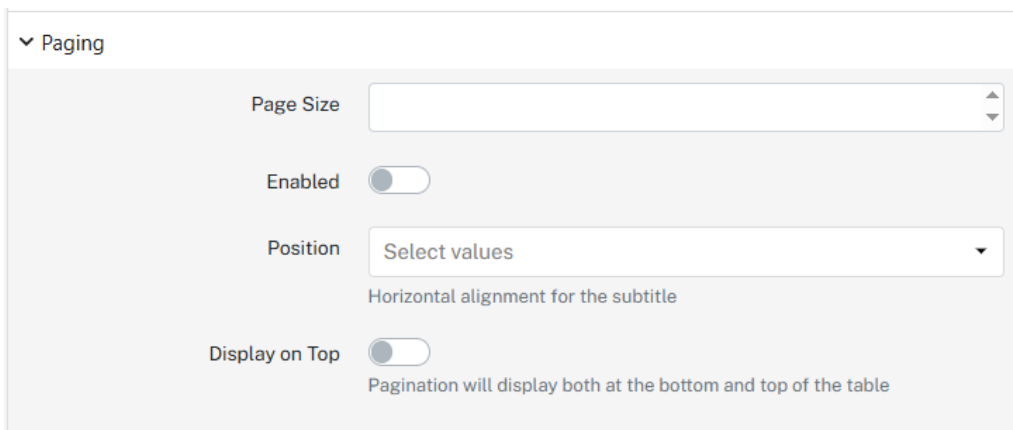
Columns can be frozen to the left and right sides of a Data Grid Visualization, selectable from the show/hide fields under the Column Display Settings tab. Only the columns present in the Visualization will be listed in the dropdown. Selecting the same column for both sides will result in the column being frozen to the left side.



The 'Columns' tab is shown with a dropdown menu. The 'Freeze Columns Left' section has a 'Select ...' dropdown. The 'Freeze Columns Right' section has a list of fields: 'Data.MS Alias Name' (with a blue icon) and 'AVG(Non/Semi Specific)' (with a blue icon). Below the list, the text 'Freeze columns so they stay on the right side of the screen while scrolling.' is displayed.

Figure 63: Columns tab for Data Grid Visualization

Paging



▼ Paging

Page Size

Enabled ☐

Position

Horizontal alignment for the subtitle

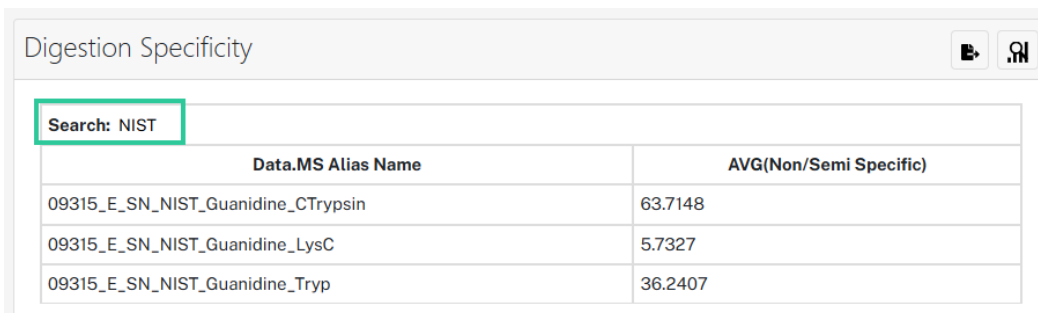
Display on Top ☐

Pagination will display both at the bottom and top of the table

Figure 64: Paging Tab for Data Grid Visualization

Within the **Paging** tab the user can designate the number of rows to be included on each page of the Data Grid. **Position** dictates where the page selector is within the Grid (can be on the left or right side). The user can also choose to display the page selector at the top of the Data Grid.

Within the Data Grid, the user can search *all* records present within the table. The search utility can be found at the top of the grid.



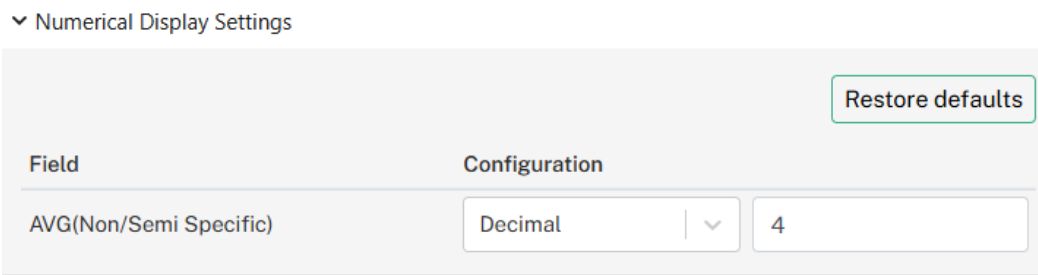
Digestion Specificity

Search: NIST

Data.MS Alias Name	AVG(Non/Semi Specific)
09315_E_SN_NIST_Guanidine_CTrypsin	63.7148
09315_E_SN_NIST_Guanidine_LysC	5.7327
09315_E_SN_NIST_Guanidine_Tryp	36.2407

Figure 65: Search result filtered based upon user query

Numerical Display Settings



▼ Numerical Display Settings

Restore defaults

Field	Configuration
AVG(Non/Semi Specific)	Decimal 4

Figure 66: Numerical Display Settings

The **Numerical Display Settings** tab allows the user to specify the configuration and number of decimal places to include for each numerical field present in the Visualization.

Gauges

Basic Data Settings

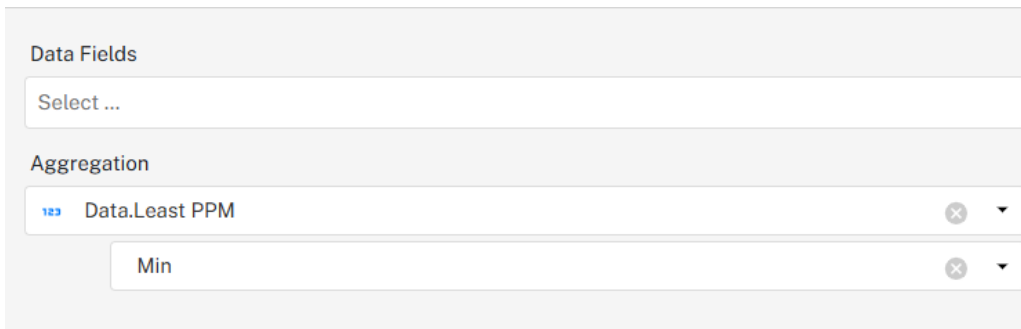


Figure 67: Basic Data Settings for the Gauge Visualization

- **Data Fields:** Data fields that can be selected in the Display Settings to be included in the Gauge Visualization
- **Aggregations:**
 - **Aggregation:** Numeric value to aggregate and display as value

Basic Display Settings

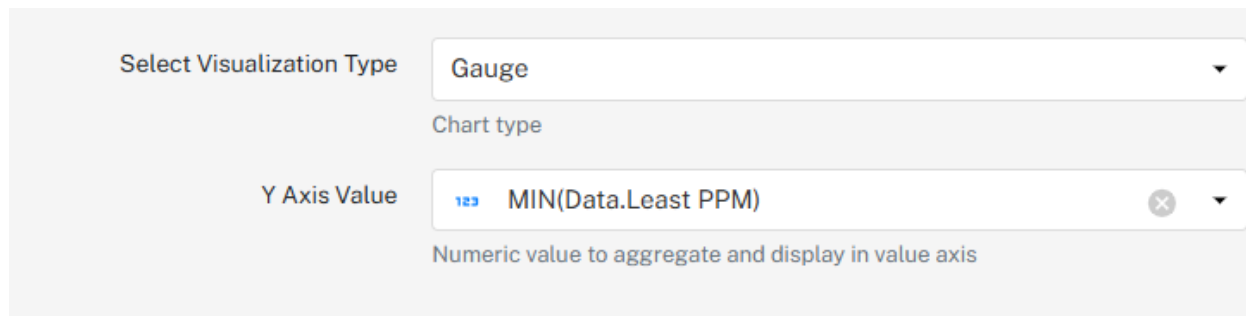


Figure 68: Basic Display Settings for Gauge Visualizations

As of release v5.10, users are directed to **Select Visualization Type** within the basic Display settings. In addition, users need to specify the Y Axis value to be used in the Gauge. Available fields are based upon the fields selected within the Data Settings.

Additional Display Settings

General

General

Mode: Number + Gauge
Mode for the chart

Value Indicator: Needle
How to indicate the value in gauge (needle vs. marker)

Needle Position: Below
Whether to set needle above or below number (if applicable)

Value Format: Select values
How to format the values displayed in the gauge

Value Format Precision:
Precision to use with value format

Subtitle: DIQMTQSPSTL
Subtitle for the chart

Font Size: 18px
Font size in pixels for the subtitle

Horizontal Alignment: 0.50
Horizontal alignment for the subtitle, from 0 (left) to 1 (right), independent of margin space

Vertical Alignment: 0.95
Vertical alignment for the subtitle, from 0 (bottom) to 1 (top), independent of margin space

Color: #a0a6a0
Color

Left Margin: 25

Right Margin: 50

Top Margin: 50

Bottom Margin: 25

Figure 69: General Settings for Gauge (Circular) Visualization

The **General** tab under **Display** allows the user to add a subtitle to the Visualization and adjust its alignment in relation to the Gauge.

The user can also determine how the gauge value is indicated with the **Value Indicator** option, which allows the user to choose either a needle indicator or a **Marker**. This number can be shown above or below the number on the gauge.

See [Margin Settings](#) for details about Margin controls.

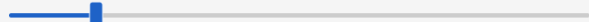
Ticks


▼ Ticks

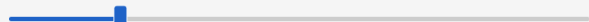
Start Value
Starting value for the gauge. It has to be lower than end value

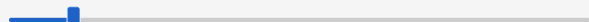
End Value
Ending value for the gauge. It has to be greater than start value

Tick Interval
Units to use for the tick interval

Font Size 
Font size in pixels for the tick mark

Location 
Location for tick marks (inside vs. outside)

Tick Length 
Length for tick marks (in pixels)

Tick Width 
Width for tick marks (in pixels)




Tick Line Color 
Color for the tick line

Figure 70: Tick Settings for Gauge Visualization

The **Tick** settings set the starting and ending value of the entire gauge, as well as the tick interval, tick color, tick length, and other characteristics.

Number

▼ Number

Font Color  
Font color for indicator number

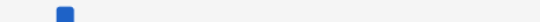
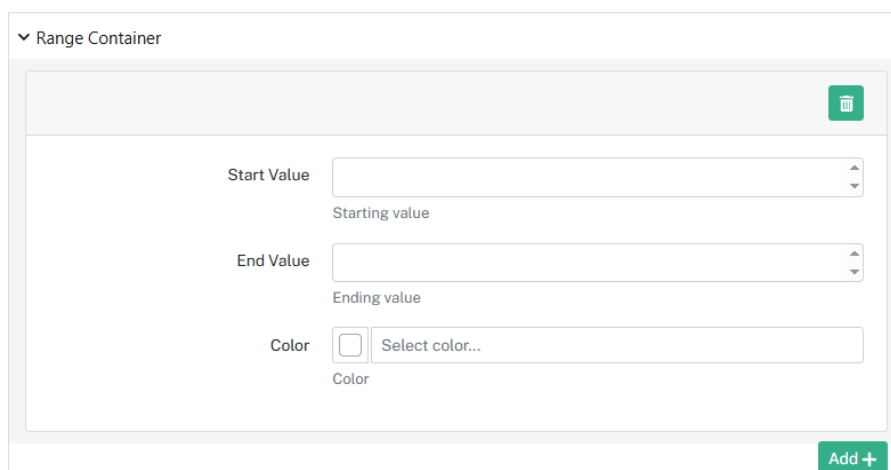
Font Size 
Font size in pixels for the indicator number

Figure 71: Number Settings for Gauge Visualization

The **Number** settings set the color and size of the font for the indicator number positioned in the center of the gauge.

Range Container



Range Container

Start Value Starting value



End Value Ending value

Color Select color... Color

Add +

Figure 72: Range Container Settings for Gauge Visualization

The **Range Container** tab allows the user to establish one or more “containers” that encompass a specific range on the gauge. For example, a user might want to create a container that encompasses the acceptable range for a value, with the **Start Value** representing the lowest acceptable value and the **End value** representing the highest acceptable value. Each range container can be distinguished by setting its **Color**.

To add an additional range container, click . An additional range container’s values can then be defined. Range containers can be deleted by clicking the trash  icon to the right of each container’s respective header.

Example:

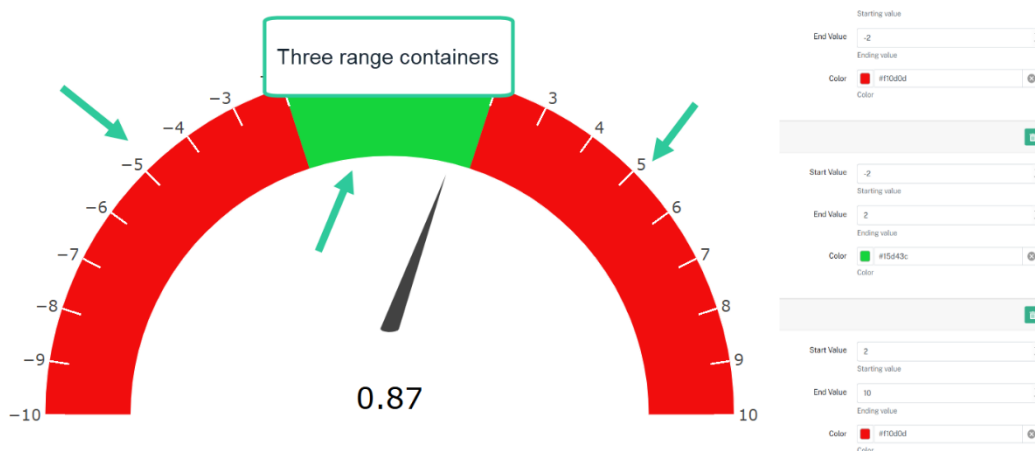
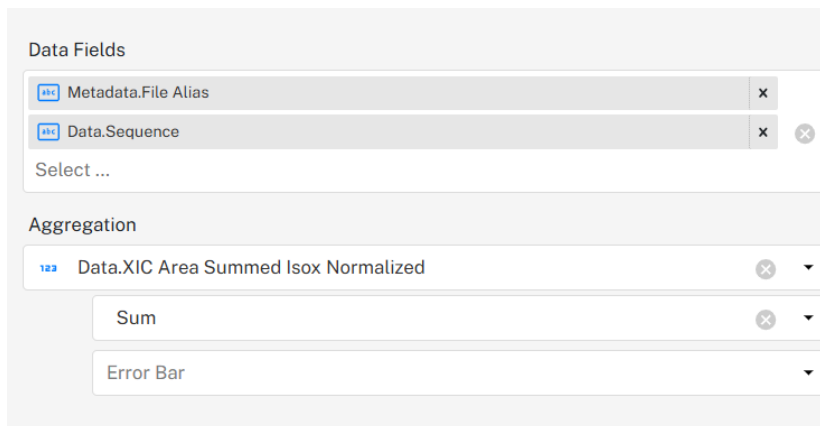


Figure 73: Range Containers within a Gauge Visualization

In the above graphic, for the green range container, the **Start Value** = -2 and the **End Value** = 2. Two additional range containers were made representing the values -10 to -2.0 and 2.0 to 10 in the color red.

Pie Charts

Basic Data Settings



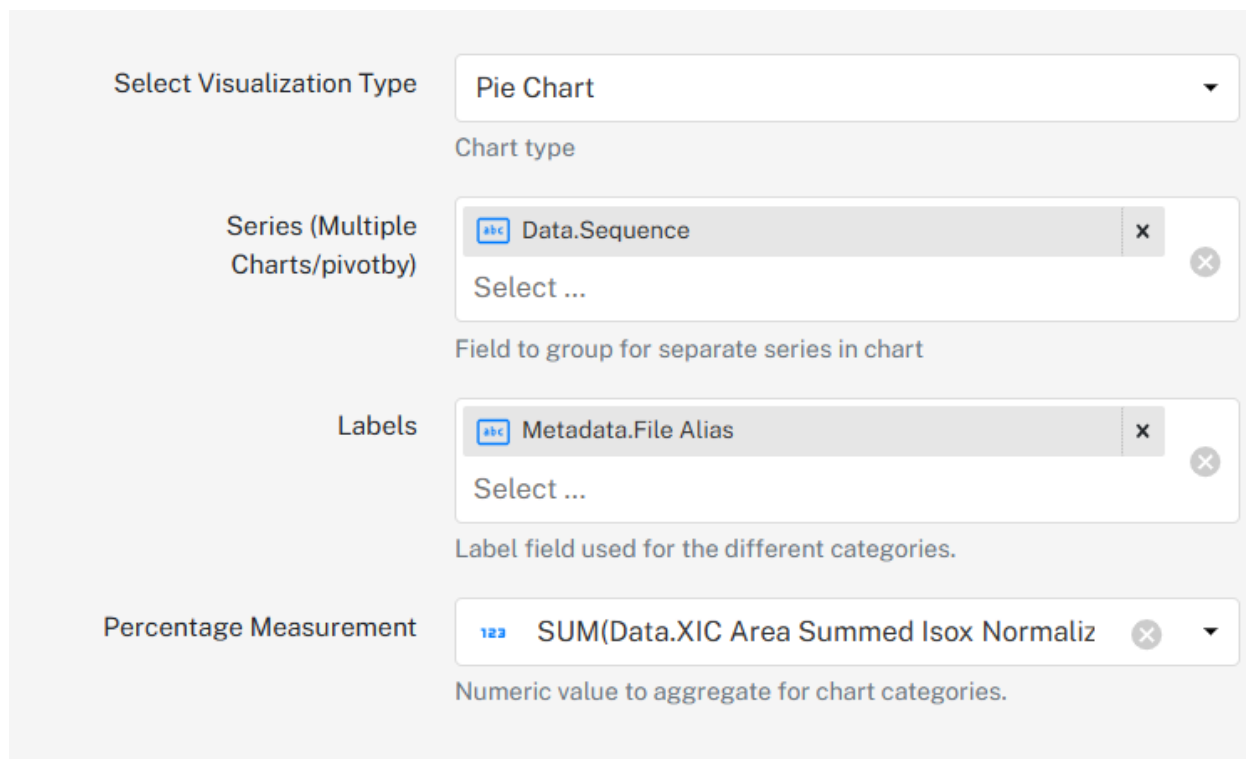
The screenshot shows the 'Basic Data Settings' for Pie Charts. It features two main sections: 'Data Fields' and 'Aggregation'. In the 'Data Fields' section, there are two items listed: 'Metadata.File Alias' and 'Data.Sequence', each with a blue 'Add' button and a close 'x' button. Below these is a 'Select ...' dropdown. The 'Aggregation' section contains a dropdown menu with 'Data.XIC Area Summed Isox Normalized' selected, a 'Sum' dropdown, and an 'Error Bar' dropdown.

Figure 74: Basic Data Settings for Pie Charts

- **Data Fields:** Data fields that can be selected in Display Settings to be included in the Pie Chart
- **Aggregation:**
 - **Aggregation:** Numeric value to aggregate and display as value
 - **Error bar:** Error bar values can be added for Min/Max, Std. Dev, 2 Std. Dev, and 3 Std. Dev. All values are + or - of the aggregation selected, with the exception of min/max. When a user selects a +/- Min/Max the error bar will function as a range (low value is the min and the highest value is the max). If Variance is used as the aggregation error bars will not be present. Note that SDTEV.P and VAR.P are used when determining error values.

Note: Manually zooming in and out of the Visualization using ctrl + mouse wheel may cause rendering issues with the Visualization. If this occurs, clicking **Apply** should reset the Visualization.

Basic Display Settings



Select Visualization Type: Pie Chart

Chart type

Series (Multiple Charts/pivotby): Data.Sequence

Select ...

Field to group for separate series in chart

Labels: Metadata.File Alias

Select ...

Label field used for the different categories.

Percentage Measurement: SUM(Data.XIC Area Summed Isox Normaliz)

Numeric value to aggregate for chart categories.

Figure 75: Basic Display Settings for Pie Chart Visualizations

As of release v5.10, users are directed to **Select Visualization Type** within the basic Display settings. In addition, the fields used to build the Visualization itself are added here, including the labels used for different categories with a single pie chart, the numerical to aggregate for chart categories, and Series specification for the generation of multiple pie charts within a single Visualization.

Additional Display Settings

General

The screenshot shows the 'General' settings panel. It includes a 'Show Series Titles' toggle (off), a 'Subtitle' text input, a 'Font Size' slider (set to 24px), 'Horizontal Alignment' (Center), 'Vertical Alignment' (Select values), 'Display Tooltip' toggle (on), 'Tooltip Value Format' (Select values), 'Precision' (input field), 'Auto Expand Margin' toggle (off), and four margin input fields: Left (40), Right (25), Top (40), and Bottom (25).

The **General** tab allows the user to add a subtitle to their Pie Chart and adjust its alignment, add and modify tooltips, and adjust the margins of the Visualization (see [Margin Settings](#)).

Internal Annotations

The screenshot shows the 'Internal Annotations' settings panel. It includes a 'Visible' toggle (off), a 'Display Mode' dropdown (Auto), and an 'Annotation Contents' dropdown (No content).

Figure 76: Internal Annotations tab

Internal Annotations options are unique to Pie Charts and, if toggled on, provide information relating to each slice within the Pie Chart. **Display mode** specifies where the annotation contents are shown. Options include **Auto**, **Horizontal**, **Radial**, and **Tangential**. **Annotation Contents** can include the data label, the

value of the slice, and the percentage of the whole each slice composes, and users also have the option to include any combination of the three (e.g., Value + Percentage, Label + Value + Percentage).

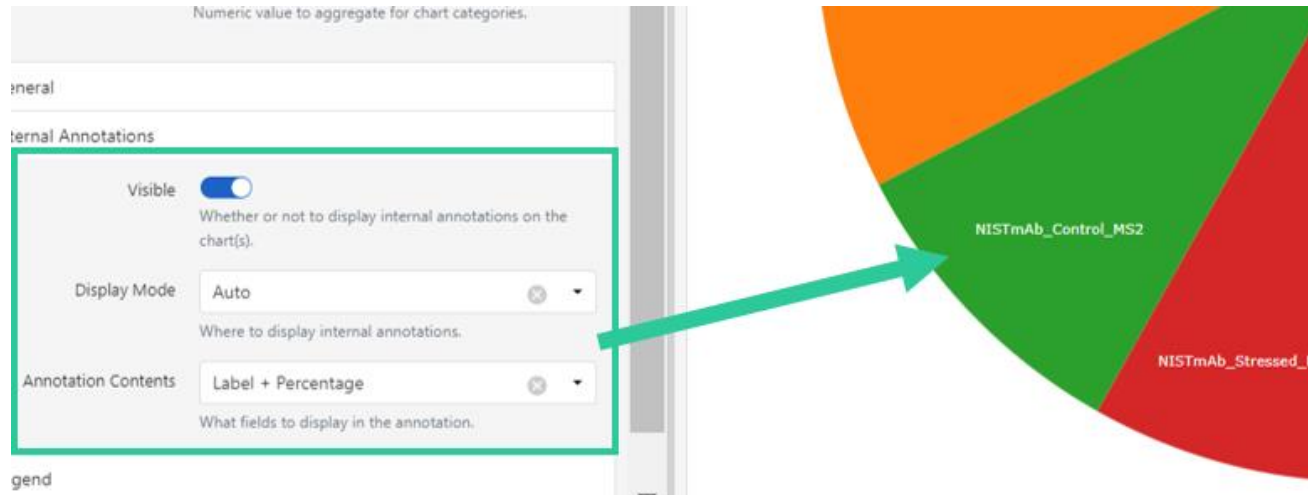


Figure 77: Example of internal annotations including data label and percentage

Legend

Legend controls are the same as those used for Chart-type Visualizations, see [Legend](#).

Chart Groupings

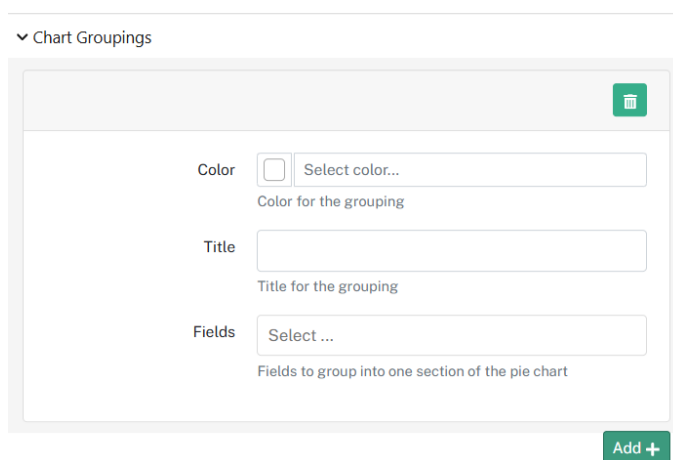


Figure 78: Chart Groupings tab

The **Chart Groupings** tab allows the user to combine multiple fields into one section of the pie chart. For example, this chart grouping contains all data fields that begin with “AD001”. Rather than displaying these data fields as independent slices, their values have been combined into a single magenta slice.

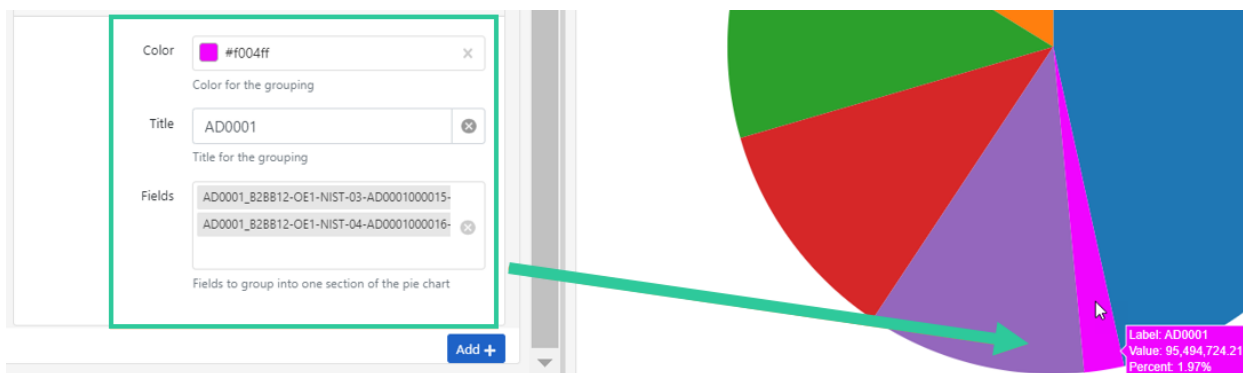


Figure 79: Chart Groupings example

Data Settings for all Visualizations

The following settings are available as tabs for all Visualization types and can be accessed by clicking on the Data block within the Visualization Builder.

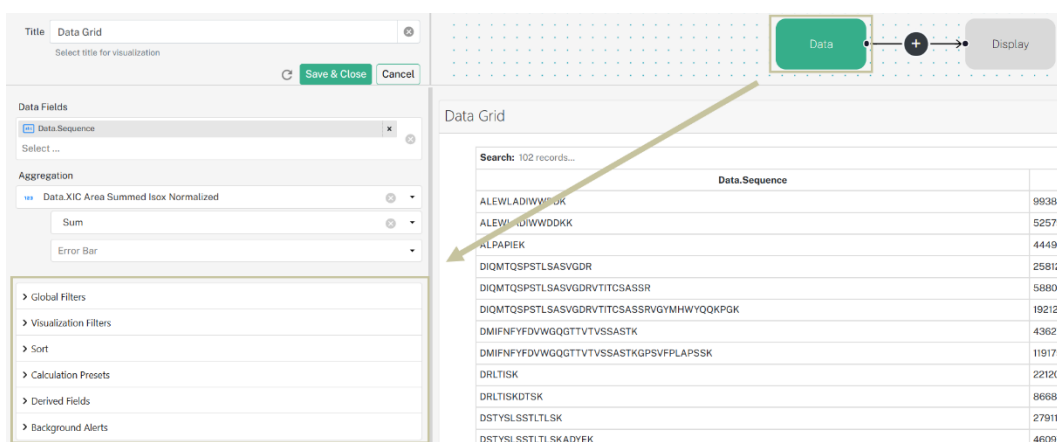


Figure 80: Data Settings

Global Filters

Global Filters are data filter settings that are applied across *all* Visualizations. Data from the selected Data Source will be filtered by these global settings before being passed to the Visualizations. Users can only *view* any **Global Filters** that have been applied, as the option to edit has been grayed out. For more information on applying Global Filters, see [Global Filters](#).

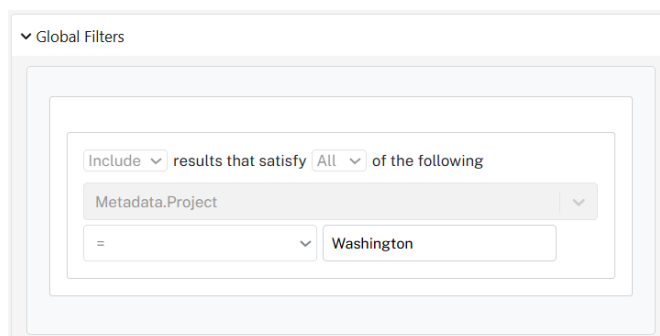


Figure 81: Global Filters tab, with options grayed out

Visualization Filters

Users can add or edit filters within a single Visualization by clicking the **Visualization filters** tab.

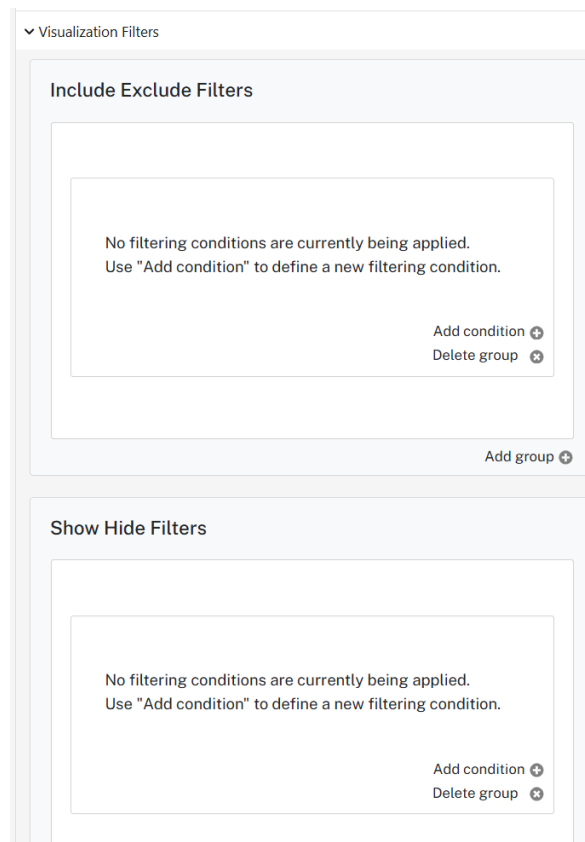



Figure 82: Visualization Filters tab

The user can also apply filters to specific Visualizations from the Dashboard by clicking the Filter  button in the header of a Visualization. This will open the same Visualization Filters page as seen in the Filter&Sort tab when editing a Visualization.

Data Grid

Search: 102 records...

Data.Sequence	SUM(Data.XIC Area Summed Isox Normaliz
ALEWLADIWWDDK	99385289.7264
ALEWLADIWWDDKK	5257951110.6648
ALPAPIEK	4449243625.9175
DIQMTQSPSTLSASVGDR	2581251138.2249
DIQMTQSPSTLSASVGDRVTITCSASSR	588082013.8833
DIQMTQSPSTLSASVGDRVTITCSASSRVGYMHWYQKPGK	19212143.3750
DMIFNFYFDVWGQGTITVTVSSASTK	436278363.6217
DMIFNFYFDVWGQGTITVTVSSASTKGPSVFPLAPSSK	11917543.6547
DRLTISK	221205894.9932
DRLTISKDTSK	866828.9655
DSTYLSSTLTLSK	2791133973.5964
DSTYLSSTLTLSKADVEK	46807015.405

Figure 83: Manage Visualization Filters from the Dashboard

To define a new filtering condition using either filter option, click **Add Condition**. This will generate a row wherein you can determine which field should be filtered (from within a dropdown), the condition it must satisfy, and a user-entered value. The user is given the option to **Include** or **Exclude** results that satisfy either **All** or **Any** specified conditions (provided more than one filter has been applied).

Include/Exclude Filters provides filtering of the data that is to be *included* or *excluded* in the calculations involved in the analysis; **Show/Hide Filters** provides filtering of the data that is to be *shown* in the analysis. If data is hidden based upon defined conditions in the **Show/Hide Filters** option, it will still be used to make calculations, but it will not be visualized.

Include Exclude Filters

Include results that satisfy All of the following

Include Created By = Morgan

Exclude

Add condition +

Delete group -

Figure 84: Include/Exclude Filters

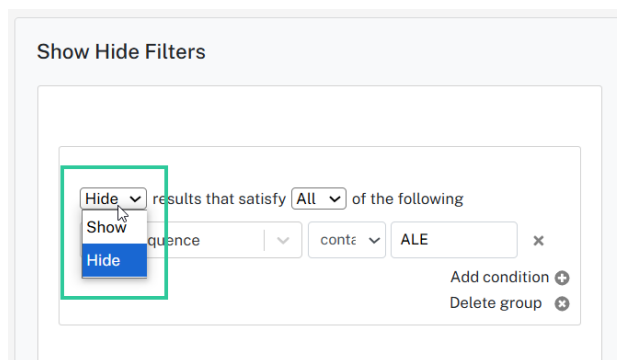


Figure 85: Show/Hide Filters

The user also has the option to create multiple conditions within a **Group**.

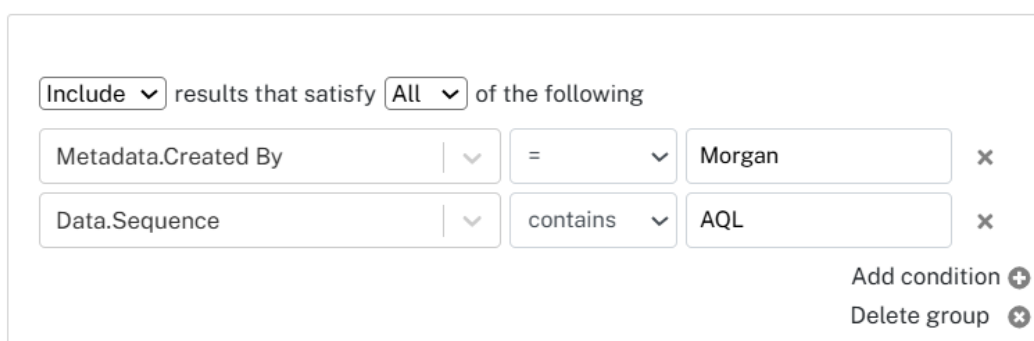


Figure 86: Multiple Conditions added to a group

The user must ensure that a filter is defined with a value if it is added and that it is not left blank. If the filter is no longer needed, the user can remove the filter by clicking the x next to the row of interest.

In the above example, the group must “**Include** results that satisfy **All** of the following [conditions]”. In this case, if three different conditions are defined, they must *all* be met by a data point for it to be included in the Visualization.

To delete a group of condition(s), click **Delete group**.

The Filters icon on a Visualization will show the number of conditions applied. The Visualization below currently has **two** filters applied.



Figure 87: Visualization with two filters applied

After performing a Deep Query search and generating a specific plot, the user can apply filters to an attribute of the data *from* the Visualization and use these filters to do the following:

1. Include/Exclude specific attributes (If **Excluded**, data is neither considered in calculations nor included in the Visualization).

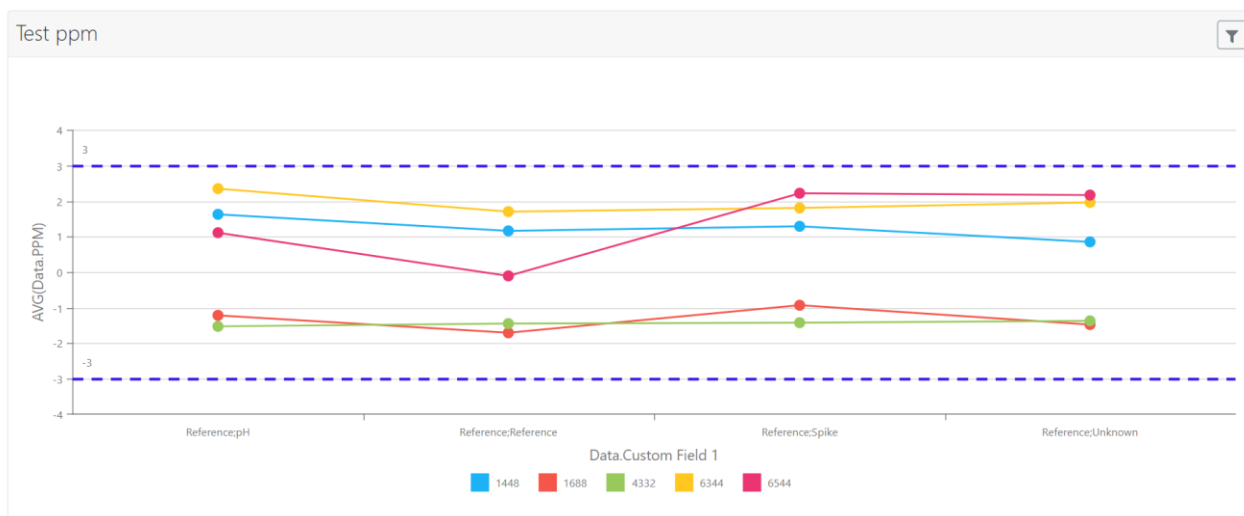


Figure 88: No filter applied

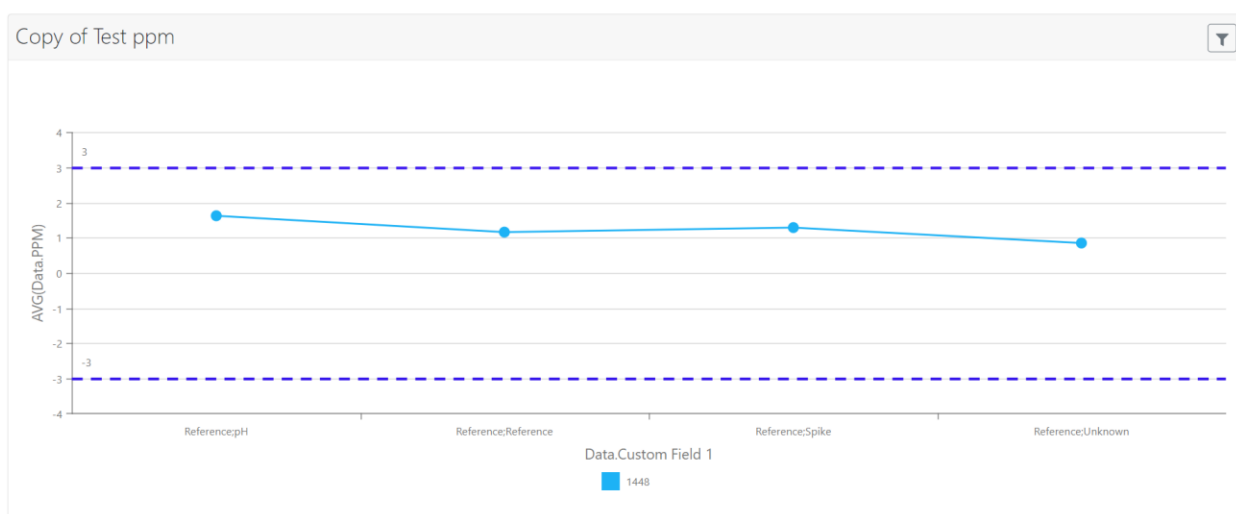


Figure 89: Exclusion filter applied

2. Show/Hide specific attributes: In this case, query results are filtered out from the Visualization, but this data is still used to perform the visualized calculations.

Additionally, the user can perform a combination of Include/Exclude and Show/Hide filters.

It is possible for too many filters to be applied or the conditions for the filters to be too narrow, which can result in the warning shown below. In this case, the user will need to try removing filters or adjust conditions (such as Any/All) to ensure that data has not been completely filtered out.

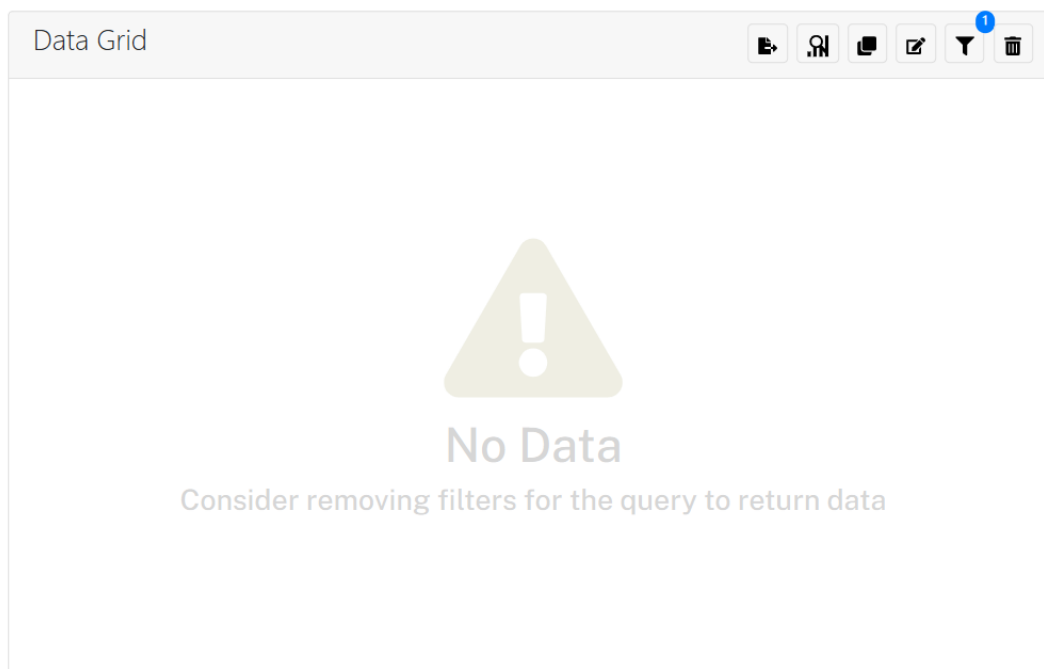


Figure 90: No Data warning

Sort

Sort orders data according to sort rules determined by the user.

Users can also order filtered data within a Visualization using the **Sort** function.



Figure 91: Sort Tab

A new Sort rule can be added to the Visualization by selecting a field from the dropdown. Multiple sort rules can be added at a time. Data fields can be sorted by ascending or descending order (selected by clicking on the ASC/DSC button to the right of the field name).

Metadata field parsing

Users can parse individual fields from “Data.Samples Custom Fields” to use in querying, filtering, visualization, and calculations. A plus sign icon displayed next to this field indicates the ability to parse.

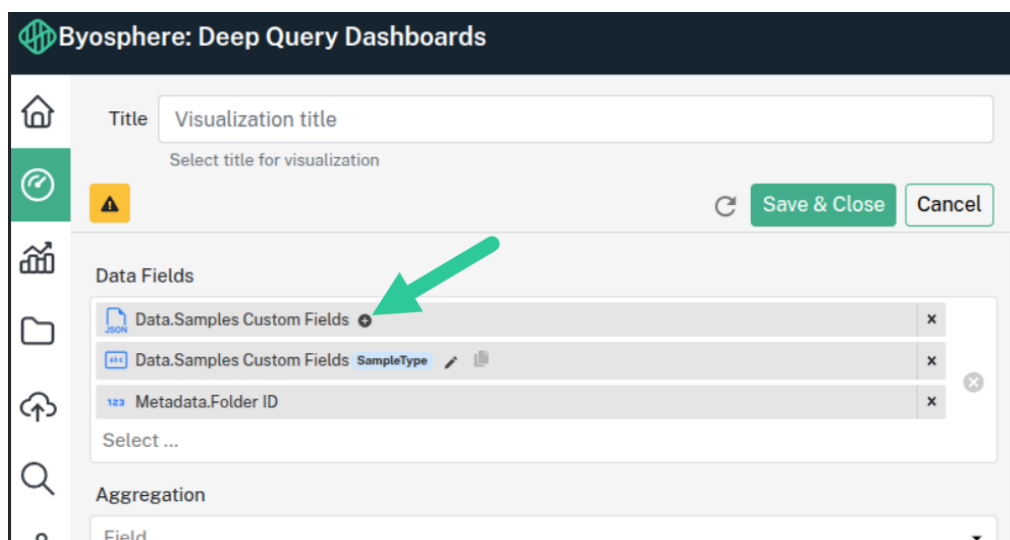


Figure 92: Users can parse metadata out of Samples Custom Fields

Clicking on this icon will open a dialog box. Within this dialog box, users can designate the property (the metadata value to parse out, based on which are available in the field) and type (Text, Date, Numeric).

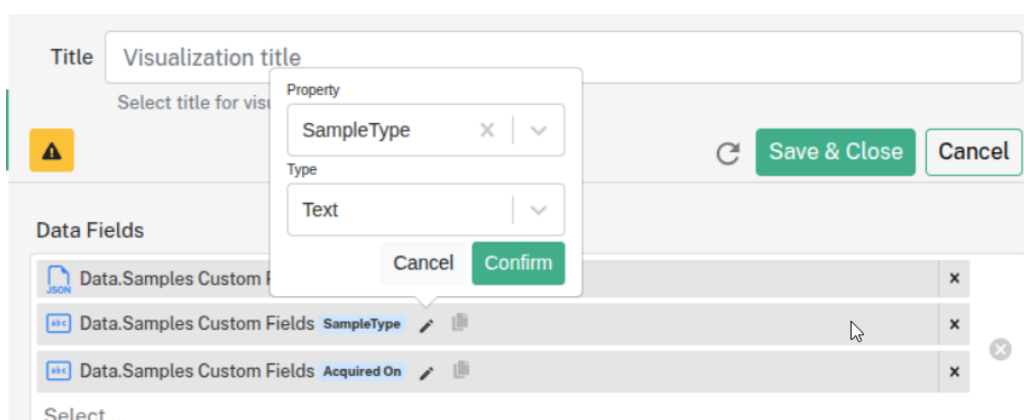


Figure 93: Metadata parsing dialog

The following example shows the mapping between parsed fields and fields available within Data.Samples Custom Fields and their subsequent parsing as individual fields as the last two columns in the table.

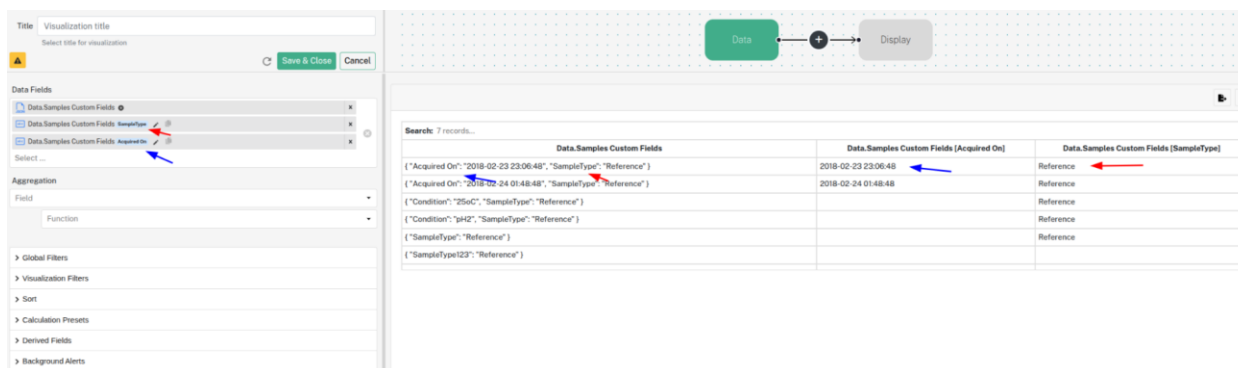


Figure 94: Result of parsing out individual metadata fields

Once a field has been created, it will remain present as a field option in the dropdown for that Visualization.

Sample-level metadata fields

Sample Metadata fields exist as a set of fields identical to the Metadata fields but are joined on the sample level (`sample_doc_id`). Users can use these fields like any other field, including filters, derived fields, etc. The prefix will show “Sample Metadata” e.g. Sample Metadata.Molecule.

These values will be updated in real-time if the user updates the Sample Metadata within Byosphere. Data is refreshed together with any other metadata field, so it will take about 1-2 minutes to propagate.

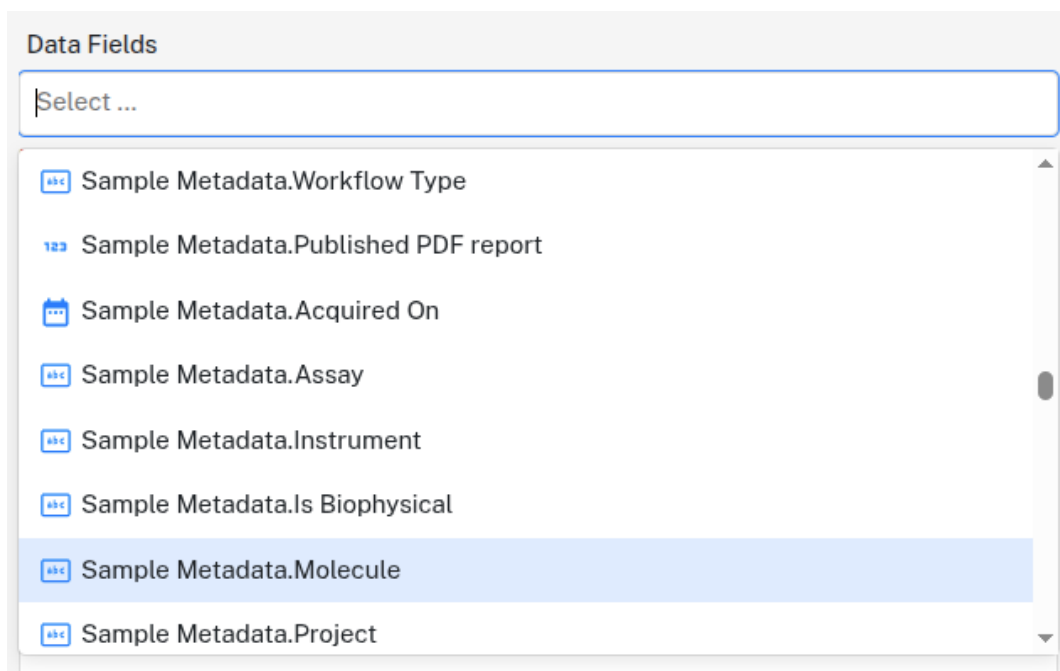


Figure 95: Sample Metadata fields

Field aggregations

When applicable, users can select an **aggregation type** for a specific numerical list field. Aggregation options include Min, Max, Average, and Sum.

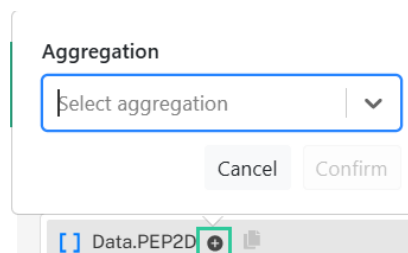


Figure 96: Adding an aggregation to a field

Once an aggregation is selected, it is listed next to the field in brackets.

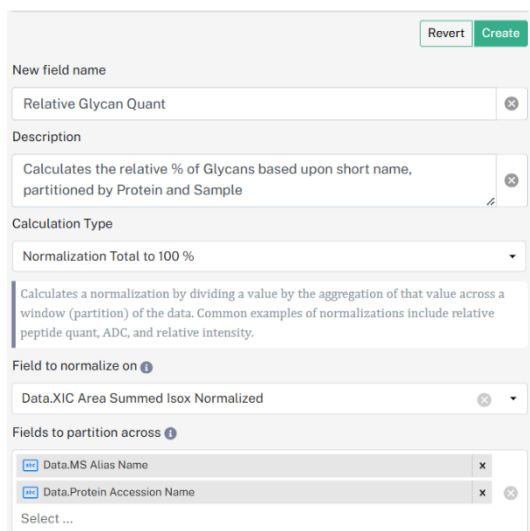
ame List	Data.Delta Score [MAX]	Data.Optimal Score [MIN]	Data.PEP1D [AVG]	Data.PEP2D [SUM]
	290.14224948806	270.231268112686	0.0034364599059979	0.0024349652893702

Figure 97: Fields with added aggregations within a Data Grid

Calculation Presets

The **Calculation Presets** tab provides the user with the ability to build calculated fields based upon Calculation Type.

When a user creates and opens a new Visualization, they will have the option to add a new Calculation Preset.



Revert Create

New field name

Relative Glycan Quant

Description

Calculates the relative % of Glycans based upon short name, partitioned by Protein and Sample

Calculation Type

Normalization Total to 100 %

Calculates a normalization by dividing a value by the aggregation of that value across a window (partition) of the data. Common examples of normalizations include relative peptide quant, ADC, and relative intensity.

Field to normalize on

Data.XIC Area Summed Isox Normalized

Fields to partition across

Data.MS Alias Name

Data.Protein Accession Name

Select ...

Figure 87: Normalization Calculation Preset options

The user will be prompted to provide a preset option from the Calculation Type dropdown list. Currently, users can use this tool to build a custom normalized field.

The inputs available are dependent upon the Calculation Type selected. The user will be required to enter values for each field. Users can consult the tooltips for more information on how to populate each field.

The **Normalization Total to 100%** calculation type provides a template for normalization calculations, which involve dividing a value across the aggregation of that value across a defined window/partition.

Advanced SQL code used to build the preset is updated in real time and can be viewed by the user underneath the Advanced option. Users can click the copy button in the corner to copy the SQL code to the clipboard.

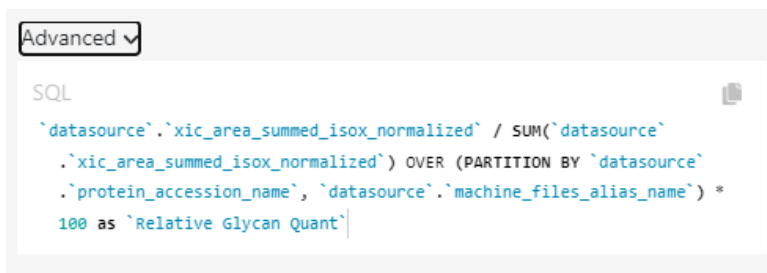
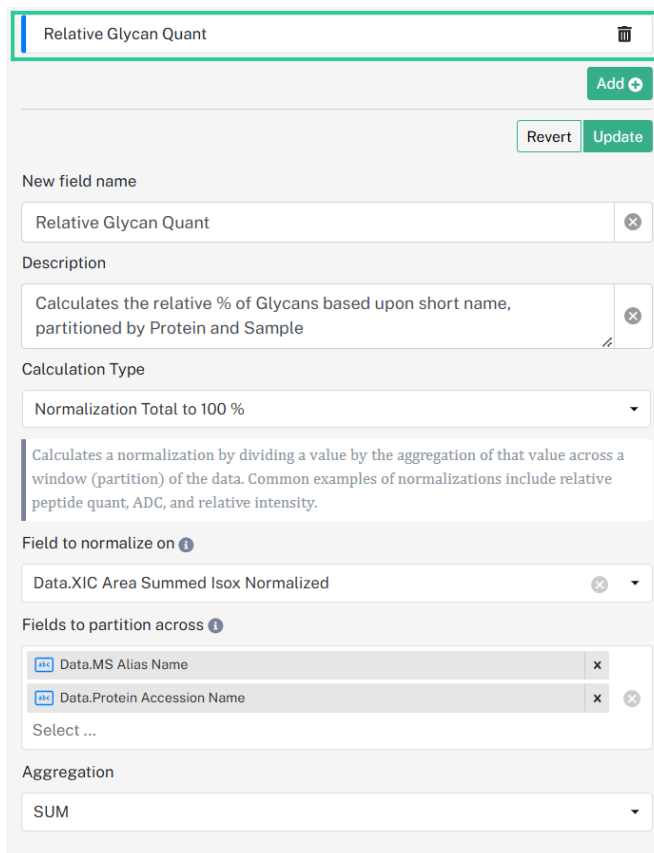






Figure 88: Advanced options can be used to preview SQL code

Some templates contain Visualizations that include calculation presets by default. For example, the Stacked Bar Chart Glycan Distribution Visualization in the PTM template contains the Relative Glycan Quant preset.




Relative Glycan Quant 


 Add

 Revert  Update


New field name

Relative Glycan Quant 


Description



Calculates the relative % of Glycans based upon short name, partitioned by Protein and Sample 


Calculation Type



Normalization Total to 100 % 




Calculates a normalization by dividing a value by the aggregation of that value across a window (partition) of the data. Common examples of normalizations include relative peptide quant, ADC, and relative intensity.

Field to normalize on 

Data.XIC Area Summed Isox Normalized  

Fields to partition across 

 Data.MS Alias Name 

 Data.Protein Accession Name  

Select ...

Aggregation


SUM 

Figure 86: Relative Glycan Quant preset

The resultant Relative Glycan Quant field is used to build the Visualization provided.

Derived Fields

Derived Fields are variables that are created from one or more existing data fields that exist in a single data source or across data sources. User-created Derived Fields can be used in local Filters, as x or y-axis Values within Visualizations, or within Background Alerts.

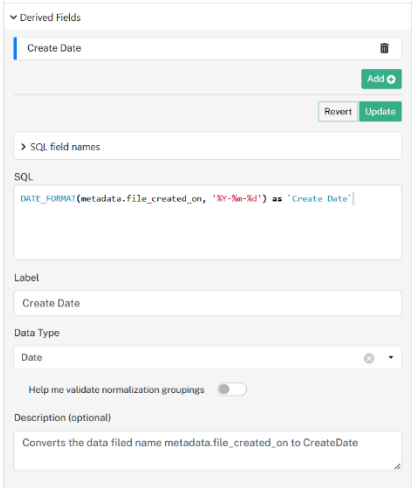
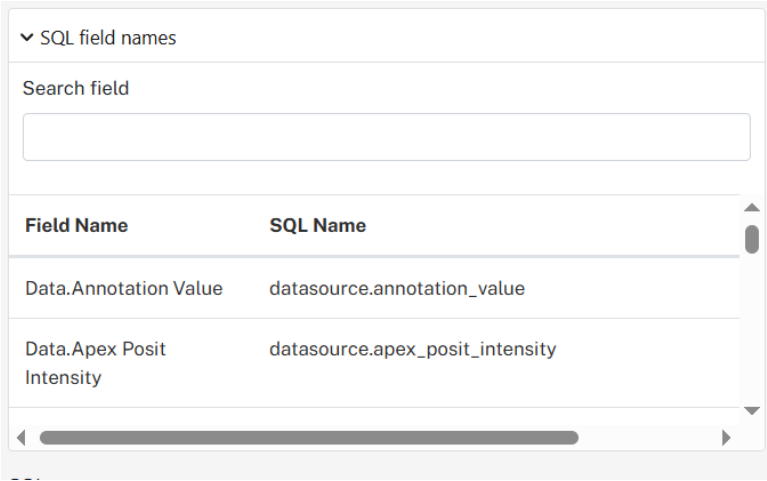


Figure 98: Derived Fields Tab

The **SQL field names** dropdown contains a searchable list of fields and their associated SQL name. Double-clicking the field of interest will populate the **SQL** text box.



Field Name	SQL Name
Data.Annotation Value	datasource.annotation_value
Data.Apex Posit Intensity	datasource.apex_posit_intensity

Figure 99: Searching SQL fields

Alternatively, the user can manually enter a SQL field into the text box themselves if an applicable field is known.

There are only certain functions available to users. If a user types in a function that does not exist, they are met with a warning:

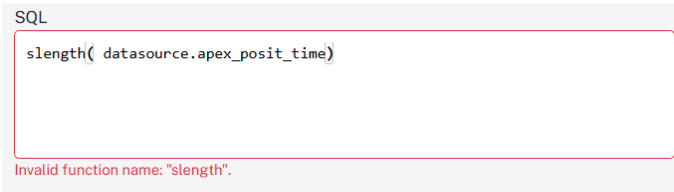


Figure 100: Invalid SQL function entry

Additionally, if a user specifies a number outside of the allowed number of arguments they are warned :

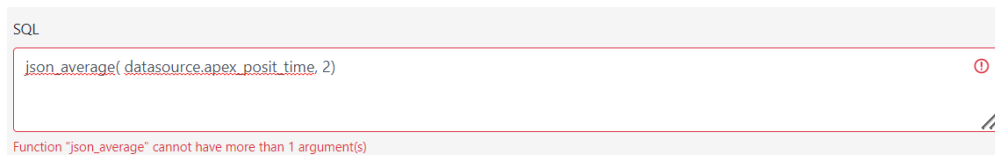


Figure 101: Invalid SQL function (too many arguments)

Label denotes the name of the generated derived field. The user can change the Label for any derived field. The user can also provide an optional **Description**.

The **Data Type** dropdown enables the user to specify the expected data type they wish to generate using SQL commands, with the options of **Date**, **Numeric**, and **Text** (which includes alphanumeric values). The default data type is numeric.

Once all required fields are filled in, clicking **Create** will add the user-created derived field to the Visualization (as an option under the X and Y-field dropdowns)

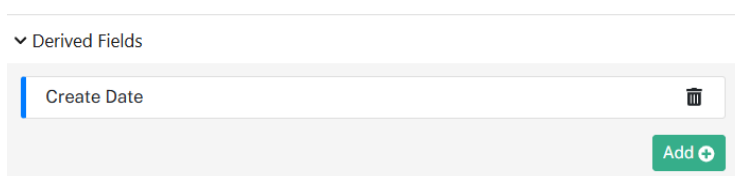


Figure 102: Created Derived Field

Once the derived field is created, it can be found within the available Data Fields within Data Settings and can be added to become available in Display Settings.

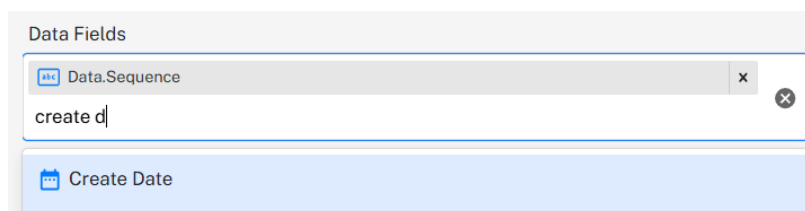


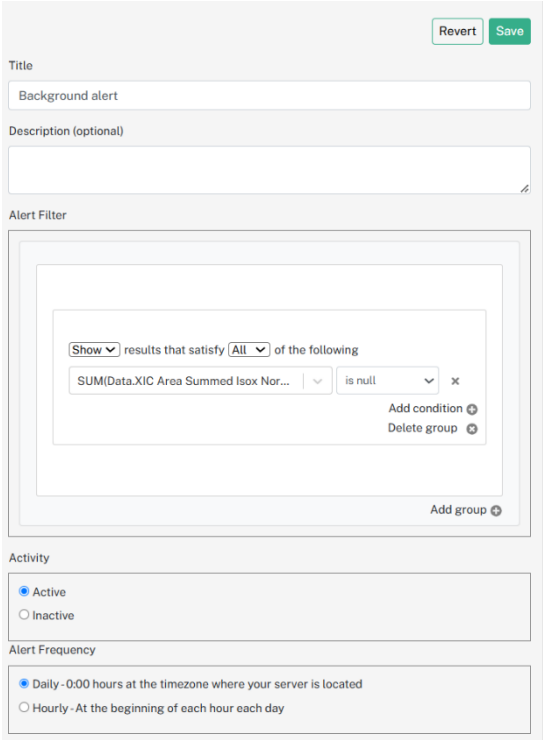
Figure 103: User-Created Derived Field available in Visualization Settings

If the user wishes to make changes to a Derived Field they created, they can click the Derived Field of interest and either **Update** to make changes or **Revert**, which will undo the last change that was made after clicking Update.

To create another Derived Field, click **Add new Derived Field**. Users can create multiple Derived Fields.

Background Alerts

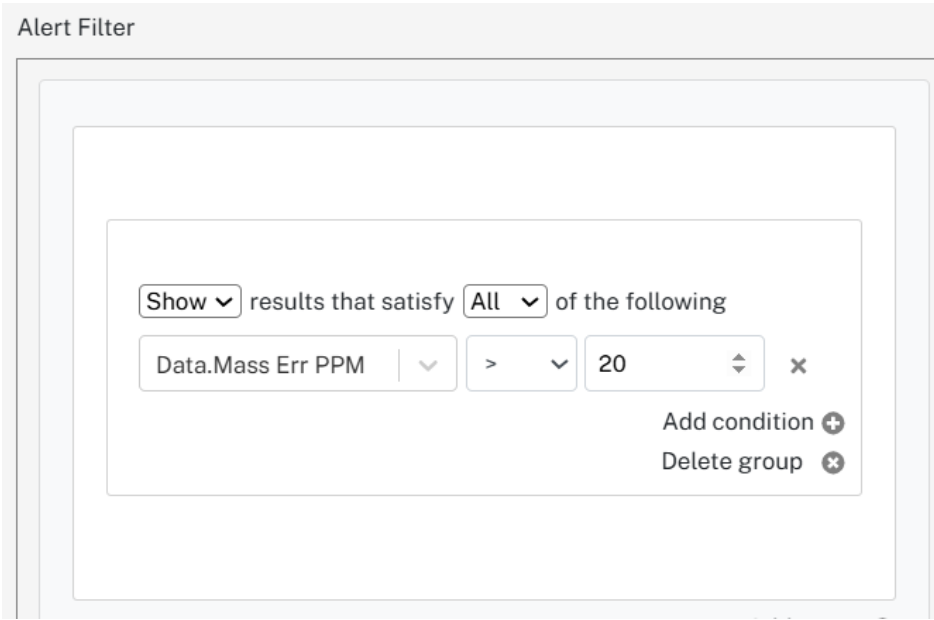
Backgrounds alerts can be set up in Deep Query that will notify the user if a value has fulfilled a condition (e.g., Obs > 5) previously assigned. To **add** a background alert, click [Add background alert](#). Background alert filters operate on top of the Global, Include/Exclude, and Show/Hide filters associated with the Visualization.



The form is titled "Background alert" and includes a "Revert" button and a "Save" button. It has a "Title" field with the text "Background alert" and a "Description (optional)" field. Below these is the "Alert Filter" section, which contains a nested box with a "Show" dropdown, the text "results that satisfy", an "All" dropdown, and the text "of the following". Inside this box is a condition: "SUM(Data.XIC Area Summed Isox Nor..." followed by a dropdown and "is null". To the right of this condition are "Add condition" and "Delete group" buttons. Below the nested box is an "Add group" button. Below the "Alert Filter" section is the "Activity" section with "Active" (selected) and "Inactive" radio buttons. At the bottom is the "Alert Frequency" section with "Daily - 0:00 hours at the timezone where your server is located" (selected) and "Hourly - At the beginning of each hour each day" radio buttons.

Figure 104: Background Alert

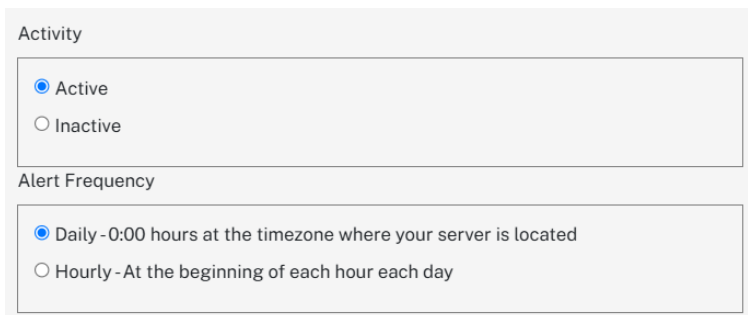
The user must provide a name to the alert and has the option to add a description. To assign a condition that must be fulfilled to trigger the background alert, click **Add Condition**.



The "Alert Filter" section shows a nested box with a "Show" dropdown, the text "results that satisfy", an "All" dropdown, and the text "of the following". Inside this box is a condition: "Data.Mass Err PPM" followed by a dropdown, ">", a dropdown, and "20". To the right of this condition are "Add condition" and "Delete group" buttons.

Figure 105: Example alert condition

In this example, an alert will be triggered for data that satisfies the following condition: For the field "Data.Mass Err PPM", the value must exceed the value of 20. Users can use both Data Source fields and Derived Fields when building conditions for Background Alerts.



The form is titled 'Activity' and 'Alert Frequency'. Under 'Activity', there are two radio buttons: 'Active' (selected) and 'Inactive'. Under 'Alert Frequency', there are two radio buttons: 'Daily - 0:00 hours at the timezone where your server is located' (selected) and 'Hourly - At the beginning of each hour each day'.

Figure 106: Activity and Alert Frequency

Alerts will not incorporate documents that the user does not have access to, and users lacking the correct roles (**Contributor** or **Advanced Viewer**) do not have permission to create a background alert.

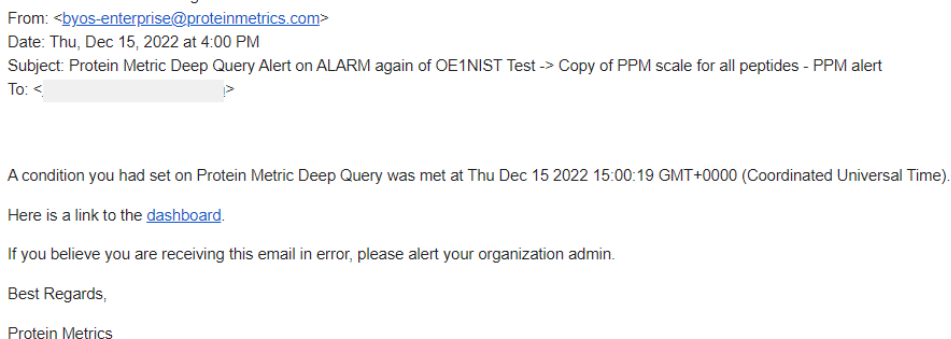
A Background Alert can be set to **Active** or **Inactive**, as shown in the above figure. If an alert is set to **Inactive**, the alert will not be run at all.

The user can also define how frequently an alert is sent out if conditions are met for a Background Alert. If **Daily**, the user will receive an alert at 0:00 in their own time zone if the alert conditions have been met within a 24 hour period. If **Hourly**, the user will receive an alert every hour if the alert conditions have been met. Alerts will only notify a user if new data has been added since the alert was last run. For example, a daily alert run yesterday will only trigger for data that has been added since the previous alert that also meets the specified alert criteria.

The user can create multiple **Groups** of conditions for an alert filter. This enables the user to set up alerts that are triggered by results that satisfy *any* of the conditions listed in the group, rather than just one criterion. Multiple conditions can be created per group and multiple groups per designated alert.

Note: Alerts will **not** be fully saved unless changes are published to the Dashboard.

A message will be sent to the user's email if the alert is triggered. The user will also receive a notification within the web client.



The email is from <byos-enterprise@proteinmetrics.com> and is dated Thu, Dec 15, 2022 at 4:00 PM. The subject is 'Protein Metric Deep Query Alert on ALARM again of OE1NIST Test -> Copy of PPM scale for all peptides - PPM alert'. The body of the email states: 'A condition you had set on Protein Metric Deep Query was met at Thu Dec 15 2022 15:00:19 GMT+0000 (Coordinated Universal Time). Here is a link to the [dashboard](#). If you believe you are receiving this email in error, please alert your organization admin. Best Regards, Protein Metrics'.

Figure 107: Background alert notification email

To **delete** an alert, the user can click the red x icon on the Alert title.

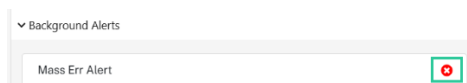


Figure 108: Deleting an Alert

If the user has not saved the alert yet, they will be prompted with a warning dialog.

Confirm deletion

You are about to delete an unsaved alert.

Cancel

Confirm

Figure 109: Unsaved alert deletion dialog

Once an alert has been saved, the user will receive a dialog warning that they are about to delete an *existing* alert.

If an alert in a project created in v5.0 contains an unsupported field or has any other issues, the user will receive an email with a link to the affected Dashboard and the background alert will be disabled.

Currently, there can only be one alert per Visualization at a time.

If the user is not the owner of a Background Alert, they are only capable of deleting it if they delete the Dashboard or Visualization it is tied to. All alerts tied to a Visualization/Dashboard are deleted when the Visualization/Dashboard is deleted. These alerts cannot be recovered even if the Visualization/Dashboard is restored. Any alert without a valid Visualization or Dashboard will be deleted automatically if it is run.

Transformations

If a user has selected either a Data Grid or Pivot Table Visualization, a plus sign icon will appear within the Visualization Builder. Clicking on this shows a list of **Transformations** which the user can apply to their data.

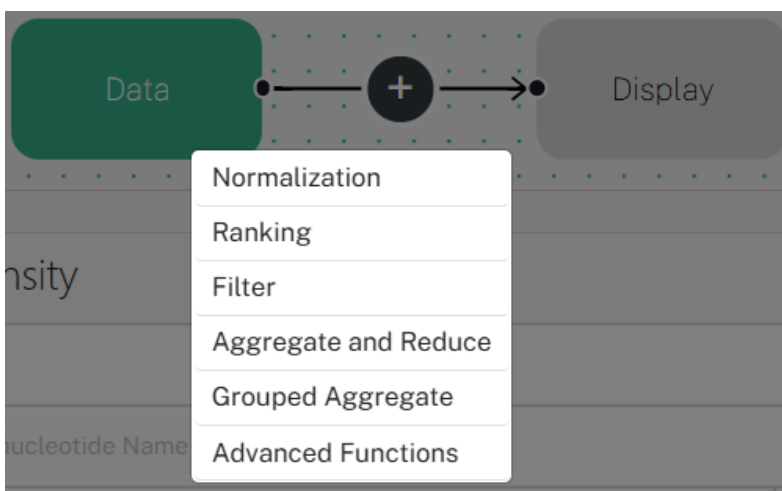


Figure 110: Transformations

Once a Transformation has been added, it will be visible within the Visualization Builder.

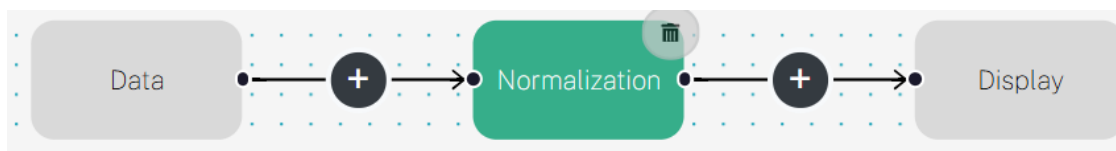


Figure 111: Transformation within Visualization Builder

Users can choose from **Normalization**, **Ranking**, **Filter**, **Aggregate and Reduce**, and **Grouped Aggregate** options. Each option has its own information that the user must populate. To perform a transformation on data, that data field must be included in the Visualization. Numeric derived fields will also be available. The way in which a grouping occurs for a transformation may be controlled by the user by utilizing the partitioning function, in much the same way as can be performed for the function “Normalization within Calculation Presets” under the Data Settings tab. The types of Transformation possible are outlined below:

- Grouped Aggregate:** This transformation will allow a user to customize a group of data and apply an aggregation to that group. In the example below, if a user wished to sum the data field “Intensity” of each Delta Mass per Protein Name (within each Sample Name), they could select the aggregation type “Sum” and determine grouping by defining the fields to partition by Sample Name and Protein Name. For transformations, only data/meta data fields present in the Visualization may be used.

The figure below shows the original Pivot Table displaying the intensity of each Delta Mass:

SUM(Data.Intensity)		Data.Sample Name			
Data.Protein Name	Data.Delta Mass Name				
Data.Protein Name	Data.Delta Mass Name	DN29_red	DN29_reddeglyc	DN32_red	DN32_reddeglyc
29HC	+Lys		4121118.2762		
	G0F	13197985.8060			
	G0F+Lys	3720682.1062			
	G0F-GlcNAc	1805375.2686			
	G1F	3472462.6772			
	G2F	616413.1983			
	Hex		1119831.9976		
	Man5	1362863.3822			
	Man5F	610930.0631			
			14595861.4616		
29LC		8951342.0869	7914232.0113		
32HC	G0F			17665752.7118	2338558.1168
	G0F-GlcNAc			4716256.0524	313890.5752
	G1F			26639927.5952	3819086.4982
	G2F			5067736.3387	715209.4129
	G2F+NeuAc			1076041.0836	
	Hex				283052.9640
					9043465.8944
32LC				9662084.9799	2402871.2190
		8165329.8535	7946099.6723	18355144.6098	4929905.6463

Figure 112: Before Transformation

The figure below outlines the details of the Grouped Aggregate Transformation being applied. The Transformation sums the intensities within each protein name group (which is also partitioned by Sample Name):

Grouped Aggregate

RevertUpdate

Field for calculation ⓘ

SUM(Data.Intensity)ⓧ▼

Fields to partition across ⓘ

Data.Sample Namex

Data.Protein Namexⓧ

Select ...

Aggregation

SUM▼

Save as separate transformation field ⓘ

☐

Transformation name

Figure 113: Detailed Grouped Aggregate Sum Transformation

The figure below shows the result of the above Transformation settings:

SUM(Data.Intensity)		Data.Sample Name			
Data.Protein Name	Data.Delta Mass Name				
Data.Protein Name	Data.Delta Mass Name	DN29_red	DN29_reddeglyc	DN32_red	DN32_reddeglyc
29HC	+ Lys		19836811.7354		
	G0F	24786712.5016			
	G0F+Lys	24786712.5016			
	G0F-GlcNAc	24786712.5016			
	G1F	24786712.5016			
	G2F	24786712.5016			
	Hex		19836811.7354		
	Man5	24786712.5016			
	Man5F	24786712.5016			
			19836811.7354		
29LC		8951342.0869	7914232.0113		
32HC	G0F			55165713.7818	16513263.4615
	G0F-GlcNAc			55165713.7818	16513263.4615
	G1F			55165713.7818	16513263.4615
	G2F			55165713.7818	16513263.4615
	G2F+NeuAc			55165713.7818	
	Hex				16513263.4615
					16513263.4615
32LC				9662084.9799	2402871.2190
		8165329.8535	7946099.6723	18355144.6098	4929905.6463

Figure 114: Resultant Visualization from the above Transformation

If a user does not wish for the data within the Pivot Table to be updated by this Transformation directly, setting the **Save as separate transformation field** toggle to **On** will save the transformation as a field.

Save as separate transformation field ⓘ

☐

Figure 115: Save as separate transformation field toggle

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- Aggregate and Reduce:** This transformation allows the user to apply a grouped aggregation in the same way as the Grouped Aggregate function, but will also reduce the data by collapsing the data field that is aggregated into a single cell (in the example below, into one row) so that the aggregated value will only appear once. In cases where multiple data fields are partitioned (in the example below, it is partitioning against Sample Name and Protein Name), it will include all the non-partitioned field results into the same cell. Here, all the values for Delta Mass Name are displayed in the same cell for each row, while Protein Name is used to partition. The aggregation applied here is the same as previously described in the Grouped Aggregate section above. The main difference between the two transformation functions is that Grouped Aggregate may report the aggregate multiple times, which could potentially impact any further calculations.

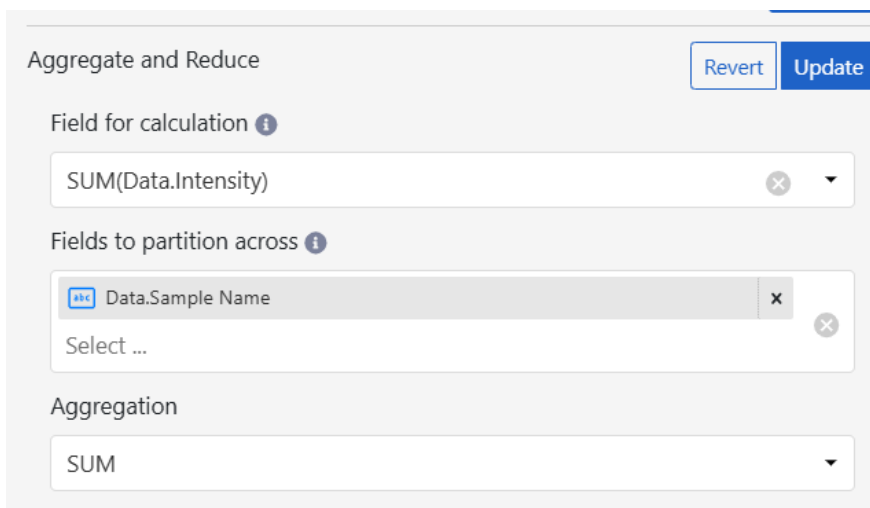


Figure 116: Example of Aggregate and Reduce Transformation

SUM(Data.Intensity)		Data.Sample Name			
Data.Protein Name	Data.Delta Mass Name				
Data.Protein Name	Data.Delta Mass Name	DN29_red	DN29_reddeglyc	DN32_red	DN32_reddeglyc
29HC, 29HC, 29HC, 29LC, null	+Lys, Hex, null, null, null		35697143.4190		
29HC, 29HC, 29HC, 29HC, 29HC, 29HC, 29LC, null	G0F, G0F+Lys, G0F-GlcNAc, G1F, G2F, Man5, Man5F, null, null	41903384.4421			
32HC, 32HC, 32HC, 32HC, 32HC, 32LC, null	G0F, G0F-GlcNAc, G1F, G2F, G2F+NeuAc, null, null			83182943.3715	
32HC, 32HC, 32HC, 32HC, 32HC, 32LC, null	G0F, G0F-GlcNAc, G1F, G2F, Hex, null, null, null				23846040.3268

Figure 117: Resultant Visualization after applying above Transformation

- Ranking:** This transformation allows the user to rank numeric values within the tables. There is an option to assign the value of 1 to correspond to the highest value (Ascending Order) vs 1 to represent the lowest numeric value (Descending Order). It is possible to choose which values to partition the ranking over. In the example below, the Ranking partitioning is based upon the data fields Sample Name and Protein Name. In this case the Ranking is based upon the numeric values within each Protein Name, within each Sample. If a user wanted to Rank the entire column, they would only partition by Sample Name.

Ranking Revert Update

Field to rank ¹

SUM(Data.Intensity)

Fields to partition across ¹

Data.Sample Name

Select ...

Sorting Order ¹

ASC

Save as separate transformation field ¹

☐

Transformation name

Figure 118: Example of Ranking Transformation

SUM(Data.Intensity)		Data.Sample Name			
Data.Protein Name	Data.Delta Mass Name				
Data.Protein Name	Data.Delta Mass Name	DN29_red	DN29_reddeglyc	DN32_red	DN32_reddeglyc
29HC	+Lys		4.0000		
	G0F	1.0000			
	G0F+Lys	4.0000			
	G0F-GlcNAc	6.0000			
	G1F	5.0000			
	G2F	8.0000			
	Hex		5.0000		
	Man5	7.0000			
	Man5F	9.0000			
			1.0000		
29LC		2.0000	3.0000		
32HC	G0F			3.0000	5.0000
	G0F-GlcNAc			6.0000	7.0000
	G1F			1.0000	3.0000
	G2F			5.0000	6.0000
	G2F+NeuAc			7.0000	
	Hex				8.0000
					1.0000
32LC				4.0000	4.0000
		3.0000	2.0000	2.0000	2.0000

Figure 119: Resultant Visualization after applying above Transformation

- Normalization:** There is an option within Transformations to perform Normalization. This is in addition to the options within Calculation Presets on the Data Settings tab. An option is provided in the Transformations tab so that a user may perform Normalizations on data that has previously been calculated using other Transformation Types. For example, a user may wish to Normalize on data that has previously been aggregated within certain groupings using either the Grouped Aggregate or Aggregate and Reduce transformation. In the figure below, there is a Normalization to the highest numeric value, and all other Normalized values are calculated relative to the highest (Max) value. As the order of operation for the transformations is based upon the sequence order in which they are set up on the transformations tab, this would mean that the Normalization (and hence determination of the highest value to use to Normalize against), is based upon the aggregated value as determined here by the Aggregate and Reduce transformation. In this example, the aggregation (summing) was applied by summing the intensity values within each Protein Name Group, per Sample Name (the same example used in the Aggregate and Reduced section above). The Normalization transformation was then applied on the entire column (in this case the partition was only applied to Sample Name) after the aggregation step, as this is the order in which they appear on the tab. The same calculated result would be obtained by using the

Grouped Aggregate Transformation, however, the value itself will be repeated within the cells within the group that is aggregated. For this particular Normalization type, the calculated value would not be impacted, however, for the Normalization type “Sum” the repeating numeric display would affect the final calculated %. In cases like this, it is recommended to use Aggregate and Reduce.

Normalization

Revert
Update

Field to normalize ⓘ

SUM(Data.Intensity)

Fields to partition across ⓘ

Data.Sample Name

Data.Protein Name

Select ...

Aggregation

MAX

Save as separate transformation field ⓘ

☐

Transformation name

Figure 120: Example of Normalization Transformation

SUM(Data.Intensity)		Data.Sample Name			
Data.Protein Name	Data.Delta Mass Name				
Data.Protein Name	Data.Delta Mass Name	DN29_red	DN29_reddeglyc	DN32_red	DN32_reddeglyc
29HC	+Lys		28.2348		
	G0F	100.0000			
	G0F+Lys	28.1913			
	G0F-GlcNAc	13.6792			
	G1F	26.3106			
	G2F	4.6705			
	Hex		7.6723		
	Man5	10.3263			
	Man5F	4.6290			
			100.0000		
29LC		100.0000	100.0000		
32HC	G0F			66.3131	25.8591
	G0F-GlcNAc			17.7037	3.4709
	G1F			100.0000	42.2303
	G2F			19.0231	7.9086
	G2F+NeuAc			4.0392	
	Hex				3.1299
					100.0000
32LC				100.0000	100.0000
		100.0000	100.0000	100.0000	100.0000

Figure 121: Result of Normalization Transformation with no Agg or Reduce

- Filter:** As with Normalization, the Filter function that is available under Data Settings is also available as part of the Transformations, so that it may be applied sequentially within, or after, other transformation calculations. In the following example a user wants to only display the Intensity values for the 3 most intense Delta Masses within each Protein, per Sample Name.

The first operation would be to Rank each of the intensities within each Protein Name Group. This may be carried out as described earlier under the Ranking section. However, in this case, as the user wishes to then add a filter, the Transformation itself must be saved as a Transformation Field, so that it will be available as an option when applying the Filtering Transformation. In this example,

the custom Transformation name that was given is “Rank”. When saved as a transformation field, it is only available for further transformation calculations, and not as an option within the Visualization itself.

When the user adds the next Transformation in the order of operations, they are able to select a filter to only display those intensities that were in the top 3 ranked.

Display Top 3 Intensity

SUM(Data.Intensity)		Data.Sample Name				
Data.Protein Name	Data.Delta Mass Name	mAb_1	mAb_2	mAb_3	mAb_4	mAb_5
Antibody	G0F/G0F	1.0000	1.0000	1.0000	1.0000	1.0000
	G0F/G0F-Fuc	3.0000	3.0000	3.0000		
	G0F/G0F-GlcNAc			7.0000		
	G0F/G1F	6.0000	6.0000	6.0000		
	G1F/G1F	1.0000	1.0000	1.0000		
	G1F/G2F	2.0000	2.0000	2.0000		
	G2F/G2F	4.0000	4.0000	4.0000		
mAb	G2F/G2F	5.0000	5.0000	5.0000		
	G0F/G0F				3.0000	
	G0F/G0F-GlcNAc				6.0000	
	G0F/G1F				1.0000	
	G1F/G1F				2.0000	
mAb 2	G1F/G2F				4.0000	
	G2F/G2F				5.0000	
	G0F/G0F					1.0000
	G0F/G0F-GlcNAc					4.0000
	G1F/G2F					2.0000
	G2F/G2F					3.0000

Figure 122: Example with ranking applied

The Filter transformation step shown below is then applied after the Ranking transformation.

Filter

Filter ⓘ

Include ▾ results that satisfy

All ▾ of the following

Rank ▾

<= ▾ 3 ▾ X

Add condition ⓘ

Delete group ⓘ

Figure 123: Filter to be applied along with Ranking transformation

Display Top 3 Intensity

SUM(Data.Intensity)		Data.Sample Name				
Data.Protein Name	Data.Delta Mass Name					
		mAb_1	mAb_2	mAb_3	mAb_4	mAb_5
Antibody	G0F/G0F	503788.9168	377888.6636	1498309.2119	598553.9637	199029.3
	G0F/G1F	1566854.3386	1228378.6293	7297505.5981		
	G1F/G1F	2714541.6706	1758500.2978	11260125.5127		
mAb	G0F/G0F	1875844.7252	1347949.3790	8065879.0623		
	G0F/G1F				2285721.1807	
	G1F/G1F				3708033.8015	
mAb 2	G0F/G0F				2621815.9349	
	G1F/G2F					884449.1
	G2F/G2F					426042.2
mAb 3	+ Hex					138103.3
	Reference					1088117.3
						1457290.9

Figure 124: Visualization with Filter and Ranking applied

Note: Unlike Visualization filters, Transformation filters will apply in the sequence that they appear in the transformations. They will act as a filter to anything at a given step at the sequence and won't impact anything before that step. Since transformations happen after the data settings step, the transformations filters apply after the major settings for global, include/exclude, show-hide filters and before any previous transformations have been applied.

Advanced Functions

If a user has selected either a **Line Chart** or **Scatter Plot** Visualization, an **Advanced Function** option is available for user selection in the dropdown of the Visualization Builder:

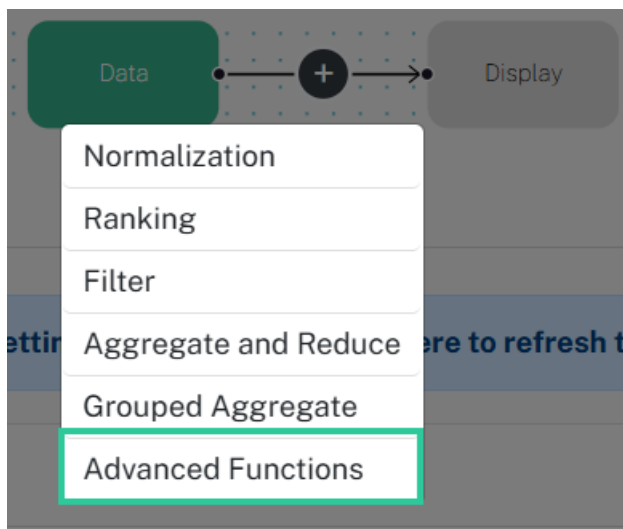


Figure 125: Advanced Functions option in dropdown

Currently, the only Advanced Function available is **Linear Regression**. Upon adding the Linear Regression Advanced Function, the user must add the Independent and Dependent Variables from the fields provided in the dropdown.

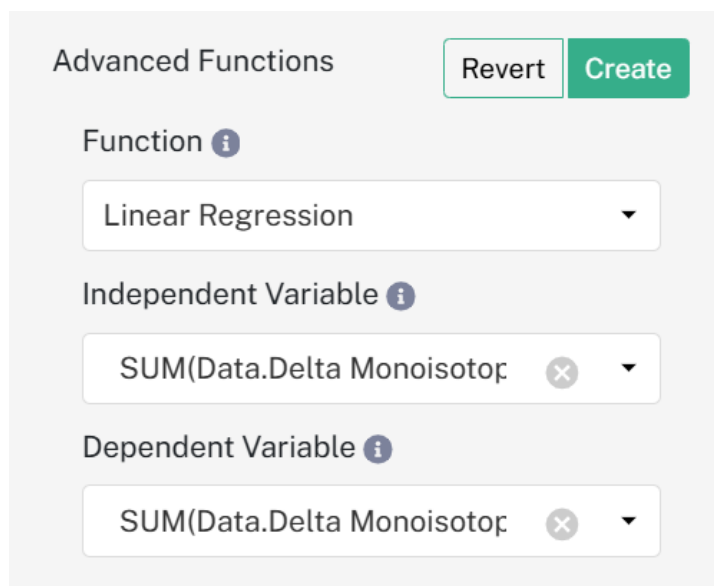


Figure 126: Linear Regression Advanced Function

Adding Linear Regression will calculate the equation for the line of best fit, the Pearson Correlation, and the R2 value. Display of these values within the Visualization can be enabled from **General > Display** settings.

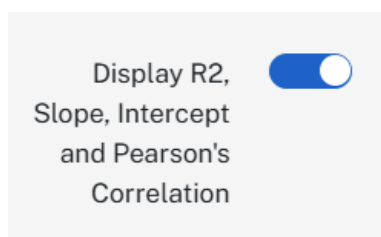


Figure 127: Linear regression display toggle

Visualization Inspection

Users can view the files present within their Dashboard by clicking the **Visualization Inspection** icon:



Data Grid

Search: 102 records...

Data.Sequence	SUM(Data.XIC Area Summed Isox I
ALEWLADIWWDDK	99385289.7264
ALEWLADIWWDDKK	5257951110.6648
ALPAPIEK	4449243625.9175
DIQMTQSPSTLSASVGDR	2581251138.2249
DIQMTQSPSTLSASVGDRVTITCSASSR	588082013.8833
DIQMTQSPSTLSASVGDRVTITCSASSRVGYMHWWYQ	19212143.3750

Figure 128: Visualization Inspection icon

This toggle shows an inspection table where users can view the Folder, Project File, and the Sample file name.

Search: 3 records...









Folder	File Name	MS Alias Name
Dashboard Template Projects 	001_001.blgc 	09315_E_SN_NIST_Guanidine_Tryp
Dashboard Template Projects 	002_001.blgc 	09315_E_SN_NIST_Guanidine_LysC
Dashboard Template Projects 	003_001.blgc 	09315_E_SN_NIST_Guanidine_CTrypsin


Figure 129: Visualization Inspection table

The **Folder**  icon will take the user to the folder browser view, opening a new tab.

The **File Search**  icon will take the user to the file search view, opening a new tab (if the user has Virtual Client enabled, they can open and review the results in the Project from within Byosphere).

Visualization Inspection views are accessible from Edit mode and the main Dashboard page and are available for *all* data sources.

Image Export

Users can click the **Image Export**  icon in View or Edit mode to export images of their graphical Visualization (excluding Pivot Table and Data Grid). Images can be exported as PNG, JPEG, or SVG.

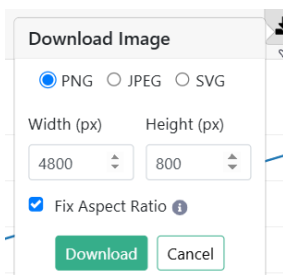


Figure 130: Users can download an image of their Visualization from View or Editor mode

Export CSV

Users can export a CSV of the data present in their **Pivot Table** and **Data Grid** Visualizations.

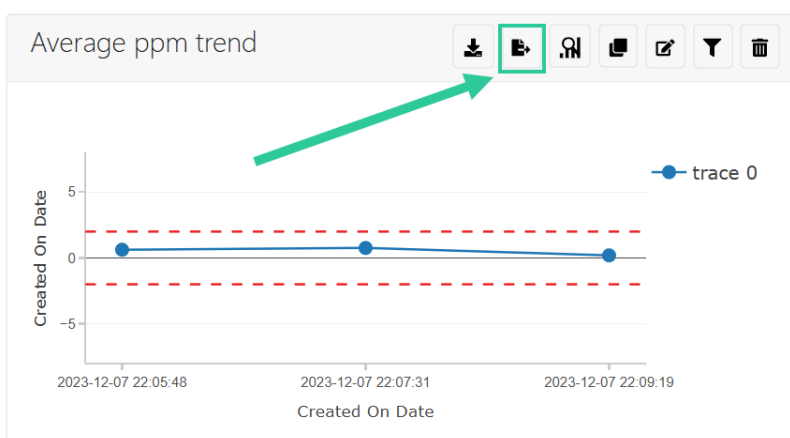



Figure 131: Export CSV

Sharing Dashboards

Clicking on the link  icon next to the Dashboard title copies a link to the Dashboard which can then be shared with others who have access to the Dashboard.

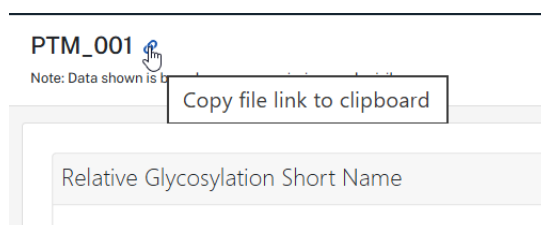


Figure 132: Copy file link to clipboard

Biophysical Data Source

The Biophysical data source, which can be used for data assessment between different orthogonal analyses, is a unique data source in several ways. Data originating from Intact, Peptide, and Chromatogram data sources can all be ingested, provided there is an association that can be made between the MS data and the Biophysical data through the fact that they are results generated for the same samples.

Ways to associate data

Mass spectrometry (MS) data must be associated with Biophysical data to be ingested. Data can be associated in one of two ways:


1. Sample Names are identical – if the value of Sample Name matches for both sets of data, data will be ingested and correlated in the Biophysical data source (Users can assure this by reviewing and editing the sample name in the Samples Table within the data analysis project)
2. A metadata value, **sample_code**, exists for the Biophysical data (saved with the project at the file level within Byosphere) and can be also found within the Sample Name of the MS data. Example:
 - The Biophysical data file, for instance, a .peaks file (a Byosphere generated file format to include previously exported 3rd party chromatographic software results), has the following metadata value, which was parsed from a .ars report file containing metadata:

Sample Code:
 - The MS raw data file, processed within a Byos Intact project, has the following associated sample name within the projects samples table and is corresponding to the same sample run on both instruments:

Sample
name
Datarun_120424 **ABC123** Run3

In this case, the user does not need to alter their sample naming conventions for either sample, which would be undesirable when there are company or laboratory standards of naming. Instead, the user must simply provide an additional metadata value in the Biophysical data that correlates with a *unique* identifier also present in the established MS sample name.

Using the Inspection Tool

Like with all other data sources, users can view the files present within their Biophysical Dashboard by clicking the **Visualization Inspection**  icon. However, due to the complexity of the Biophysical data source, there are additional fields present to accommodate identification of all contributing data points.

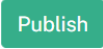

Field	Data Source	Description
Biophysical Folder	Biophysical	The folder from which the Biophysical data file originates
Biophysical File Name	Chromatogram	The file name of the Chromatogram project from which Biophysical data is processed
Biophysical Sample Name	Chromatogram	The name of the Biophysical data within the Chromatogram project
Chromatogram Sample Name	Biophysical	Sample Name originating from the Biophysical report (.ars)
Sample Code	Biophysical	Metadata value originating from Biophysical report (.ars)

Peptides Folder	Peptides	The folder from which the Peptides data originates
Peptides File Name	Peptides	The file name of the Peptides project from which Peptide MS data is processed
Peptides MS Sample Name	Peptides	The name of the Peptides MS sample within the Peptides project
Intact Folder	Intact	The folder from which the Intact data originates
Intact File Name	Intact	The file name of the Intact project from which Intact MS data is processed
Intact MS Sample Name	Intact	The name of the Intact MS sample within the Intact project

Figure 133: Visualization Inspection fields for Biophysical Data

Publishing a Dashboard

Clicking **Save and Close** after changing Visualization settings, adding Filters/Sort, Derived Fields, or Background Alerts will update the Dashboard in real-time for the user. However, this will **not** save the contents of the Dashboard and any changes will be lost if the page is closed and reopened.

To ensure any changes made to the Dashboard have been saved, the user must **Publish** the Dashboard by clicking the  icon on the right-hand side of the Dashboard. Note that this button only becomes available once the user has clicked  when initially entering the Dashboard.

Note that the Publish button will be disabled if the user tries to change the name of the Dashboard to a preexisting name that is already saved within the same Folder.

If publishing a Dashboard fails for some reason (such as having an invalid or blank Title or Location), the Dashboard will remain in Edit mode so the user can try again. If the Publish is successful, the Dashboard Editor will close, and the Dashboard will display in Viewer mode.

If the user clicks Cancel prior to Publishing a Dashboard that has changes, they will be met with a dialog asking if they would like to proceed and discard any unsaved changes.

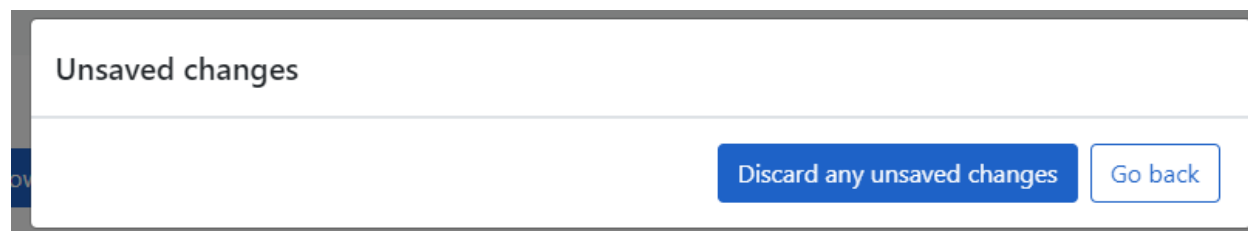


Figure 134: Discard any unsaved changes dialog