

USER GUIDE

Proteograph™ Analysis Suite

Notice

© 2021 Seer, Inc. All rights reserved. Information in this document is subject to change without notice. Seer assumes no responsibility for any errors or omissions in this document. Duplication and/or reproduction of all or any portion of this document without the express written consent of Seer is strictly forbidden. Seer does not convey any license under its patent, trademark, copyright, or common-law rights nor similar rights of any third parties by this document.

Nothing contained herein shall constitute any warranty, express or implied, as to the performance of any products described herein, or any warranties of merchantability, fitness for a particular purpose or non-infringement. The use of products described herein is subject to certain restrictions as set forth in the applicable terms and conditions of sale or license accompanying the purchase of such product and any written agreements between Seer and user. Seer may refer to products or services offered by other companies by their brand names or company names solely for clarity and does not claim any rights in those third party marks or names. All products and services described herein are intended FOR RESEARCH USE ONLY and NOT FOR USE IN DIAGNOSTIC PROCEDURES.

The instructions in this document must be strictly and explicitly followed by qualified and properly trained personnel in order to ensure the proper and safe use of the product(s) described herein. All of the contents of this document must be fully read and understood prior to using such product(s).

Failure to completely read and explicitly follow all of the instructions contained herein may result in damage to the product(s), injury to persons, including to users or others, and damage to other property, and will void any warranty applicable to the product(s). Seer does not assume any liability arising out of the improper use of the product(s) described herein (including parts thereof or software).

BUYER IS NOT LICENSED OR AUTHORIZED TO, AND AGREES NOT TO, USE ANY SEER PRODUCT FOR ANY CLINICAL OR DIAGNOSTIC PURPOSES.

Revision history

DOCUMENT	DATE	DESCRIPTION OF CHANGE
CF-1003 B (PAS version 1.5)	October 2021	<p>Per <i>Proteograph Analysis Suite Release Notes</i> (CF-1018 A)</p> <p>New analyses to visualize differences in peptide/protein group intensities between samples and groups</p> <ul style="list-style-type: none"> • New interactive table containing peptide/protein group intensities across samples/groups • New heatmap plot for visualizing peptide/protein group intensities across samples/groups <p>New analysis to identify peptide/protein groups with significantly different intensities between groups (e.g., healthy vs. disease samples)</p> <ul style="list-style-type: none"> • Added new "Group analysis" sections to 'Analysis' section • Guided comparison setup providing data filtering, normalization, imputation, and statistical test options • Toggle for viewing only 'Significant Peptides/Proteins' in dataset • Interactive plots and tables for exploratory expression analysis of significantly regulated targets with dynamic fold-change and p-value options • New group analysis plots to visualize peptides/protein groups with statistically different intensities <ul style="list-style-type: none"> - Volcano plot – fold-change vs. statistical significance with coloring options to highlight proteins-of-interest - Coverage viewer – Amino acid sequence coverage by peptides display, including PTM detection - Clustered heatmap – visualizing peptide/protein group intensities across samples/groups with rows (peptide/protein groups) and columns (samples) ordered using hierarchical clustering - Protein-protein interaction – Visualization of PPIs (STRING db) of significant proteins - Intensity box plots – Compare significant peptide/protein group intensities between groups <p>Changes to plot visualizations</p> <ul style="list-style-type: none"> • Added ability to export plot source data to .csv files • Improved plot rendering speeds • Added user preferences to modify plots <p>New analysis protocols</p> <ul style="list-style-type: none"> • Integration of DIA-NN database search engine <ul style="list-style-type: none"> - Pre-installed DIA-NN library-based protocol (DIANN – System Provided DIA Protocol) - Expanded Seer human plasma spectral library file (4,011 protein groups; 62,687 precursors) - Optional in silico predicted library-free protocol

DOCUMENT	DATE	DESCRIPTION OF CHANGE
Changes to results summary		
<ul style="list-style-type: none">• Simplified peptide and protein group results tables<ul style="list-style-type: none">- Panel level summary- NP level summary		
Changes to help content		
<ul style="list-style-type: none">• Updated user guide• Indexed online help• Tooltips		
New data file management		
<ul style="list-style-type: none">• New AutoUploader application allows automatic data transfer from LC-MS system to PAS account		
CF-1003 A (PAS version 1.0)	May 2021	Initial release

Contents

Notice	2
Revision history	3
Contents	5
Chapter 1 Welcome to PAS	9
Access the PAS application	10
Tour of the PAS application	11
Sidebar menu	11
Top bar and User Account menu	11
Work with PAS tables	12
Show or hide table columns	12
Add custom columns	12
Sort a table	13
Filter a table; search for a specific item	13
Control how many items are shown per table page	13
Navigate among table pages	13
Access item details and/or sub-items	13
Set color preferences in PAS graphs	14
Get help with PAS	14
Manage your user profile	14
Input files	15
Plate map file format	15
Sample description file format	16
Output files	17
Quality control	18
Application settings	19
Change the appearance of the user interface	19
Configure application settings	19
Configure two-factor authentication for yourself	19
Configure default display settings for analysis results	20
User management	21
Users and Permissions page	21
Add a user	21
Edit a user	22
Delete a user	22
Chapter 2 Analysis Setup	23
Analysis setup workflows	24
Setup workflow: Add a plate	25
Add one or more MS data files	25
Add the plate map file	25
Specify plate information	26
Add a sample description file (optional)	26
Add the samples to a project	26
Start the analysis	27
Setup workflow: Link to a plate	28
Review the MS data files to be linked a plate	28
Add the plate map file	28

Specify plate information	29
Add a sample description file (optional)	29
Add the samples to a project	29
Start the analysis	30
Setup workflow: Select samples or controls for analysis	31
Analyze selected samples	31
Analyze controls only	32
Chapter 3 Analysis Results	33
Access analysis results	34
Review analysis results	35
Data visualization	36
Analysis Summary tab	37
Open an analysis's Analysis Summary tab	37
Summary section	37
Protein Group Counts section	37
Set Protein Group Counts preferences	38
Peptide Counts section	38
Set Peptide Counts preferences	39
Distribution of Detected Proteins in Plasma Proteome section	39
Set Distribution of Detected Proteins in Plasma Proteome preferences	40
Protein Group Overlap Sets section	40
Set Protein Group Overlap Sets preferences	41
Sample Comparability section	42
Set Sample Comparability preferences	42
Analysis Metrics tab	44
Open an analysis's Analysis Metrics tab	44
Intensities section	44
Set Intensities preferences	45
Plate Map Grid section	45
Set Plate Map Grid preferences	46
Lamppost Proteins' Concentration section	46
Set Lamppost Proteins' Concentration preferences	47
PCA Analysis section	48
Change the PCA Analysis color scheme	48
Peptide Counts Distribution and Protein Group Counts Distribution sections	49
Protein Group Counts of Nanoparticles and Peptide Counts of Nanoparticles sections	50
Set Protein Group Counts of Nanoparticles and Peptide Counts of Nanoparticles preferences	51
Hierarchical Clustering section	52
QC Charts tab	53
Open and filter an analysis's QC Charts tab	54
Set QC Charts preferences	55
Manage user-defined and calculated control limits	55
Define and use user-defined control limits	56
Define and use calculated control limits	56
Delete a calculated control limit date range	56
Exclude a sample	56
Annotate control charts	57
Add an annotation	57
Edit an annotation	57

Delete an annotation	57
Generate reports of control results	57
Download summarized control results	57
Generate a detailed PDF report of control results	58
Analysis Output Files tab	59
Chapter 4 Analysis Interpretation	60
Open an analysis's Group Analysis tab	61
Export raw data to a file	62
View a raw protein group data heatmap	63
Set up and start a group analysis	64
Specify the quantitation level and grouping of samples	64
Filter out (exclude) samples and groups	64
Filter out (exclude) proteins or peptides	64
Normalize values and impute sparse or missing values	65
Select the statistical test and the groups to compare	65
Group Analysis tab	66
Raw Data section	66
Clustered Heatmap section	68
Volcano section	69
Coverage section	70
Filtered PPI Network section	71
Enrichment section	72
Box Plots section	73
Chapter 5 Data Management	75
Plates and samples	76
Plates page	76
Review a plate	77
Edit a plate	77
Delete a plate	77
Plate Samples section	78
Add samples to an existing plate	79
Add sample descriptions	80
Edit sample information	80
Delete a sample from a plate	81
Plate Grid section	81
Edit or delete samples in wells	81
Upload a custom file containing sample information	82
Projects	83
Projects page	83
Add a project	84
Delete a project	84
Sample List section	84
Add samples to a project	85
Analyses	86
Analyses page	86
Download an analysis log	87
Download an analysis's protein groups and peptides results	87
Edit an analysis	87

Delete one or more analyses	88
MS data files	89
Data Files page	89
Create a folder	90
Upload MS data files	90
Move MS data files	90
Rename MS data files or folders	90
Delete MS data files or folders	91
Download and install the Seer AutoUploader application	91
Analysis protocols	92
Protocols page	92
View an analysis protocol's search engine parameters	93
Upload an analysis protocol	93
Copy an analysis protocol	94
Download an analysis protocol	94
Delete an analysis protocol	94
Glossary	95
Index	99
Technical Support	102
Contact Information	102
Telephone	102

Chapter 1

Welcome to PAS

Introduces you to the Seer Proteograph™ Analysis Suite (PAS) software application, part of the Seer Proteograph™ Product Suite.

With this dedicated software solution, you can process, analyze, and visualize proteomics data sets generated by liquid chromatography-mass spectrometry (LC-MS). PAS includes an integrated search engine for identification and annotation of LC-MS data.

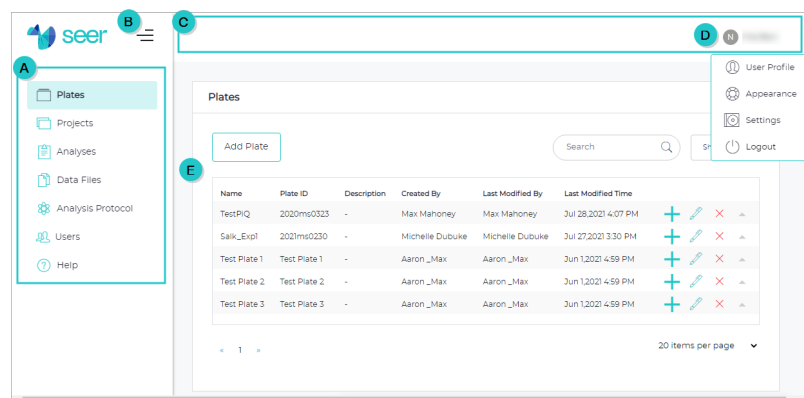
Access the PAS application

To access the PAS application, point your web browser to pas.seer.software. Compatible browsers include Chrome, Chromium, Edge, Firefox, and Safari.

When prompted to log in, enter your username and password. In the future, if you configure two-factor authentication, you will also need to enter a code generated by an authenticator app on your mobile device. (For details for setting up two-factor authentication, see [Configure two-factor authentication for yourself \(page 19\)](#).)

Tour of the PAS application

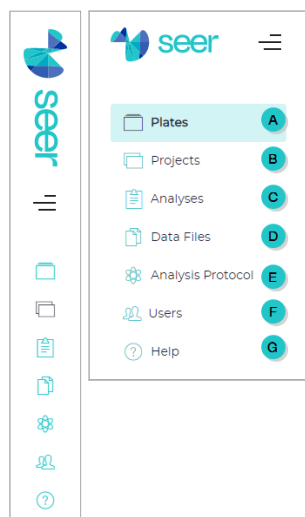
The PAS application window has several main parts.



- A** Sidebar menu
- B** Button to expand and collapse the sidebar menu
- C** Top bar
- D** User Account menu, accessible from your username
- E** Page with table items. For general table techniques, see [Work with PAS tables \(next page\)](#).

Sidebar menu

Use the sidebar menu to access PAS functionality and data.



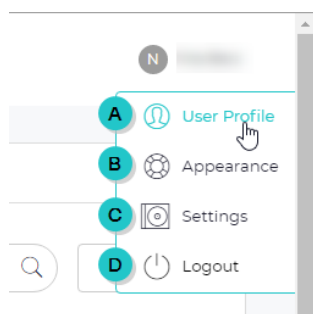
- A Plates** — For importing sample metadata from the Proteograph Assay method and associated MS data files. See [Plates and samples \(page 76\)](#).
- B Projects** — For grouping Proteograph Assay plates at the experimental project level and submitting data analysis jobs. See [Projects \(page 83\)](#).
- C Analyses** — For accessing data analysis jobs, data analysis results, and data visualizations. See [Analyses \(page 86\)](#).
- D Data Files** — For accessing the repository of MS data files and managing your data. See [MS data files \(page 89\)](#).
- E Analysis Protocol** — For accessing a collection of database search analysis protocols. See [Analysis protocols \(page 92\)](#).
- F Users** — (Admin only) For viewing, adding, editing, and deleting users. See [User management \(page 21\)](#).
- G Help** — For accessing PAS documentation including the user guide (PDF), web-based Help system, and videos. See [Get help with PAS \(page 14\)](#).

Top bar and User Account menu

The top bar of the PAS application window has just one component, the **User Account** menu, at the far right. To open the menu, select your username.

NOTE

When the sidebar menu is collapsed, the top bar — including your username — is hidden.



- A** User Profile — For managing your user information, such as your telephone number. See [Manage your user profile \(page 14\)](#).
- B** Appearance — For selecting a light or dark theme for the PAS user interface. See [Change the appearance of the user interface \(page 19\)](#).
- C** Settings — For configuring various application settings, including which DDA and DIA protocols will be used by default for data analysis. See [Configure application settings \(page 19\)](#).
- D** Logout — Logs you out of PAS.

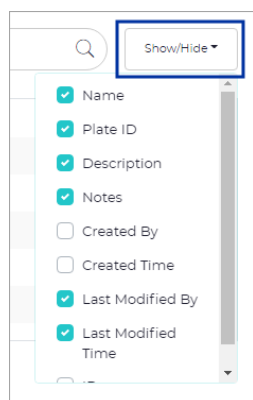
Work with PAS tables

Information in PAS is organized into tables. For example, the [Projects page \(page 83\)](#) offers a table of all projects, while the [Users and Permissions page \(page 21\)](#) offers a table of all PAS users.

Use the following techniques when working with tables.

Show or hide table columns

Some tables offer a **Show/Hide** list from which you can show and hide columns by selecting and clearing checkboxes.



Add custom columns

You can add custom columns to the [Plate Samples section \(page 78\)](#) and [Sample List section \(page 84\)](#). Any custom column you add to one of these tables is available for the other table. You can show and hide custom columns like any other column.

To add a custom column:

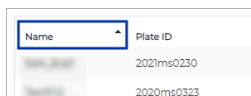
1. Select **Show/Hide**, scroll to the bottom of the list, and select **Add Custom** to open the **Add Custom Field** dialog.
2. Complete the fields.
 - **Custom Name** — A unique name for this custom field, within this table and with no spaces.
 - **Description** — The description of the custom field.
 - **Notes** — Additional information about the custom field.

3. Select **Create**.

The custom field (column) appears at the bottom of the **Show/Hide** column with the prefix `custom_`.

Sort a table

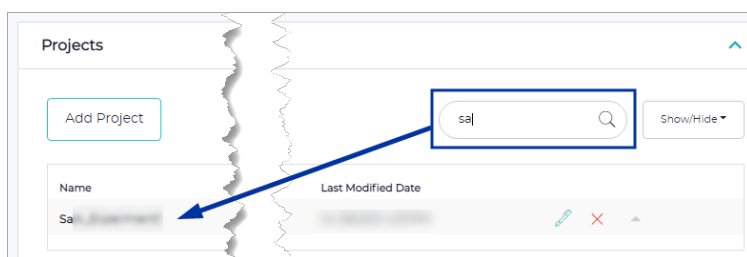
Sort table items by selecting the heading of the column you want to sort by. PAS sorts in descending order by default. To reverse the order, select the heading again. To turn off sorting entirely, select the heading one more time.



Name	Plate ID
2021ms0230	
2020ms0323	

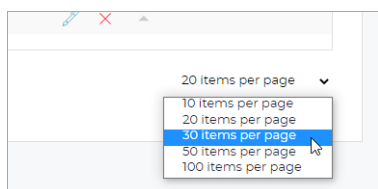
Filter a table; search for a specific item

Filter a table to show only specific items — and to find a specific item — by typing a string of characters in the **Search** field. As you type, PAS refreshes the table to show only matching items. To show all items again, clear the **Search** field.



Control how many items are shown per table page

To control how many table items PAS shows per page, select an option from the **Items per page** list, located at the lower right below the table.



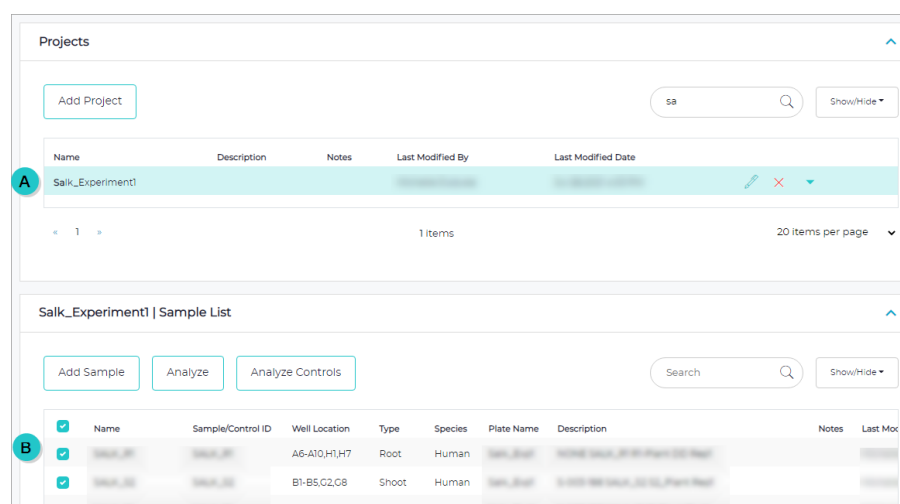
Navigate among table pages

Depending on how many items are shown per page, some tables may be broken into several pages. To navigate among the pages, use the left and right arrows located at the lower left below the table.



Access item details and/or sub-items

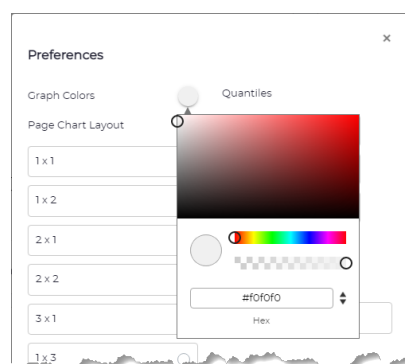
Some tables offer access to item details and/or related sub-items. To access an item's details or its sub-items, select that item's row. For example, on the **Projects** page, selecting a project row to access its related samples.



- A** Selected item
- B** Table of sub-items associated with the selected item

Set color preferences in PAS graphs

Many **Preferences** dialogs for PAS graphs offer controls with which you can set colors to suit your preferences. These controls open a color picker from which you can select a color.




To set a color preference:


1. Select the color control, such as **Graph Colors** as shown here, to open the color picker.
2. Select a color on the color spectrum or enter a color's hexadecimal value.
3. Click outside color picker to close it.

Get help with PAS

PAS offers many in-application resources where you can learn how to get the most out of it.

1. On the sidebar menu, select  **Help** to open the **Help** page.
2. Select the resource you're interested in: PAS web-based Help, the PDF of the user guide, or training videos.

Manage your user profile

1. On the **User Account** menu, select  **User Profile** to open the **User Profile** page.
2. Edit the fields as needed. (Depending on your role and organization, the fields may vary.)
 - **User Profile** — Edit your first name, last name, and phone number.
 - **Tenant Info** — Edit information about your organization and your address.
3. Select **Save**.

Input files

PAS accepts the following files as input for analysis.

- **Analysis protocol** (.xml, .json) — (Optional) The parameters for an MS database search. PAS includes preinstalled analysis protocols for both data-dependent acquisition (DDA) and data-independent acquisition (DIA) data files.
- **MS data files** (.raw, .wiff, .wiff.scan) — The results of MS analysis for each sample or control in a plate. Each sample or control is associated with one MS data file.
- **Plate map file** (.csv) — The location of each sample in a plate with information on each sample, control, nanoparticle, and peptide.
- **Sample description file** (.csv) — Metadata for each sample in a plate, such as sample name and IDs, type, species, and condition.

Plate map file format

The Proteograph™ Instrument Control Software (ICS) generates the plate map file (.csv). All columns are prefilled except for MS file name, which you must define.

COLUMN	DESCRIPTION
MS file name	The name of the MS data file, including extension (for example, EXP20101_2020ms0321X83_A.raw)
Sample name	A unique identifier for the sample, typically the biological sample name ¹
Sample ID	A unique identifier for the sample ¹
Well location	The column and row of the well the sample occupies
Nanoparticle	The nanoparticle name (nanoparticle 1–5)
Nanoparticle ID	The nanoparticle lot (kit ID)
Control	The control type: Process Control, Digestion Control, MPE Control, or MS Peptide Control
Control ID	The control lot
Instrument name	The name of the liquid handler that converted the samples into peptides
Date sample preparation	The date the method ended
Sample volume	The volume of sample in the indicated well ²
Peptide concentration	The concentration of peptide in the well ²
Peptide mass sample	The mass of peptide in the well ²
Recon volume	The volume of Peptide Reconstitution Buffer added to the well ²
Kit ID	The ID of the assay kit used to convert the samples into peptides
Plate ID	A unique identifier for the plate
Plate Name	A descriptive name for the plate

¹The sample name links the plate map and sample description files, while the sample ID groups the nanoparticles in an assay.

²The file shows the numeric value only, without unit of measure.

Sample description file format

The sample description file (.csv) contains the following information about each sample in a plate. The file can also include custom (user-defined) columns. These columns must include the prefix `custom_`.

Table 1. Columns in a sample description file

COLUMN	DESCRIPTION
Sample Name	A unique identifier for the sample, typically the biological sample name
Sample Type	The type of sample, such as plasma or tissue lysate
Species	The species (human or mouse) from which the sample was collected
Description	A description of the sample
Sample Receipt Date	The date your laboratory received the sample
Sample Collection Date	The date the sample was collected
Condition	The categorical group the sample belongs to
Biological Replicate	The biological replicate number
Technical Replicate	The technical replicate number

Output files

An analysis generates several results files, which record search results for each sample in .txt and .xml formats.

Quality control


A plate includes prepared samples and the following controls for quality control (QC) purposes. The control results provide insight into the variation and reproducibility of experiments and LC-MS analysis.

- **Process Control** — A reference sample added before protein corona formation.
- **Digestion Control** — A reference sample added before trypsin digestion.
- **MPE Control** — Reference peptides added before desalting cleanup.
- **MS Peptide Control** — Reference peptides added before LC-MS analysis.

Application settings


You can configure several PAS application settings, including the default analysis protocols for controls and samples. You can also change the appearance of the PAS user interface. These settings are global and apply to all analyses and pages. Finally, you can configure two-factor authentication for yourself.

Change the appearance of the user interface

1. On the **User Account** menu, select  **Appearance** to open the **Appearance** page.
2. Select the theme you want to use:
 - **Light** (default) — Makes the background of the user interface white.
 - **Dark** — Makes the background of the user interface black.
3. Select **Save**.

Configure application settings


Follow these steps to configure PAS application settings. See also [Configure two-factor authentication for yourself \(below\)](#).

1. On the **User Account** menu, select  **Settings** to open the **Settings** page.
2. In the **Settings** section, configure settings as needed.
 - **Default Analysis Protocol** — Select the DDA-based and DIA-based analysis protocols you want to use for controls and for samples.
 - **Remove MS data files when plate is deleted** — Select either:
 - . *No (default)* to have PAS retain the MS data files linked to the plate.
 - . *Yes* to have PAS delete the MS data files linked to the plate.
 - **Receive email notifications on analysis updates** — Select either:
 - . *Yes (default)* to have PAS send you an email whenever an analysis status changes.
 - . *No* to have PAS not send emails about analysis updates.
3. Select **Save**.

Configure two-factor authentication for yourself

You can configure PAS to require two-factor authentication when you log in. That means that PAS will prompt not only for your username and password, but also for a generated authentication code.

Before continuing, you will need to have already installed an authentication app on your mobile device. PAS is compatible with many such apps, including Google Authenticator, Duo Mobile, 1Password, Auth, and Microsoft Authenticator.

1. On the **User Account** menu, select  **Settings** to open the **Settings** page.
2. In the **Two-factor Authentication** section, select **Use Authenticator App** to open the **Authenticator verification** dialog.


3. Using the authenticator app on your mobile device, either scan the QR code or enter the key shown on-screen into the authenticator app.
4. In PAS, enter the generated code.
5. Select **Submit** and then select **OK** to close the success message.

NOTE

Notice that the **Use Authenticator App** button now reads **Disable Authenticator App Security**. To turn two-factor authentication off, follow the same steps as above, select that button, and follow the on-screen prompts.

Configure default display settings for analysis results

In addition to configuring PAS application settings (see [Configure application settings \(previous page\)](#)), you can also configure display settings for analysis results. These display settings determine which analysis results are shown and how they are grouped and sorted. The settings are global and apply to all analyses.

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. Select any analysis.
3. Below the **Analyses** table, locate and select **Display Settings** to open the **Display Settings** dialog.
4. Configure settings as needed.
 - **Group by** — Select an option for grouping protein group and peptide counts.
 - **Sort by** — Select an option for sorting data on the **Analysis Summary** tab.
 - **<list of wells>** — Select or clear checkboxes to show or hide wells. Scroll to see all wells.
 - **Hide Controls** — Set the toggle key to **ON** to hide controls.
 - **Visualization graphs** — Select each toggle key to **ON** or **OFF** to show or hide the corresponding graph.
5. Select **Continue** to apply the settings.

User management



If you are a PAS administrator, you can add, edit, and delete users.

Users and Permissions page

If you are an Admin, use the **Users and Permissions** page to manage PAS users.

- To open this page, select  **Users** on the sidebar menu.

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.

Toolbar items



- Add User** — Select to add a new user. See [Add a user \(below\)](#).
- Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).

Table columns


- Name** — The user's name.
- Email** — The user's email address.
- Role** — The user's role, which grants access to specific PAS functionality.
 - User* — Can add plates, create projects, create analysis protocols, view MS data files, and view results files.
 - Admin* — In addition to *User* functionality, can also manage users.
- Group** — The group or groups the user is assigned to.

NOTE

- Use group assignments to limit user access to specific plates, projects, and analyses.
- Members of a user group can access and view the plates, projects, and analyses of everyone in the group.

- Status** — The user's status (e.g., *Confirmed*, meaning acceptance of the invitation to join PAS).
-  (**Edit**) — Select to edit the selected user. See [Edit a user \(next page\)](#).
-  (**Delete**) — Select to delete the selected user. See [Delete a user \(next page\)](#).

Add a user

- On the sidebar menu, select  **Users** to open the **Users and Permissions** page.
- Select **Add User** to open the **Invite User** dialog.
- Complete the fields. Required fields are marked on-screen with an asterisk.
 - Username** — Enter a unique identifier for the user.
 - Email** — Enter the user's email address.

- **Role** — From the list, select the user's role: *User* (the default) or *Admin*.
- **User Groups** — (For a user of *User* role) From the list, select one or more existing user groups. To add a new group, enter its name.



NOTE

- Use group assignments to limit user access to specific plates, projects, and analyses.
- Members of a user group can access and view the plates, projects, and analyses of everyone in the group.
- By default, PAS excludes the user from all groups.



4. Select *Send*.

The user will be sent an email invitation with the assigned username, a temporary password, and a link to PAS.

Edit a user

1. On the sidebar menu, select  **Users** to open the **Users and Permissions** page.
2. Find the user you want to edit and select  (**Edit**) to open the **Edit User** dialog.
3. Edit the fields as needed.
4. Select **Save**.

Delete a user

1. On the sidebar menu, select  **Users** to open the **Users and Permissions** page.
2. Find the user you want to delete and select  (**Delete**).
3. Select **OK** to confirm.



Chapter 2

Analysis Setup

Offers step-by-step guidance for different setup workflows for getting ready for analysis.

Analysis setup workflows

PAS offers several workflows for getting ready for data analysis.

To set up a new plate and initiate a new analysis, follow:

- [Setup workflow: Add a plate \(next page\)](#) — This is the most straightforward setup workflow. Begin on the **Plates** page and add a plate.
- [Setup workflow: Link to a plate \(page 28\)](#) — Begin on the **Data Files** page, add MS data files, and then link the files to a plate.

To analyze existing plate data, follow:

- [Setup workflow: Select samples or controls for analysis \(page 31\)](#) — Begin on the **Projects** page to analyze samples. Choose this workflow when you have more than one plate whose samples you want to analyze in a single analysis. You can also choose this workflow when you want to reanalyze samples.

Setup workflow: Add a plate

When you set up analysis by adding a plate, PAS guides you through the workflow with the **Add Plate** dialog. In this workflow, you add a new plate to PAS and then add samples to a new or existing project. Depending on your choices during the workflow, the analysis will start immediately or will be deferred for later.

To begin this workflow:

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Select **Add Plate** to open the **Add Plate** dialog.




Add one or more MS data files

In the **MSData Files** section, you add one or more MS data files.

1. Select the MS data files.

NOTE

Supported file formats are .raw, wiff, or .wiff.scan. Supported folders are RAW and D.

- To add a single file, select **Files** to open the **Add Files** dialog.
 - To add multiple files, select **Folder** to open the **Add Folder** dialog.
2. Either drag the file or folder into the drag-and-drop area or use **Browse** to navigate to and select it.
 3. Select **Add**.
 4. Review the selected files.
 - To remove a file, select  (**Delete**).
 - To remove all files, select **Clear**.
 5. Select **Next** to advance.

Add the plate map file

In the **Plate Map File** section, you add a plate map file, which specifies the locations of samples.

1. If you don't have a plate map file, create one before continuing.
 - a. Select the on-screen link from which you can download an example plate map file (.csv).
 - b. Open the file and edit it as needed.

The **MS file name**, **Sample ID**, and **Plate ID** columns are required. (See [Plate map file format \(page 15\)](#) for detailed descriptions of the columns in the file.)
 - c. Save as a .csv file.
2. Select **Add File** or **Add** to open the **Add File** dialog.

3. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.
4. Select **Add**.
5. Select **Next** to advance.

Specify plate information

In the **Plate ID and Name** section, you link the MS data files to a new or existing plate.

1. Do either of the following:
 - To link to an existing plate, select **Use Existing Plate**, and then select a plate from the **Select Existing Plate** list.
 - To set up a new plate, complete the fields.
 - **Plate ID** — A unique identifier for the plate.
 - **Plate Name** — A descriptive name for the plate.
2. Select **Next** to advance.

Add a sample description file (optional)

In the **Sample Description File** section, you upload metadata for each sample in the plate.

NOTE

This part of the workflow is optional. To skip it, select **Next** to advance.

1. Select **Add** or **Add File** to open the **Add Files** dialog.
2. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.
3. Select **Add**.
4. Select **Next** to advance.

Add the samples to a project


In the **Add to Project** section, you add samples to a new or existing project. Depending on your choices, the analysis will start immediately or will be deferred for later.


1. Create or select a project:
 - To create a new project, select **New Project**, enter a project name, and select **Add**.
 - To use an existing project, select it from the **Select Project** list.
2. Select or clear the applicable checkboxes. (To defer analysis, clear both checkboxes.)
 - **Analyze samples after addition** — Select to analyze samples.
 - **Analyze controls after addition** — Select to analyze controls.
3. Select the MS method:
 - **DDA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.

- *DIA* — Derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.
4. From the **Analysis Protocol** list (which shows only protocols compatible with the selected MS method), select a protocol.
 5. Select **Add Plate**, and then select **Close**.
 - If you had selected either or both **Analyze...** checkboxes earlier, the analysis starts immediately.
 - If you deferred analysis, you must start it manually. See [Start the analysis \(below\)](#).

Start the analysis

If you deferred analysis during the setup workflow, follow these steps to start the analysis.

1. On the sidebar menu, select  **Projects** to open the **Projects** page.
2. Select the applicable project.
3. Select one of the following options:
 - **Analyze** — Opens the **Analysis** dialog from which to analyze all selected samples in the project.
 - **Analyze Controls** — Opens the **Analyze Controls** dialog from which to analyze the controls only.
4. If you are analyzing all selected samples, in the **Analysis Name** field, enter a name for the analysis.
5. Select the MS method:
 - *DDA* — Derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.
 - *DIA* — Derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.
6. From the **Analysis Protocol** list (which shows only protocols compatible with the selected MS method), select a protocol.
7. In the **Description** field, enter a description of the analysis.
8. In the **Notes** field, optionally enter any additional information about the analysis.
9. If you are analyzing all selected samples and want to exclude the controls, select the **Exclude controls** checkbox.
10. If you are analyzing only controls, under **Analysis Name Pattern**, review the MS data file name format and list of controls to analyze.
11. Select **Start**, and then select **OK**.

The samples or controls are queued for analysis.
12. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
13. Confirm that the new analysis appears on the **Analyses** page.


Setup workflow: Link to a plate

When you set up analysis by linking to a plate, PAS guides you through the workflow with the **Link to Plate** dialog. In this workflow, you link MS data files and associated sample information to a new or existing plate. Depending on your choices during the workflow, the analysis will start immediately or will be deferred for later.

NOTE

If you have not already uploaded the MS data files you want to work with, follow the steps in [Upload MS data files \(page 90\)](#) before starting this workflow.

To begin this workflow:

1. On the sidebar menu, select  **Data Files** to open the **Data Files** page.
2. Select the folder that holds the files you want to work with.
3. Select the checkbox of each MS data file to include in the analysis. Each MS data file represents one sample.
4. Select **Link to Plate** to open the **Link to Plate** dialog.



Review the MS data files to be linked a plate

In the **MSData Files** section, you review the selected MS data files to be linked to a plate.

1. Review the selected MS data files.
 - To remove a file, select its **X (Delete)** button.
 - To remove all files, select **Clear**.
2. Select **Next** to advance.

Add the plate map file

In the **Plate Map File** section, you add a plate map file, which specifies the locations of samples.

1. If you don't have a plate map file, create one before continuing.
 - a. Select the on-screen link from which you can download an example plate map file (.csv).
 - b. Open the file and edit it as needed.

The **MS file name**, **Sample ID**, and **Plate ID** columns are required. (See [Plate map file format \(page 15\)](#) for detailed descriptions of the columns in the file.)
 - c. Save as a .csv file.
2. Select **Add File** or **Add** to open the **Add File** dialog.
3. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.

4. Select **Add**.
5. Select **Next** to advance.

Specify plate information

In the **Plate ID and Name** section, you link the MS data files to a new or existing plate.

1. Do either of the following:
 - To link to an existing plate, select **Use Existing Plate**, and then select a plate from the **Select Existing Plate** list.
 - To set up a new plate, complete the fields.
 - **Plate ID** — A unique identifier for the plate.
 - **Plate Name** — A descriptive name for the plate.
2. Select **Next** to advance.

Add a sample description file (optional)

In the **Sample Description File** section, you upload metadata for each sample in the plate.

NOTE

This part of the workflow is optional. To skip it, select **Next** to advance.

1. Select **Add** or **Add File** to open the **Add Files** dialog.
2. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.
3. Select **Add**.
4. Select **Next** to advance.

Add the samples to a project


In the **Add to Project** section, you add the samples to a new or existing project. Depending on your choices, the analysis will start immediately or will be deferred for later.


1. Create or select a project:
 - To create a new project, select **New Project**, enter a project name, and select **Add**.
 - To use an existing project, select it from the **Select Project** list.
2. Select or clear the applicable checkboxes. (To defer analysis, clear both checkboxes.)
 - **Analyze samples after addition** — Select to analyze samples.
 - **Analyze controls after addition** — Select to analyze controls.
3. Select the MS method:
 - **DDA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.
 - **DIA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.

4. From the **Analysis Protocol** list (which shows only protocols compatible with the selected MS method), select a protocol.
5. Select **Add Plate**, and then select **Close**.
 - If you had selected either or both **Analyze...** checkboxes earlier, the analysis starts immediately.
 - If you deferred analysis, you must start it manually. See [Start the analysis \(below\)](#).

Start the analysis

If you deferred analysis during the setup workflow, follow these steps to start the analysis.

1. On the sidebar menu, select  **Projects** to open the **Projects** page.
2. Select the applicable project.
3. Select one of the following options:
 - **Analyze** — Opens the **Analysis** dialog from which to analyze all selected samples in the project.
 - **Analyze Controls** — Opens the **Analyze Controls** dialog from which to analyze the controls only.
4. If you are analyzing all selected samples, in the **Analysis Name** field, enter a name for the analysis.
5. Select the MS method:
 - **DDA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.
 - **DIA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.
6. From the **Analysis Protocol** list (which shows only protocols compatible with the selected MS method), select a protocol.
7. In the **Description** field, enter a description of the analysis.
8. In the **Notes** field, optionally enter any additional information about the analysis.
9. If you are analyzing all selected samples and want to exclude the controls, select the **Exclude controls** checkbox.
10. If you are analyzing only controls, under **Analysis Name Pattern**, review the MS data file name format and list of controls to analyze.
11. Select **Start**, and then select **OK**.

The samples or controls are queued for analysis.
12. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
13. Confirm that the new analysis appears on the **Analyses** page.

Setup workflow: Select samples or controls for analysis

The **Projects** page is the starting point for the sample selection method of analysis setup.

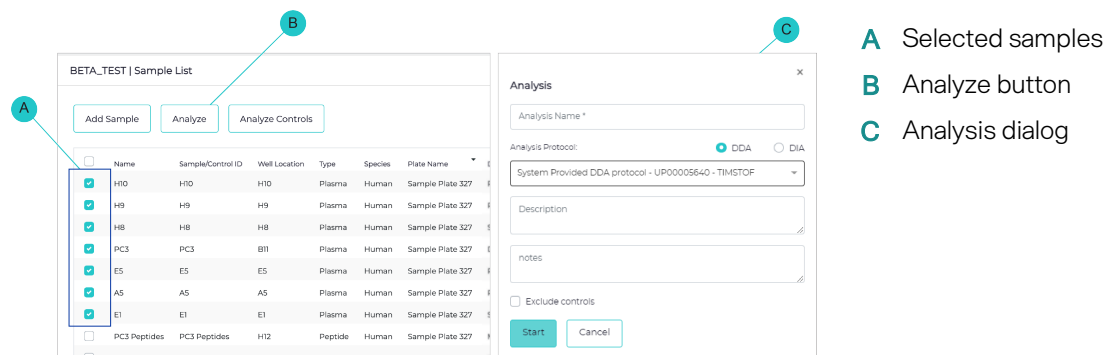
Choose this workflow when you have more than one plate whose samples you want to analyze in a single analysis. You can also use this workflow to reanalyze samples. See [Analyze selected samples \(below\)](#).

Use this workflow also to analyze controls only. See [Analyze controls only \(next page\)](#).

NOTE

For this workflow, PAS must already contain the applicable plate and MS data files in a project.


Figure 1. Projects page (left) and Analysis dialog (right)




Analyze selected samples

- On the sidebar menu, select **Projects** to open the **Projects** page.
- Select the applicable project.
- Select the checkbox of each sample to analyze.
- Select **Analyze** to open the **Analysis** dialog.
- In the **Analysis Name** field, enter a name for the analysis.
- From the **Analysis Protocol** list (which shows only protocols compatible with the selected MS method), select a protocol.
- In the **Description** field, enter a description of the analysis.
- In the **Notes** field, optionally enter any additional information about the analysis.
- If you want to exclude the controls, select the **Exclude controls** checkbox.
- Select **Start**, and then select **OK**.
The samples are queued for analysis.
- On the sidebar menu, select **Analyses** to open the **Analyses** page.
- Confirm that the new analysis appears on the **Analyses** page.

Analyze controls only

1. On the sidebar menu, select  **Projects** to open the **Projects** page.
2. Select the applicable project.
3. Select samples, and then select **Analyze Controls** to open the **Analyze Controls** dialog.
4. Select the MS method:
 - *DDA* — Derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.
 - *DIA* — Derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.
5. From the **Analysis Protocol** list (which shows only protocols compatible with the selected MS method), select a protocol.
6. In the **Description** field, enter a description of the analysis.
7. In the **Notes** field, enter any additional information about the analysis.
8. Under **Analysis Name Pattern**, review the MS data file name format and the list of controls to analyze.
9. Select **Start**, and then select **OK**.

The samples are queued for analysis.
10. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
11. Confirm that the new analysis is listed.



Chapter 3

Analysis Results

Describes analysis results (exclusive of Group Analysis) and offers step-by-step guidance for working with them.

Access analysis results

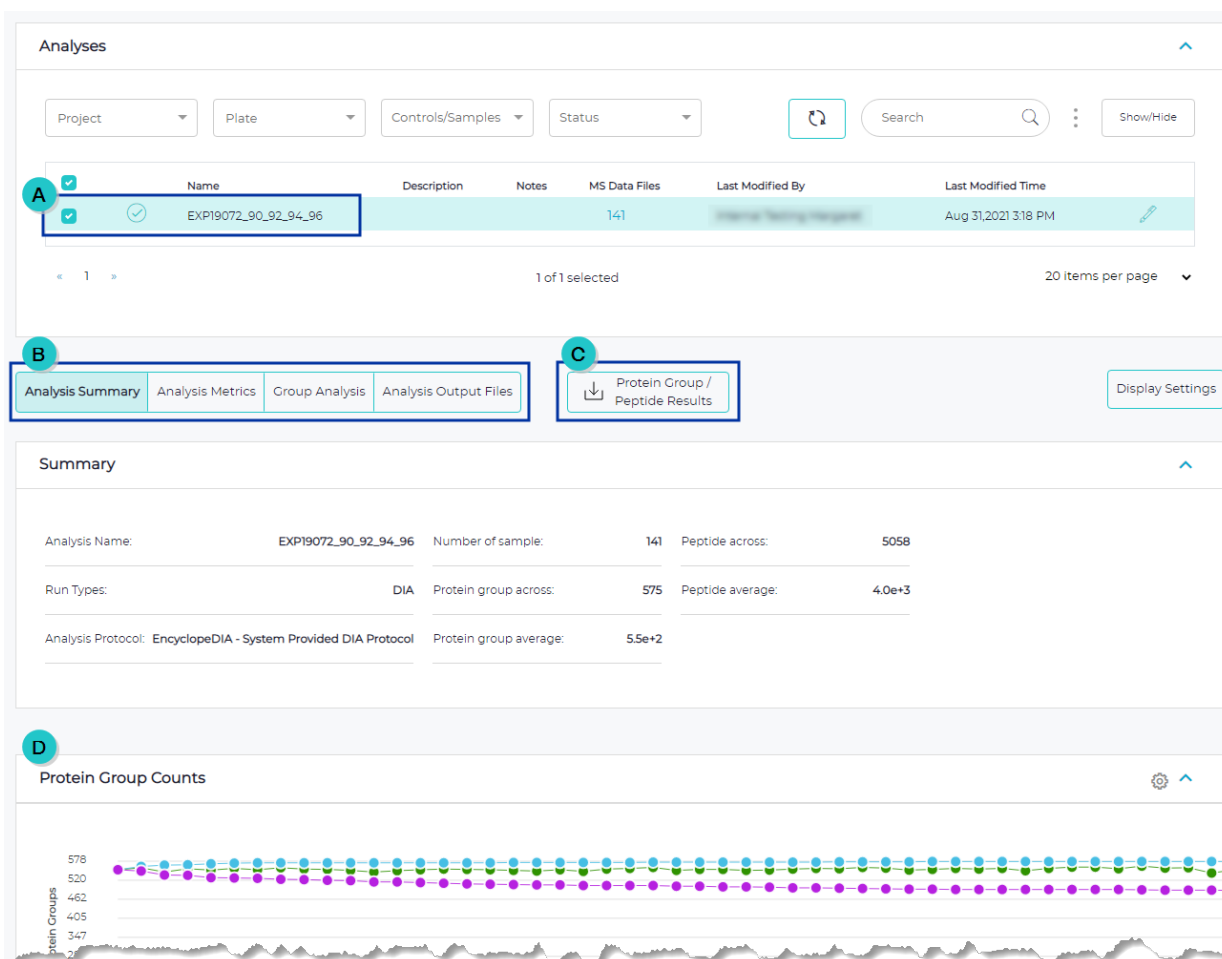
Access analysis results on the **Analyses** page, where you can review data in a variety of graphs and download results files. The results of the selected analysis are arranged in up to five tabs, each presenting a subset:

Analysis Summary, **Analysis Metrics**, **Group Analysis**, **QC Charts**, and **Analysis Output Files**.

NOTE

Depending on the selected analysis, the **QC Charts** tab might not be shown.

Figure 2. Analyses page




A Select an analysis

B Select tabs to view subsets of the analysis's results

C Download the analysis's protein groups and peptide results


D A results graph

Review analysis results

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. From the **Status** list, select *Completed*.
3. To apply additional filters, select options from any of the following lists:
 - **Project** — Shows analyses for specified projects.
 - **Plate** — Shows analyses for specified plates.
 - **Controls/Samples** — Shows analyses for controls only or samples only.
4. Select an analysis.

NOTE

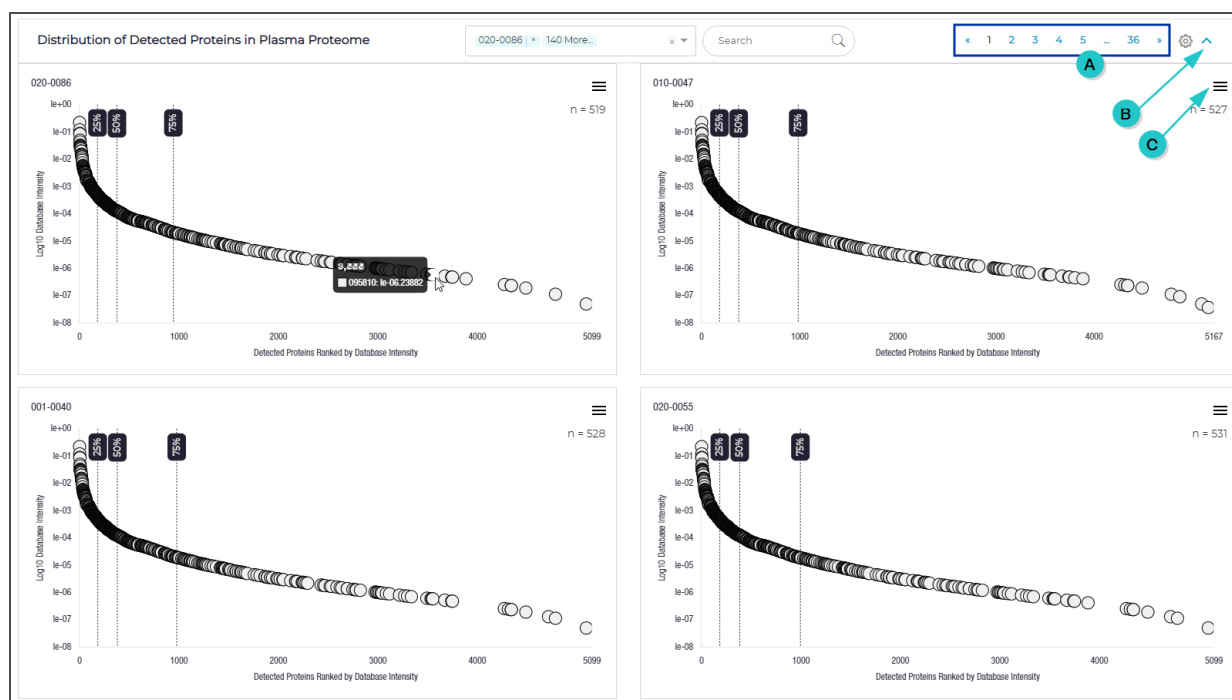
If you select multiple analyses, PAS does not show an analysis summary or results files and, instead, groups all data in the graphs on the remaining tabs.

5. On the **Analysis Summary** tab, compare samples and review a summary of the analysis, counts of peptides and protein groups, the dynamic range distribution of detected proteins, sample overlap, and sample correlation. To learn more about this tab, begin at [Analysis Summary tab \(page 37\)](#).
6. On the **Analysis Metrics** tab, review the intensities, sample clusters, nanoparticle counts, and other QC metrics. To learn more about this tab, begin at [Analysis Metrics tab \(page 44\)](#).
7. If the analysis included controls, select the **QC Charts** tab to review the control results. To learn more about this tab, begin at [QC Charts tab \(page 53\)](#).
8. On the **Analysis Output Files** tab, review results files.
9. (Optional) Use  **Protein Group / Peptide Results** to download the analysis's protein groups and peptide results. See [Download an analysis's protein groups and peptides results \(page 87\)](#).

Data visualization

Several tabs of the [Analyses page \(page 86\)](#) are divided into expandable and collapsible sections. Some sections include a menu for downloading graph data as a .svc, .png, or .csv file. Sections with many graphs include scroll arrows for accessing all the graphs.

Figure 3. Example section





- A** Scroll arrows and page numbers to move through all graphs
- B** Arrow to expand or collapse the section
- C** Menu for downloading data in the section

Analysis Summary tab


An analysis's **Analysis Summary** tab (on the **Analyses** page) offers an overall view of analysis results, organized into sections.

For some sections, you can modify labels, reorganize layouts, and otherwise adjust display preferences. These modifications are temporary and apply only to the select analysis. When you leave the **Analyses** page, each section returns to the default view. (To configure display preferences for all analyses in PAS, see [Configure default display settings for analysis results \(page 20\)](#).)

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.

Open an analysis's Analysis Summary tab

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. From the **Status** list, select *Completed*.
3. Select an analysis to open its analysis results.
4. Select the **Analysis Summary** tab.

Summary section

The **Summary** section shows the following information.

- **Analysis name** — The name of the analysis.
- **Number of samples** — The number of samples analyzed.
- **Peptides across** — The total number of distinct peptides across samples.
- **Run types** — The analysis protocol type, either *DDA* or *DIA*.
- **Protein group across** — The total number of distinct protein groups across samples.
- **Peptide average** — The average number of peptides per sample.
- **Analysis protocol** — The name of the analysis protocol applied to the analysis.
- **Protein group average** — The average number of protein groups per sample.

Protein Group Counts section

The **Protein Group Counts** section graphs the number of proteins in each sample. The y-axis plots the number of identified protein groups and the x-axis plots each well. Three lines compare protein group trends for the plate:

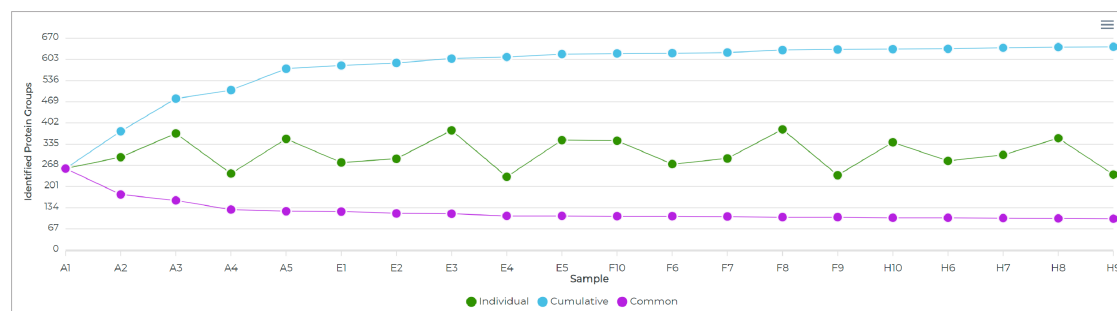
- The individual line traces the total number of protein groups observed in each sample.
- The cumulative line traces the cumulative number of protein groups observed with each successive sample. For example, the A3 value reflects the number of protein groups detected at least one time among A1, A2, and A3.
- The common line traces the proteins in common for each successive sample. For example, the A3 value reflects the number of proteins in common with A1, then A2.

Dots along each line identify values for each well.

- Hover over a dot on the line graph to view the exact value.
- Select a dot in the legend to hide the corresponding line.
- Hover over a dot in the legend to hide the lines corresponding to the other dots.


To customize this section for the selected analysis, see [Set Protein Group Counts preferences \(below\)](#).

Figure 4. Line graph showing protein group counts



Set Protein Group Counts preferences

You can customize the appearance of the [Protein Group Counts section \(previous page\)](#). The next time you view the section, it will have reverted to its default view.

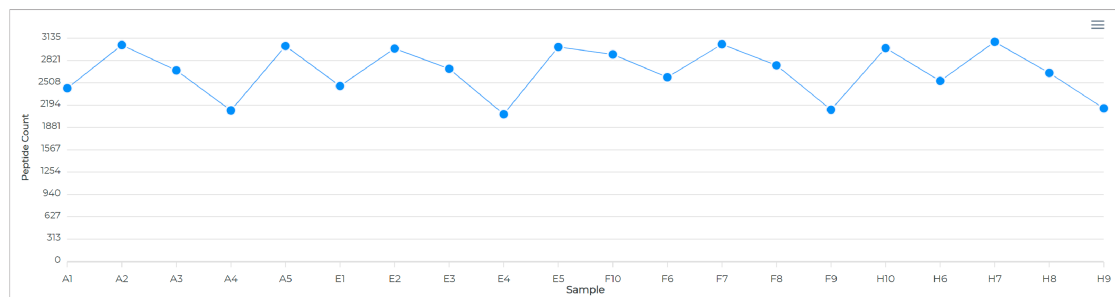
1. Open the **Analysis Summary** tab. (See [Open an analysis's Analysis Summary tab \(previous page\)](#).)
2. In the **Protein Group Counts** section, select  (**Settings**) to open the **Preferences** dialog.
3. Set preferences as needed.
 - **X Tick Label** — Select the label to show along the x-axis, e.g., *Sample Name*, *Plate Name*, *Sample ID*.
 - **Y Axis Range** — Select the range for the y-axis.
 - *Min is 0 and Max Data Dependent* — The minimum value is set at 0 and the maximum value depends on data.
 - *Min and Max Data Dependent* — Both the minimum and maximum values depend on data.
 - *User Defined* — Enter the minimum and maximum values.
4. Select **Continue** to apply the settings.

Peptide Counts section

The **Peptide Counts** section graphs the number of peptides in each sample. The y-axis plots the peptide count, and the x-axis plots each sample. You can update the x-axis label, but the values remain the same. Hover over a dot on the line graph to view the exact value.


To customize this section for the selected analysis, see [Set Peptide Counts preferences \(next page\)](#).

Figure 5. Line graph showing peptide counts



Set Peptide Counts preferences

You can customize the appearance of the [Peptide Counts section \(previous page\)](#). The next time you view the section, it will have reverted to its default view.

1. Open the **Analysis Summary** tab. (See [Open an analysis's Analysis Summary tab \(page 37\)](#).)
2. In the **Peptide** section, select  (**Settings**) to open the **Preferences** dialog.
3. Adjust the settings as you prefer.
 - **X Tick Label** — Select the label to show along the x-axis, e.g., *Sample Name*, *Plate Name*, *Sample ID*.
 - **Y Axis Range** — Select the range for the y-axis.
 - *Min is 0 and Max Data Dependent* — The minimum value is set at 0 and the maximum value depends on data.
 - *Min and Max Data Dependent* — Both the minimum and maximum values depend on data.
 - *User Defined* — Enter the minimum and maximum values.
4. Select **Continue** to apply the settings.

Distribution of Detected Proteins in Plasma Proteome section

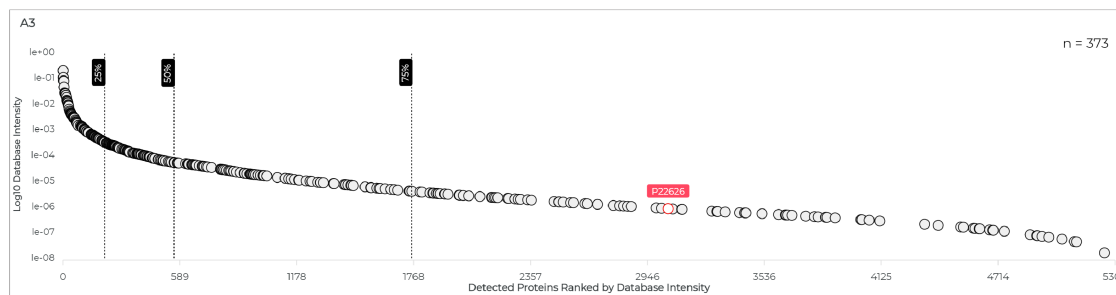
The **Distribution of Detected Proteins in Plasma Proteome** section shows the dynamic range of proteins identified in each sample compared to a deep reported human plasma proteome index.¹ The n-value equals the number of proteins detected in the sample that were also detected in the index.

The x-axis plots the number of identified proteins ranked by database intensity. The y-axis plots the intensity calculated in the database using the logarithm base 10 (log10) function. Each protein appears as a circle on the plot.

- Hover over a circle to view the name of the protein and the exact intensity values.
- Use the scroll arrows and numbers to move through all the graphs.
- Select or clear wells in the Samples list to show or hide the corresponding graphs.
- Enter a keyword or term in the Search field to find specific graphs.
- Annotate proteins you want to highlight, as shown in red in the following figure.

To customize this section for the selected analysis, see [Set Distribution of Detected Proteins in Plasma Proteome preferences \(next page\)](#).



Figure 6. Graph comparing the proteins detected in sample A3 to the plasma proteome



¹Keshishian, Hasmik, Michael W. Burgess, Michael A. Gillette, Philipp Mertins, Karl R. Clauser, D. R. Mani, Eric W. Kuhn, et al., "Multiplexed, Quantitative Workflow for Sensitive Biomarker Discovery in Plasma Yields Novel Candidates for Early Myocardial Injury," 14, no. 9 *Molecular & Cellular Proteomics* (September 2015): 2375–2393, <https://doi.org/10.1074/mcp.M114.046813>.

Set Distribution of Detected Proteins in Plasma Proteome preferences

You can customize the appearance of the [Distribution of Detected Proteins in Plasma Proteome section](#) (previous page). The next time you view the section, it will have reverted to its default view.

1. Open the **Analysis Summary** tab. (See [Open an analysis's Analysis Summary tab](#) (page 37).)
2. In the **Distribution of Detected Proteins in Plasma Proteome** section, select  (**Settings**) to open the **Preferences** dialog.
3. Adjust the settings as you prefer.
 - **Graph Colors** — Use the color picker to select graph colors. (See [Set color preferences in PAS graphs](#) (page 14).)
 - **Page Chart Layout** — Select an option for how many graphs appear on a page and the layout. For example, the 2 × 2 option shows four graphs per page, two down and two across.
 - **Quantiles** — Adjust the frequency distribution. The default quantiles are 0.25, 0.5, and 0.75.
 - To add a quantile, select **Add** and enter its value.
 - To modify existing quantiles, update the values in each field.
 - To delete a quantile, select  (**Delete**).
 - **Proteins** — Annotate proteins of interest by entering their names, separated by commas (e.g., P35579, F5H7Y6, Q5VZ73). The dots representing the annotated proteins will appear on each graph in red with the protein names above.
4. Select **Continue** to apply the settings.

Protein Group Overlap Sets section

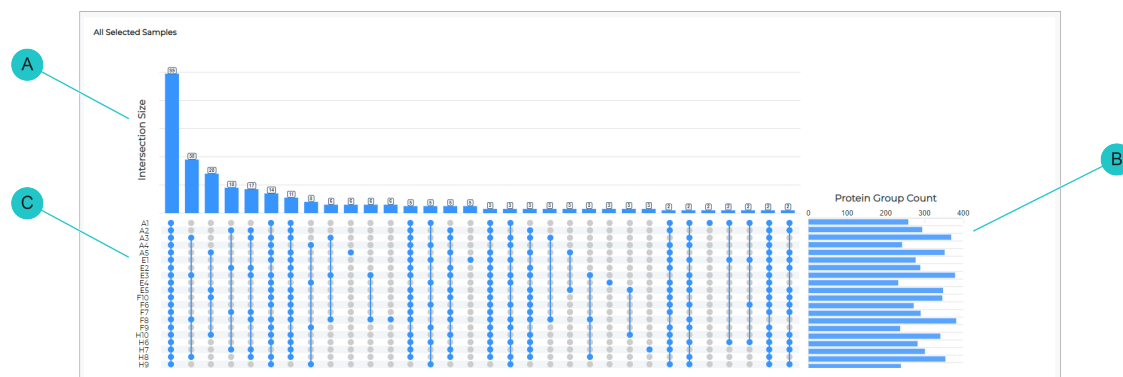
The **Protein Group Overlap Sets** section is divided into two bar graphs and a matrix that together show protein group intersections. The **Within Samples** checkbox shows intersection size and protein group count as standalone graphs for each sample with a dot representing the MS data file.

- Hover over a vertical bar to view the intersection size for the group of samples as an integer and the percentage of the total it represents.

- Hover over a horizontal bar to view the sample and the exact number of protein groups it contains.
- Select or clear wells in the Samples list to show or hide the corresponding bars.

To customize this section for the selected analysis, see [Set Protein Group Overlap Sets preferences \(below\)](#).


Figure 7. *Graphs and a matrix show protein group overlaps*



- A** Intersection Size bar graph **C** Matrix
B Protein Group Count bar graph

Set Protein Group Overlap Sets preferences

You can customize the appearance of the [Protein Group Overlap Sets section \(previous page\)](#). The next time you view the section, it will have reverted to its default view.

1. Open the **Analysis Summary** tab. (See [Open an analysis's Analysis Summary tab \(page 37\)](#).)
2. In the **Protein Group Overlap Sets** section, select  (**Settings**) to open the **Preferences** dialog.
3. Adjust the settings as you prefer.
 - **Horizontal Bar Position** — Select an orientation for the graph.
 - *Left* — The graph is positioned left.
 - *Right* — The graph is positioned right.
 - *None* — The graph is hidden.
 - **Vertical Height Rate** — Enter a value for the relative bar height in the graph.
 - **MS file's name length** — Enter the character limit for the MS data file name.
 - **Display Top N Intersection** — Select which bars appear on the graph.
 - *All* — Shows intersection sizes for all samples.
 - *4* — Shows the intersection sizes of the top four largest samples only.
 - *8* — Shows the intersection sizes of the top eight largest samples only.
 - *16* — Shows the intersection sizes of the top 16 largest samples only.
 - *32* — Shows the intersection sizes of the top 32 largest samples only.
 - **Display Percentage** — Select to show percentages on top of each bar in the Intersection Size graph.

- **Page Chart Layout** — Select an option for how many graphs appear on a page and the layout. For example, the 2 × 2 option shows four graphs per page, two down and two across.

By default, this section consolidates information for all samples into two bar graphs and a matrix for easy comparison. You can divide these elements into graphs for individual samples and change the page layout accordingly.

- **<colors>** — Set colors for the various parts of the graph, such as for the vertical and horizontal bars. Use the techniques in [Set color preferences in PAS graphs \(page 14\)](#).

4. Select **Continue** to apply the settings.

Sample Comparability section

The **Sample Comparability** section shows the degree of statistical correlation between samples based on the Pearson correlation coefficient (PCC) and the similarity in protein groups between samples based on the Jaccard Index, which measures the linear correlation of data. You can switch between the PCC and Jaccard index.

Each matrix is color-coded for easy reference. Samples on the green end of the spectrum have high correlation. Samples on the red end of the spectrum have low correlation.


To customize this section for the selected analysis, see [Set Sample Comparability preferences \(below\)](#).

Figure 8. A color-coded matrix shows sample comparability data using PCC (left) or the Jaccard index (right)



Set Sample Comparability preferences

You can temporarily customize the appearance of the [Sample Comparability section \(above\)](#). The next time you view the section, it will have reverted to its default view.

1. Open the **Analysis Summary** tab. (See [Open an analysis's Analysis Summary tab \(page 37\)](#).)
2. In the **Sample Compatibility** section, select  (**Settings**) to open the **Preferences** dialog.
3. Adjust the settings as you prefer.



- **Similarity Score** — To change how sample intensity data are compared, select either:
 - *Pearson's correlation coefficient* — Shows data calculated by normalizing the covariance measurement.
 - *Jaccard index* — Shows data calculated by dividing the intersection size by the union size.
 - **Color Labels By** — To change the matrix label colors, select an option, e.g., *Sample Name*, *Sample ID*, *Plate Name*. To not use colors for labels, select *Disabled*.
 - **Label Font Size** — Select the point size text of the label.
4. Select **Continue** to apply the settings.

Analysis Metrics tab


An analysis's **Analysis Metrics** tab (on the **Analyses** page) shows the QC metrics for an analysis result, organized into sections. The metrics indicate how well an analysis method performed.

For some sections, you can modify labels, reorganize layouts, and otherwise adjust display preferences. These modifications are temporary and apply only to the select analysis. When you leave the **Analyses** page, each section returns to the default view. (To configure display preferences for all analyses in PAS, see [Configure default display settings for analysis results \(page 20\)](#).)

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.

Open an analysis's Analysis Metrics tab

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. From the **Status** list, select *Completed*.
3. Select an analysis to open its analysis results.
4. Select the **Analysis Metrics** tab.

Intensities section

The **Intensities** section graphs the protein and peptide intensities and the distribution of protein sequence coverage for each sample, including the coefficient of variation (CV). You can update the default chart type, a density plot, to a violin plot.

On a density plot, the x-axis plots intensity and the y-axis plots density.

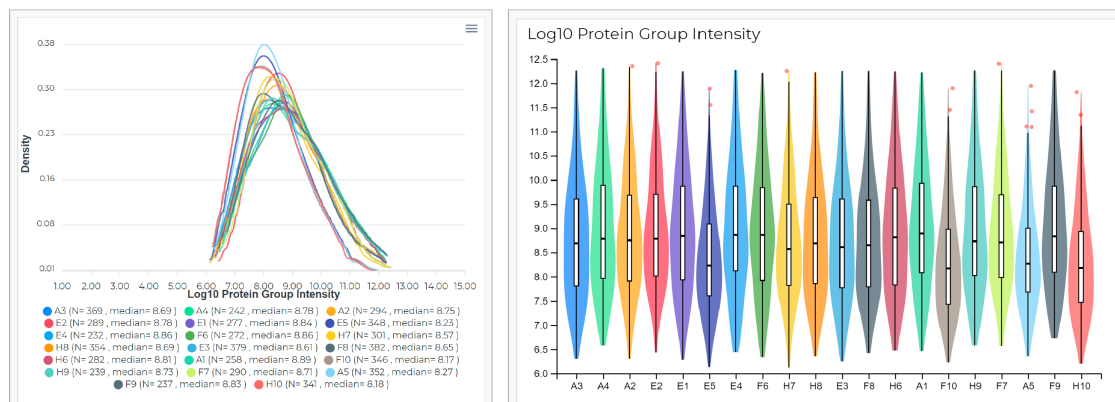
- Move the pointer along a curve to view the exact intensity value at each point in the curve.
- Select a sample in the legend to hide the corresponding line.
- Hover over a sample in the legend to hide the lines corresponding to the other samples.

On a violin plot, the sample appears along the x-axis and the y-axis plots intensity. Box plots represent quantile ranges with box plots with density on either end. Red dots represent outliers.

- Hover over a box plot to view the quantile for the sample.
- Hover over a dot to view the exact outlier value.

To customize this section for the selected analysis, see [Set Intensities preferences \(next page\)](#).

Figure 9. Density plot (left) and violin plot (right) showing the intensity distribution for a sample



Set Intensities preferences

You can temporarily customize the appearance of the [Intensities section \(previous page\)](#). The next time you view the section, it will have reverted to its default view.


1. Open the **Analysis Metrics** tab. (See [Open an analysis's Analysis Metrics tab \(previous page\)](#).)
2. In the **Intensities** section, select  (**Settings**) to open the **Preferences** dialog.
3. Adjust the settings as you prefer.
 - **Page Chart Layout** — Select an option for how many graphs appear on a page and the layout. For example, the 2 × 2 option shows four graphs per page, two down and two across.
 - **Chart Type** — Select an option.
 - *Density plot* — Shows the full distribution of data for each sample as a continuous curve.
 - *Violin plot* — Shows data for each sample as quartiles with the full distribution of data.
4. Select **Continue** to apply the settings.

Plate Map Grid section

The **Plate Map Grid** section shows metrics for each sample in the format of 96-well plates. Each plate represents one of the following metrics. Hover over a well to view the value. Alternatively, you can consolidate these data into a single table with one column for each metric.

- **Protein group counts** — The number of protein groups identified per well.
- **Peptide counts** — The number of peptides identified per well.
- **Peptide quant mass** — The mass of peptide in the well as calculated by the peptide quantification assay.
- **Miscleavage rate** — The fraction of peptides identified as having missed cleavages based on the maximum allowable missed cleavages set in the analysis protocol.
- **Oxidation ratio** — The fraction of peptides identified with methionine oxidation.
- **ID rate** — The rate at which an MS/MS scan is converted into a database peptide identification.


To customize this section for the selected analysis, see [Set Plate Map Grid preferences \(next page\)](#).

Figure 10. Grids for each metric showing results for each sample



Set Plate Map Grid preferences

You can temporarily customize the appearance of the [Plate Map Grid section \(previous page\)](#). The next time you view the section, it will have reverted to its default view.

1. Open the **Analysis Metrics** tab. (See [Open an analysis's Analysis Metrics tab \(page 44\)](#).)
2. In the **Plate Map Grid** section, select  (**Settings**) to open the **Preferences** dialog.
3. Adjust the settings as you prefer.
 - **Graph Types** — Select each toggle key to show or hide a graph or table column (depending on the **Display Type**).
 - **Scaling** — Select *Each graph* or *Each type* scaling for reviewing multiple plates.
 - **Display Type** — Select an option:
 - *Plate Map Grid* — Shows each metric in a separate grid.
 - *Table* — Shows the protein group counts, peptide counts, and other metrics in one table.
 - **Page Chart Layout** — Select an option for how many graphs appear on a page and the layout. For example, the 2 × 2 option shows four graphs per page, two down and two across.
4. Select **Continue** to apply the settings.

Lamppost Proteins' Concentration section

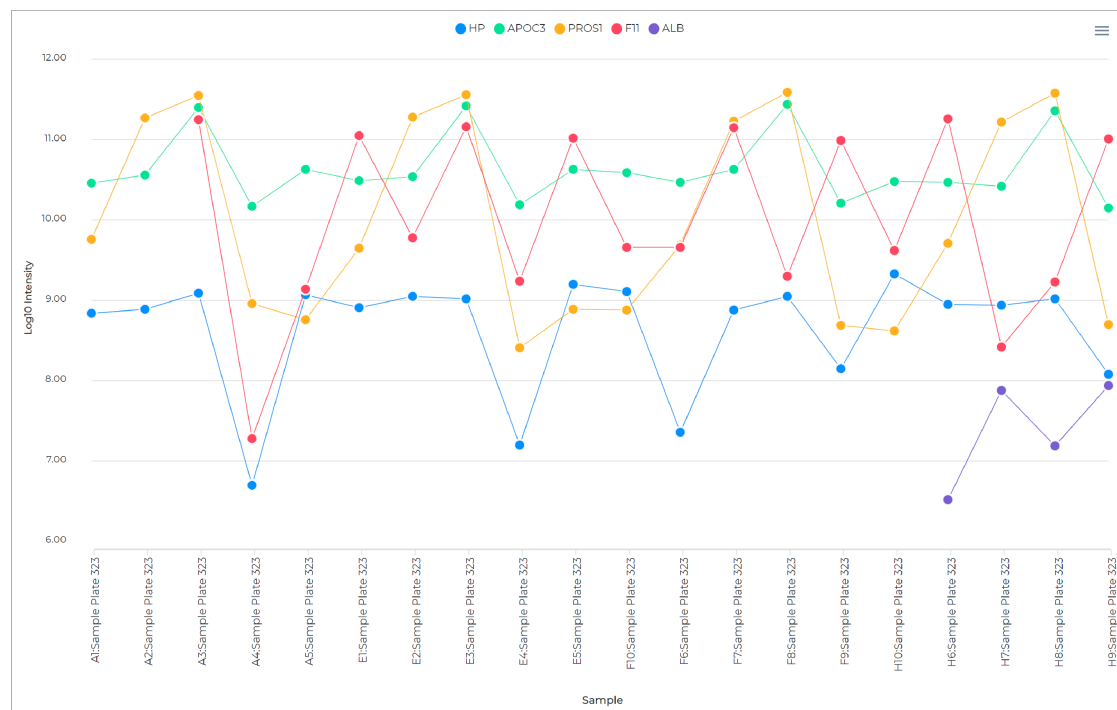
The **Lamppost Proteins' Concentration** section graphs the intensity of landmark proteins in each sample. The x-axis plots each well and plate and the y-axis plots log10 intensity.

Five lines compare intensities for the proteins HP, APOC3, PROS1, F11, and ALB. Dots along each line identify the intensity value for each protein in the sample.

- Hover over a dot on the line graph to view the exact value for all five proteins.
- Select a dot in the legend to hide the corresponding line.
- Hover over a dot on the legend to hide the lines corresponding to the other dots.


To customize this section for the selected analysis, see [Set Lamppost Proteins' Concentration preferences \(below\)](#). Specifically, you can add, edit, and delete proteins.

Figure 11. Line graph showing intensities for landmark proteins



Set Lamppost Proteins' Concentration preferences

You can temporarily customize the appearance of the [Lamppost Proteins' Concentration section \(previous page\)](#). Specifically, you can add, edit, and delete proteins to use instead of the default QC landmark proteins. The next time you view the section, it will have reverted to its default view.



1. Open the **Analysis Metrics** tab. (See [Open an analysis's Analysis Metrics tab \(page 44\)](#).)
2. In the **Lamppost Proteins Concentration** section, select  (**Settings**) to open the **Lamppost Proteins** dialog.
3. To add a protein or group of proteins:
 - a. Select **Add Proteins** to open the **Add Proteins** dialog.
 - b. In the **Name** field, enter a label for a detected protein or group of proteins.
 - c. In the **Proteins** field, enter a protein name or enter multiple names separated by commas.
 - d. Select **Add**.

Notice that the label you entered for the protein or group of proteins is now selected.

TIP

To revert to using the default QC landmark proteins, select **Abundance monitoring**.

4. To edit a protein or group of proteins:

- a. Select its  (**Edit**) button to open the **Edit Proteins** dialog.
 - b. Change the fields as needed.
 - c. Select **Edit** to save the changes.
5. To delete a protein or group of proteins:
 - a. Select its  (**Delete**) button.
 - b. Select **OK** to confirm.
6. Select **Continue** to apply the settings.

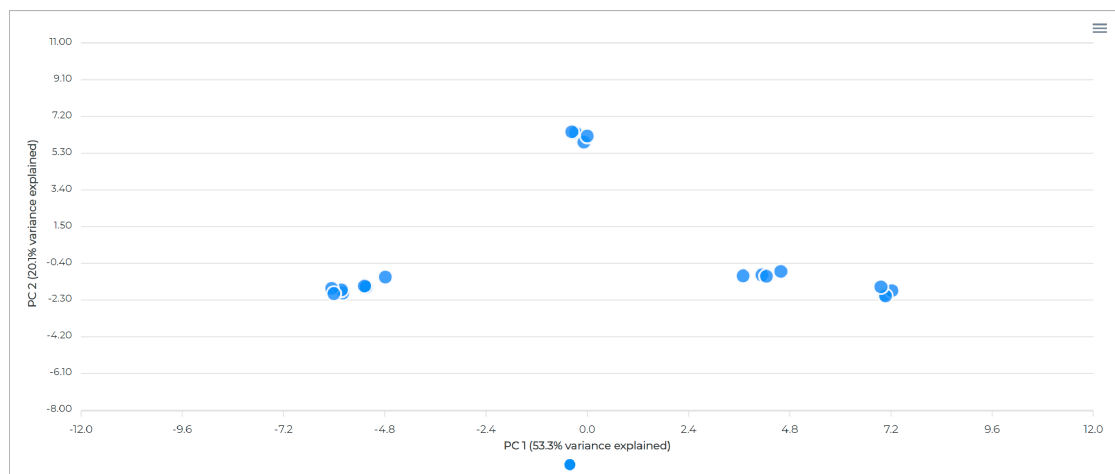
PCA Analysis section

The **PCA Analysis** section clusters similar samples in a scatter plot. The x-axis plots principal component 1 (PC1) analysis scores and the y-axis plots principal component 2 (PC2) analysis scores. Each dot represents one sample.

- Select a dot under the x-axis to hide the corresponding sample.
- Hover over a dot to view the sample and plate names.

To customize this section for the selected analysis, see [Change the PCA Analysis color scheme \(below\)](#).

Figure 12. Scatter plot showing clusters of similar samples



Change the PCA Analysis color scheme

You can temporarily change the color scheme of the [PCA Analysis section \(above\)](#). The next time you view the section, it will have reverted to its default view.

1. Open the **Analysis Metrics** tab. (See [Open an analysis's Analysis Metrics tab \(page 44\)](#).)
2. In the **PCA Analysis** section, select an option from the **Color By** list:
 - *Condition* — Applies the same color to all data points. The color represents sample quality.
 - *Sample Name* — Applies a unique color to each sample.
 - *Plate Name* — Applies the same color to all data points. The color represents the sample plate.
 - *Sample ID* — Applies a unique color to each sample.

3. Set colors as you prefer.
 - a. Select a label box next to or below the **Color By** list. For example, if you selected *Sample ID* above, you can adjust the color for each sample.
 - b. Use the color picker to select a color. (See [Set color preferences in PAS graphs \(page 14\).](#))
 - c. Repeat for other label boxes.

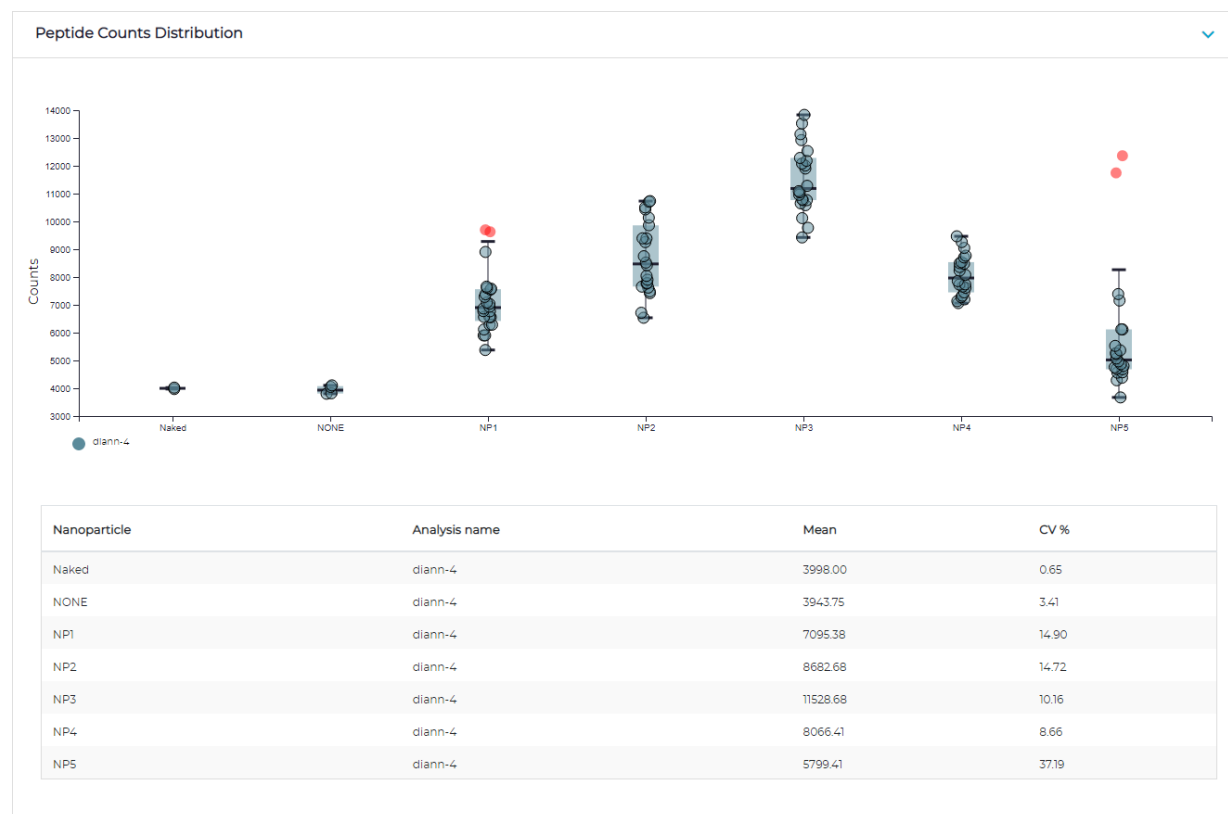
Peptide Counts Distribution and Protein Group Counts Distribution sections

The **Peptide Counts Distribution** and **Protein Group Counts Distribution** sections show the peptide and protein counts for the five nanoparticles as box plots. A table below each plot shows the analysis name, mean value, and CV percentage for each nanoparticle. Each box plot and table represent one plate.

- Hover over a dot to view the peptide or protein count, file, and sample name.
- Hover over a box to view the quantile for the nanoparticle.

Figure 13. Box plots showing peptide counts distribution



Figure 14. Box plots showing protein group counts distribution

Protein Group Counts of Nanoparticles and Peptide Counts of Nanoparticles sections

The **Protein Group Counts of Nanoparticles** and **Peptide Counts of Nanoparticles** sections offer two charts:

- **Protein Group Counts** — Shows the sample protein group counts identified by each nanoparticle. Each dot represents a sample. The x-axis plots samples and the y-axis plots the number of peptides.
- **Peptide Counts** — Shows the sample peptide counts identified by each nanoparticle. Each dot represents a sample. The x-axis plots samples and the y-axis plots the number of peptides.

To use these charts:

- Hover over a dot to view the well, nanoparticle that occupies the well, and the peptide count.
- Select a dot under the x-axis to remove the corresponding well from the plot.

To customize this section for the selected analysis, see [Set Protein Group Counts of Nanoparticles and Peptide Counts of Nanoparticles preferences \(next page\)](#).

Figure 15. Scatter plot showing protein group counts of nanoparticles

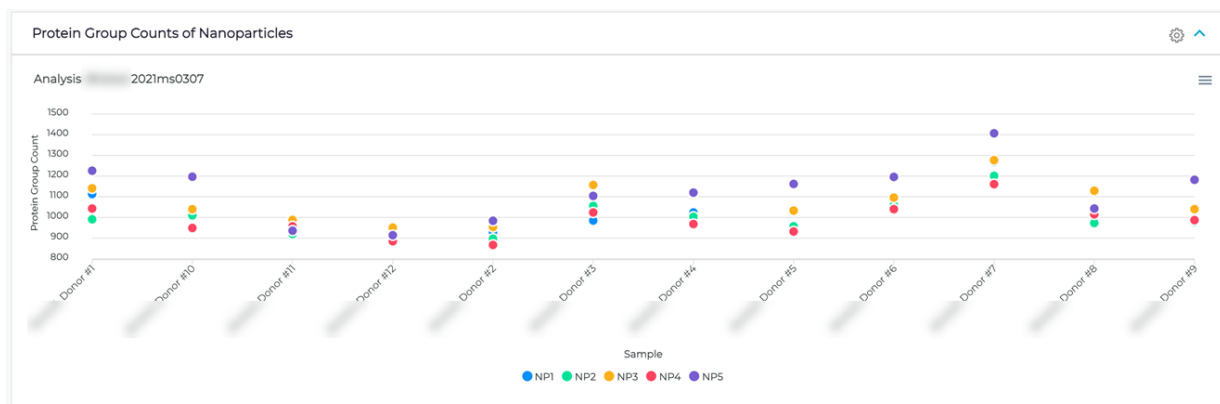
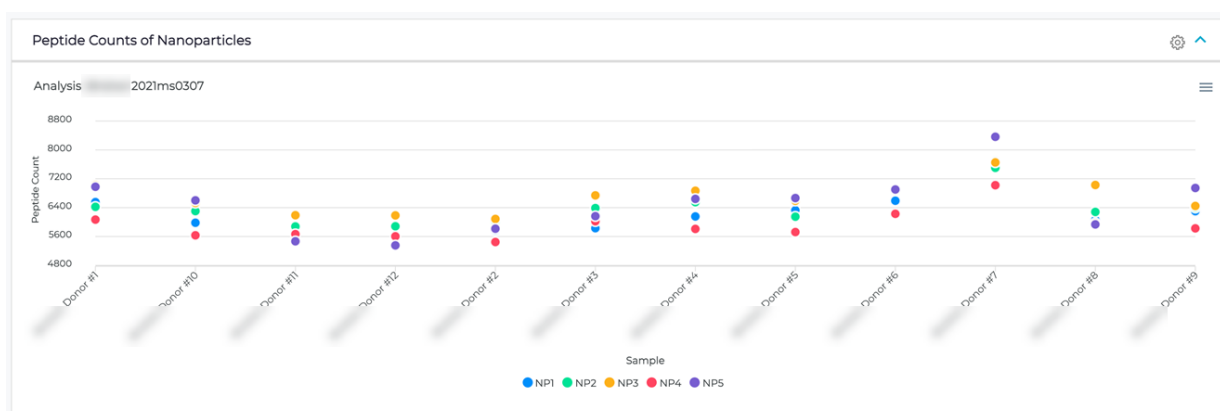



Figure 16. Scatter plot showing peptide counts of nanoparticles



Set Protein Group Counts of Nanoparticles and Peptide Counts of Nanoparticles preferences

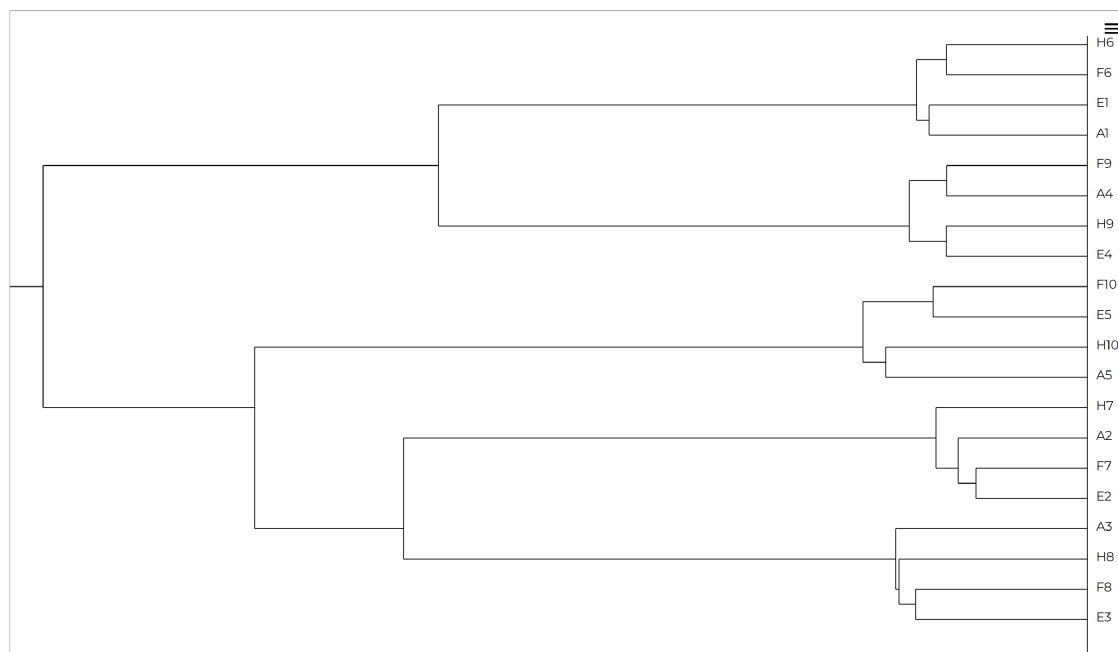
You can temporarily customize the appearance of the [Protein Group Counts of Nanoparticles](#) and [Peptide Counts of Nanoparticles](#) sections (previous page). The next time you view the section, it will have reverted to its default view.

1. Open the **Analysis Metrics** tab. (See [Open an analysis's Analysis Metrics tab \(page 44\)](#).)
2. In the **Protein Group Counts of Nanoparticles** or **Peptide Counts of Nanoparticles** section, select  (**Settings**) to open the **Preferences** dialog.
3. Adjust the settings as you prefer.
 - **Y Axis Range** — Select the range for the y-axis.
 - *Min is 0 and Max Data Dependent* — The minimum value is set at 0 and the maximum value depends on data.
 - *Min and Max Data Dependent* — Both the minimum and maximum values depend on data.
 - *User Defined* — Enter the minimum and maximum values.
4. Select **Save**.

Hierarchical Clustering section


The **Hierarchical Clustering** section shows a cluster analysis based on agglomerative nesting, which groups samples in clusters based on similarity. Each sample starts a single cluster. Pairs of clusters are then successively merged until all clusters are merged into a dendrogram.

Figure 17. Dendrogram successively grouping similar samples





QC Charts tab





An analysis's **QC Charts** tab (on the **Analyses** page) shows assay control data for an analysis. Each chart plots one metric for one assay control category. Charts are organized in a grid, with the same metric across each row and the same control type down each column. The x-axis is labeled with the date of analysis and the y-axis depends on the metric.

- Select a status icon (e.g., ) in the summary table above the control charts to jump to the corresponding control chart.
- Hover over a dot on a control chart to view general information about the control, such as well and plate.

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.

Toolbar items

- **<control filters>** — By default, all controls are included. Select another option to filter by a specific control type.
 - **Process Control** — Results for the process controls only.
 - **Digestion Control** — Results for the digestion controls only.
 - **MPE Control** — Results for the MPE controls only.
 - **MS Peptide Control** — Results for the mass spec controls only.
- **MS Instrument** — The instruments listed vary depending on your organization. Select up to six instruments to aggregate their data.
- **Color By** — (Available when only one MS instrumented is selected.) Select your preferred coloration for the graphs, e.g., *Gradient*.
- **Start Date** — Enter or select the earliest date of data you want to see.
- **End Date** — Enter or select the latest date of data you want to see
- **Control Limits** — Select how you want control limits to be defined.
 - *Preinstalled* — Use the preinstalled control limits.
 - *User Defined* — Define your own control limits. See [Define and use user-defined control limits \(page 56\)](#).
 - *Calculated* — Calculate control limits from data within one or more date ranges, which you define with the  **Calculate** button (see below).
-  **Limits** — Select to view the calculated control limit date ranges. From here, you can also delete a range. See [Delete a calculated control limit date range \(page 56\)](#).
-  **Exclusion** — Select to exclude an outlier or other data point from the control limit calculation. Selecting one data point (sample) in a plot excludes the corresponding sample from the other plots. A well containing the mass spec control has 10 reported QC metrics. All other control wells have 11 reported QC metrics. See [Exclude a sample \(page 56\)](#).
-  **Calculate** — Select to define a calculated control limit based on a range of dates. See [Define and use calculated control limits \(page 56\)](#).



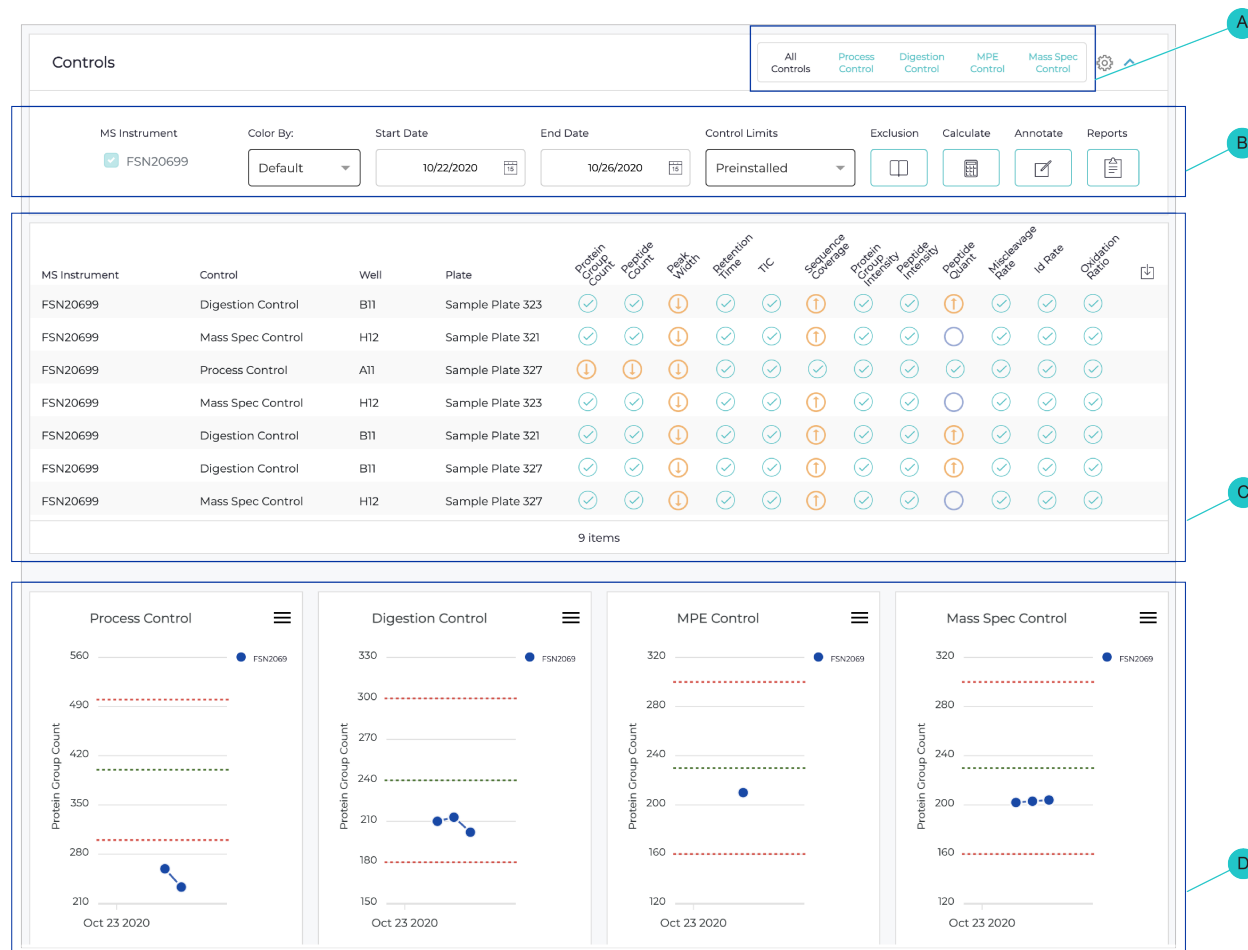

-  **Annotate** — Select to annotate all control charts for a specific date. See [Annotate control charts \(page 57\)](#).
-  **Reports** — Select to generate a PDF report of control results, with specific criteria. See [Generate a detailed PDF report of control results \(page 58\)](#).

Figure 18. Results for controls



- A** Filters for viewing charts for all controls or a selected control type
- B** Toolbar with additional filters and functions
- C** Summary of control data for the selected analysis time frame
- D** QC charts with metrics of each control

Open and filter an analysis's QC Charts tab

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. From the **Status** list, select *Completed*.
3. From the **Controls/Samples** list, select *Samples included*.
4. Select the checkbox of each applicable analysis whose QC charts you want to work with.
5. Select the **QC Charts** tab.


The [QC Charts tab \(page 53\)](#) presents each control with metrics for assay and MS performance.

6. Under **MS Instrument**, select up to six instruments.

The tab aggregates data from the selected instruments and hides the **Color By** menu.

7. To filter the results for a specific control type, select an option:
 - **Process Control** — Results for the process controls only.
 - **Digestion Control** — Results for the digestion controls only.
 - **MPE Control** — Results for the MPE controls only.
 - **MS Peptide Control** — Results for the mass spec controls only.
8. To filter results for a specific time frame, enter the MS injection time frame in the **Start Date** and **End Date** fields.

Set QC Charts preferences

1. Open and filter the **QC charts** tab for an analysis. (See [Open and filter an analysis's QC Charts tab \(previous page\)](#).)
2. Select  (**Settings**) to open the **Preferences** dialog.
3. Complete the fields as needed.
 - **Show Annotations** — Select to show or hide annotation. See [Annotate control charts \(page 57\)](#).
 - **Show Historical Data** — Select to show or hide historical data. By default, each control chart shows values from historical data. Although independent of the selected analyses, these data points are sourced from previous analyses that exist in the user group.
 - **Show Variables** — Select the checkbox of each variable of interest, e.g., *Protein Group Count*, *Peak Width (seconds)*. Clear the checkbox of any you're not interested in.
 - **Process Variables Y Axis Range** — Select the range for the y-axis for processed variables.
 - *Min and Max Data Dependent* — Both the minimum and maximum values depend on data.
 - *Min is 0 and Max Data Dependent* — The minimum value is set at 0 and the maximum value depends on data.
 - *User Defined* — Enter the minimum and maximum values.
4. Select **Save**.

Manage user-defined and calculated control limits


Depending on the MS injection time frame, filtering results on the **QC Charts** tab by time frame shows a summary that presents each control with metrics for assay and MS performance. Each metric is color-coded to indicate whether it is within the control limits (teal) or outside the control limits (orange).

Control limits help determine whether results are expected. The mean provides a historical average, while the upper and lower control limits indicate normal variation. PAS includes default control limits calculated using two standard deviations above and below the mean. Calculated control limits are generated from user data.

Define and use user-defined control limits


1. On the **Controls** section's toolbar, select the **Control Limits** list and select *User Defined* to open the **Control Limits** dialog.
2. Along the top of the dialog, select the tab of the control whose limits you want to define, e.g., *MPE Control*. Use the scroll arrows to view all tabs.
3. For each control limit, enter a value.
 - *Mean* — The value to serve as the historical mean.
 - *UCL* — The value to serve as the upper control limit.
 - *LCL* — The value to serve as the lower control limit.
4. Select **Save**.

Define and use calculated control limits

1. On the **Controls** section's toolbar, select  **Calculate** to open the **Calculate Control Limits** dialog.
2. In the **Start Date** and **End Date** fields, enter or select the applicable dates.
3. Select **Save**.



A teal background appears on the plots, indicating that data are shown with modified control limits.

NOTE

The new control limit date range has been added to the **Calculate Control Limits Range** dialog, which you can open with the  **Limits** button.



4. On the toolbar, select the **Control Limits** list and select *Calculated* to use the calculated control limits.

Delete a calculated control limit date range

1. On the **Controls** section's toolbar, select  **Limits** to open the **Calculate Control Limits Range** dialog.
2. Find the date range you want to delete and select its  **(Delete)** button.
3. Select **Yes** to confirm.
4. Select **Save**.

Exclude a sample


Exclude an outlier or other data point from the control limit calculation. Selecting one data point (sample) in a plot excludes the corresponding sample from the other plots. A well containing the mass spec control has 10 reported QC metrics. All other control wells have 11 reported QC metrics.

1. Select  **Exclusion** to open the **Control Limit Exclusion** dialog and display a list of samples that are being excluded.
2. Find the data point (sample) you want to remove and select its  **(Delete)** button.
3. Select **Yes** to confirm.
4. Select **Close**.


Annotate control charts

You can add an annotation that will be applied to all control charts for a specific date. An annotation is indicated by a dot above a control chart with the full annotation below the chart. Select an annotation dot to view its annotation type, date, and accompanying message.


Add an annotation

1. Open and filter the **QC charts** tab for an analysis. (See [Open and filter an analysis's QC Charts tab \(page 54\)](#).)
2. Select  **Annotate** to open the **Annotate** dialog.
3. Complete the fields.
 - **Annotation Type** — Do either of the following:
 - . To select an existing annotation type, select it from the list.
 - . To add a new annotation type, select **Add Annotation Type**, enter the annotation, and select **Add**.
 - **Date** — Enter or select the date the event occurred.
 - **Message** — Enter more information about the annotation.
4. Select **Save**.

Edit an annotation

1. Select the annotation dot for the annotation you want to edit.
2. In the annotation pop-up, select  **(Edit)** to open the **Annotate** dialog.
3. Edit the annotation as needed.
4. Select **Save**.

Delete an annotation


1. Select the annotation dot for the annotation you want to delete.
2. In the annotation pop-up, select  **(Delete)**.
3. Select **OK** to confirm.

Generate reports of control results


Summarize and output control results in a .csv file or generate a more detailed report as a .pdf file. The summary lists each QC metric with the control, well, plate, value, and result. The report summarizes results and shows a table for each control. Each table includes the well and plate and lists values for each QC metric with optional notes.

Download summarized control results

1. Open and filter the **QC charts** tab for an analysis. (See [Open and filter an analysis's QC Charts tab \(page 54\)](#).)

2. In the summary table above the control charts, select  (**Download CSV**) to open the **Download CSV** dialog.
3. Select the checkbox of each field to add to the summary:
 - **File name** — The full name of the MS data file, including extension.
 - **Assay instrument name** — The name of the liquid handler that prepared the assay.
 - **Mass spec instrument name** — The name of the MS instrument that analyzed the assay output.
 - **Injection time** — The month and day of MS injection.
 - **Gradient** — The duration of the LC gradient.
4. Select a format:
 - **One line per metric** — Organizes the summary by metric.
 - **One line per control** — Organizes the summary by control.
5. Select **Download** to generate the summary.

Generate a detailed PDF report of control results

1. Open and filter the **QC charts** tab for an analysis. (See [Open and filter an analysis's QC Charts tab \(page 54\)](#).)
2. Select  **Reports** to open the **Controls Report** dialog.
3. Complete the fields.
 - **Assay Equipment ID** — Select the name of the liquid handler used to prepare the assay.
 - **Mass Spec ID** — Select the name of the MS instrument that analyzed the assay output.
 - **Report By** — (Read-only) Shows your username.
 - **Report Date** — (Read-only) Shows the current date and time.
4. Select **Create** to generate the report.

Analysis Output Files tab


An analysis's **Analysis Output Files** tab (on the **Analyses** page) lists all outputs of the search engine results for the analysis. You can download an output file simply by selecting it.

Chapter 4

Analysis Interpretation


Describes techniques for interpreting analysis results, specifically for group analyses, performed from the **Group Analysis** tab of the **Analyses** page.

Open an analysis's Group Analysis tab

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. From the **Status** list, select *Completed*.
3. Select an analysis to open its analysis results.
4. Select the **Group Analysis** tab. (See [Group Analysis tab \(page 66\)](#).)


Export raw data to a file

Prior to doing a group analysis, you can export raw data to a .csv file.

1. Open the **Group Analysis** tab. (See [Open an analysis's Group Analysis tab \(previous page\)](#).)
2. Select  **Export**.
3. Navigate to the location on your computer where you want to save the file and select **Save**.

View a raw protein group data heatmap

Prior to doing a group analysis, you can visualize a heatmap of raw protein group intensity.


1. Open the **Group Analysis** tab. (See [Open an analysis's Group Analysis tab \(page 61\)](#).)
2. Select  **Heatmap**.

PAS prepares the data and then displays the heatmap.

Set up and start a group analysis

Follow these steps to prepare to conduct a group analysis in which you visualize differences in proteins detected between groups.

To begin this workflow:

1. Open the **Group Analysis** tab. (See [Open an analysis's Group Analysis tab \(page 61\)](#).)
2. Select  **Setup Group Analysis** to open the **Setup Group Analysis** dialog.



Continue to the next section.



Specify the quantitation level and grouping of samples

In the **Feature and Grouping** section, you specify the parameters for the differential expression analysis between groups of samples.

1. For **Feature**, select the quantitation level, either *Protein* or *Peptide*.
2. For **Group By**, select the category by which you want to group samples, e.g., by a condition or custom field. The options vary based on the metadata imported from the sample description file.
3. Select **Next** to advance.

Filter out (exclude) samples and groups

In the **Filter Samples and Group** section, you specify the individual samples or whole groups of samples to be filtered out of (excluded from) the final comparison.

1. (Optional) From **Select Sample**, select one or more samples.
 - If you change your mind about an excluded sample, select its  **(Delete)** button.
2. (Optional) From **Select Groups**, select one or more groups of samples.
 - If you change your mind about an excluded group, select its  **(Delete)** button.
3. Select **Next** to advance.

Filter out (exclude) proteins or peptides

In the **Filter Peptides / Proteins** section, you specify measurement completeness thresholds for the final comparison.

1. Complete the fields.

NOTE

PAS will use whichever minimum (percentage or specific value) yields the larger number of samples.

- **Minimum % of valid values in at least one group** — Enter the minimum percentage of samples to consider. For example, if there are 24 samples and you enter 50, a minimum of 12 samples will be considered. The default is 0.
 - **Minimum number of valid values in at least one group** — Enter the exact minimum number of samples to consider. The default is 2.
 - **Remove peptides / proteins with complete missing values in at least one group** — Select to exclude peptides / proteins for which data is entirely missing (i.e., all table cells that show –).
 - **Remove peptides / proteins with missing values** — Select to exclude peptides / proteins with one or more missing values (i.e., some table cells that show –).
2. Select **Next** to advance.

Normalize values and impute sparse or missing values

In the **Normalization and Imputation** section, you specify the processes by which raw measurement values are normalized and sparse and missing values are handled.

1. For **Normalization**, select either:
 - *Median* — Raw MS intensity values are normalized on a run-by-run basis. This will account for potential measurement bias and make samples more comparable.
 - *None* — No normalization of raw measurements will occur.
2. For **Imputation**, select either:
 - *Minimal Probability* — Substitute missing values with random values from a normal distribution using a mean that is down-shifted from the sample mean and a standard deviation (SD) that is a fraction of the SD of the sample distribution.
 - *None* — No imputation of raw measurements will occur.
3. Select **Next** to advance.

Select the statistical test and the groups to compare

In the **Statistical Test and Group Comparison** section, you select the statistical test to use for comparison analysis and then select the groups of samples you want to compare.












1. For **Statistical Test**, select the appropriate test to use for comparison analysis.
 - *T Test* — A parametric test. Select this if you previously elected to normalize data.
 - *Wilcoxon* — A non-parametric text rank-based test. Select this if you previously elected not to normalize data.
2. Under **Groups for Comparison**, select the checkbox of each set of groups you want to compare. The groups offered vary, based on selections you made earlier in the setup workflow.
3. Select **Start**.

The group analysis begins immediately. When it is finished, the analysis results are shown on the **Group Analysis** tab, organized into sections, with the **Volcano** section being shown. To explore all the sections, begin at [Group Analysis tab \(next page\)](#).

Group Analysis tab

An analysis's **Group Analysis** tab (on the **Analyses** page) shows the analysis and results from comparing two user-defined groups, organized into sections. You can visualize differences in proteins detected between the groups and explore initial biological insights into the data.

Toolbar items

- Before you run a group analysis, the toolbar includes:
 - **Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).
 - **Feature** — Select *Protein* or *Peptide* to filter the **Raw Data** table.
 - **Group By** — Select the categorical grouping by which you want to group raw data.
 -  **Heatmap** — (Not applicable to peptides.) Select to visualize a heatmap of raw protein group data. See [View a raw protein group data heatmap \(page 63\)](#)
 -  **Export** — Select to export raw data to a .csv file. See [Export raw data to a file \(page 62\)](#).
 -  **Setup Group Analysis** — Select to set up groups for and start a comparative analysis. See [Set up and start a group analysis \(page 64\)](#).
- After you run a group analysis, the toolbar includes these additional items:
 -  **Raw Data / Results** — Use to switch back and forth between the raw data and group analysis results.
 - **Significant Proteins** — Select to show only significant proteins.
 -  **Volcano Plot** — Select to view the [Volcano section \(page 69\)](#).
 -  **Coverage** — (Available when at least two proteins are selected.) Select to view the [Coverage section \(page 70\)](#).
 -  **Clustered Heatmap** — Select to view the [Clustered Heatmap section \(page 68\)](#).
 -  **PPI Network** — (Available only for significant proteins.) — Select to view the [Filtered PPI Network section \(page 71\)](#).
 -  **Enrichment** — (Available only for significant proteins.) — Select to view the [Enrichment section \(page 72\)](#).
 -  **Box Plots** — (Available only for significant proteins.) — Select to view the [Box Plots section \(page 73\)](#).
 -  **Preferences** — Select to set threshold preferences. e.g., *High Regulation Threshold*.

Raw Data section

The **Raw Data** section shows a table consisting of protein groups (rows) identified across the analyzed samples (columns) and their corresponding intensity levels (values). Samples for which a protein group was detected show a numerical value. However, samples for which a protein group was not detected show a hyphen – character.


- Search for the protein (protein group) to extract intensity values across samples.
- Select the protein to visualize the distribution of abundances between samples corresponding to each group as an Intensity Plot box plot.
- Select the  **Heatmap** button to visualize a heatmap of raw protein group data.

Figure 19. Raw Data table listing proteins and Intensity Plot for the selected protein

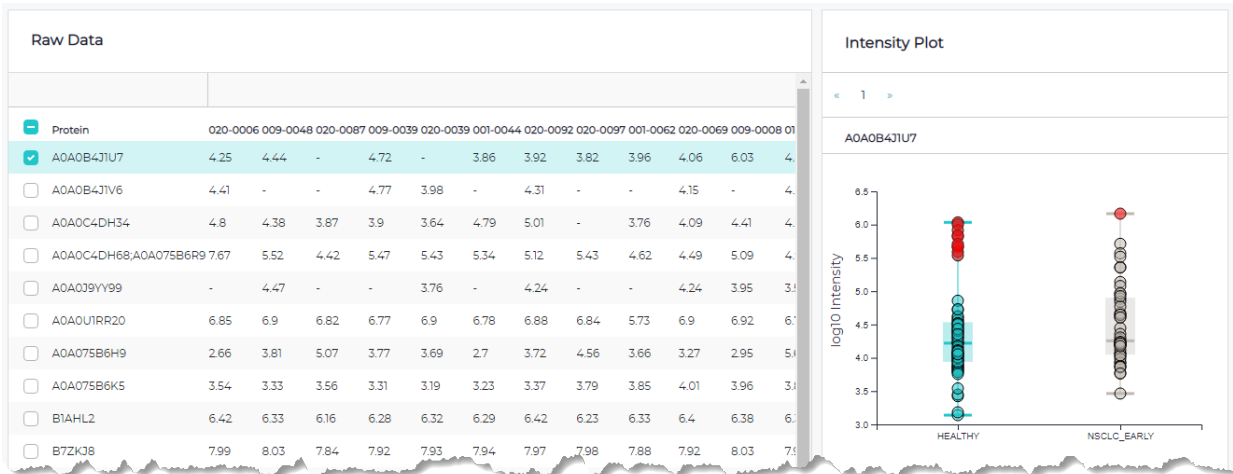
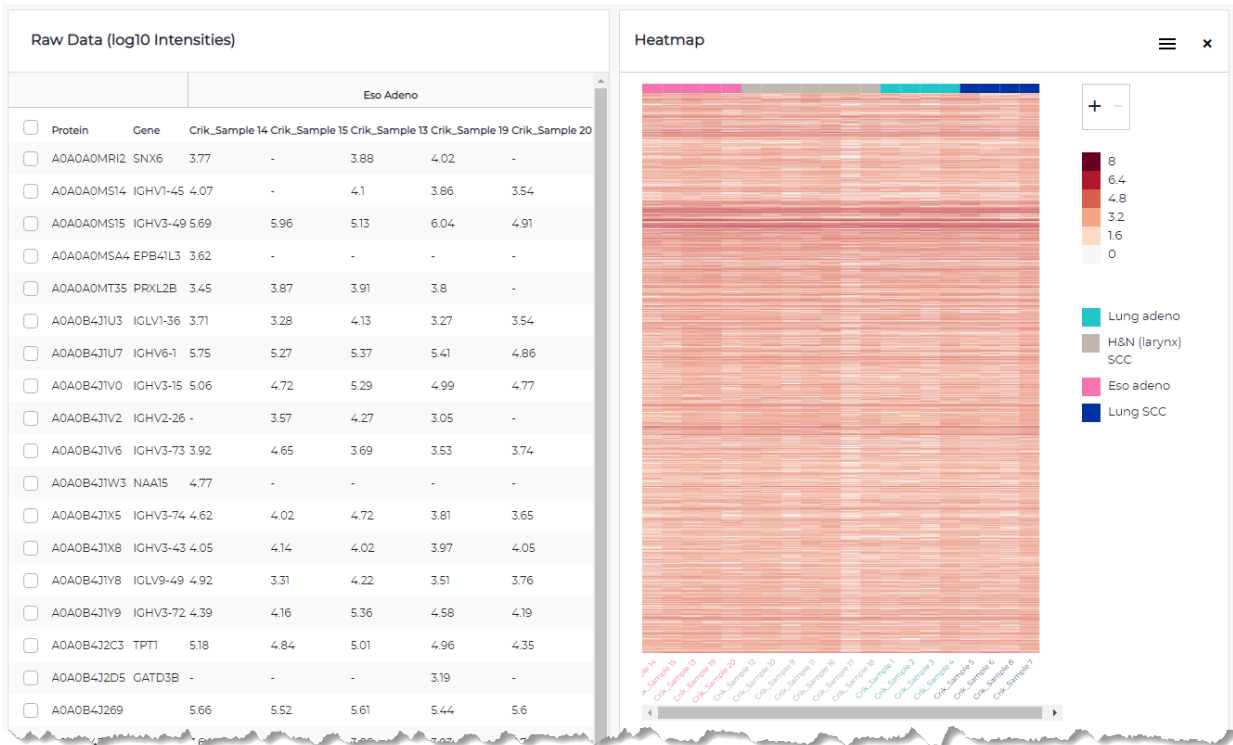


Figure 20. Raw data table listing proteins and heatmap for all proteins



Clustered Heatmap section

After doing a group analysis, you can view the **Clustered Heatmap** section.

Here you can visualize protein abundances across samples, with both proteins (rows) and samples (columns) clustered based on agglomerative nesting. Cell colors range from blue (lowly abundant) to red (highly abundant).


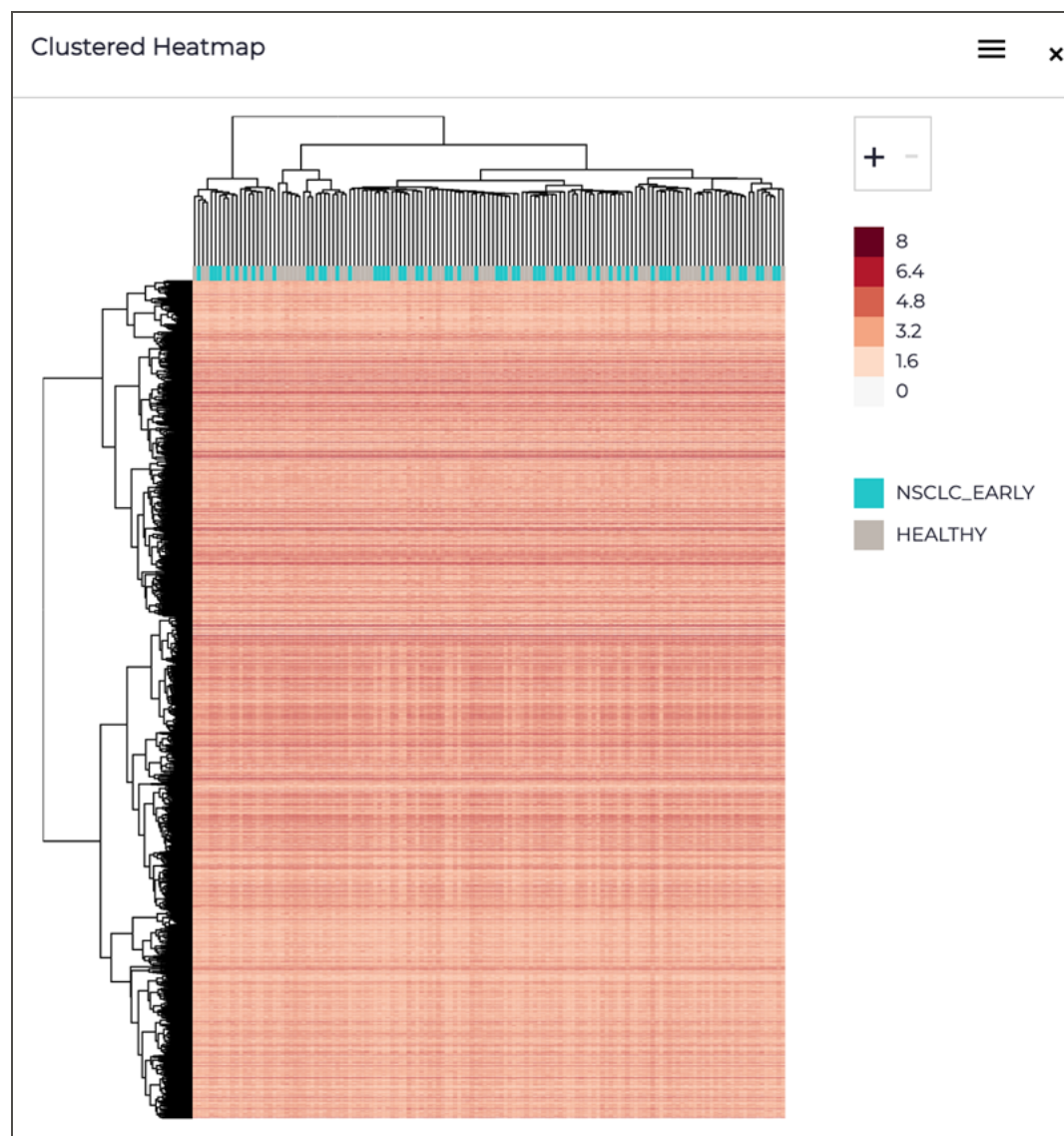
- Use the + and - buttons to zoom in and out of the graph.
- Hover over a cell to reveal the protein name, sample name, and abundance.
- Select  ("hamburger menu") to download the graph as .svg or .png.

Figure 21. Clustered heatmap graph



Volcano section

After doing a group analysis, you can view the **Volcano** section.

Here you can visualize a scatter plot showing the statistical significance (p-value) in abundance differences between your compared groups versus the magnitude of the change (Fold Change). Highlighted in the teal quadrants are proteins with large fold changes (default: ± 2) and statistically significant (default: $p < 0.05$). Data displayed in the plot are shown in detail in the table on the left of the plot.



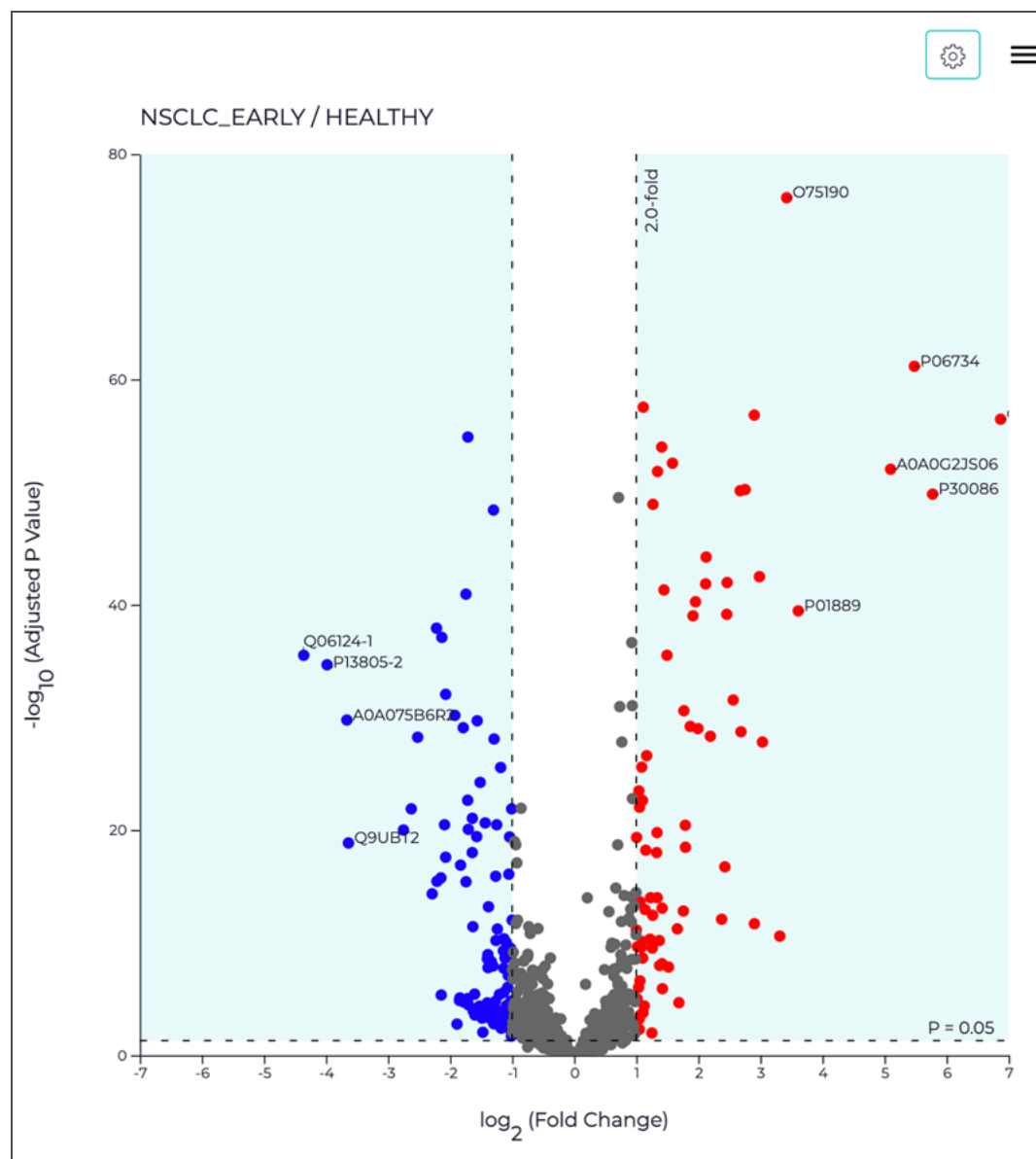
- Each point in the plot represents a protein. Hover over each point to display the protein group, fold change, and p-value.
- Clear the **Significant Proteins** checkbox in the **Group Analysis** section's toolbar to display both significant and non-significant proteins.
- Select this section's  (**Settings**) button to highlight a protein of interest.
- Select  ("**hamburger menu**") to download the graph as .svg or .png.

Figure 22. Volcano graph



Coverage section

After doing a group analysis, you can view the **Coverage** section.

Here you can visualize the amino acid sequence of your selected protein and the regions where measured peptides map. You must select at least one protein in the list to the left of this section.

Coverage is represented as percent (%) of sequence observed by measured peptides.



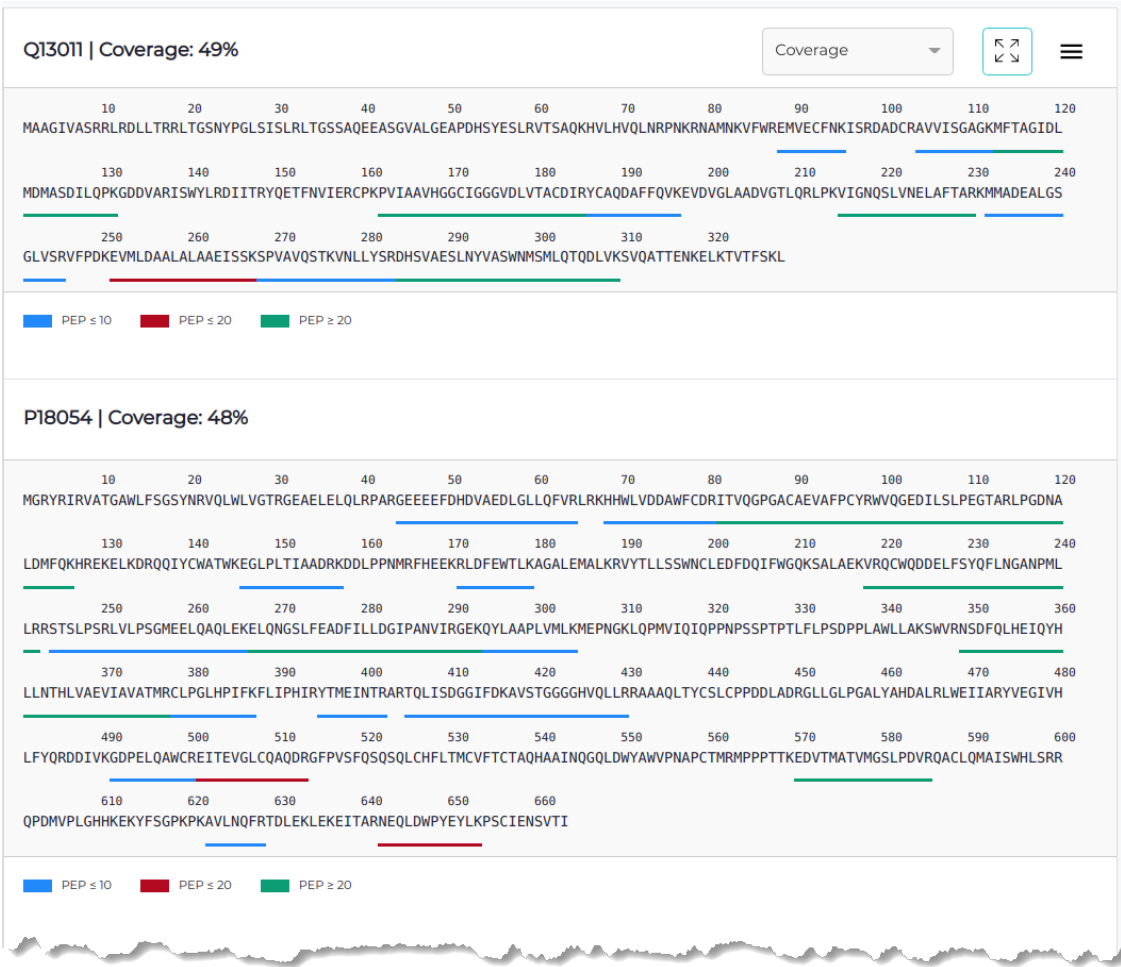
- In cases where a PTM is detected for your selected protein, use the **Coverage** list to change to PTM to view where the PTM occurs.
- Select  (**Expanded View**) to expand the section so you can see data more easily, without its wrapping
- Select  ("**hamburger menu**") to download the graph as .svg or .png.

Figure 23. Coverage graph



Filtered PPI Network section

After doing a group analysis and with the **Significant Proteins** checkbox selected, you can view the **Filtered PPI Network** section.

Here you can visualize a network plot showing protein–protein interactions between proteins with significantly different abundances between groups compared.


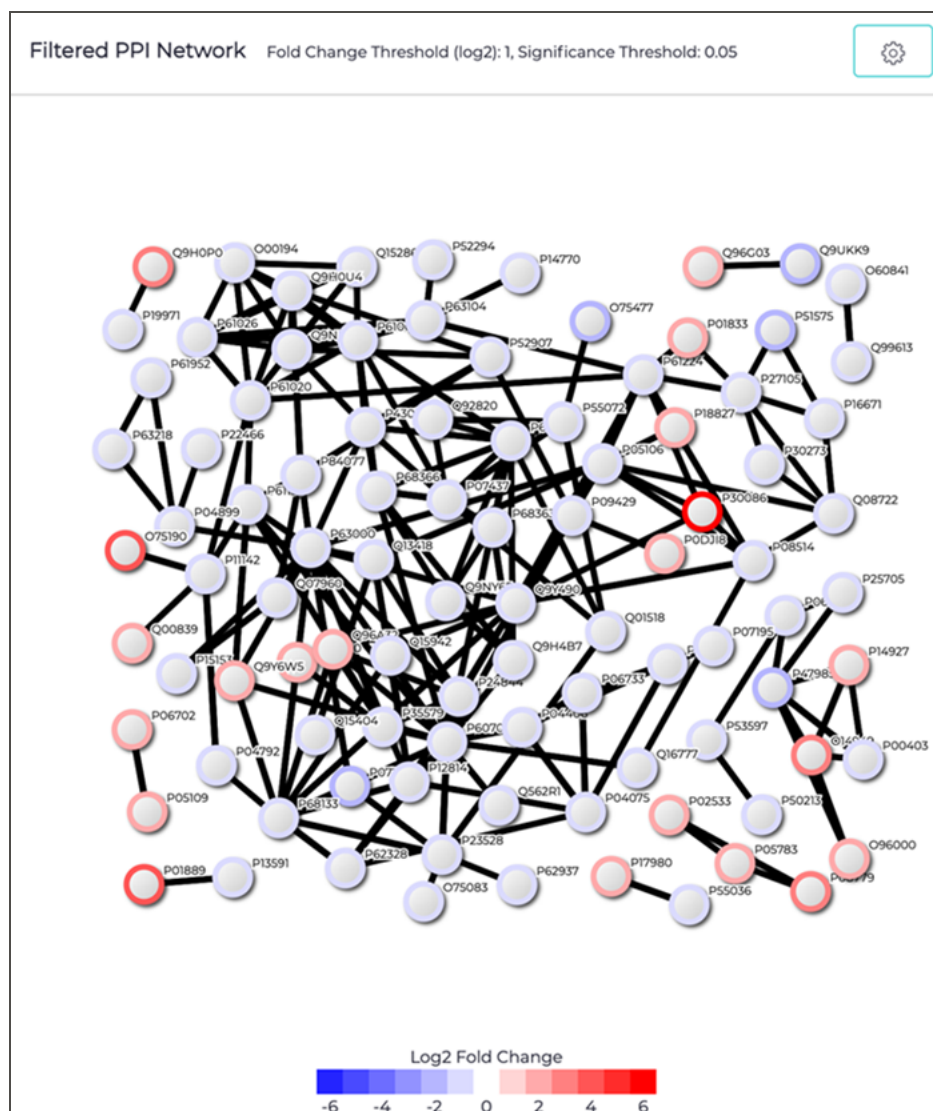
- Select this section's  (**Settings**) button to adjust the confidence of the Minimum Interaction Score.
- Nodes in the graph are selectable to view protein description and can be moved around.



Figure 24. Filtered PPI Network graph



Enrichment section

After doing a group analysis and with the **Significant Proteins** checkbox selected, you can view the **Enrichment** section.

Here you can functionally characterize proteins showing abundance difference between groups compared by performing gene ontology (GO) enrichment.

- Use the list to switch between GO categories: *Molecular Function*, *Biological Process*, and *Cellular Compartment*.
- Select this section's  **Chart Settings** button to set the cutoff (adjusted p-value upper limit).
- Display the GO term enrichment as either:
 -  **Dot Plot** — To "condense" similar terms by family (i.e., condense all children from each superfamily), select **Summarize Terms**.


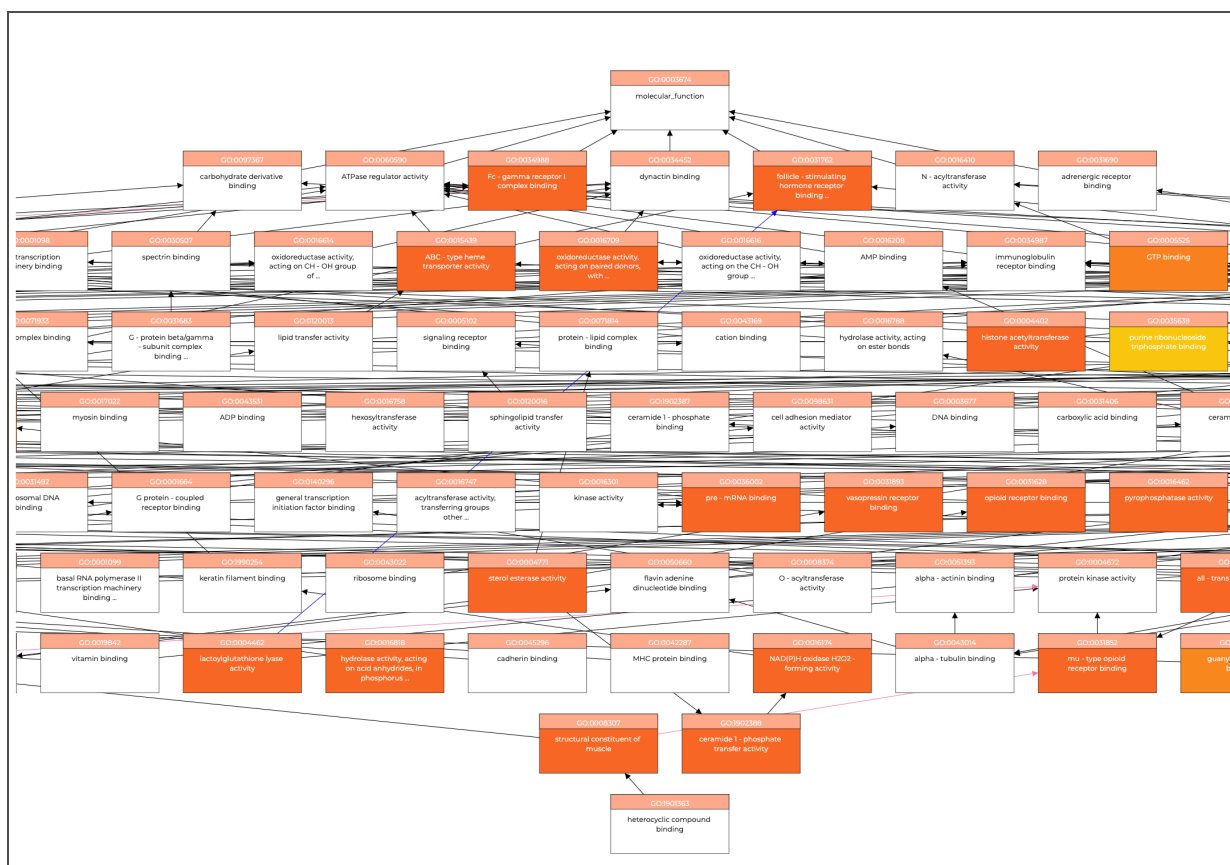
-  **Ontology Plot** (hierarchical tree)
 - Hover over a box to view its GO information.
 - Use the mouse wheel to zoom into and out of the plot.
 - Drag the plot to reposition it so that you can examine different areas.

Figure 25. Enrichment plot, shown as an ontology plot (hierarchical tree)



Box Plots section

After doing a group analysis and with the **Significant Proteins** checkbox selected, you can view the **Box Plots** section.

Here you can visualize the intensity differences between groups of significantly different proteins.


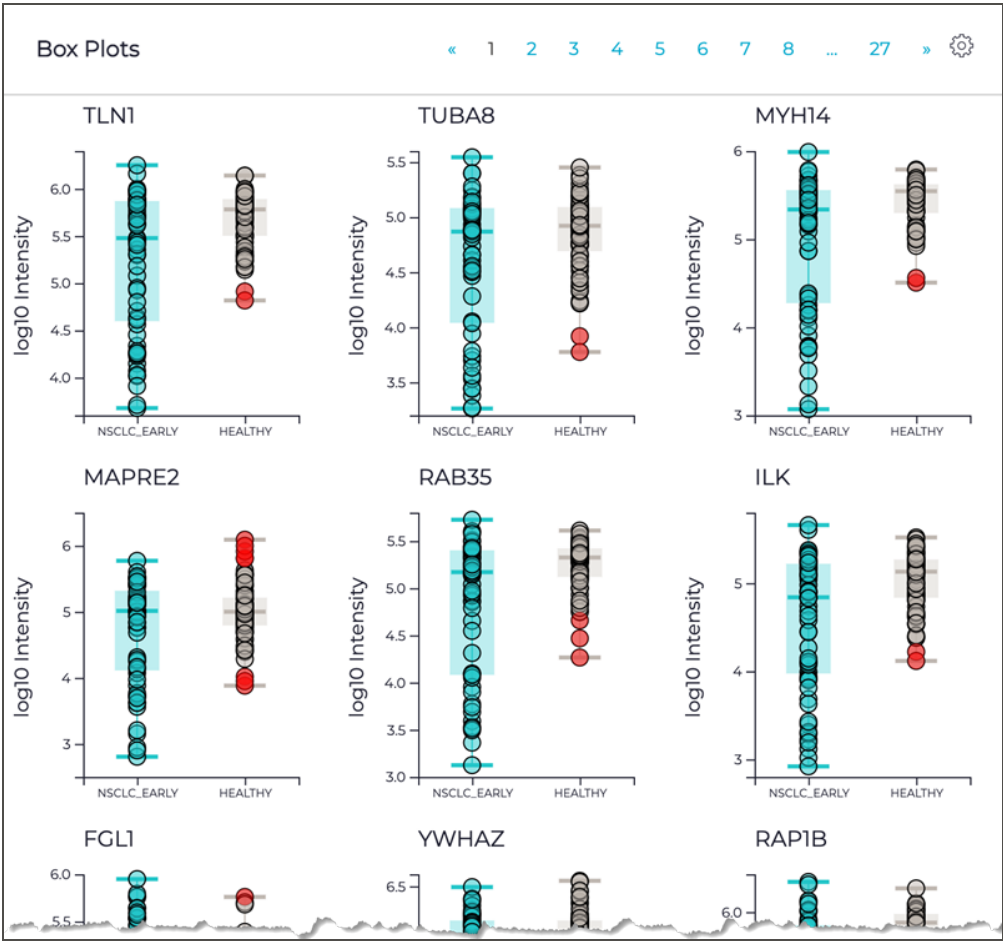
- Select this section's  (**Settings**) button to set layout preferences for the charts.
- Hover over a dot to view a sample's count and name.

Figure 26. Box plots





Chapter 5

Data Management

Covers the components of and how to work with PAS's main pages.

Plates and samples



A plate in PAS represents a Peptide Collection Plate, which is the output of the Proteograph Assay method analyzed with MS. A plate contains the samples, controls, and nanoparticles from a method run with the corresponding metadata.

Plates page

Use the **Plates** page to manage plates and sample information and to upload custom files.

- To open this page, select  **Plates** on the sidebar menu.



TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.

Toolbar items

- Add Plate** — Select to add a plate to PAS when setting up an analysis. See [Setup workflow: Add a plate \(page 25\)](#).
- Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).
- Show/Hide** — Select or clear checkboxes to show or hide table columns. See [Show or hide table columns \(page 12\)](#).


Table columns

- Name** — The name of the plate.
- Plate ID** — The unique identifier of the plate.
- Description** — The description of the plate.
- Notes** — Additional information about the plate.
- Created By** — The user who created the plate.
- Created Time** — The date and time the plate was created.
- Last Modified By** — The user who last modified the plate.
- Last Modified Time** — The date and time the plate was last modified.
- ID** — The unique, internal identifier of the plate.
-  (**Add Sample**) — Select to add samples to the selected plate. See [Add samples to an existing plate \(page 79\)](#).
-  (**Edit**) — Select to edit the selected plate. See [Edit a plate \(next page\)](#).



Other page sections

- Plate Samples** — Shows a table of samples associated with the plate selected in the **Plates** section. For detailed information about this section, see [Plate Samples section \(page 78\)](#).
- Plate Grid** — Shows a grid or table of wells associated with one or more samples selected in the Plate Samples section. For detailed information about this section, see [Plate Grid section \(page 81\)](#).

Review a plate

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Select a plate to review.
The **Plate Samples** table appears, listing the samples in the selected plate.
3. (Optional) Adjust the table view as needed:
 - To adjust the number of visible table rows, scroll to the bottom of the table and select the number of items per page.
 - To sort a table column, select the column heading to sort in descending order. To sort in ascending order, reselect the column.
 - To filter samples, enter a keyword or term in the **Search** field.
4. Select samples for review:
 - To review all samples, select the checkbox in the column heading.
 - To review selected samples, select each sample's checkbox.The **Plate Grid** appears, showing the plate with yellow wells indicating the selected samples.
5. Review sample details:
 - To individually review sample details, select a yellow well.
 - To simultaneously review details for all samples, select **Table View**.
 - To modify sample details, see [Edit or delete samples in wells \(page 81\)](#).

Edit a plate

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Find the plate you want to edit and select its  (**Edit**) button to open the **Edit Plate** dialog.
3. Edit the fields as needed.
 - **Plate ID** — Enter a unique identifier for the plate.
 - **Plate Name** — Enter a descriptive name for the plate.
 - **Description** — (Optional) Enter a description of the plate.
 - **Notes** — (Optional) Enter additional information about the plate.
4. Select **Confirm** to save.

Delete a plate




1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Find the plate you want to delete and select its  (**Delete**) button.
3. Select **OK** to confirm.

Plate Samples section

The **Plate Samples** section is part of the [Plates page \(page 76\)](#).

- To open it, select  **Plates** on the sidebar menu and then select a plate. You may need to scroll down to see the **Plate Samples** section.



Toolbar items

- Link to Sample Description File** — Select to link a sample description file to the selected plate. See [Add sample descriptions \(page 80\)](#).
- Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).
- Show/Hide** — Select or clear checkboxes to show or hide table columns. See [Show or hide table columns \(page 12\)](#).

TIP



You can add custom columns to this table. See [Add custom columns \(page 12\)](#).

Table columns

- Name** — The descriptive name of a sample.
- Sample/Control ID** — The unique identifier of a sample or control.
- Well Location** — The location of a sample or control in the selected plate.
- Type** — The type of sample: *Plasma* or *Peptide*.
- Species** — The species a sample was collected from: *Human* or *Mouse*.
- Sample Collection Date** — The date the sample was collected.
- Sample Receipt Date** — The date your laboratory received the sample.
- Condition** — The categorical group the sample belongs to.
- Biological Replicate** — The biological replicate number.
- Technical Replicate** — The technical replicate number.
- Description** — The description of the sample.
- Notes** — Additional information about the sample.
- Created By** — The user who created the sample.
- Created Time** — The date and time of the sample was created.
- Last Modified By** — The user who last modified the sample.
- Last Modified Time** — The date and time the sample was last modified.
- ID** — The unique, internal identifier of the sample.
- Plate ID** — The unique identifier of the plate.
- Plate Name** — The descriptive name of the plate.
-  **(Edit)** — Select to edit information about the selected sample. See [Edit sample information \(page 80\)](#).
-  **(Delete)** — Select to delete the selected sample. See [Delete a sample from a plate \(page 81\)](#).


Add samples to an existing plate

Adding samples to an existing plate follows a similar workflow to the add-a-plate workflow of analysis setup (described in [Setup workflow: Add a plate \(page 25\)](#)). The difference is that in the add-a-plate workflow, you add a new plate and its samples to PAS, whereas you can also add samples to an existing plate, as described below.

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Find the plate to which you want to add sample and select its  (**Add Sample**) button to open the **Add Sample** dialog.
3. In the **MSDATA Files** section, you add one or more MS data files.
 - a. Select the MS data files.

NOTE

Supported file formats are .raw, wiff, or .wiff.scan. Supported folders are RAW and D.

- To add a single file, select **Files** to open the **Add Files** dialog.
 - To add multiple files, select **Folder** to open the **Add Folder** dialog.
- b. Either drag the file or folder into the drag-and-drop area or use **Browse** to navigate to and select it.
 - c. Select **Add**.
 - d. Review the selected files.
 - To remove a file, select  (**Delete**).
 - To remove all files, select **Clear**.
 - e. Select **Next** to advance.
4. In the **Plate Map File** section, you add a plate map file, which specifies the locations of samples.
 - a. If you don't have a plate map file, create one before continuing.
 - A. Select the on-screen link from which you can download an example plate map file (.csv).
 - B. Open the file and edit it as needed.


The **MS file name**, **Sample ID**, and **Plate ID** columns are required. (See [Plate map file format \(page 15\)](#) for detailed descriptions of the columns in the file.)
 - C. Save as a .csv file.
 - b. Select **Add File** or **Add** to open the **Add File** dialog.
 - c. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.
 - d. Select **Add**.
 - e. Select **Next** to advance.
 5. In the **Plate ID and Name** section, you link the MS data files to an existing plate.
 - a. Select **Use Existing Plate**, and then select the applicable plate.
 - b. Select **Next** to advance.
 6. (Optional) In the **Sample Description File** section, you upload metadata for each sample in the plate.

NOTE

This part of the workflow is optional. To skip it, select **Next** to advance.


- a. Select **Add** or **Add File** to open the **Add Files** dialog.
 - b. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.
 - c. Select **Add**.
 - d. Select **Next** to advance.
7. In the **Add to Project** section, you add the samples to a new or existing project.
- a. Create or select a project:
 - To create a new project, select **New Project**, enter a project name, and select **Add**.
 - To use an existing project, select it from the **Select Project** list.
 - b. Select or clear the applicable checkboxes. (To defer analysis, clear both checkboxes.)
 - **Analyze samples after addition** — Select to analyze samples.
 - **Analyze controls after addition** — Select to analyze controls.
 - c. Select the MS method:
 - **DDA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.
 - **DIA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.
 - d. From the **Analysis Protocol** list (which shows only protocols compatible with the selected MS method), select a protocol.
 - e. Select **Add Plate**, and then select **Close**.
 - If you had selected either or both **Analyze...** checkboxes earlier, the analysis starts immediately.
 - If you deferred analysis, you must start it manually. See [Start the analysis \(page 27\)](#).


Add sample descriptions

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. In the **Plates** table, select a plate to add sample descriptions to.
3. On the **Plate Samples** section's toolbar, select **Link to Sample Descriptions File** to open the **Upload File** dialog.
4. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.
5. Select **Upload**.

The information from the uploaded file appears in the **Plate Samples** section of the **Plates** page.

Edit sample information

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Select the plate for which you want to edit information about a sample.

3. In the **Plate Samples** table, find the sample you want to edit and select its  **(Edit)** button to open the **Edit** window.
4. Complete the fields as needed.
5. Select **Confirm** to save.

Delete a sample from a plate



1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Select the plate from which you want to delete a sample.
3. In the **Plate Samples** table, find the sample you want to delete and select its  **(Delete)** button.
4. Select **OK** to confirm.



Plate Grid section


The **Plate Grid** section of the **Plates** page shows the selected plate with yellow wells indicating the samples selected in the **Plate Samples** list.

The section offers two views of the same information.  **Grid View** facilitates editing and deleting samples one well at a time, while  **Table View** offers a more efficient means to work with samples in multiple wells. For detailed instructions, see [Edit or delete samples in wells \(below\)](#).



If you have created a custom .csv, .tsv, .xls, or .xlsx file containing sample information, you can upload it to the **Plates** page from the **Plate Grid** section. See [Upload a custom file containing sample information \(next page\)](#).

Edit or delete samples in wells

The **Plate Grid** section of the **Plates** page offers two views for editing samples in and deleting samples from wells.  **Grid View** facilitates editing and deleting samples one well at a time, while  **Table View** offers a more efficient means to work with samples in multiple wells.

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
2. Select the plate whose samples you want to edit or delete.
3. In the **Plate Samples** table, select the checkbox of each sample you want to work with.
The **Plate Grid** appears below the **Plate Samples** table and shows the selected samples as yellow wells in a 96-well plate.
4. Edit or delete samples as described below.

Grid view

1. Select  **Grid View** if it is not already selected.
2. To edit a sample in a well:
 - a. Select a yellow well to open its details and then select its  **(Edit)** button.
 - b. Edit values in the editable fields. PAS saves each change as you work.










- c. When finished editing, select the  (**Edit**) button again to save all the changes.
3. To delete a sample from a well :
 - a. Select a yellow well to open its details and then select its  (**Delete**) button.
 - b. Select **OK** to confirm.

Table view

1. Select  **Table View**.
2. To edit samples in a well:
 - To edit an individual cell, enter a value, and then press **Enter**.
 - To apply the same value to all cells in a column, select the column heading's  (**Update**) button, enter a value, and then select **Apply**.
 - To copy and paste a row, scroll all the way to the right and select  (**Copy**). Edit the copied row as needed and then select  (**Save Copy**).
3. To delete a sample from a well, select the well's  (**Delete**) button. Select **OK** to confirm.

Upload a custom file containing sample information

You can create a custom .csv, .tsv, .xls, or .xlsx file containing sample information and upload it from the **Plates** page. To create the file, match the columns in the file to the columns in the table view.

1. On the sidebar menu, select  **Plates** to open the **Plates** page.
 2. Select the applicable plate.
 3. In the **Plate Samples** table, select the checkbox of at least one sample to open the **Plate Grid** sections.
 4. Select  (**Upload File**) to open the **Upload File** dialog.
 5. Either drag the file into the drag-and-drop area or use **Browse** to navigate to and select it.
 6. Select **Upload**.
- PAS populates the plate grid with imported sample information.

Projects



When you set up an analysis, PAS creates a corresponding project and adds it to the **Projects** page. The project lists all samples in an analysis with sample information. On the **Projects** page, you can add samples to the analysis and then start the analysis.

Projects page

Use the **Projects** page to manage projects, to manage the samples associated with a project, and to view the MS data files associated with a specific sample.

- To open this page, select  **Projects** on the sidebar menu.

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.



Toolbar items

- Add Project** — Select to add a new project. See [Add a project \(next page\)](#).
- Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).
- Show/Hide** — Select or clear checkboxes to show or hide table columns. See [Show or hide table columns \(page 12\)](#).

TIP

You can add custom columns to this table. See [Add custom columns \(page 12\)](#).

Table columns


- Tenant ID** — The user identification.
- Name** — The name of the project.
- Description** — The description of the project.
- Notes** — Additional information about the project.
- Created By** — The user who created the project.
- Created Date** — The date and time of project was created.
- Last Modified By** — The user who last modified the project.
- Last Modified Date** — The date and time the project was last modified.
- ID** — The unique, internal identifier of the project.
-  (**Edit**) — Select to edit the selected project's name, description, and/or notes.
-  (**Delete**) — Select to delete the selected project (one that you originally added). See [Delete a project \(next page\)](#). You cannot delete someone else's project (unless you are an Admin).

Other page sections

- Sample List** — Shows a table of samples associated with the project selected in the **Projects** section. For detailed information about this section, see [Sample List section \(next page\)](#).



- **MS Data files** — Shows a read-only table of MS data files associated with the sample selected in the **Samples List** section. You can show or hide columns and can search for a specific data file.

Add a project

1. On the sidebar menu, select  **Projects** to open the **Projects** page.
2. Select **Add Project** to open the **Create Project** dialog.
3. Complete the fields.
 - **Project Name** — Enter a unique name for the project.
 - **Select Plate** — Select a plate to add to the project.
 - **Add** — Select to add another plate to the project. Repeat as needed.
 - **Description** — Enter a description of the project.
 - **Notes** — Enter any additional information about the project.
4. Select **Save**.


Delete a project

You can delete any project that you originally created. You cannot delete someone else's project unless you are an administrator.

1. On the sidebar menu, select  **Projects** to open the **Projects** page.
2. Find the project you want to delete and select its  **(Delete)** button.
3. Select **Yes** to confirm.

Sample List section

The **Sample List** section of the [Projects page \(previous page\)](#) shows a table of samples associated with the selected project.

- To open it, select  **Projects** on the sidebar menu and then select the project whose samples you want to manage.

Toolbar items

- **Add Sample** — Select to add samples to the project. See [Add samples to a project \(next page\)](#).
- **Analyze** — Select to select samples for analysis, as described in [Setup workflow: Select samples or controls for analysis \(page 31\)](#).
- **Analyze Controls** — Select to select controls only for analysis. See [Analyze controls only \(page 32\)](#).
- **Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).
- **Show/Hide** — Select or clear checkboxes to show or hide table columns. See [Show or hide table columns \(page 12\)](#).


TIP

You can add custom columns to this table. See [Add custom columns \(page 12\)](#).

Table columns

- **Tenant ID** — The user identification.
- **Name** — The descriptive name of a sample.
- **Sample/Control ID** — The unique identifier of a sample or control.
- **Well Location** — The location of a sample or control in the selected plate.
- **Type** — The type of sample: *Plasma* or *Peptide*.
- **Species** — The species a sample was collected from: *Human* or *Mouse*.
- **Sample Collection Date** — The date the sample was collected.
- **Sample Receipt Date** — The date your laboratory received the sample.
- **Condition** — The categorical group the sample belongs to.
- **Biological Replicate** — The biological replicate number.
- **Technical Replicate** — The technical replicate number.
- **Plate Name** — The descriptive name of the plate.
- **Description** — The description of the sample.
- **Notes** — Additional information about the sample.
- **Created By** — The user who created the sample.
- **Created Date** — The date and time of the sample was created.
- **Last Modified By** — The user who last modified the sample.
- **Last Modified Date** — The date and time a sample was last modified.
- **ID** — The unique, internal identifier of the sample.

Add samples to a project

1. On the sidebar menu, select  **Projects** to open the **Projects** page.
2. Select a project to add samples to.
3. Above the **Sample List** table, select **Add Sample** to open the **Add Sample** dialog.
4. Complete the fields.
 - **Select Plate** — Select the plate to add samples to.
 - **Select Sample** — Select a sample to add.
 - **Add** — Select to add another sample.
5. Select **Save** to add the selected samples.

Analyses



When you set up an analysis, PAS adds the analysis to the Analyses page with general information about the analysis: the number of MS data files in the analysis, who last modified the analysis and when, and optional notes and descriptions. An icon to the left of the analysis name indicates the status. Selecting an icon opens the analysis log.

Analyses page



Use the **Analyses** page to manage analyses and to view and download analysis results and logs.

- To open this page, select  **Analyses** on the sidebar menu.

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.



Toolbar items



- Project** — Select the project whose analysis data you want to work with.
- Plate** — Select the plate whose analysis data you want to work with.
- Controls/Samples** — Select whether to show controls or samples on the list.
- Status** — Select the status of analyses that you're interested in, e.g., *Completed*.
-  **Refresh** — Select to refresh the table.
- Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).
-  (**Menu**) — Select to open a menu of options (e.g., *Delete*) to use when multiple analyses are selected. See [Delete one or more analyses \(page 88\)](#).
- Show/Hide** — Select or clear checkboxes to show or hide table columns. See [Show or hide table columns \(page 12\)](#).

TIP




You can add custom columns to this table. See [Add custom columns \(page 12\)](#).

Table columns

- <status>** — The status of an analysis:  (**Succeeded**),  (**Failed**).
- Name** — The name of an analysis.
- Description** — The description of the analysis.
- Notes** — Additional information about the analysis.
- Protocol** — The protocol used for the analysis.
- MS Data Files** — The number of MS data files associated with the analysis.
- Analyzed By** — The user who created the analysis.
- Analysis Start** — The date and time the analysis started.
- Analysis End** — The date and time the analysis ended.

- **Last Modified By** — The user who last modified the analysis.
- **Last Modified Time** — The date and time the analysis was last modified.
- **ID** — The unique, internal identifier of the analysis.
-  **(Edit)** — Select to edit the selected analysis. See [Edit an analysis \(below\)](#).
-  **(Delete)** — Select to delete the selected analysis. See [Delete one or more analyses \(next page\)](#).

Download an analysis log



1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. Find the analysis whose log you want to download and select the status icon (e.g.,  **(Succeeded)**) that precedes its name.
The **Analysis Log** dialog opens, listing all analysis events from oldest to newest.
3. Select  **(Download Log)**.
4. Depending on your browser or browser preferences, the file may download immediately, or you may be prompted where to save the file. Follow any on-screen prompts.

Download an analysis's protein groups and peptides results



You can download results for protein groups and peptides for a selected analysis. The results are organized into several files, each offering simplified data tables containing summarized results.

- **Peptide_NP.tsv** — Peptides, abundances, and other metadata across nanoparticles.
- **Peptide_Panel.tsv** — Peptides, abundances, and other metadata with nanoparticle values rolled up.
- **Protein_Group_NP.tsv** — Protein groups, abundances, and other metadata across nanoparticles.
- **Protein_Group_Panel.tsv** — Protein groups, abundances, and other metadata with nanoparticle values rolled up.

To download analysis results:

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. Select the analysis whose results you want to download.
3. Select  **Protein Group / Peptide Results**, located to the right of the analysis's tabs.
4. Depending on your browser or browser preferences, the file may download immediately, or you may be prompted where to save the file. Follow any on-screen prompts.



Edit an analysis

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. Find the analysis you want to edit and select its  **(Edit)** button to open the **Edit Analysis** dialog.
3. Edit the fields as needed.



- **Analysis Name** — Enter a name of the analysis.
 - **Description** — (Optional) Enter a description of the analysis.
 - **Notes** — (Optional) Enter additional information about the analysis.
4. Select **Save**.

Delete one or more analyses

To delete a single analysis:

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. Find the analysis you want to delete and select its  (**Delete**) button.
3. Select **OK** to confirm.

To delete multiple analyses:

1. On the sidebar menu, select  **Analyses** to open the **Analyses** page.
2. Select the checkbox of each analysis you want to delete.
3. Select  (**Menu**) and then select **Delete**.
4. Select **OK** to confirm.

MS data files

When you upload MS data files during analysis setup, PAS creates a folder to contain the files. From the **Data Files** page, you can customize any folder and manually create folders.

Use the following filters to refine your view of the **Data Files** page.



- **Start Date** and **End Date** — Filter for folders and files created within a specified date range.
- **Last Uploaded** — Filter for folders and files uploaded within the last day, last five days, or last month.

Data Files page

Use the **Data Files** page to create, move, and delete MS data files and folders and to download an application for automatic file updates.

- To open this page, select  **Data Files** on the sidebar menu.

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.

Toolbar items












- **Link to Plate** — (Available when one or more files or folders are selected.) Select to link the selected files or folders to a plate when setting up an analysis. See [Setup workflow: Link to a plate \(page 28\)](#).
-  **New** — Select to add a new, empty folder.
-  **Upload** — Select to upload data files. See [Upload MS data files \(next page\)](#).
-  **Refresh** — Select to refresh the table.
- **Start Date** — Set the earliest creation date for the files you want to view.
- **End Date** — Set the latest creation date for the files you want to view.
- **Last Uploaded** — Select a filter the list to show only those files created or uploaded within the last day (1D), last five days (5D), or last month (1M). To clear the active filter, select it again.
-  **(Menu)** — Select to move, rename, or delete the selected files or folders. See [Move MS data files \(next page\)](#), [Rename MS data files or folders \(next page\)](#), and [Delete MS data files or folders \(page 91\)](#).
-  **Uploader** — Select to download the Seer AutoUploader application with which you can automatically transfer new MS data files to PAS. You may find it a more convenient means of uploading a large set of files rather than using the  **Upload** button. See [Download and install the Seer AutoUploader application \(page 91\)](#).

Table columns




- **<folders/files>** — Initially shows the top level of folders into which data files are organized. Select a folder to view its contents. The column's heading shows the breadcrumb (path) to the folder whose contents are listed. To return to another folder in the path, select its link in the breadcrumb. To return to the top-level folders, select  (**Home**).
- **Filepath** — Shows the location where a file or folder is stored.
- **Date** — Shows the date the file or folder was added to PAS.

- **Time** — Shows the time the file or folder was added to PAS.
- **Size** — Shows the disk size of the file or folder.
-  **(Download)** — Select to download the selected file.
-  **(Delete)** — Select to delete the selected file or folder. See [Delete MS data files or folders \(next page\)](#).



Create a folder

1. On the sidebar menu, select  **Data Files** to open the **Data Files** page.
2. Select  **New** to open the **Create Folder** dialog.
3. Enter the name of the new folder.
4. Select **Create**.


Upload MS data files


1. On the sidebar menu, select  **Data Files** to open the **Data Files** page.
2. Select  **Upload** to open the **Add Raw MSDATA Files** dialog.
3. Select the MS data files.
 - To upload a single file, select **Add Files** to open the **Add Files** dialog.
 - To upload multiple files, select **Add Folder** to open the **Add Folder** dialog.
4. Either drag the file or folder into the drag-and-drop area or use **Browse** to navigate to and select it.
5. Select **Upload**.
6. Review the uploaded files.
 - To remove a file, select  **(Delete)**.
 - To remove all files, select **Clear**.

Move MS data files



1. On the sidebar menu, select  **Data Files** to open the **Data Files** page.
2. Select the folder where the MS data files you want to move are stored.
3. Select the checkbox of each file you want to move.
4. Select  **(Menu)** and then select **Move**.
5. Select a destination folder, and then select **Move Here**.
6. Select **OK** to confirm.

Rename MS data files or folders


1. On the sidebar menu, select  **Data Files** to open the **Data Files** page.
2. Navigate to the folder where the folder or file you want to rename is stored.
3. Select the checkbox of the folder or file you want to rename.



4. Select  (**Menu**) and then select **Rename**.
5. Enter a new name for the folder or file.
6. Select **Save**, and then select **OK**.

Delete MS data files or folders

1. On the sidebar menu, select  **Data Files** to open the **Data Files** page.
2. Navigate to the folder where the folder or file you want to delete is stored.
3. Find the folder or file you want to delete and select its  (**Delete**) button.
4. Select **OK** to confirm.

Download and install the Seer AutoUploader application


The Seer AutoUploader is an application that runs on your MS computer to automatically upload new MS data files to your PAS account. You may find it a more convenient means of uploading a large set of files rather than using the  **Upload** button on the **Data Files** page.

1. On the sidebar menu, select  **Data Files** to open the **Data Files** page.
2. Select  **Uploader** to open the **Download AutoUploader** dialog.
 - a. From **Select file to download**, select the version of the AutoUploader you want to download.
 - b. In the **Save As** window, navigate to the folder in which you want to save the installation package and select **Save**.
 - c. Select **Done**.
3. In your computer's file system, navigate to and double-click the installation package to launch it. Follow the prompts to install the software.

Analysis protocols

An analysis protocol specifies search parameters for the MS database search engine.

- For DDA-based analyses, PAS uses the MaxQuant¹ protocol.
- For DIA-based analyses, PAS uses either the EncyclopeDIA² or DIA-NN³ protocol.

PAS includes several preinstalled analysis protocols, identified on the [Protocols page \(below\)](#) by the  (star) icon. You can also create custom protocols by copying an existing protocol or by uploading a protocol.

¹Cox, Jürgen, and Matthias Mann, "MaxQuant enables high peptide identification rates, individualized p.p.b.-range mass accuracies and proteome-wide protein quantification," 26 *Nature Biotechnology* (November 2008): 1367–1372, <https://doi.org/10.1038/nbt.1511>.

²Searle, Brian C., Lindsay K. Pino, Jarrett D. Egertson, Ying S. Ting, Robert T. Lawrence, Brendan X. MacLean, Judit Villén, et al., "Chromatogram libraries improve peptide detection and quantification by data independent acquisition mass spectrometry," 9 *Nature Communications* (December 2018): 5218, <https://doi.org/10.1038/s41467-018-07454-w>.



³Demichev, V., Messner, C.B., Vernardis, S.I. et al., "DIA-NN: neural networks and interference correction enable deep proteome coverage in high throughput." 17 *Nat Methods* (January 2020): 41–44, <https://doi.org/10.1038/s41592-019-0638-x>.

Protocols page

Use the **Protocols** page to manage analysis protocols and to view analysis parameters.

- To open this page, select  **Analysis Protocol** on the sidebar menu.

TIP

Use  (**Collapse**) and  (**Expand**) (where available) to selectively collapse and expand sections as you work.

Toolbar items




- **Copy** — (Shown when a protocol is selected.) Select to copy a custom (user-defined) or preinstalled protocol. See [Copy an analysis protocol \(page 94\)](#).
- **Upload** — Select to upload a protocol. See [Upload an analysis protocol \(next page\)](#).
- **Search** — Use to filter the table or find a specific item. See [Filter a table; search for a specific item \(page 13\)](#).
- **Show/Hide** — Select or clear checkboxes to show or hide table columns. See [Show or hide table columns \(page 12\)](#).

TIP


You can add custom columns to this table. See [Add custom columns \(page 12\)](#).

Table columns

- **Name** — The name of the protocol.
- **Type** — Whether the associated MS method is DDA or DIA.


- **Species** — Whether the analyzed sample is from a human or mouse.
- **Version** — The version of the protocol, useful if you want to keep track of different versions (updates) of protocols.
- **Description** — The description of the protocol.
- **Notes** — Additional information about the protocol.
- **Created By** — The user who created the protocol.
- **Created Time** — The date and time the protocol was created.
- **Parameters** — The name of the file in which the search engine parameters are defined. To view the search engine parameters for a protocol, select its row. See [View an analysis protocol's search engine parameters \(below\)](#).
- **Preinstalled** — Shows which protocols are preinstalled (indicated by  **(star)**). You may copy but not delete preinstalled protocols.
- **ID** — The unique, internal identifier of the protocol.
-  **(Download)** — Select to download a protocol. See [Download an analysis protocol \(next page\)](#).
-  **(Delete)** — Select to delete selected protocol. See [Delete an analysis protocol \(next page\)](#).

View an analysis protocol's search engine parameters

1. On the sidebar menu, select  **Analysis Protocol** to open the **Protocols** page.
2. Select the analysis protocol whose search engine parameters you want to view.

A panel opens to the right of the **Protocols** table to display the selected protocol's parameters, which are read in from the protocol's parameters file.

Upload an analysis protocol

1. On the sidebar menu, select  **Analysis Protocol** to open the **Protocols** page.
2. Select **Upload** to open the **Analysis Protocol** dialog.
3. Complete the fields.

- **Name** — Enter a unique name for the protocol.
- **Analysis Type** — Select an MS method.

From the **DDA** list, select the MS method:

- **DDA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.
- **DIA** — Derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.


- **Analysis Engine** — Select an analysis engine, e.g., *Max Quant*.

For information about the analysis engines supported by PAS, see [Analysis protocols \(previous page\)](#).

- **Species** — Select the species to analyze: *Human* or *Mouse*.

- **Description** — Enter a description for the protocol.
 - **Notes** — Enter any additional information about the protocol.
4. When ready to upload the protocol:
 - a. Select **Upload** to open the **Upload File** dialog.
 - b. Drag-and-drop the file or select **Browse** to navigate to and select the file.
 - c. Select **Upload**.
 5. On the **Analysis Protocol** dialog, select **Save**.

Copy an analysis protocol

1. On the sidebar menu, select  **Analysis Protocol** to open the **Protocols** page.
2. Select the protocol you want to copy and select **Copy**.
 - For a DDA-based protocol, be sure to copy a DDA protocol.
 - For a DIA-based protocol, be sure to copy a DIA protocol.



The **DDA** and **DIA** fields cannot be modified in a copied protocol.
3. In the **Edit Protocol** dialog, edit fields for the new protocol.

NOTE



The search engine parameter fields vary, depending on the search engine being used, e.g., *MaxQuant*, *Andromeda*.

4. Select **Save**.

Download an analysis protocol

1. On the sidebar menu, select  **Analysis Protocol** to open the **Protocols** page.
2. Find the protocol you want to download and select its  (**Download**) button.
3. On the **Save As** dialog, navigate to the folder where you want to save the protocol and select **Save**.

Delete an analysis protocol

1. On the sidebar menu, select  **Analysis Protocol** to open the **Protocols** page.
2. Find the custom protocol you want to delete and select its  (**Delete**) button.
3. Select **OK** to confirm.

Glossary

A

Admin

Role that allows adding plates, creating projects, creating analysis protocols, viewing MS data files, viewing results files, and adding and deleting users.

analysis

A search for identification and annotation of LC-MS data.

Analysis Metrics

Tab that provides the QC metrics for an analysis result.

analysis protocol

The parameters for an MS database search in a .xml or .json file.

Analysis Summary

Tab that provides an overall view of analysis results.

annotation

A highlight or explanatory note added to a chart.

C

CO-RE

Compressed O-ring expansion.

consumables

Reagents and plasticware.

control limits

Parameters that help determine whether results are expected. The mean provides a historical average, and the upper and lower control limits indicate normal variation.

custom file

Optional sample information in a .csv, .tsv, .xls, or .xlsx file.

CV

Coefficient of variation.

D

data-dependent acquisition

MS method that derives an MS/MS spectra from selection, isolation, and fragmentation of an individual precursor ion.

data-independent acquisition

MS method that derives an MS/MS spectra from selection, isolation, and fragmentation of all precursor ions in a defined m/z range.

DDA

Data-dependent acquisition.

DIA

Data-independent acquisition.

Digestion Control

A reference sample added before nanoparticle incubation.

distribution of detected proteins in plasma proteome

The dynamic range of proteins identified in each sample compared to a deep reported human plasma proteome index.

E

equipment

Reusable laboratory equipment.

H

hierarchical clustering

Cluster analysis based on agglomerative nesting, which groups samples in clusters based on similarity.

I

intensities

Protein and peptide intensities and the distribution of protein sequence coverage for each sample, including the coefficient of variation.

L

lamppost protein concentration

The intensity of landmark proteins in each sample.

LC

Liquid chromatography.

LC-MS

Liquid chromatography-mass spectrometry.

LCL

Lower control limit.

M

Mass Spec Control

Reference peptides added before LC-MS analysis.

materials

Consumables and equipment.

MPE

Monitored multi-flow positive pressure evaporative extraction.

MPE Control

Reference peptides added before desalting cleanup.

MS

Mass spectrometry.

MS data file

The results of MS analysis for each sample or control in a plate in a .raw, .wiff, .wiff.scan file.

N

NCT

Nested conductive tips.

NP

Nanoparticle.

NTR

Nested tip rack.

P

PC1

Principal component 1.

PC2

Principal component 2.

PCA

Principal component analysis.

PCA analysis

Clusters of similar samples based on PC1 and PC scores.

PCC

Pearson correlation coefficient.

Pearson correlation coefficient

A measure of the linear correlation of data.

peptide counts

The number of peptides in each sample.

peptide counts distribution

Peptide counts for the five nanoparticles processed with the samples.

peptide counts of nanoparticles

Sample counts plotted by nanoparticle.

plate

The samples, controls, and nanoparticles from a Proteograph Assay method run.

plate map file

The location of each sample in a plate in a .csv file.

plate map grid

Metrics for each sample in the format of 96-well plates.

Plate Samples

Table listing all samples in a plate selected on the Plates page.

Plates

Table on the Plates page listing all plates in PAS.

Process Control

A reference sample added before nanoparticle incubation.

project

All samples in an analysis with sample information.

Projects

Table on the Projects page listing all projects in PAS.

protein group counts

The number of proteins in each sample.

protein group counts distribution

Protein group counts for the five nanoparticles processed with the samples.

protein group overlap sets

Protein group intersections, including intersection size and protein group counts.

Proteograph Analysis Suite

Seer software used to process, analyze, and visualize LC-MS data.

Proteograph

Descriptive product term.

Proteograph Assay Kit

The reagents and labware for preparing samples on the SP100.

Proteograph Instrument Control Software

Software onboard the SP100 used to operate the instrument.

Proteograph Product Suite

The bundle of Seer kit, instrument, and analysis software.

Protocols

Table on the Protocols page listing all analysis protocols in PAS.

Q**QC**

Quality control.

QC charts

Charts presenting process control data for an analysis.

QC metrics

Metrics indicating how well an analysis performed.

R**report**

A summary of control results in a .pdf file.

results file

The output of an analysis in .txt or .xml file format.

S**sample comparability**

The degree of statistical correlation between samples based on the Pearson correlation coefficient or Jaccard index.

sample description file

Metadata for each sample in plate in a .csv file.

Sample list

List of all samples in a project selected on the Projects page.

Seer AutoUploader

An application that runs on the MS computer and automatically transfers new MS data files to PAS.

SP100 Automation Instrument

The Seer liquid handling instrument.

summary

A list of each QC metric with the control, well, plate, value, and result in a .csv file.

U**UCL**

Upper control limit.

User

Role that allows adding plates, creating projects, creating analysis protocols, viewing MS data files, and viewing results files.

user group

A group of users that can access and view the plates, projects, and analyses of all other users in the group.

Index

A

accounts 9, 14, 21
add
 users 21
adding
 custom table columns 12
adjusting tables 77
Analyses page 9, 34, 36, 86
analysis
 DDA-based 92
 DIA-based 92
 metrics 44
 performance 44
 results 20, 37, 44
 settings 20, 54
 starting 26, 29, 79-80, 83
 status 86
 summaries 37
analysis interpretation 60
analysis logs 86-87
analysis metrics 34, 36
Analysis Metrics
 Hierarchical Clustering section 52
 Intensities section 44-45
 Lamppost Proteins' Concentration section 46-47
 PCA Analysis section 48
 Peptide Counts Distribution section 49
 Peptide Counts of Nanoparticles section 50-51
 Plate Map Grid section 46
 Protein Group Counts Distribution section 49
 Protein Group Counts of Nanoparticles section 50-51
 Set Plate Map Grid section 45
analysis output files 59
Analysis Output Files tab 59
Analysis Protocol page 9, 92
analysis protocols 15, 19, 37, 79, 92
 creating 92-94
 defaults 19
 parameters 92-94
 selecting 31
analysis summary 34, 36
Analysis Summary
 Distribution of Detected Proteins in Plasma Proteome section 39-40
 Peptide Counts section 38-39
 Protein Group Counts section 37-38
 Protein Group Overlap Sets section 40-41
 Sample Comparability section 42
 Summary section 37

annotations 9, 39-40, 57
appearance, user interface 19
applications 91
assay controls 9
auto updater 91

B

bar graphs 40
box plots 44, 49
Box Plots 73
browsers 10

C

calculated control limits 55
calculations 39, 45, 55-56, 92
Chart Type preference 45
charts 44, 53
citations 39, 92
Clustered Heatmap 68
clusters 48, 52
coefficient of variation 44, 49
color codes 42, 55-56
Color Labels By preference 43
color scheme
 PCA Analysis 48
columns
 custom 16
 descriptions 76, 83
 plate map files 15
 required 25, 28, 79
 sample description files 16
 showing and hiding 46
 sorting 77
common proteins 37
comparing samples 52
compatible browsers 10
contact information, Seer 102
control charts 53, 55, 57
control software 15
controls
 analyzing 27, 30-31
 information 53
 metrics 55, 57-58
 results 53, 55, 57-58
 types 15, 18, 53-54
Coverage 70
creating folders 90
creating projects 26, 29, 79-80, 84
cumulative protein groups 37
custom analysis protocols 92-94
custom columns 16
custom table columns 12
customer support 102

D

dark theme 19
data
 distribution 44-45
 hiding 55
 reanalyzing 24, 31
Data Files page 9, 28, 89
default control limits 55
delete
 users 22
deleting annotations 57
deleting folders 91
dendrograms 52
density 44
density plots 44-45
detected proteins 37, 39, 47
differences in proteins between groups 66
digestion controls 18, 54
directories 28, 83, 89
disable authenticator app security 20
Display Percentage preference 41
Display Top N Intersection preference 41
Display Type preference 46
Distribution of Detected Proteins in Plasma Proteome 39-40
distributions 44-45

E

edit
 users 22
emails 19
EncyclopeDIA 92
Enrichment 72

F

field descriptions 76, 83
fields, custom 12
file extensions 15
file formats 15, 17, 87
file management 28, 89
file names 15
Filtered PPI Network 71
filters 53-56, 77, 89
folders 28, 89-91
functions 9, 41

G

Graph Colors preference 40

Graph Types preference 46
 graphs 20
 group analysis
 differences between groups 66
 Group Analysis
 Box Plots section 73
 Clustered Heatmap section 68
 Coverage section 70
 Enrichment section 72
 Filtered PPI Network section 71
 Raw Data section 66
 Volcano section 69
 Group Analysis tab 60, 66
 grouping data 20

H

Heatmap 67
 help, technical 102
 Hierarchical Clustering 52
 historical means 56
 Horizontal Bar Position preference 41

I

icons 86
 ICS 15
 identification rates 45
 index 39
 injection 54-55
 input files 24-25, 28, 79, 82, 93
 instruments 15, 45, 54, 57-58, 76
 intensities 39, 46
 Intensities 44-45
 Intensity Plot 67
 interpretation of analysis results 60
 intersections 40

J

Jaccard index 42-43

L

labels 37-38, 44
 Lamppost Proteins' Concentration 46-47
 landmark proteins 46-47
 layouts 37, 44
 LC-MS 9, 45
 LCLs 56
 light theme 19
 line graphs 37-38, 46
 link, PAS 10
 links 19
 log10 39, 46
 logs 86-87
 lower control limits 56

M

mass spec controls 18, 54, 56
 matrices 40, 42
 MaxQuant 92
 MaxQuant analysis protocol 92
 means 37, 49, 56
 method runs 76
 metrics, displaying 34, 36, 46
 miscleavage rates 45
 moving files 89
 MPE controls 18, 54
 MS computer 91
 MS controls 18, 54
 MS data files 19, 28, 31, 40
 automatic upload 91
 file formats 15
 file names 15
 links 19, 24, 89
 number of 86
 removing 19, 25, 28, 79, 90
 MS database 15, 39, 45, 92
 MS file's name length preference 41

N

n-values 39
 nanoparticles 49-50, 76
 navigation 9

O

optional inputs 26-27, 29-31, 57
 orange, meaning 55
 outliers 56
 output files 57-59
 oxidation ratios 45

P

Page Chart Layout preference 40, 42, 45-46
 pages
 Analyses 86
 Data Files 89
 Plates 76
 Projects 83
 Protocols 92
 Users and Permissions 21
 parameter files 93
 PAS link 10
 PC1 48
 PC2 48
 PCA Analysis 48
 PCC 42
 Pearson correlation coefficient 42
 Pearson's correlation coefficient 43
 Peptide Collection Plate
 contents 76

peptide counts 50
 Peptide Counts 38-39
 Peptide Counts Distribution 49
 Peptide Counts of Nanoparticles 50-51
 peptides 37-38, 45
 performance 44, 55
 permissions 21
 Plate Grid section 81
 plate map files 15, 79
 Plate Map Grid 46
 Plate Samples tables 77, 80
 plates
 contents 15, 76
 naming 26, 29, 77
 removing 77
 Plates page 9, 25, 76
 Plates table 76
 PPI Network 71
 preferences
 Distribution of Detected Proteins in
 Plasma Proteome 40
 Intensities 45
 Lamppost Proteins' Concentration 47
 PCA Analysis 48
 Peptide Counts 39
 Plate Map Grid 46
 Protein Group and Peptide Counts of
 Nanoparticles 51
 Protein Group Counts 38
 Protein Group Overlap Sets 41
 Sample Comparability 42
 principal component analysis 48
 process controls 18, 53-54
 projects
 creating 26, 29, 79-80, 83-84
 removing 84
 revising 85
 Projects page 9, 31, 83
 Projects table 83
 Protein Group Counts 37-38
 Protein Group Counts Distribution 49
 Protein Group Counts of
 Nanoparticles 50-51
 Protein Group Overlap Sets 40-41
 protein groups 37, 40, 45
 comparisons 42
 intersections 40
 protein names 40, 46-47
 proteins 39
 adding 47
 annotated 40
 counts 49
 distribution 39-40
 highlighting 40
 Proteins preference 40
 Proteograph Assay method
 output 76
 Proteograph Instrument Control
 Software 15
 proteome 40
 Protocols page 92

Q

QC charts 34, 54-55
 quality control 44, 47, 54, 66
 quantification 45
 quantiles 40, 44
 Quantiles preference 40
 quartiles 44-45

R

ranges, control limits 56
 Raw Data 66
 reanalyzing data 24, 31
 red proteins 39
 reference peptides 18
 reference samples 18
 references 39, 92
 renaming files 89
 renaming folders 90
 required columns 25, 28, 79
 results 9, 34, 36
 results files 17, 34
 results, interpretation of 60
 runs 37, 76

S

Sample Comparability 42
 sample description files 15, 79-80
 sample information 16, 26, 29, 37, 82-83
 samples
 adding 83
 analyzing 27, 30-31
 correlations 42
 grid view 81
 nanoparticles 50
 number of peptides 38, 45
 number of proteins 39, 45
 reviewing 77, 81-82
 similar 48, 52
 table view 81
 scaling 46
 Scaling preference 46
 scatter plots 48, 50
 search engine 9, 92
 search engine parameters 93
 Search field 21, 66, 76, 78, 83-84, 86, 92
 search parameters 15, 92
 search results 17
 Seer contact information 102
 Set Plate Map Grid 45
 settings 37, 40, 44, 54-55
 Default Analysis Protocol 19
 Receive email notifications on analysis updates 19
 Remove MS data files when plate is deleted 19
 Use Authenticator App 19
 Show/Hide dropdown 76, 78, 83-84, 86,

92

sidebar 9
 Similarity Score preference 43
 similarity scores 42
 sorting 20, 77
 starting analysis 26, 29, 79-80, 83
 starting points 25, 28, 31
 status, analysis 86
 summaries 53, 57-58
 Summary 37

T

table view 82
 tables
 adjusting 77
 teal, meaning 55-56
 technical assistance 102
 templates 25, 28, 79
 tenants 14
 theme 19
 trends 37
 turn two-factor authentication on or off 20
 two-factor authentication 19

U

UCLs 56
 upper control limits 56
 user groups 55
 user interface 9
 customizing 19-20, 37, 41, 44
 light or dark 19
 navigation 9
 scaling 46
 User menu 21
 user roles 21
 Users and Permissions page 21
 Users menu 21
 Users page 9, 21

V

Vertical Height Rate preference 41
 violin plots 44-45
 Volcano 69

X

X Tick Label preference 38-39

Y

Y Axis Range preference 38-39, 51, 55
 yellow wells 77, 81

Technical Support

For technical assistance, contact Seer.

Contact Information

Seer, Inc.
3800 Bridge Pkwy #102
Redwood City, CA 94065
Email: support@seer.bio
seer.bio

Telephone

650.453.0000

Seer, Inc.
3800 Bridge Pkwy #102
Redwood City, CA 94065
650.453.0000
info@seer.bio
seer.bio

