MyAssays Desktop
User's Guide

MyAssays

www.myassays.com

Notices

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Introducing MyAssays Desktop

MyAssays Desktop is an easy-to-use data analysis tool for bioassays.

MyAssays Desktop is the only desktop tool with an integrated search-and-download feature providing direct access to the growing online database of protocols from myassays.com. The preconfigured data analysis protocols cover popular applications and support for commercial assay kits (backed by leading kit manufacturers); these are all ready to download and integrate into your lab's workflow.

Beyond this, if your application is not already supported, the software provides a powerful yet easy-to-use system to build and customize your own data analysis protocols.

MyAssays Desktop provides first-class tools for:

- Data Import
- Data Visualization
- Data Analysis (including advanced Curve Fitting)
- Reporting
- Export
- Workflow Integration

How to Use This Guide

We have arranged this guide to help you get started quickly and to simplify how you can find the information and details that you need.

This **Introduction** contains a summary of the key features and editions of the software.

The **Getting Started** section covers installation and general orientation information. It also includes a Quick Start section to show you where the basics are and to walk you through your first data analysis. It also provides links to further information and online video guides.

The **Working with MyAssays Desktop** section dives into further detail, covering each element in more detail with the content arranged into logical sections. This includes:

- getting around the various applications

- protocols

- common tasks (such as importing, exporting, curve fitting, marking outliers to exclude, and much more)

The final **Reference** section provides a more complete description of each facet. Here the content is arranged to simplify quick retrieval.

What Should I Read?

We encourage all new users to read through all of the **Introduction** and **Getting Started** sections.

You will find more information about the topics and get a better understanding from the **Working with MyAssays Desktop** section. Feel free to skip sections here that are not relevant to your applications. If you're working with particular protocols or need to perform specific tasks, be sure to follow the relevant sections under **Protocols** and **Common Tasks**.

We don't expect you to read through the **Reference** section in order; it is more useful to consider it a resource for providing further details as and when you need them.

Features

Supported Measurements

MyAssays Desktop is designed to process measurement data from any microplate or rack-based reader. In addition, it can import and analyze data from any scientific measurement device.

The software supports measurements from any type of detection technology (such as absorbance, luminescence, fluorescence, counts, counts-per-minute), with data collected from each sample as:

- **Endpoint** – A single measurement value
- **Kinetic** – Values measured over time (data can be processed with or without time stamps)
- **Spectral** – Data measured at various multiple wavelengths
- **Multiplex** – Multiple analyte measurements from each sample
- **Well Scan** - Data where each position contains multiple measurements on a 2D grid

Data can be collected and processed together in any combination. For example, dual endpoint measurements read at both 665nm and 620nm can be imported and analyzed (perhaps with a ratio calculation). Even more exotic measurement combinations are possible with features to process multiple endpoint, kinetic, and spectral data all together within the same analysis.

Multiple Plate Measurements

Data can be captured and processed from measurements made from a single microplate or from across multiple plates. Data to process together can be arranged in a single file or in separate files that can be imported and merged together. Curve fitting can be performed with standards defined on some or all plates, with curves computed using averages of standard measurements across plates or from the measurements on the same plate.

Data Import

For maximum flexibility, MyAssays Desktop provides a number of ways to get your data into the system. These are designed to help you get started quickly and to streamline your workflow:

- In the simplest case, copy and paste your data from any source for quick and convenient analysis.

- The included extensive Import Script library can automatically detect and import data from many proprietary instrument formats. Simply select the file to import; if it's supported, the data and any metadata (data accompanying the read such as measurement date/time, barcode, etc.) are imported automatically. (For the latest list of currently supported formats, see: **https://www.myassays.com/supported-file-formats.html**.)

- If your data is in an Excel document, the import wizard will guide you through the process of importing the relevant data and meta data from the cells in your workbook. Mark the cells to import the data (with these settings saved to your protocol).

- For other files, use the intuitive and familiar import wizard to specify how to process and import the data from your files.

If your data is spread across multiple files, the import wizard can import your data together for a combined analysis.

Importing Other Types of Data

In addition to first-class support for handling your measurement data, MyAssays Desktop supports importing other types of data, including:

- Measurement metadata (data associated with your readings, such as date/time, plate ID, operator ID, etc.)

- Worklist (e.g., containing sample IDs, dilution factors, standard concentrations)

- Plate name/IDs, barcodes, analyte names, etc.

Beyond this, it is also possible to import any data analysis parameters (including layout, calculation settings, fit method, etc.) from data stored or produced by other systems. In this way, your data analysis process can be fully automated or controlled by other software.

Data Visualization

MyAssays Desktop provides a rich modern user interface to clearly present data, configuration, and analysis results, including:

- 2D and 3D interactive views of your measurement data

- Heatmap

- Histogram

- Interactive charts

  - Overlay charts (e.g., by fit, by sample, by replicate) in any combination for convenient visual comparison

  - Zoom in/out

  - Mark outliers (to exclude from analysis) directly from a chart or plate (including outliers in endpoint, spectral, kinetic, and multiplex data)

  - Specify data analysis ranges interactively (e.g., mark subsets of data to process for kinetic or spectral analysis)

- Sample labels for data

  - By name

  - By colour

  - By graphical value bars

Data Analysis

Beyond the online database of ready-to-use preconfigured protocols, MyAssays Desktop provides a comprehensive data analysis engine supporting a wide range of applications.

The system provides a toolbox of preconfigured components (including over 30 transforms) ready to bolt together in any combination. Each transform performs a single mathematical task on measurement or calculated data. Transforms include endpoint, kinetic/spectral, and kinetic/spectral reduction.

Transforms include:

- Blank Correction – Subtract a specified background value (or values) from all samples
- %CV – Calculate percentage coefficient of variation of replicates
- Standard Curve Fit – Calculate concentrations from a standard curve fit
- Maximum Slope – Find the maximum slope and report its values (such as slope/time to onset/response)

For a complete list of the 30+ available transforms, see Transforms.

Transforms are linked to your sample layout. If your sample layout changes between assay runs (or even to correct a preparation error), the analysis takes this into account. No reconfiguration of analysis is required to work with different layouts.

The transforms parameters are completely customizable. In addition, a rich expression-based language enables you to specify parameters and methods as mathematical operations using an expressive familiar (Excel-like) syntax.

Results with Labels

Label your results using your own text and highlights. For example, perhaps samples with a response or calculated concentration greater than a specified amount should be clearly indicated as such; use labels to define your own rules accordingly.

Validation

Add automatic checking of measurements and results. For example, check that your samples are within an expected range by defining your own validation rules. These are evaluated with each run of your assay, with the results clearly presented as pass or fail in the report.

Curve Fitting

MyAssays Desktop provides the curve fitting tools you would expect, plus more, including:

- Quantitative tools – Weighted and unweighted 4-parameter logistic, 5-parameter logistic, and linear regression (plus legacy methods such as cubic spline, smoothed spline, cubic regression, point-to-point, and many more)

- Fit data to your own user-defined curve fitting equation

- Best Fit feature automatically compares multiple fit methods and applies the best (with customizable scoring methods)

- Goodness of fit measures reported – R^2, aR^2, SE, F-statistic, P-value, AIC, AICc, BIC and more (and available for further automatic scrutiny such as validation messages or best fit scoring)

- Automatic computation of LLOQ, ULOQ, and LOD based on customizable precision and accuracy thresholds

- View computed curve fit equations in mathematical symbolic notation

Reporting

For some applications, the most convenient type of report to work with is sheet-based; for other scenarios, a page-based structure is more suitable.

- Sheet – A spreadsheet structure comprising of a workbook of worksheets of cells
- Page – Structured ties to a fixed sized printed format (e.g., A4)

For these reasons, MyAssays Desktop supports both. Easily switch between report views to best work with your content as you need to.

Excel Objects

Exported Excel content features native Excel objects (e.g., chart content). This means that you can edit and extend the output using the full power of Excel.

MyAssays Desktop protocols reports can be configured to include power-features such as value bars for enhanced viewing and visualization of content.

Report Templating with Word

For page-based reporting, use the full power of Word to define a reporting template to apply to your MyAssays Desktop output. This can include any content you can create in Word, such as headers, footers, custom images, fonts, macros, signature line, etc.

Analysis results are merged into your Word template for maximum user-customizable reporting output.

Export

MyAssays Desktop provides a wide variety of export options and settings:

- Export to XLS/XLSX/PDF/DOCX/TXT/CSV/HTML/XML.

- XSLT support is provided, enabling custom export definitions to be created for exacting output as required by your existing system.

- Specify the export destination folder.

- Specify the naming convention of the output files, including references to imported meta data (for example, name your output files to match a barcode imported along with your measurement data).

- Configure a protocol to automatically export with these settings so no user intervention is required.

Workflow Integration

MyAssays Desktop has been designed with your workflow in mind and provides a number of features and tools to integrate with other systems and streamline your process.

For routine data analysis, your reports can be generated without any user interaction required at all. For example, MyAssays Desktop data analysis can be performed completely automatically, with data (including any combination of measurement data, sample IDs, parameters, etc.) being imported, analyzed, exported, or printed as soon as a new measurement file is detected from your reader software.

Command Driven

MyAssays Desktop analysis provides a complete command-line interface. Launch the analysis directly from another application or process. Specify measurements files to process, worklists to use, output options. All data analysis parameters can be sent from the command line.

Launcher

To facilitate working with the command line, the user-friendly Launcher utility simplifies building your command line with a point-and-click interface.

Folder Poll

To integrate more effectively with other systems (such as instrument control software), use the integrated Folder Poll tool to automatically launch MyAssays Data analysis as soon as a new data file is detected.

XSLT Export

For integration with other systems, such as LIMS which might have very specific data formatting requirements, utilize the XSLT feature to output data in the exact format required. Example XSLT files are installed to help you get started.

Advanced XML Configuration and Tooling

Inside the system, a well-design XML structure is used to define the data analysis of every assay. Most users will not need know about its existence, but for those specialist scenarios, advanced users can configure data analysis using a powerful built-in XML editor complete with inline help and auto-complete features.

Which Edition is Right for Me?

To satisfy different needs and budgets, MyAssays Desktop is available in both **Basic** and **Pro** editions. Also, optional Add-Ons are available to cater for working with specific applications and environments.

MyAssays Desktop Basic

The Basic version is suitable for working with the preconfigured assays that are installed as part of MyAssays Desktop or those available for download from the growing assay database at MyAssays.com. With the Basic edition, it is easy to:

- Find and use an assay protocol
- Provide measurement data (via copy-and-paste or import)
- Input sample IDs
- Tweak basic protocol parameters such as fit method, sample concentrations, layout, etc.
- Calculate results
- Mark outliers to exclude from analysis
- Generate reports
- Export to Word/Excel/PDF
- Save versioned results

MyAssays Desktop Pro

The Pro edition includes all of the Basic features plus a wealth of tools and functions to simplify building and integrating powerful data analysis and reporting into the workflow of the most demanding laboratory.

A key benefit with the Pro edition is the capability to build data analysis protocols from scratch or by adapting existing protocols. This is achieved through the provision of a well-designed toolbox of data analysis components ready to bolt together to meet the needs of a wide range of data analysis applications. This toolbox includes:

- Transforms – Utilize a library of over 30 transforms.
- Matrices – Configure each layer of the analysis, including numerical formatting, sample labels, and value bars.

- Evaluation – Specify custom evaluations using powerful expression-based library.
- Validation – Define rules to verify each time analysis is performed (e.g., checking raw or computed control values are in range, checking the %CV of samples). The results are clearly presented as pass or fail.
- Report Elements – Customize the report content by adding the report elements that you need, including histograms, multiple sample tables, matrices, text, macros, and many more.

Also, the Pro edition provides power-features designed for the busy lab professional to improve productivity, including:

- Best Fit – Perform multiple fit methods and weight models on a single assay and automatically pick the best (the definition of "what is the best" can be customized).
- Standard Curve Fit from Library – Utilize a standards curve measured in a previous assay run (to save costs of reagents).
- Folder Poll – Streamline your workflow so that data analysis (or other operations) are performed automatically as soon as new measurement files are detected using the integrated folder polling tool.
- Multiple Plate Support – Analyze measurement data that spans more than one plate.
- Custom Export – Configure the export for working with third-party systems such as LIMS.

Beyond that, Pro Add-Ons are available to target specific assay and instrument types, enhance data security, or streamline inter-assay quality control.

> ℹ To view complete list of features available for each edition, see Feature Comparison Matrix.

Licensing

Single, multiple seat, and site licenses are available for all editions and add-ons.

Pro Add-Ons

MyAssays offers a range of optional tools that provide data analysis solutions tailored to your lab. Add-ons extend Pro functionality customizing it to fit your laboratory's exact needs.

Enhanced Security

For those users working under GxP or 21CFR11, the Enhanced Security edition offers the features that are necessary to achieve compliance. The software provides protected and tracked access to system features inside a secure environment with:

- Access control – Authentication and authorization are used to permit or deny access to MyAssays Desktop Pro functions.
- Operating-system-level security-data storage protection – Only authorized users can make changes to MyAssays Desktop Pro data files and settings.
- Audit trail and login log – All activity is stored against the logged-in user with a date/time stamp.
- Data certification – Restrict the system to handle only certified data (eliminating the processing of tampered data).
- Password protected and locked outputs (e.g., locked Excel and Word outputs).

Multiplex

Quickly and easily perform multiplex data analysis on your multiplex data:

- Calculate results from multiple analytes within a single analysis step.
- For quantitative analysis, apply the same curve-fitting method to each analyte or use the Best Fit option to automatically apply the most appropriate fit method for each analyte.
- Specify concentration values as a series (defining the starting concentration of each analyte and the series) or enter specific concentrations for each analyte.
- Specify units per analyte or common units.
- Paste in or import measurement data, analyte names, starting concentration values, or specific concentration values.
- Includes import methods to automatically extract multiplex measurement data and analyte names from Luminex® xPONENT and Meso Scale Discovery Workbench® CSV and TXT formats.

QC

The QC option provides a range of inter-assay analysis features to support the continuous-monitoring automatic validation that your assay remains in control:

- Monitor, track, and chart observations across assay runs.

- Any numerical result can be tracked. For example, monitor raw or calculated control values, %CVs, or curve R^2 values.

- Include Levey-Jennings, CUSUM, and Control Charts as part of each assay report to compare and visualize the latest results with historical data.

- Generate QC reports on-the-fly as and when needed.

- Automatic validation can ensure that the monitored observations are within defined acceptance parameters. Violations are clearly indicated in the report. For example, an acceptance rule can be defined to test whether a control result of a particular assay run is within a range of +/- 2*SD of the historical observations.

Rack Layouts

If your reader measures samples in tubes or vials (rather that microplates), then the Rack Add-On is for you:

- Rack Layout Editor – Define layouts in accordance with racks of tubes or vials.

- Dynamic sample layouts – Layouts are automatically adjusted based on the number of samples actually measured.

- Support for microplate layouts included (for the multifunctional lab).

Feature Comparison Matrix

Please refer to the table below to learn which features are available with your edition.

Feature	Basic	Pro
Downloadable Protocols (from myassays.com)	✔	✔
Installed Protocols:	✔	✔
• 4PL (Constrained by B0 and NSB) Quantification	✔	✔
• 4PL Quantification	✔	✔
• Alpha 384-well Screening	✔	✔
• ATP Lite	✔	✔
• Best-Fit Quantification	▬	✔
• Cell Confluency Assay Development	✔	✔
• DNA 260nm	✔	✔
• DNA Quantification	✔	✔
• Dual DPM	▬	✔
• Dose–Response Curves for EC50	▬	✔
• ELISA	✔	✔
• ELISA - Single Page Report	✔	✔
• LANCE cAMP	✔	✔
• Linearized (Logit-Log) Quantification	✔	✔
• Liquid Handling QC	✔	✔
• Multiplex	▬	✔
• OQ Absorbance	✔	✔
• Standards Curve with Titres and Parallelism Plots (Dual)	▬	✔
• Z-Factor	✔	✔
Import Script Support	✔	✔
Excel Import	✔	✔
Worklist Import	✔	✔
Data Visualization (3D View/Heatmap/Kinetic Overlay/Spectral Plot)	✔	✔
Versioned Analysis	✔	✔
Export to XLSX/DOCX/PDF	✔	✔
Edit Protocols	Limited	✔
Report Customization	Limited	✔
Custom Export (e.g., for LIS/LIMS)	▬	✔
Multiple Plate Support	▬	✔

Feature	Basic	Pro
Create New Protocols (New Protocol Wizard)	▬	✔
Matrix-Transform Data Analysis	▬	✔
Custom Validation Rules	▬	✔
Custom Evaluation Expressions	▬	✔
Best Fit	▬	✔
Fit to Library Curve	▬	✔
Folder Poll	▬	✔
PLA	▬	✔

Getting Started

Installation

System Requirements

MyAssays Desktop runs successfully on the minimum system configuration listed below. If your computer does not meet the technical requirements, you may be not able to use MyAssays Desktop.

CPU:	Intel/AMD 2 GHz or faster processor (32-bit or 64-bit)
Memory:	2GB RAM
Available disk space:	300MB
Operating systems:	Windows 10, Windows 8.x, Windows 7
Other software:	Microsoft .NET 4.7.2 or later
Display:	1024 x 768 or higher resolution

Software Requirements

Microsoft .NET 4.7.2 or later must be installed (this is pre-installed on newer Windows 10 systems). For earlier versions of Windows, if it is not already installed on your system or you are not sure, please download and install from:
http://go.microsoft.com/fwlink/?LinkId=863262.

More information about the .NET 4.7.2 installation can be found at:
https://support.microsoft.com/en-gb/help/4054530/microsoft-net-framework-4-7-2-offline-installer-for-windows.

Installation Process

The latest version of MyAssays Desktop can be downloaded here.

Upon downloading the installation package:

1. Double-click the installation package file to launch MyAssays Desktop Setup Wizard and click **Next** to continue.

2. To proceed with installation on your computer, you must accept the terms of End-User License Agreement. Please read the license agreement carefully, then select **I accept the terms of the license agreement** and click **Next**.
If you do not agree with terms of the license agreement, click **Cancel** to exit the wizard.

3. If you are content with the default path, click **Next**. To pick another destination folder, click **Change** and set preferable root.

4. Select the choices you made and click **Install**. The process will take a few moments.

5. Click **Finish** to complete the installation. Select **Launch MyAssays Explorer on exit** to start working with the software immediately.

6. [Activate MyAssays Desktop](#) with your product serial code and activate your license in order to start working with the application.

> MyAssays Desktop can be installed and run alongside the legacy software WorkOut. Refer to [Installing Alongside WorkOut](#) for further details.

Launching

After installation, you will see the MyAssays Desktop Explorer icon on your desktop. To launch the application, click it or:

On Windows 10:

Select **Start**, then scroll down to and click the MyAssays Desktop Explorer icon.

For earlier versions of Windows:

- **Windows 8.1 or Windows 8:** Swipe up or choose the arrow at the bottom of the **Start** screen to see a list of all your applications. You might need to scroll left or right to see the MyAssays Desktop Explorer.

- **Window 7:** Choose **Start > All Programs** to see a list of all your applications and click the MyAssays Desktop Explorer icon.

> To access MyAssays Desktop Explorer more conveniently, you can pin it to your Start menu or taskbar. Right-click the desktop icon and click **Pin to Start** or **Pin to Taskbar**.

Product Licensing

MyAssays Desktop requires a valid license to activate the application. You can obtain a trial, temporary, or permanent license from MyAssays Ltd.

A serial code represents your license or licenses (for multiple seat site licenses) to use the software. When you first launch the software, you must enter a valid serial code and activate your license.

> A single license can be transferred between systems but can only be active on one system at a time.

License Activation

On launching MyAssays Desktop, if there is no valid license already installed, then the Licensing Activation Wizard will appear.

> ℹ️ An administrator account is required to activate (or deactivate) a license.

If you have a serial code, select **I have a serial code to activate** and click **Next**.

> 📝 If you do not yet have a serial code, then you can obtain a trial serial code from https://www.myassays.com/download-and-install-myassays-desktop.html by clicking the **Claim Key** option.

Paste in the serial code along with your email address into the Licensing Activation Wizard and click **Next**.

> 📝 A working valid email address is required to administer your license. Access to this email account will be required to transfer your license to another system in the future.

Online Activation

If your PC is connected to internet:

1. Select **Use internet connection for activation** and click **Continue** to proceed.

2. Fill in your personal details and click **Activate**.

3. When prompted to grant **User Account Control** permission to access the licensing settings, confirm by selecting **Yes**.

4. If the license activation is accessed, a confirmation window appears.

5. Click **Close** to exit the **License Activation Wizard** and start the application.

Offline Activation

If your PC is not connected to internet, it is still possible to activate MyAssays Desktop using a separate internet-connected device. In this case:

1. Clear the **Use internet connection for activation** check box and click **Continue** to proceed.

2. A QR code will appear; if you have a network-connected device (such as a smartphone or tablet) capable of reading this, then scan the QR code and follow the instructions. Alternatively, copy and paste the provided link and open it on a system with internet connection (perhaps by transferring via USB memory device).

3. On successful activation of your serial code from your internet-connected device, a **license key** text string will be generated (with a copy sent to the provided email address).

4. Transfer this text string to your PC where MyAssays Desktop is installed and paste in the **License Activation Wizard** under the **license key** setting.

5. When prompted, grant **User Account Control** permission to access the licensing settings and confirm by selecting **Yes**.

6. If the license activation is accessed, a confirmation window appears.

7. Click **Close** to exit **License Activation Wizard** and start the application.

Multiple Seat Licenses

A multiple seat license can be used to install and use the software on multiple PCs at the same time.

With a multiple seat license, the same serial code is used to activate MyAssays Desktop Pro on up to as many seats as you have purchased.

In this case, the email address used to activate the first seat will be treated as the primary email address. Supply this address when activating other seats with the same license. It's not possible to activate other seats with a different email address.

> We recommend using a permanent email address of an administrator as the primary email address for activating each seat.

Licensed Features

There are various editions of MyAssays Desktop as well as optional add-ons. The features available to you will depend on your license. To see which features are included in your license:

1. Launch **MyAssays Desktop Explorer**.

2. Click the **File** tab to open MyAssays Backstage view and click the **Information** tab.

The availability of licensed features is marked with the following icons:

✅ for active features.

❌ for features not supported by your current license.

To learn more about additional features, which are not included in your existing MyAssays Desktop license, click the **Upgrade License** button.

License Deactivation

If you need to transfer an activated license to another PC, it must first be deactivated from the PC where it is in use.

To deactivate MyAssays Desktop on your PC, launch the Deactivation Wizard as follows:

1. Launch **MyAssays Desktop Explorer**.

2. Click the **File** tab to open MyAssays Backstage view.

3. On the **Information** tab, click **Deactivate License**.

Follow the steps of the **License Deactivation Wizard** as described below to deactivate the license:

Online Deactivation

If your PC is connected to internet:

1. Keep the **Use internet connection for deactivation** selected and click **Continue** to proceed with deactivation.

2. Confirm deactivation and click **Deactivate**.

3. When prompted to grant **User Account Control** permission to access the licensing settings, confirm by selecting **Yes**.

4. On successful deactivation, a copy of the license serial code will be sent to the email address it is associated with, ready for activation on another system.

5. Click **Finish** to close the **License Deactivation Wizard**.

Offline Deactivation

If your PC is not connected to internet, it is still possible to deactivate MyAssays Desktop using a separate internet-connected device. In this case:

1. Clear the **Use internet connection for deactivation** check box and click **Continue** to proceed with deactivation.

2. Confirm deactivation and click **Deactivate**.

3. When prompted to grant **User Account Control** permission to access the licensing settings, confirm by selecting **Yes**.

4. A QR code will appear; if you have a network-connected device (such as a smartphone or tablet) capable of reading this, then scan the QR code and follow the instructions.

Alternatively, copy and paste the provided link and open it on a system with internet connection (perhaps by transferring via USB memory device).

5. On successful deactivation of your serial code, a confirmation message will appear in the browser and a copy of the license serial code will be sent to the email address it is associated with, ready for activation on another system.

6. Confirm that the email has been received in the **License Deactivation Wizard** and click **Finish**.

> After successful deactivation, the application will be closed and will not be usable until it is reactivated. The deactivated license will be immediately available for activation on another system.

Activate New License

When you obtain a new serial code (perhaps as the result of a purchased upgrade or support extension), it will be necessary to replace an existing license with a new one.

Follow these steps to activate your new license:

1. Launch **MyAssays Desktop Explorer**.

2. Click the **File** tab to open MyAssays Backstage view.

3. On the **Information** tab, click **Activate New License**.

4. Click **Yes** to confirm the removal of the existing license.

5. When prompted to grant **User Account Control** permission to access the licensing settings, confirm by selecting **Yes**.

6. Follow the steps of the **License Activation Wizard** as described in the License Activation section to activate new license.

7. On completion of the wizard, any new license updates will be applied to your installation and any new features or support extensions will be available.

Update Existing License

If new features have been added to your existing license (perhaps as the result of a purchased upgrade or support extension), then it will be necessary to update your activated license with the latest information.

1. Launch **MyAssays Desktop Explorer**.

2. Click the **File** tab to open MyAssays Backstage view.

3. On the **Information** tab, click **Update Existing License**.

4. If your PC is connected to the internet, then select **Update my license online in one click**. Otherwise, select **Get a unique link to my activation code** and activate using a separate device that is online (as described in License Activation).

5. When prompted to grant **User Account Control** permission to access the licensing settings, confirm by selecting **Yes**.

6. On completion of the wizard, any new license updates will be applied to your installation and any new features or support extensions will be available.

Quick Start

MyAssays Desktop – The Basics

This section introduces the basics of the MyAssays Desktop system by providing a summary of the key features and functions and where to find them.

This section is intended to be short to help equip you with the basics so that you can start to be productive with the software quickly and feel comfortable to explore further functions yourself.

Firstly, MyAssays Desktop provides two key applications to help organise and work with your data:

- MyAssays Desktop Explorer (MADE) – For arranging, locating, discovering, and launching your assay data
- MyAssays Analysis (MAA) – For performing the assay data analysis

The following subsections provide orientation details for working with both of these applications.

- Introducing MyAssays Desktop Explorer
- Introducing MyAssays Analysis

Introducing MyAssays Desktop Explorer

Orientation

The **Welcome** screen is displayed on launching MADE. Its main area provides shortcut links to:

- Previously used protocol and results files

- Online resources including video tutorials

- The protocols and results folders

- The **New Protocol** wizard (Pro versions only)

Along the left side of the MADE window, you will see tabbed sections to conveniently access the folders that contain the various types of assay data.

Along the top of the MADE window, you will see the ribbon providing various commands and functions for navigating and managing your data.

Here you can find the **Search MyAssays.com** control, which provides a convenient function to search the online database of preconfigured protocols. Simply enter any appropriate search term such as assay or kit name, product or kit manufacturer name to search for available downloadable content.

Assay Data

If you've just installed MyAssays Desktop, you will find some installed assay protocols and layouts under their respective tabs. The results and reports tabs will be empty until you've ran some analyses and created some reports.

As you run analyses and create various content, MyAssays Desktop will automatically store content in the associated folders.

Where is My Data?

It is worth noting that all of your MyAssays data is stored under a single parent folder. This makes backing up your data a simple process of copying all of the data in this folder. The default location of MyAssays data is the subfolder located under your Windows **Documents** folder.

You may prefer to store your data in a location different to this default location. For example, you may want to:

- Use a common location shared with your colleagues

- Store your data in another location

To access this location setting, select **File | Data**, the **Assay Data Folder Root** section reports the current setting. Use the **Select Folder Root** option to change this as required. This setting is stored with your Windows login account (so will be remembered the next time you log in).

You can of course access all of your data outside of MADE and in Windows Explorer, simply navigate to assay data folder root directory.

Introducing MyAssays Analysis

Orientation

The MAA application is displayed when launching an assay protocol or opening an existing assay results file.

The **Overview** tab is typically selected when launching MAA. This tab displays name and any description of the launched assay. It might also include a link to online content (such as kit manufacturer's product insert).

Along the left side of the MAA window, you will see various tabbed sections for providing and reviewing the data and results for the analysis. All assays will contain the tabs:

- **Overview**
- **Measurements** – From here you can provide and review your measurements (and any metadata). Various subtabs are provided for viewing your data in different formats.
- **Results** – After performing calculations, the results of the analysis will appear in this tab. This will include the report. If the report is arranged as multiple worksheets, you will see worksheet tabs at the bottom of this area for navigating between worksheets. Also, depending on the analysis performed, you might see various subtabs appearing to the right of a **Report** subtab; these provide interactive controls for working with your data in various ways (such as flagging outliers from a **Standard Curve Fit**).

In addition to the **Overview**, **Measurements** and **Results** tabs, your assay protocol might be configured to include further tabs such as:

- **Microplate** – For defining, reviewing, and managing the sample layout.
- **Sample IDs** – For providing ID values for each unknown sample.
- **Dilution Factors** – For providing dilution factors for each unknown sample. These will be applied to the concentration value computed from the curve.
- **Standard Concentrations** – For providing known concentration values for each standard (calibrator) sample.

There might also be further tabs displayed for providing data specific to the assay.

Assay Protocol and Assay Results

When an assay protocol is launched, MAA operates in *protocol mode*. In protocol mode you can provide the data for your analyses and optionally save the settings to the protocol file.

Provide your analysis assay parameters along with your measurement data (or use the provided example data) and then click **Calculate** to create the first set of results.

> For all assay protocols, typical example data is provided to help you familiarise yourself with the analysis when you don't have any data to hand.

Clicking the **Calculate** button:

- Performs the calculations

- Generates the report

- Performs any configured export operations

For the first set of calculations, some additional steps are automatically performed as MAA transitions from protocol to *results mode*:

- The results appear in the **Results** tab.

- An assay results file is created. This contains a copy of the assay protocol that was launched and all of the data provided (measurements and analysis parameters).

- The assay results file is automatically named and saved on the first calculation.

> The file naming method can be changed under **File | Save | Results Naming**.

Results

The calculated results can be found under the **Results** tab. If the analysis generates charts, then these will also appear in subtabs under **Results**.

When there are multiple subtabs, the report can be found under the **Report** subtab. If the report is arranged into multiple worksheets (in **Sheet View**), then the sheet can be selected using the sheet names appearing at the bottom of the **Report** subtab.

Page View or Sheet View

The report can be displayed as **Sheet View** or **Page View**; these settings are available through the Ribbon's **Report** tab.

When getting started, we suggest using the Sheet View so that your outputs are not confined by the limitations of a printed page. Use the Page View only if and when the layout of the printed page is important (For page-based reporting, you can define a reporting template to apply to your MyAssays Desktop output).

Save the Changes to the Protocol?

Before the first calculation is performed (protocol mode) any interactions performed apply to the launched protocol. If you perform the **Save** operation at this point, then the changes will be saved, updating the original protocol file. Also, on the first set of calculations the settings are automatically saved, updating the protocol.

This workflow might be useful if you want your changes to apply to future runs of the protocol (so you don't need to repeat the configuration again next time). Alternatively, you might want the changes to only apply to this particular analysis.

For example, perhaps you are running a routine assay but have used a slightly different sample layout than you usually use. You might want to apply this change to the current run only, or you may decide to use this layout in future runs too.

To configure the behaviour that best suits you, select **File | Save** and set the **Save changes to the protocol** option as you require. With this option set, any changes you make to the launched protocol are saved to the protocol. The changes are also save to the protocol on the first calculation (as the system transitions from protocol to results mode). Any further changes in results mode will then only apply to the results.

> This **Save changes to the protocol** setting is stored across sessions so it will apply to any other protocols you launch in the future.

Further Save Options

Under the **File | Save** area, you will see further self-explanatory save options:

- **Save**
- **Save Results As**
- **Save Protocol As**

Note that the **Save Protocol As** option can be used when viewing results to extract all of the current configuration settings to a new protocol file. This is useful to package up all of your recent changes made to a results file to a new protocol file.

Results Naming

Before any calculations are performed (protocol mode), the **Results Naming** option is available to enable you to specify how the created assay results file is named and stored. For example, you could name the results file using metadata imported from the measurements data file and/or customize the subfolder where it is stored.

Save the changes to the protocol so any future runs of the protocol will follow the naming convention you have specified.

Calculate

Click the **Calculate** button when you are ready to calculate the results. In case this is not obvious, if you make any changes to the data or parameters, you will be reminded to perform the calculations when you are ready.

> MAA does not perform calculations automatically on every setting change because this could impact on your experience of working with the software. With larger data sets (such as multiplex, kinetic or multiple plate assays) it might take a few seconds to perform the analysis.

Result Versions

Each time the **Calculate** button is clicked, a new version of results is created. You can find the version controls including the full version history of the results in the **Home | Versions** ribbon group.

To view a different version, use the **Current Version** selector. Changing a version will update the whole of the MAA application to reflect the newly selected version; all data views reflect the data and results for the selected version.

If you have made changes but not yet calculated the results of these changes, then the **Current Version** selector will display the new version number with the text **(pending)** following it. This is to indicate that the new results are pending calculation. Click **Calculate** to create the new results version.

If you change version when results are pending calculation, then those changes will be lost (a warning message will prompt for confirmation before this action is completed).

> You cannot make changes to an earlier previously calculated version; any changes made will apply to a new result versions pending calculation.

In addition, you can remove unwanted versions using:

- **Purge** – Removes all versions except the one currently selected.
- **Rollback** – Removes all versions that follow the selected version.

Video Tutorials

For the latest video content please visit https://www.myassays.com/myassays-desktop-training-course.html

Selected video links are provided here:

Getting Started

- https://www.myassays.com/video/myassays-desktop-installation (3 min 23 sec)
- https://www.myassays.com/video/licensing-myassays-desktop-with-internet-connectivity (2 min 17 sec)
- https://www.myassays.com/video/licensing-myassays-desktop-without-internet-connectivity (3 min 18 sec)
- https://www.myassays.com/video/get-started-with-myassays-desktop-(concepts-and-processes) (9 min 53 sec)
- https://www.myassays.com/video/get-started-with-myassays-desktop-(using-the-software) (5 min 24 sec)
- https://www.myassays.com/video/myassays-desktop-explorer (4 min 30 sec)
- https://www.myassays.com/video/download-protocols-for-myassays-desktop (3 min 47 sec)
- https://www.myassays.com/video/create-a-protocol-with-myassays-desktop (11 min 33 sec)
- https://www.myassays.com/video/introduction-to-assay-validation-(elisa) (12 min 13 sec)
- https://www.myassays.com/video/introduction-to-assay-validation-(ria) (6 min 58 sec)
- https://www.myassays.com/video/whats-new-in-myassays-desktop-r4 (8 min 7 sec)
- https://www.myassays.com/video/whats-new-in-myassays-desktop-r5 (6 min 20 sec)
- https://www.myassays.com/video/whats-new-in-myassays-desktop-r6 (8 min 12 sec)
- https://www.myassays.com/video/whats-new-in-myassays-desktop-r7 (7 min 8 sec)
- https://www.myassays.com/video/upgrading-myassays-desktop-versions (2 min 23 sec)
- https://www.myassays.com/video/whats-new-in-myassays-desktop-r8 (6 min 6 sec)

Essentials

- https://www.myassays.com/video/get-started-with-myassays-desktop-(concepts-and-processes) (9 min 53 sec)

- https://www.myassays.com/video/get-started-with-myassays-desktop-(using-the-software) (5 min 24 sec)

- https://www.myassays.com/video/myassays-desktop-plate-layout-editor (4 min 57 sec)

- https://www.myassays.com/video/myassays-desktop-rack-layout-editor (5 min 46 sec)

- https://www.myassays.com/video/import-data-with-myassays-desktop (9 min 33 sec)

- https://www.myassays.com/video/create-a-protocol-with-myassays-desktop (11 min 33 sec)

- https://www.myassays.com/video/myassays-desktop-standard-curve-fit-transform (8 min 45 sec)

- https://www.myassays.com/video/myassays-desktop-fit-methods (9 min 16 sec)

- https://www.myassays.com/video/myassays-desktop-transforms (7 min 2 sec)

- https://www.myassays.com/video/best-fit-with-myassays-desktop (4 min 29 sec)

- https://www.myassays.com/video/reporting-with-myassays-desktop-(an-introduction) (2 min 20 sec)

- https://www.myassays.com/video/data-export-with-myassays-desktop (5 min 14 sec)

- https://www.myassays.com/video/elisa-analysis-with-myassays-desktop (11 min 45 sec)

- https://www.myassays.com/video/ria-data-analysis-with-myassays-desktop (6 min 15 sec)

- https://www.myassays.com/video/qualitative-assays-and-data-qualification-with-myassays-desktop (3 min 33 sec)

- https://www.myassays.com/video/myassays-desktop-sample-labels (5 min 15 sec)

- https://www.myassays.com/video/configuring-multiple-exports-in-myassays-desktop (4 min 13 sec)

- https://www.myassays.com/video/myassays-desktop-expressions (7 min 29 sec)

- https://www.myassays.com/video/kinetic-and-spectral-data-analysis-with-myassays-desktop (4 min 52 sec)

- https://www.myassays.com/video/myassays-desktop-with-folder-poll (4 min 33 sec)

- https://www.myassays.com/video/migrating-from-a-legacy-system-to-myassays-desktop (12 min 25 sec)

- https://www.myassays.com/video/collecting-diagnostic-logs-with-myassays-desktop (1 min 37 sec)

Basics

- https://www.myassays.com/video/download-protocols-for-myassays-desktop (3 min 47 sec)
- https://www.myassays.com/video/import-data-with-myassays-desktop (9 min 33 sec)
- https://www.myassays.com/video/create-a-protocol-with-myassays-desktop (11 min 33 sec)
- https://www.myassays.com/video/myassays-desktop-standard-curve-fit-transform (8 min 45 sec)
- https://www.myassays.com/video/myassays-desktop-fit-methods (9 min 16 sec)
- https://www.myassays.com/video/myassays-desktop-transforms (7 min 2 sec)
- https://www.myassays.com/video/myassays-desktop-expressions (7 min 29 sec)
- https://www.myassays.com/video/myassays-desktop-sample-labels (5 min 15 sec)
- https://www.myassays.com/video/configuring-multiple-exports-in-myassays-desktop (4 min 13 sec)
- https://www.myassays.com/video/reporting-with-myassays-desktop-(an-introduction) (2 min 20 sec)
- https://www.myassays.com/video/data-export-with-myassays-desktop (5 min 14 sec)
- https://www.myassays.com/video/quality-control-with-myassays-desktop (8 min 22 sec)
- https://www.myassays.com/video/introducing-myassays-desktop-qc-control-chart (4 min 21 sec)
- https://www.myassays.com/video/myassays-desktop-with-folder-poll (4 min 33 sec)
- https://www.myassays.com/video/qualitative-assays-and-data-qualification-with-myassays-desktop (3 min 33 sec)
- https://www.myassays.com/video/myassays-desktop-dynamic-worklist-import (6 min 34 sec)
- https://www.myassays.com/video/introduction-to-assay-validation-(elisa) (12 min 13 sec)
- https://www.myassays.com/video/introduction-to-assay-validation-(ria) (6 min 58 sec)
- https://www.myassays.com/video/edit-overview-and-resource-references-in-myassays-desktop (1 min 58 sec)
- https://www.myassays.com/video/constraining-a-custom-curve-fit-in-myassays-desktop (2 min 1 sec)

Working with Microplate Assays

- https://www.myassays.com/video/myassays-desktop-plate-layout-editor (4 min 57 sec)
- https://www.myassays.com/video/myassays-desktop-plate-layout-editor-(for-multiple-plate-analysis) (7 min 54 sec)
- https://www.myassays.com/video/elisa-analysis-with-myassays-desktop (11 min 45 sec)
- https://www.myassays.com/video/multiple-plate-analysis-with-myassays-desktop (6 min 25 sec)
- https://www.myassays.com/video/multiple-plate-analysis-with-myassays-desktop-(different-standard-concentrations-per-plate) (3 min 16 sec)
- https://www.myassays.com/video/myassays-desktop-fit-methods (9 min 16 sec)
- https://www.myassays.com/video/troubleshooting-multiple-samples-outside-curve-limits-with-myassays-desktop (5 min 10 sec)
- https://www.myassays.com/video/quality-control-with-myassays-desktop (8 min 22 sec)
- https://www.myassays.com/video/introducing-myassays-desktop-qc-control-chart (4 min 21 sec)

Working with Multiplex Assays

- https://www.myassays.com/video/multiplex-data-analysis-with-myassays-desktop (9 min 25 sec)
- https://www.myassays.com/video/luminex-xponent-multiplex-data-analysis-with-myassays-desktop (10 min 12 sec)
- https://www.myassays.com/video/intelliflex-qualitative-data-analysis-protocol-creation-with-myassays-desktop (19 min 32 sec)
- https://www.myassays.com/video/intelliflex-qualitative-data-analysis-protocol-with-myassays-desktop (4 min 38 sec)
- https://www.myassays.com/video/intelliflex-quantitative-data-analysis-protocol-creation-with-myassays-desktop (9 min 46 sec)
- https://www.myassays.com/video/intelliflex-quantitative-data-analysis-protocol-with-myassays-desktop (4 min 44 sec)
- https://www.myassays.com/video/intelliflex-data-file-export-for-myassays-desktop (2 min 46 sec)
- https://www.myassays.com/video/intelliflex-field-data-import-into-myassays-desktop (6 min 22 sec)

Working with RIA

- https://www.myassays.com/video/migrating-from-a-legacy-system-to-myassays-desktop (12 min 25 sec)

- https://www.myassays.com/video/ria-data-analysis-with-myassays-desktop (6 min 15 sec)

- https://www.myassays.com/video/myassays-desktop-rack-layout-editor (5 min 46 sec)

- https://www.myassays.com/video/myassays-desktop-fit-methods (9 min 16 sec)

- https://www.myassays.com/video/wizard2-data-import-with-myassays-desktop (7 min 41 sec)

- https://www.myassays.com/video/introduction-to-assay-validation-(ria) (6 min 58 sec)

- https://www.myassays.com/video/quality-control-with-myassays-desktop (8 min 22 sec)

- https://www.myassays.com/video/introducing-myassays-desktop-qc-control-chart (4 min 21 sec)

- https://www.myassays.com/video/wizard2-integration-with-myassays-desktop-(1-of-3) (2 min 48 sec)

- https://www.myassays.com/video/wizard2-integration-with-myassays-desktop-(2-of-3) (7 min 9 sec)

- https://www.myassays.com/video/wizard2-integration-with-myassays-desktop-(3-of-3) (7 min 28 sec)

Kinetic/Spectral Analysis

- https://www.myassays.com/video/kinetic-and-spectral-data-analysis-with-myassays-desktop (4 min 52 sec)

- https://www.myassays.com/video/myassays-desktop-xy-data-analysis-range (3 min 36 sec)

- https://www.myassays.com/video/curve-fitting-to-xy-data-with-myassays-desktop (4 min 13 sec)

- https://www.myassays.com/video/myassays-desktop-xy-reduction-peak-transform (10 min 19 sec)

- https://www.myassays.com/video/enzyme-kinetics-with-myassays-desktop (11 min 55 sec)

- https://www.myassays.com/video/myassays-desktop-xy-reduction-transforms (17 min 16 sec)

- https://www.myassays.com/video/myassays-desktop-xy-plot-report-element (3 min 35

sec)

- https://www.myassays.com/video/myassays-desktop-xy-replicates-function-transform (2 min 16 sec)

- https://www.myassays.com/video/myassays-desktop-xy-reduction-function-transform (3 min 23 sec)

Scan Well Analysis

- https://www.myassays.com/video/well-scan-data-analysis-with-myassays-desktop (7 min 23 sec)

- https://www.myassays.com/video/myassays-desktop-scan-blank-correction-transform (2 min 33 sec)

Configuring Data Calculations

- https://www.myassays.com/video/myassays-desktop-transforms (7 min 2 sec)
- https://www.myassays.com/video/myassays-desktop-matrices (5 min 35 sec)
- https://www.myassays.com/video/myassays-desktop-sample-labels (5 min 15 sec)
- https://www.myassays.com/video/myassays-desktop-evaluations (10 min 43 sec)
- https://www.myassays.com/video/validation-with-myassays-desktop (6 min 40 sec)
- https://www.myassays.com/video/myassays-desktop-expressions (7 min 29 sec)
- https://www.myassays.com/video/myassays-desktop-expression-transforms (9 min 29 sec)

- https://www.myassays.com/video/myassays-desktop-sample-label-expressions (6 min 48 sec)

- https://www.myassays.com/video/using-isflagged-in-myassays-desktop-pro-sample-labels (6 min 23 sec)

- https://www.myassays.com/video/myassays-desktop-validation-expressions (7 min 11 sec)

- https://www.myassays.com/video/myassays-desktop-evaluation-expressions (7 min 51 sec)

- https://www.myassays.com/video/myassays-desktop-reference-curve-overlay (5 min 11 sec)

- https://www.myassays.com/video/myassays-desktop-custom-fit (2 min 55 sec)

- https://www.myassays.com/video/troubleshooting-multiple-samples-outside-curve-limits-with-myassays-desktop (5 min 10 sec)

- https://www.myassays.com/video/quality-control-with-myassays-desktop (8 min 22 sec)

- https://www.myassays.com/video/myassays-desktop-scatter-plot-xy-report-element (5 min 53 sec)

- https://www.myassays.com/video/myassays-desktop-multiple-standard-curve-fits-on-a-single-plate (14 min 37 sec)

- https://www.myassays.com/video/adding-conditional-transforms-with-myassays-desktop (3 min 47 sec)

- https://www.myassays.com/video/adding-ec-and-ic-values-with-myassays-desktop (4 min 57 sec)

- https://www.myassays.com/video/adding-ec-and-ic-values-with-myassays-desktop-r7 (4 min 37 sec)

- https://www.myassays.com/video/add-evaluations-to-dose-response-curves-in-myassays-desktop (4 min 40 sec)

- https://www.myassays.com/video/reference-limits-of-quantification-in-myassays-desktop (5 min 12 sec)

- https://www.myassays.com/video/myassays-desktop-posvaluebyindex-function (3 min 57 sec)

- https://www.myassays.com/video/macros-in-myassays-desktop (4 min 51 sec)

- https://www.myassays.com/video/myassays-desktop-quick-protocol-editor (3 min 13 sec)

- https://www.myassays.com/video/constraining-a-custom-curve-fit-in-myassays-desktop (2 min 1 sec)

Reporting

- https://www.myassays.com/video/reporting-with-myassays-desktop-(an-introduction) (2 min 20 sec)

- https://www.myassays.com/video/myassays-desktop-report-elements (4 min 55 sec)

- https://www.myassays.com/video/sheet-reports-with-myassays-desktop (6 min 38 sec)

- https://www.myassays.com/video/page-reports-with-myassays-desktop (7 min 24 sec)

- https://www.myassays.com/video/sample-table-ordering-with-myassays-desktop (4 min 42 sec)

- https://www.myassays.com/video/myassays-desktop-sample-labels (5 min 15 sec)

- https://www.myassays.com/video/myassays-desktop-matrix-references-in-sample-labels (4 min 28 sec)

- https://www.myassays.com/video/sample-labels-column-with-myassays-desktop (5 min 2 sec)

- https://www.myassays.com/video/ordering-field-data-with-myassays-desktop (4 min 12 sec)

- https://www.myassays.com/video/myassays-desktop-reference-curve-overlay (5 min 11 sec)

- https://www.myassays.com/video/chart-appearance-editor-in-myassays-desktop (3 min 59 sec)

- https://www.myassays.com/video/myassays-desktop-results-naming-with-meta-data (5 min 11 sec)

- https://www.myassays.com/video/myassays-desktop-scatter-plot-xy-report-element (5 min 53 sec)

- https://www.myassays.com/video/myassays-desktop-curve-overlay (6 min 27 sec)

- https://www.myassays.com/video/myassays-desktop-xy-plot-report-element (3 min 35 sec)

- https://www.myassays.com/video/editing-multiple-matrices-and-report-elements-with-myassays-desktop (3 min 21 sec)

- https://www.myassays.com/video/myassays-desktop-report-scaling-and-sheet-ordering (3 min 37 sec)

Transforms

- https://www.myassays.com/video/myassays-desktop-standard-curve-fit-transform (8 min 45 sec)

- https://www.myassays.com/video/myassays-desktop-general-curve-fit-transform (7 min 2 sec)

- https://www.myassays.com/video/dose-response-curve-analysis-with-myassays-desktop (6 min 3 sec)

- https://www.myassays.com/video/dose-response-curve-parameters-with-myassays-desktop (2 min 19 sec)

- https://www.myassays.com/video/updates-to-dose-response-curves-in-myassays-

- [desktop](https://www.myassays.com/video/...) (6 min 25 sec)

- https://www.myassays.com/video/curve-fitting-to-xy-data-with-myassays-desktop (4 min 13 sec)

- https://www.myassays.com/video/myassays-desktop-xy-reduction-peak-transform (10 min 19 sec)

- https://www.myassays.com/video/myassays-desktop-expression-transforms (9 min 29 sec)

- https://www.myassays.com/video/myassays-desktop-xy-reduction-transforms (17 min 16 sec)

- https://www.myassays.com/video/adding-conditional-transforms-with-myassays-desktop (3 min 47 sec)

- https://www.myassays.com/video/myassays-desktop-dose-by-position (3 min 14 sec)

- https://www.myassays.com/video/myassays-desktop-import-to-expression-by-sample-group (5 min 57 sec)

- https://www.myassays.com/video/add-evaluations-to-dose-response-curves-in-myassays-desktop (4 min 40 sec)

- https://www.myassays.com/video/myassays-desktop-xy-reduction-function-transform (3 min 23 sec)

- https://www.myassays.com/video/well-scan-data-analysis-with-myassays-desktop (7 min 23 sec)

Automating Data Analysis

- https://www.myassays.com/video/myassays-desktop-with-folder-poll (4 min 33 sec)

- https://www.myassays.com/video/myassays-desktop-analysis-launcher (5 min 12 sec)

- https://www.myassays.com/video/myassays-desktop-analysis-launcher-with-tweak-files (3 min 11 sec)

- https://www.myassays.com/video/kaleido-3-0-data-analysis-automation-with-myassays-desktop (4 min 43 sec)

- https://www.myassays.com/video/folder-poll-impersonation-wizard (4 min 24 sec)

Protocols

- https://www.myassays.com/video/download-protocols-for-myassays-desktop (3 min 47 sec)

- https://www.myassays.com/video/create-a-protocol-with-myassays-desktop (11 min 33 sec)

- https://www.myassays.com/video/dose-response-curve-analysis-with-myassays-desktop (6 min 3 sec)

- https://www.myassays.com/video/dose-response-curve-parameters-with-myassays-desktop (2 min 19 sec)

- https://www.myassays.com/video/liquid-handling-quality-control-with-myassays-desktop (1 min 52 sec)

- https://www.myassays.com/video/introduction-to-parallel-line-analysis-with-myassays-desktop (4 min 33 sec)

Parallel Line Analysis

- https://www.myassays.com/video/introduction-to-parallel-line-analysis-with-myassays-desktop (4 min 33 sec)

- https://www.myassays.com/video/create-a-parallel-line-analysis-protocol-with-myassays-desktop (9 min 42 sec)

- https://www.myassays.com/video/multiple-plate-parallel-line-analysis-with-myassays-desktop (7 min 36 sec)

- https://www.myassays.com/video/myassays-desktop-parallel-line-analysis-acceptance-criteria (14 min 11 sec)

Data

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- https://www.myassays.com/video/wizard2-integration-with-myassays-desktop-(1-of-3) (2 min 48 sec)
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- https://www.myassays.com/video/wizard2-data-import-with-myassays-desktop (7 min 41 sec)
- https://www.myassays.com/video/ria-data-analysis-with-myassays-desktop (6 min 15 sec)

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Working with MyAssays Desktop

Key Concepts

Throughout MyAssays Desktop, various concepts and terms are used to communicate and reference the different types of data related to assay data analysis. This section introduces these fundamental concepts.

Measurements

The measurements are the data points acquired from your scientific instrumentation (e.g., microplate reader).

The software supports measurements from any type of detection technology (such as absorbance, luminescence, fluorescence, counts, counts-per-minute), with data collected from each sample as:

- **Endpoint** – A single measurement value
- **Kinetic** – Values measured over time (data can be processed with or without time stamps)
- **Spectral** – Data measured at various multiple wavelengths
- **Multiplex** – Multiple analyte measurements from each sample

Measurement data is typically accompanied with other types of data; examples include date/time of measurements, plate ID, and user ID. We refer to this data as meta data. The software can import and report this alongside your measurement data.

Import

The import process gets your measurement and any meta data into the software. The software supports a variety of methods including:

- Copy and paste
- Excel selection import
- Automated import for supported third-party proprietary formats

Protocol

An assay protocol defines all of the parameters necessary for performing the data analysis required for any assay. This includes:

- Expected measurement data (e.g., endpoint, kinetic, spectral, multiplex, etc.)
- Layout – How samples are arranged
- Calculations
- Report content and configurations

Also, the protocol can define:

- Import settings (exactly how and what data to import)
- Export settings (how to export the data, e.g., to Excel/PDF or a custom file such as CSV/TXT)
- Quality control settings (intra and inter-assay calculations and settings)

With MyAssays Desktop, the settings for a particular assay protocol are stored in an assay protocol file. These files use the **.assay-protocol** file extension.

> An assay protocol file is a self-contained file with no dependencies on any database, making it easy to transfer protocols between systems and to share protocols with colleagues.

Results

Each time an assay protocol is launched and results are calculated, an assay results file is automatically created. The assay results file contains the results of the analysis including the measurements and meta data and any data specific to the run. This could include:

- Sample IDs
- User-entered notes
- Calculation log
- Any changes to the configuration such as:

  - New sample layout
  - Calculation settings
  - Any flagged data (i.e., marked as outliers)

Assay result files use the **.assay-results** file extension.

> An assay results file also contains its own copy of the assay protocol. This is important so that any changes to the original assay protocol file will not impact the results already calculated. This structure also simplifies sharing data and transferring

results between systems.

In addition, an assay results file can contain the whole version history of changes made to the analyses. Each time results are recalculated, a new set of results is created and stored within the same results file. The full-version history is available so you can go back to earlier versions of the results.

Reports

The report is the primary output of interest of the data analysis. A report is generated each time the assay results are calculated.

Typically, the report will contain a table listing the measurement data and results for each sample. The report might also contain charts and other content. MyAssays Desktop Pro provides a wealth of features and functions for tailoring the report content to your exact needs.

Report Views

Depending on your data or preferences there are two types of report, each with their own benefits:

- Sheet view
- Page view

Exports

MyAssays Desktop can export the report content to a variety of formats, including Excel/Word/PDF. In addition, content can be easily output to popular text-based formats such as CSV using preconfigured export methods. Beyond this, XSLT support is provided to enable you to export your content in any format to exactly match you output requirements.

Sample Layout

The sample layout (or simply layout) defines how the samples are arranged on the container or containers from where they were or will be measured.

> Here we use the general term "container" because the samples could be measured in a microplate or a rack of vials; in fact, any vessel for your samples is supported.

Getting Around

MyAssays Desktop provides two key applications to help organize and work with your data:

- MyAssays Desktop Explorer – For arranging, locating, discovering, and launching your assay data
- MyAssays Analysis – For performing the assay data analysis

MyAssays Desktop Explorer (MADE)

MADE is the application launched when you click the MyAssays Desktop Explorer icon installed on your desktop. This application is the starting point for all MyAssays Desktop functionality. From here you can:

- Search and download preconfigured assays from MyAssays.com
- Access useful videos and training guides
- Access technical support
- Manage your product license
- Access your assay data
- Create new assay protocols (requires Pro version)

MyAssays Desktop Analysis (MAA)

If you launch a protocol or open a results file, MAA opens. MAA provides the user interface for working with your assay data analysis. From here you can access all of the various options, including:

- Import/export data
- Provide assay parameters
- Enter sample IDs
- Generate report
- Calculate new results

MyAssays Desktop Explorer

MyAssays Desktop Explorer is the first application of MyAssays Desktop you interact with.

With MADE, you can:

- [Find, download, and launch assay protocols from MyAssays.com database](#)
- View existing assay [layouts](#), [results](#), and [reports](#)
- Run assay [protocols](#) and open [results](#)
- [Create](#) or [request](#) an assay protocol

> ℹ️ Assay protocols and results can also be launched directly from Windows Explorer

MADE Ribbon

Ribbon extends across the top of the main area of the MADE.

Ribbon Tabs:

Home

This tab consists of several groups for operating with data files inside MADE directly.

- **Navigation** includes three main options for moving around tabs, folders, and subfolders inside the application.
  As you continue working on your data analysis, you may prefer to divide and arrange your data in folders by its measurements or features. Therefore, the number of folders and subfolders in tabs will grow. You may use the **Back**, **Forward**, and **Up** navigation commands on **Ribbon** or **Quick Access Toolbar** to change your current location quickly.

- **Clipboard** provides better management of your stored data. You may prefer to rearrange the way your files or folders are stored by using **Paste**, **Cut**, and **Copy** commands. This way you can simply move around data files between various storage folders.

> ℹ️ Clipboard data is automatically deleted when the computer shuts down or restarts, so remember to save important information.

- **File** consists of two commands: **New**, which launches [New Protocol Wizard](#), and **Open**, which launches data from MADE's tabs.

- **Search MyAssays.com** can be of the maximum use for finding and downloading specific preconfigured assays from the MyAssays online database. This tab consists of **Search text box** and **Search button**.

Tools

This tab embodies **Utilities** you may find useful.

- **Analysis launcher** is a tool for advanced launching of the MAA.
- **Folder Poll Manager** launches MyAssays Folder Poll Manager.

Support

This tab provides connection between MyAssays and the end users.

Assistance group has a Request Protocol command, which you may find useful if the assay template you are looking for is not yet in the MyAssays database.

It also features a backstage view for additional use of application scenarios and configuration.

Backstage Area:

File Tab

File Tab gives you access to MADE's important tasks.

- **Information** contains details about your MyAssays Desktop personal use. This includes product version, current license details, and features.

> You may want to change some features of your MyAssays Desktop (i.e., activate, deactivate, or update license). The Product Licensing describes further details for these options.

- **View** defines whether the Measurements Tab is displayed on the Folder Side Bar and the Launch Assay Protocol with Options setting is displayed on preview pane in the Protocols tab.

- **Data** displays the storage path for persisting your assay data files and Welcome Screen's **Recent** feature options.

- **Drivers**

- **Exit** closes the application.

Quick Access Toolbar

Quick Access Toolbar contains shortcuts to commands and functions to make your work on MyAssays Desktop Explorer easier and personalized.

> You can Customize the Work Area to fully adjust it to your needs.

Application Button

Click the logo in the upper left corner of the MADE to:

- **Restore** – Return window size to the previous one
- **Move** – Change windows on-screen' locations, if they are not full screen
- **Size** – Widen or narrow the window
- **Minimize** – Put the window in taskbar
- **Maximize** – Make the window full screen
- **Exit** – Close the program

Navigation Shortcuts

The other default commands of Quick Access Toolbar are the ones from **Navigation group**, namely **Back**, **Forward**, and **Up**, which are useful for switching between the tabs you currently work with quickly.

Advanced Options

You can set the Quick Access Toolbar position in this drop-down menu. Click **Show Quick Access Toolbar Below/Above the Ribbon** (depending on its current location), **Minimize the Ribbon**, and change the Quick Access Toolbar view by adding or excluding some options in **More Commands** menu.

Folders Tab

MADE provides a hierarchical view of the organized data and presents its preview if it is available. MyAssays Desktop stores different types of data in separate subfolders in the MyAssays **Data Folder Root**. These tabs point to actual Windows folders.

In MADE, you can access information from every subdirectory easily in the appropriate left side bar tab.

> MyAssays Desktop arranges your data automatically in correspondent folders so that you can easily manage, share, and back up your assets. You may prefer to customize how results files are named and where your data is stored.

Folders Tab Content

Tab	Contains Files
Search Results	Assay protocol titles that match search query
Protocols	Assay protocol files with .assay-protocol extension
Measurements	Measurement data files in **supported file formats** (*.TXT, *.CSV, *.XML, *.DAT, *.XLS, *.XLSX, and others)
Results	Assay results files with .assay-results extension
Layouts	Layout files with .assay-samplelayout extension
Reports	Report files with supported **report extension** (*.DOC, *PPT, *.XLS, *DOCX, *XLSX, *PPTX, *.MHT, *.HTM, *.PDF)

Selecting a tab displays its content in the main window.

File and Preview Panes

The File and Preview panes are populated with the content of the selected tab.

File Pane

A list of available data files displays on the left side of the active tab. It is a visualization of the folder that persists data, that was used to launch, or is a result of performing a particular assay analysis.

In the File Pane, files can be selected using normal Windows procedures. Right-click to display the default Windows Explorer context-sensitive pop-up menu. Relevant MADE Ribbon options are available when a single file is selected.

Sort and View

The default view of content is **Details**. To change it, right-click active tab's empty space > **View** > select preferable view from the drop-down list.

Files are sorted by name by default. To change the file sorting order:

- Right-click the empty space of the active tab > **Arrange Icons By** > choose preferable option form the drop-down list.

OR

- If File List is displayed in default view, click the column headings **Name**, **Size**, and **Date Modified**.

Subfolders

Tabs may contain subfolders (subdirectories). Creating subfolders in tabs comes in handy when working with big data sets or with multiple versions of analyses. All subfolders will be of the same type as their primary parent. To create a new subfolder, right-click anywhere on the File Pane and select **New** > **Folder**.

The File Pane may be navigated using the relevant buttons on the MADE Ribbon.

Preview Pane

Select a single file from the list to see its preview and available actions on the right side of the active window.

The contents of the preview pane depend on the type of file selected:

Folder Tab	Preview Pane Contents
Search Results Protocols	A summary of assay protocols, including the name, the instrument settings, the position used and layout, and any configured transformations
Measurements	Precanned and custom raw data files
Results	Two panes: - **Overview** with the assay protocol summary - **Latest Report** with the latest report of the results
Layouts	A microplate control showing each plate layout in the layout
Reports	The preview of the PDF reports

Welcome Screen

This is the screen that displays as you launch MADE. It contains some useful options for a proficient start. Get acquainted with MyAssays Desktop Explorer's basic functions and begin your work at full speed.

The left pane of Welcome screen consists of:

- **Start** – Shortcuts to basic data analysis options, particularly New Protocol, Launch Protocol, and Open Results

- **Recent** – A specified number of assay protocols and results you have worked with last

(the particular title will be launched in MAA upon selection)

> You can customize a number of entries in the **Recent** list or clear the file history in Data options.

The right pane comprises of two subpanes:

- Upper subpane **Discover MyAssays Desktop** displays links to a detailed review of MyAssays tools and the desktop application specifically. Visit **MyAssays Home Page** or **What's New in MyAssays Desktop?** and get to know latest information about desktop version.
- Lower subpane contains:
  - **Product Videos** – Links to video materials that will help you familiarize yourself with MyAssays Desktop and its components
  - **Support** – A link to the **MyAssays Support** contact form and the Request an Assay Protocol dialog box

Recent Used Files Feature

The number of files displayed under the **Recent** subpane of the Welcome Screen may vary from 0 to 20.

To change the number of Recent files, type it in the corresponding box or use the arrows to adjust it.

Press the **Clear Recently Used File list** button if you want to erase the history.

Search Results Tab

This tab displays on the Folder Tab after you submit a Search MyAssays.Com.

It displays a File List and Preview of the assay protocols that match search query.

When this tab is active, multiple search results options are available.

Search and Download Preconfigured Protocols from MyAssays.com

Using MyAssays Desktop, you can access the constantly evolving database of preconfigured assay protocol templates from MyAssays.com.

Use the Search tool and explore search results options.

About Preconfigured Assays

MyAssays.com allows users to quantify their data with growing base of online assay tools. Using MyAssays Desktop, you can search the protocol database and download ready-to-use data analysis protocols on your PC. The preconfigured assays include:

- Commercially available kits
- Common analysis methods
- Tailor-made protocols per request

The database supports wide range of microplate and rack-based instrumentation and contains high-quality templates that simplify assay data evaluation.

Finding Assay by Search Term

You can search the database by any keyword or term such as kit manufacturer name, study type (in vivo, in vitro, qualitative, quantitative, etc.), assay type (ELISA, HTRF, etc.), or fit method (4PL, 5PL, etc.).

Find an Assay Protocol from MyAssays.com

1. Launch MADE.

2. On the **Home** ribbon tab, in **Search MyAssays.com** group, in the **Enter Assay Name** field, enter or paste the search term.

   > ℹ️ You can also use a **CTRL + E** keyboard shortcut.

3. Click **Search** or press **Enter** on keyboard.

   The list of preconfigured assay protocols that match your query will appear in the Search Results tab.

How the Search Results Are Displayed

Upon submitting the search, you will see the list of assay protocols that match the entered keyword. To help you choose a protocol that will suit your needs, select an item from the list to view a description of the analysis performed in the right-hand Preview pane.

Some assays also contain the Kit Booklet with the instructions and notes provided by the manufacturer. To launch the booklet with your default browser, click **View Assay PDF** link under the assay summary.

Download and Launch Options

When you select an assay protocol, the following options are available:

- **Download and Launch** – To save a single assay protocol to your Protocols tab and automatically launch it in MAA.

  > **ⓘ** You can also double-click the file from the list to download and launch it in MAA automatically.

- **Download** – To save one or more assay protocols to your Protocols tab.
  To select multiple protocols, use the **(Ctrl+Shift+Arrow Keys)** keyboard shortcut or **Ctrl+A** to select all search results.

  > **ⓘ** When selecting multiple protocols from the list, only this option is available.

- **Launch Assay Protocol** – Appears if you have downloaded a particular assay protocol previously. The above actions are then not displayed. To enable redownloading, click the **Click here** hyperlink in the message below **Visit on MyAssays.Com**.

- **Visit on MyAssays.Com** – Directs you to the online MyAssays.Com webpage of the selected assay protocol.

If No Assays Match Your Search

If the assay you are looking for is not yet in the MyAssays database, our experts can provide data analysis solutions specific to your needs. To learn more, see Request an Assay Protocol.

Protocols Tab

The **Protocols Tab** displays a File List and Preview of the assay protocols that are persisted to your PC.

> **ⓘ** Only data files with an .assay-protocol or .apr extension are visible through this folder.

Upon selecting a particular assay title from the list, you will see its summary on the Preview pane and, if it is available, a detailed Booklet Kit from the kit manufacturer.

In the **Protocols Tab**, you can:

MyAssays Desktop Pro edition allows creating new protocols for your data with the New Protocol Wizard.

To start the wizard, launch MADE and do one of the following:

- On the **Welcome** screen, click **New Protocol**.

- On the **Protocols** tab, in **File** group of the ribbon, click **New**.

You also can launch the wizard from command line. For further details, see Command Line Arguments.

How to: Launch Assay Protocol File

Select the Protocols tab, then select a single assay result file to open and do one of the following:

- Double-click its title.

- Right-click the title and click **Run with MyAssays Desktop Analysis**.

- Click **Launch Assay Protocol** in the lower right corner of the Preview pane.

By doing this, you will launch the file in MAA.

> You can also launch an assay protocol directly from Search Results.

Launch Assay Protocol with Options

This feature will open the Analysis Launcher tool with the selected protocol.

Click the **Launch Assay Protocol with Options** button to launch an assay protocol with command-line options for more control over the analysis.

How to: Launch Assay Protocol with Command Line Options

1. Launch MADE.

2. Click the **File** tab to open MyAssays Backstage view and click the **View** tab.

3. Select **Show Launch Assay Protocol with Options**.

> The **Show Launch Assay Protocol with Options** state persists between sessions.

If it is selected, a corresponding option appears on the Preview pane of the Protocols tab upon protocol file selection.

How to Request Assay Protocol

Launch MADE and do one of the following:

- In the Welcome tab, on **Support** subpane, click **Request an Assay protocol**.

- On the ribbon, in the **Support** tab, click **Request an Assay protocol**.

When this option is selected, a **Request Protocol** dialog box will appear. Fill in the fields to specify what kind of an assay you want to be included in the MyAssays knowledge base.

Please mention any information that can be of use in **Other Significant** field.

You can and are welcome to attach any applicable files, such as Example Raw Data, Kit Insert PDF, and Other files (in zipped files).

After you have provided details of an assay, click the **Submit Request** button to send your requirements to MyAssays Support.

Measurements Tab

How to: View the Measurements Tab

1. Launch MADE.

2. Select the **File** tab of the MADE Ribbon.

3. Select the **View** screen.

4. Select the **View Measurements** check box.

> The **View Measurements** state persists between sessions.

If it is selected, an additional tab is displayed on the Folder Side Bar.

The measurements tab contains a default **Examples** folder with a 12x8 Endpoint.txt file. For each assay, a text file containing your measurement settings data can be uploaded and processed for analysis. To upload a file, paste it in the **Measurements** folder in your MyAssays Folder Root.

The New protocol wizard can automatically identify and import the relevant readings from a file saved in many supported file formats, including TXT, CSV, or other proprietary formats.

Visit MyAssays Supported File Formats (http://www.myassays.com/supported-file-formats.html) to see list of supported measurements data formats.

Results Tab

The **Results Tab** displays a File List and Preview of the results of previously run data analyses. Select a single Assay Results file from the File List to see the Preview of the report.

Results files generate when you have launched a particular assay protocol and performed a data analysis. It is empty on your first time launching MADE and will fill as you work with the application. By default, these files are named after a protocol, but you can change the name (i.e., after incoming measurements, current date, etc.).

> Only assay results data files with an .assay-results or .ars extension are visible through this folder.

When you select a title, two information insets appear on the Preview pane. The **Overview** shows an assay summary and may contain a link to the Booklet Kit from manufacturer. The **Latest Report** contains the report of the selected Assay Results file.

> To enlarge the Preview view, hold down **Ctrl** button and push the mouse scroll wheel upward.

In the **Results Tab**, you can Open Results in MAA.

Open Existing Results

How to: Launch Assay Results File

On the Results tab, select a single assay result file and do one of the following:

- Double-click its title
- On the **Home** ribbon tab, in the **File** group, click **Open**
- On the Preview pane, in **Latest Report** inset, click **Open**

By doing this you will launch the file in MAA.

Layouts Tab

The Layouts tab displays a File List and Preview of the assay layouts persisted to your PC. Vice versa, only files persisted to this tab may be used in running assays by MyAssays Desktop Analysis. Select a single Assay Layout file to view it on the Preview pane.

> Only data files with an .assay-samplelayout or .mlo extension are visible through this folder.

Assays in MyAssays Desktop Analysis are initially set up to use a default layout for your samples. You will most likely prefer to use your own sample layouts in your data analyses.

Use the Plate Layout Editor to edit existing or create new layouts.

Reports Tab

All assay result data exported into a report file is stored to this folder. Double-click the title to open it in a relevant application.

Customize the Work Area

You can configure **Work Area** to fully match your preferences and enhance your experience. Learning about its potential may be useful for taking full advantage of the features, tools, and options of the application.

Customizing the Quick Access Toolbar

The Quick Access Toolbar displays tools that you have bookmarked. For making use of its full potential, you may prefer to rearrange and manage these tools.

Location

You may prefer the Quick Access Toolbar to be displayed above or below the Ribbon. Right-click any spot of the Ribbon and hit on the **Show Quick Access Toolbar Below the Ribbon** command. If the toolbar is already below, you can configure it to be vice versa.

Adding or Excluding Tools

To add a command to the Quick Access Toolbar, choose the one you want from the **Home**, **Tools**, or **Support** tab and right-click on it. In the drop-down menu that will appear, click **Add to Quick Access Toolbar**. Upon doing that, the command will be displayed in the Quick Access Toolbar.

To exclude a command from the Quick Access Toolbar, right-click on it and click **Remove from Quick Access Toolbar**.

Advanced Customizing

You may consider customizing the Quick Access Toolbar to fully match your preferences. To call up a **Customize Quick Access Toolbar** options menu, do one of the following:

• Right-click anywhere on the Ribbon and click **Customize Quick Access Toolbar** on the context menu.

• Click **Advanced** on the Quick Access Toolbar and click the **More Commands** command.

Upon doing this, a dialog box will appear. Select tools you prefer and add or remove them from the list.

You can add or remove commands from a list or from a specific tab. You can also determine their on-screen order by pressing the arrows on the right side of the **Quick Access Toolbar** list.

When you have finished customizing toolbar, click **OK** to save changes or **Cancel** to undo them.

To return the toolbar to its default configuration, click **Reset** in the **Customize Quick Access Toolbar** dialog box.

Customizing the Ribbon

The Ribbon is designed to make finding and working with commands convenient and easy. You may consider the capability to personalize and customize the Ribbon in the way you want useful. With this feature, you can change the default Ribbon and create custom tabs and groups with your preferred commands.

To customize the Ribbon, right-click anywhere on the Ribbon and then choose the **Customize Quick Access Toolbar** context menu to bring out the dialog box. Select the **Customize Ribbon** option and personalize your Ribbon view for your convenience.

Minimize Ribbon

This option may be useful to expand your on-screen view of the application. If the **Ribbon** is minimized, tabs appear on click and hide when you click on any other spot of the screen. To do this, right-click anywhere on the Ribbon and select **Minimize Ribbon** in the drop-down list. To undo minimizing, repeat these actions and clear the command.

Layout Rules

Layout rules are requirements that can be defined as part of the layout. An assay of a particular type may require certain specifications to be complied. For example, a quantitative assay that uses a curve fit may require a certain number of standard samples to be measured (at least 2 would be required for linear regression, more for other fit methods). Similarly, an assay protocol developed by a kit manufacturer may insist on using a specific number of replicates.

When creating or editing a layout according to layout rules, the system will check that the new layout satisfies these rules on save. If these rules are not satisfied, then the new layout cannot be saved or used with the associated protocol.

Layout Filtering

The layout rules are also used to filter out irrelevant layouts for selection; this helps to find only useful layouts that apply to the assay you are working with. For example, if there are many layouts defined on your system, when working with a specific protocol the system will automatically exclude any layout that does not satisfy these rules.

Layout References in Expressions

Data analysis is linked to and relies on the sample layout to perform required calculations. The layout itself and its components can be referred to in expressions for more accurate and flexible coordination of the assay analysis.

Sample Group References

In all cases (except Standard Curve Fit using the Curve option **Average** with multiple plates), a reference to a specific group implies to the replicates of that group on the container (analyte/plate) it is associated with. In configuration, the group numbering is always local-based.

For example, during configuration of microplate assays, **Blank1** refers to the first blank group on the layout. It does not consider replicates on other plates/analytes. The Standard Curve Fit using the Curve option **Average** with multiple plates is a special case that enables the standard curve to be created using samples across plates. Thus, **Blank1** will only refer to the replicates in the first group of the current container.

> Note the distinction between group numbers that are reported (i.e., in the report and group numbers during configuration). They are different for multiple plate.

More details on referencing sample groups is provided in the Operands subsection.

References of the Positions and Layout in Expressions

Over and above sample references, the layout itself and even single positions can be useful when configuring data analysis. For example, the layout function is used for By-Row Blank Correction Example.

Further information on this topic is provided in Layout Analysis Functions.

Plate Layout Editor

Most assays allow you to specify your own layout for processing and distinguishing various types of measurement data. The editor is used to create new layouts or modify existing layouts.

You can freely position your samples and change the number of sample groups providing the requirements of the assay are met. Certain assays allow you to provide measurement data ran across multiple plates.

In addition to being used to define a layout before data is collected, the editor can be used after data collection to correct for preparation errors.

> If your samples are measured in tubes or vials, then use the Rack Layout Editor to define the sample arrangement.

Using the Plate Layout Editor

The Plate Layout Editor is displayed when you click **Create** to create a new layout or **Edit** to edit an existing layout on the Layout Selection pane of MAA **Microplate** tab. You can also create a new layout as a step of the New Protocol Wizard.

Editor Flexibility

The actual flexibility available in your custom layout depends on an assay's requirements. Most assays require a certain number of positions of a particular type to be defined (e.g., **Blank** or **Standard** groups). In most cases, however, you may set up the layout as you prefer providing your layout meets an assay's requirements.

Once your new layout is created, you can select it to be applied to future calculations of an assay. By making calculations or saving settings, your new layout is saved under MyAssays/Layouts in your MyAssays folder root.

Creating Multiple Plate Layouts

A layout can be defined for each real-world physical container. The Plate Layout Editor can be used to define layouts across multiple containers. The group numbering of samples is contiguous and sequential for each type.

There are a number of different ways that standards and samples of an assay might be arranged across multiple plates. Plate Layout Editor allows you to specify for each plate:

1. How samples are arranged

2. Which standards measurements should be used to construct a standard curve

3. Which curve to use to calculate concentrations from

Plate Layout Editor Settings

With the following options, you can specify how samples are arranged on a plate.

There are two modes for specifying an assay layout:

- **Erase** – For removing samples that you are not measuring
- **Fill** – For defining the layout by selecting areas to fill
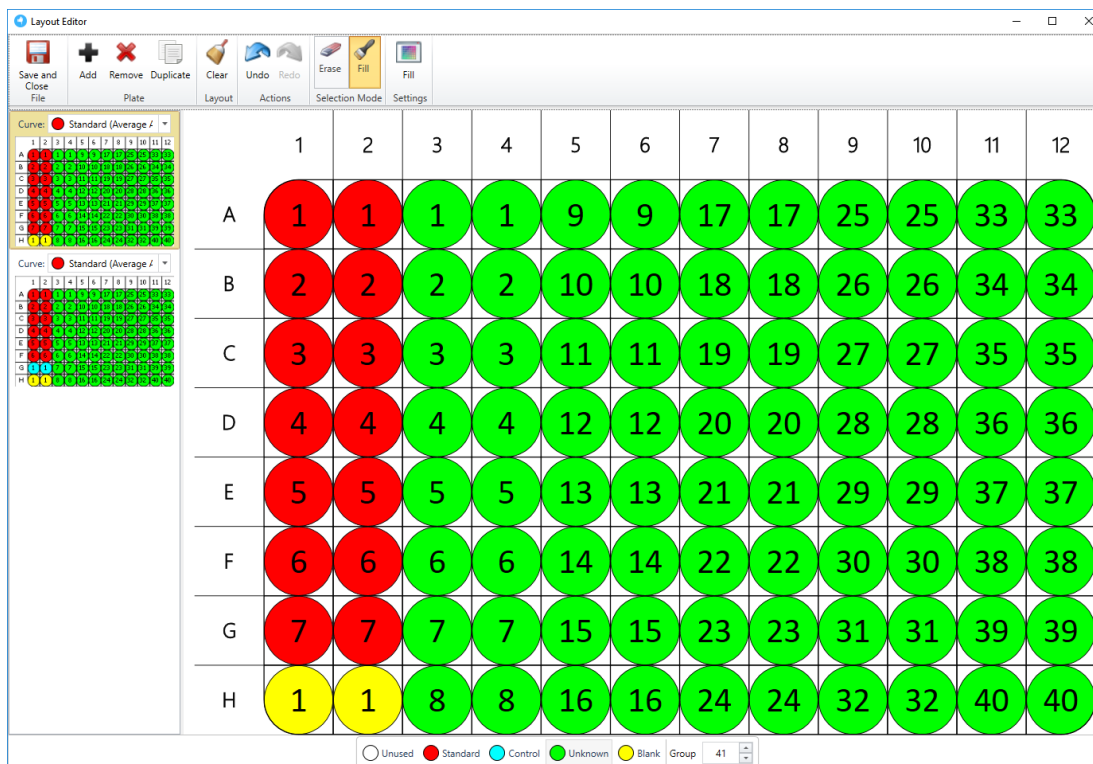
Erase Edit Mode

Erase mode allows you to remove samples that you are not measuring (i.e., mark them **Unused**).

To remove a position:

1. Select the **Erase** icon on the toolbar.
2. Move the mouse pointer over a defined position.
3. Left-click to remove all positions of this sample group.

> If the sample group contains more positions than you want to remove, select **Unused** type on the type and group selector and fill the position(s) with it.

Sample numbering will be adjusted to ensure that the group numbering remains contiguous.

Fill Edit Mode

Fill Edit mode allows greater flexibility in layout arrangement. To enter **Fill Edit** mode, click **Fill**. The **Fill Settings** button will appear, enabling you to specify how the positions you select are filled.

Also, the type and group selector can be used to select the next group to fill with your chosen settings.

To change the sample at a position, simply left-click your mouse pointer on the position. To fill an area, left-click at the first position and hold and drag to the last position. The **Fill Settings** dialog window appears, allowing you to change how this fill operates. You can specify the fill direction and number of positions for your selected group. The following fill options are available:

- **By Row**
- **By Column**
- **Rectangle Mode**

If **Rectangle Mode** is selected, you can choose whether the replicates fill **By Row** or **By Column**. You can specify the number of positions per group using the entry box.

Group numbering must start at 1 and be contiguous for each sample type.

Undo/Redo

Use these buttons to cancel the last change or re-apply it.

Save + Close

When you are satisfied with your changes, click **Save + Close**. This will save the new layout to your Layouts folder and make it available to relevant assay analyses.

Multiple Plate Options

If you have selected the Multiple Plate option or are editing a multiple plate layout, the Plate Layout Editor's functionality expands with options applicable only to multiple plate layouts. Also, you can switch between plates and choose curve-fit generation properties.

Options

The toolbar for multiple plate expands with following options:

- **Add Plate** – Adds an empty plate
- **Remove Plate** – Removes a selected plate

- **Duplicate plate** – Copies a selected plate with all defined changes

Curve Selection

Curve selection describes how the multiple layout is arranged and behaves (i.e., defines if and how a curve can be selected).

> For multiplex assays, only single layouts can be applied.

Multiple Plate Group Numbering

When defining the layout (in the Plate Layout Editor), the numbering for each sample group on every plate should always start at 1.

This might seem counter-intuitive, however, this is intentional to make things easier when working with multiple plates. With this approach, if you decide to change the number of samples on the first plate you do not need to update the numbering on all plates that follow. For example, being able to refer to, for example, **Control1** to reference all **Control1** replicates is much simpler than having to remember or decode the measurement data.

To handle multiple plate assay operations efficiently, you can refer to sample group either on certain container(s) precisely or with regard to whole measured data. This is described further in the Sample References in Multiple Container Assays.

When the data analysis is performed, the software will apply the group numbers across plates contiguously. This assures the results (for non-calibrator groups types) are presented sequentially and each sample group has a unique number. For example, if the layouts for plate 1 and plate 2 are both defined with **Unknown1-Unknown10**, when the analysis is performed, plate 1 will include **Unknowns1-10** and plate 2 would include **Unknowns11-20**.

Multiple Plate Standard/Calibrator

With **Standard/Calibrator (Control)** sample types, it does not make sense for numbering to be sequential across plates as this would imply that the data for a single curve is spanned across plates. Also, it is possible to configure standard replicates across plates (e.g., every plate has a **Standard1**, etc.). Therefore, for these sample types, numbering always starts at 1 for each plate.

> The number of plates defined in the layout may or may not correspond to the actual number of plates measured. See Trimming and Padding subsection.

Multiple Plate Rules

The number of plates defined in the layout may or may not be equivalent to the number of data containers measured. For example, the layout might only define one container whereas 50 containers' worth of data are provided. Equally, there may be less containers measured than there are defined in the layout. In these cases MAA will rely on the following rules:

Trimming

The layout contains more plates than data containers.

When there are more plates defined in the layout than containers measured, for each data container the layout with the same index will be applied. The extra layouts will be ignored.

Example: Let's assume that we have a layout made up of 3 plates and 2 containers of data. The analysis will be performed in the following way: **Plate1** on **Container1**, **Plate2** on **Container2**. The **Plate3** will not be used for analysis.

Padding

The layout contains more plates than data containers.

When there are more containers measured than there are defined in the layout, the last defined layout plate will be reused. For each data container will be applied the layout with the same index. The excessive measurements data will be analyzed using the layout with the last index.

Example: Let's assume that we have layout made up of 3 plates and 5 containers of data. The analysis will be performed in the following way: **Plate1** on **Container1**, **Plate2** on **Container2**, **Plate3** on **Container3**, **Plate3** on **Container4**, and **Plate3** on **Container5**.

> The data analysis evaluation results are presented sequentially, with a unique number for each sample group.

Multiple Plate Analysis

The multiple plate features greatly simplify processing measurement data when your samples span more than one plate.

For multiple plate layouts, the layout can contain one or more plates with different positioning (and curve-fitting options) of the samples on each. Each layout in a collection has the same dimensions (width and height). For example, all containers in a collection might be 12x8.

> 📝 While different layouts may be applied on different containers, the same layout is applied on all matrices of a specific container unconditionally.

Plate Layout Editor allows you to freely define how your samples are arranged on each plate. For example, the following multiple plate layout uses a different sample arrangement on each plate:

For quantitative assays, your standards might be arranged on every plate in the batch or you may decide to measure standards only on some of the plates in the batch. You can specify how the standard curve is generated and which curve to use to calculate the concentrations for each plate.

Plate 1

Plate 2

Plate 3

Partial Standards

When running an assay across multiple plates, you might decide that it is not necessary to measure the full range of standards on every plate. Instead you could read the full range of standards on only one plate and measure a subset of the standards on other plates, then visually compare the curve fits to ensure they are usable. This allows you to:

- Save costs on standards

- Save preparation time

- Measure more samples per plate

MyAssays makes this process easy by allowing you to define layouts with partial standard groups. We use this term to define a layout that includes the full range of standards on one or

more plates of the layout with other plates featuring only a subset of the full range of standards.

Multiple Plate Layout Curve Fit Settings

The Plate Layout Editor provides a method for selecting the curve to use for each plate. The layout configuration defines how the standard groups are arranged on each plate. This can be the curve generated from either:

- the average (of calibrator groups measured across separate plates)
- a specific plate

Example

With a layout that comprises of 3 plates, the following options for creating a curve are available:

- **Standard** (Average Across Plates)
- **Standard** (Plate 1)
- **Standard** (Plate 2)
- **Standard** (Plate 3)

For more details about curve fitting on multiple plate assays, see Multiple Plate Standard Curve Fit Analysis.

Rack Layout Editor

This section provides information about creating and editing custom rack layouts with the Rack Layout Editor.

The Rack Layout Editor is used to define the sequence of samples when assay data is measured from tubes or vials. The editor is used to create new layouts or modify existing layouts.

Racks are used to represent the sample data on-screen. The editor allows you to define and arrange the sequence of your samples.

In addition to being used to define a layout before data is collected, the editor can be used after data collection to correct for preparation errors.

> 📝 If your samples are measured on a microplate, then use the Plate Layout Editor to define the sample arrangement.

Rack Layout

With rack layouts, the number of samples that can be measured in each rack is fixed, this is the rack width and it is the same for all racks measured in an assay. Each rack is measured from left-to-right. For example, the following layout illustrates the racks used to measure 26 samples with each rack containing up to 10 samples.

With rack layouts the actual number of samples may vary at each run. To simplify the configuration of rack layouts, a sequence based editor is used to define the sequence of samples to measured. This is then converted to a layout to apply for samples that are actually read on each run of the assay.

Using the Rack Layout Editor

The Rack Layout Editor is displayed when you click **Create** to create a new layout or **Edit** to edit an existing layout on the Layout Selection pane of MAA **Layout (Racks)** tab. You can also create a new layout as a step of the New Protocol Wizard.

Rack Layout Editor Settings

The Rack Layout Editor is arranged into two panes:

- **Definition** – For defining the sequence of samples to measure and for specifying any dynamic section

- **Preview** – A visual representation of the rack layout using sample sequence with a specified number of samples to measure

Initially the Preview pane will not be displayed. It can be displayed by pressing the **Preview** button.

For example, here we can see the Rack Layout Editor showing a sequence definition of B0, Standards, Controls and Unknowns. The left-hand side shows the definition with the right-hand side showing the preview for 48 samples:

Sequence Definition

A rack assay might be fixed or dynamic:

- **Fixed** – The resulting sequence will contain only the samples specified in the definition pane

- **Dynamic** – The sample layout adjusts in accordance of number of positions measured

A fixed layout is only useful if you plan to run the exact same number of samples each time the assay is used.

A dynamic layout allows you to specify a common layout that can automatically be applied to different runs of the assay where a different number of samples is measured in each case. With a dynamic layout one or more adjacent sample groups are marked as dynamic; these appear highlighted in yellow in the definition pane. The resulting sequence will contain n copies of the groups in the sample (where n depends on the total number of samples). More...

Definition Pane

In this pane, you specify the order in which your samples will be measured.

Add Sample(s) settings

The Add Sample(s) controls are located on the bottom of the Sample Sequence Grid and are used to specify the type and number of samples to add. It comprises of:

- **Type Selector** – Select the sample type from a drop-down list
- **Number of Groups** – The number of sample groups to add
- **Number of Replicates** – The number of replicates in the sample group

After specifying the options, click **Add Sample(s)**. The ordering in which samples are added reflects the order in which they will be added to the layout.

In case the grid already contains any samples specified, the **Add Sample(s)** expands with a drop-down menu of insertion settings. Select a sample on the grid and select **Before Selection** or **After Selection** option to specify insertion of a new sample. To add a sample at the end of the list, select the **Append** option.

> Group numbering must start at 1 and be contiguous for each sample type.

Sample Sequence Grid

While the width of the racks is fixed (as defined by protocol settings), the actual number of samples may vary at each run. Thus, you can define the sequence in which the samples will be added by specifying state of sample sections:

- **Fixed** – The resulting sequence will contain these samples in the exact number as they are defined in the section
- **Dynamic** – Adjusts in accordance of number of positions measured. The resulting sequence will contain n copies of the groups in the sample (where n depends on the total number of samples). More...

The defined sequence of groups is listed in the grid, where each row corresponds to a sample. The attributes of each sample are editable.

Set Dynamic

One or more adjacent rows can be set as dynamic. Select one or more adjacent rows in the table and click **Set Dynamic**. Rows in the dynamic selection are highlighted with a yellow background. To return the row to the fixed state, select it and click **Remove Dynamic**.

> To select multiple rows to mark as dynamic, press and hold the Shift key when selecting rows with the mouse.

Undo/Redo

Use these buttons to cancel the last change or reapply it.

Clear

This button removes all **Sample** configurations (i.e. remove all Fixed and Dynamic sections)

Delete

This button removes selected sample(s) from the table. Sample group numbering may be prompted to be adjusted to ensure that it remains contiguous.

Save + Close

When you are satisfied with your changes, click **Save + Close**. This will save the new layout to your Layouts folder and make it available to relevant assay analyses.

Preview Pane

The Preview Pane displays the layout arrangement sequenced using the specified number of samples. To display the preview settings, click **Preview**. The **Number of Samples:** edit-box will appear, enabling you to specify how many positions to display on the preview. To apply this setting click the ▶ icon to the right of the edit box.

Racks

When working with assays that measure samples in tubes or vials (rather than microplates), MyAssays Desktop presents the measurement data on screen using "racks of samples".

Each rack is represented on screen with a fixed number of samples and are filled left-to-right. For example, the following graphic illustrates a rack-layout for 26 measured samples. These samples are represented across 3 racks.

The rack representation provides a convenient method for presenting data measured from multiple samples in a 2D view.

Rack Width

Within an assay a fixed rack width is used. If your reader or workflow works with racks, then use a rack width that corresponds to the actual number of tubes or vials per rack.

> The rack width is the number of samples measured in each rack.

I'm Not Working With Racks

If your reader or workflow does not use racks but instead reads any number of tubes or vials, then adopt a rack width that is a practical size to present your data onscreen. A rack width of 10 is a good choice, but as you work with the software you may prefer a different width.

Dynamic Layouts

When working with rack-based assays, the actual number of samples (tubes or vials) to measure may vary considerably between assay runs. Typically, there will be samples that are always read on each assay run (such as standards, controls, blanks) however there will also be sample types (such as unknowns) that will be measured in different volumes on each run of the assay.

For flexibility and ease-of-use, MyAssays Desktop supports the definition of "dynamic" layouts. The main benefit of working with a dynamic layout is that you do not need to redefine the sample layout each time the assay is ran. The sample layout is automatically inferred from the actual number of samples measured and the dynamic sample layout definition.

A dynamic layout defines one or more sample groups as dynamic. Each time the assay is ran, the number of samples allocated for the dynamic section on the layout will be automatically adjusted based on the total number of samples measured.

Example 1:

In this example, the **Unknown** group (in duplicate) is marked as dynamic. This means that the number of **Unknowns** on the layout will depend on the number of samples measured. This particular layout will ensure that a **Control** group is read before and after the **Unknowns**.

Type	Group	Replicates
B0	1	2
Standard	1	2
Standard	2	2
Standard	3	2
Standard	4	2
Standard	5	2
Standard	6	2
Control	1	2
Unknown	1	2
Control	2	2

For example, with 26 samples, the resulting layout comprises of 4 automatically assigned **Unknown** groups:

Using the same layout measured with 40 samples, 11 **Unknown** groups are automatically assigned.

Example 2:

In this example, the dynamic section defines a singlet **Blank** followed by an **Unknown** in duplicate.

Type	Group	Replicates
B0	1	2
Standard	1	2
Standard	2	2
Standard	3	2
Standard	4	2
Standard	5	2
Standard	6	2
Blank	1	1
Unknown	1	2

> To select multiple rows to mark as dynamic, press and hold the Shift key when selecting rows with the mouse.

For example, with 26 samples, the resulting layout comprises of 4 automatically assigned **Unknown** groups each with an associated blank.

Using the same layout measured with 38 samples, 8 **Unknown** groups each with an associated blank are automatically assigned.

Analysis

Versioned Analysis

Overview

When you launch an assay protocol and click **Calculate**, an assay-results file is created with the first calculated version of results (**Version 1**). A result version contains all of the settings and results for a specific **Calculation**. You can select to view a different version of results at any point.

> Each time the **Calculate** button is clicked, a new version of results is created and stored to the .assay-results.

Changing Versions

When there is more than one version of results available, you can freely switch between them.

How to: Switch Between Versions of the Results

1. Open a results file.

2. On the ribbon, in **Home** tab, hover to the **Versions** group.

3. From the **Current version** drop-down list, select the version you want to switch to.

Changing the version of results updates all settings and results views to display the data relevant for the selected results view. Any changes made to the currently selected version will be saved as a new version.

> Clicking **Calculate** will create a new version (with version number 1+ the current highest version number).

For example, if there are 3 versions of results and you go back to **Version 1** and make changes, then **Version 4 (pending)** is created. If you then click **Calculate**, the **Version 4** will be stored. This is the new set of results based on **Version 1** with those changes made to **Version 1** (as **Version 4**).

Purge Versions and Rollback

Purge Versions

The Purge operation will delete all version data except the current selected version. This setting is available if your assay contains more than one version.

Rollback

The Rollback operation will delete all data that follows the selected version. It is active if the current version is not the newest version of the results.

> ℹ️ The **Purge Versions** and **Rollback** operations cannot be undone; however, the changes are not committed to the file until the **Save** operation is performed.

Uncalculated Version

When you make changes to a results file after the last set of calculations and before the **Calculate** button is clicked again, the **Version {n} (pending)** label is displayed in the **Current Version** selector.

Unsaved Changes

If you made changes without calculating them (i.e., a pending version) and want to exit MAA, you will be advised to **Save these settings** on exit. These settings will be saved to the assay-results file as new uncalculated version and also to the assay protocol if that option is selected.

This also applies to assay protocol with no calculated changes.

> 📝 When the assay-results file with uncalculated changes is opened in MAA, the first set of results will be calculated automatically.

Save Options

You can save data you are working with as an:

- **Assay protocol** – To save only the settings representing the assay analysis to be performed
- **Assay results** – To save the settings representing the assay analysis and versioned results of its performance

Save Changes To Protocol

This check box appears if you have launched MAA with an assay-protocol file. It indicates whether the changes (i.e., layout to use, measurements data, sample IDs) should be stored in the assay-protocol file, overwriting its default properties.

> ℹ️ The **Save Changes to Protocol** check box state persists between sessions.

Save Commands

- **Save**

  To simplify the different types of save options, there is one master **Save** command.

  The master **Save** command is accessible from:

  - Quick Access Toolbar

  - On the **File** MyAssays Backstage View, in the **Save** tab

  This option saves results of the analysis to the directory it was launched from. It also optionally saves changes to a protocol, if the **Save Changes to Protocol** check box is selected.

- **Save Results As**

  With this command you can save the assay results with all changes to a new .assay-results file. When you click **Save Results As**, a dialog box appears. You can provide a new filename and a location for it to be stored in.

- **Save Protocol As**

  With this command you can save the modified assay protocol to a new .assay-protocol file. When you click **Save Protocol As**, a dialog box appears. You can provide a new filename and a location for it to be stored in.

Naming Results

> This setting is only available if MAA was launched with an assay-protocol file.

With this you can specify a custom target path to save a file to and how save filenames are automatically generated (e.g., to arrange all results into subfolders based on the protocol name).

When you click **Results Naming**, a dialog window with the following options appears:

1. **Default** (automatically named and stored in Results folder).
   This means a default file naming convention is used and applied by default; this default method is based on the protocol name of the related assay protocol. **Example**: For "ELISA.assay-protocol," the first time it is ran a results file "ELISA (1).assay-results" is created in the Results folder.

2. **Custom**
   You can customize the naming method and target path manually, by using macros, or by combining these approaches.

How to: Set Custom Results Naming

If you choose the **Custom** option in the **Results Naming** dialog window, the following text boxes will appear:

Folder. With this you can provide a custom path to store your files in. The options are:

- Provide a full path to the folder in the text box (manually or from clipboard).

- Click **Browse** to provide the full path to the folder in **Browse for Folder** tree view. Click **OK** to save the path or **Cancel** to close the dialog box without any updates.

- Click **Manage** to insert any number of supported macros from the list. Click **Update** to save changes or **Discard** to cancel.

Also, you can combine these options. **Example**: Provide path to a parent folder via the **Browse** option and use the <ProtocolName><CurrentDateShort> macros from **Manage** to specify folder name.

Filename. This specifies the title of assay results files. The options are:

- Type a name in the textbox.

- Click **Manage** to insert any number of supported macros from the list. Click **Update** to save changes or **Discard** to cancel.

Also, you can combine these options. **Example**: type in "Experimental results for" and use <ProtocolName><CurrentDateShort> macros from **Manage** to specify the analysis type and date it was performed.

> If the **Test settings when OK is clicked** check box is selected, MAA checks the accessibility of specified target path and verifies if the file can be created.

When these are provided, click **OK** to apply changes or **Cancel** to close the dialog box without any updates.

New Protocol Wizard

How to: Launch New Protocol Wizard

Launch the MADE and do one of the following:

- On Welcome Screen, click **New Protocol**.

- On the **Protocols** tab, in the **File** ribbon group, click **New**.

The New Protocol Wizard provides a way to easily create a new assay protocol by entering only the minimum and most important information.

It guides you through the steps you can move between by clicking **Next** and **Back** to configure the following assay parameters:

- Measurement data specifics

- Layout and sample types settings

- Administrative properties (metadata)

- A name and (optionally) a description for the protocol

> At any step, you can click the cross icon at the upper right of the New Protocol Wizard window to discard all changes and exit.

At the end of the wizard, the .assay-protocol file with defined configuration is added to your default **Protocols** folder.

Analysis Launcher

The Analysis Launcher tool simplifies building up the command line arguments to launch a protocol with a specified set of options in MAA. It provides visual controls and validation to predetermine data analysis with no user intervention required. Also, it comes in handy when configuring multiple runs of a certain data analysis (via assay protocol) with various measurements data.

The Launcher includes:

- Controls for browsing and selecting an assay protocol, measurement data, Sample IDs, and protocol tweaks files

- Various user-friendly controls for selection of command line arguments

- A text box showing the full command line of the current selection

- The **Copy to clipboard** button, which copies a built command line with selected controls to the clipboard

- The **Launch** button, which launches the command line

The built command line is displayed as changes are made. When valid, the command line can be launched directly from **Launcher**.

How to: Open Analysis Launcher

You can open this tool in one of the following ways:

- On the **Tools** tab of MADE, in the **Utilities** group, click **Analysis Launcher**.

- In MADE, enable the Launch Assay Protocol with Options feature, and then click **Launch Assay Protocol with Options**.

- Launch the **MyAssays.Desktop.Analysis.Launcher** application under the **MyAssays/MyAssays Desktop/** installation root folder.

> If you run the application from the installation root, specify the protocol file path to see all applicable controls.

Installed Protocols

The default MyAssays Desktop installation includes a number of preconfigured protocols; these protocols are stored in the **Protocols** folder.

What About Commercial Kits?

If you are performing your assay using a commercially available kit, use Search to find a preconfigured assay protocol available at MyAssays.com. You can search by manufacturer or analyte, and if your protocol isn't currently available, you can request it using the **Request Protocol** button.

Tips for MyAssays Desktop Pro

If you are using Pro edition, you can review and edit the various settings of the installed protocols. This is a good way to see how the components of an assay protocol (including transforms, evaluations, validations, and report content) fit together to perform data analysis and reporting for real-world applications. To explore how an assay protocol is configured, follow these steps:

1. Launch an assay protocol.
   (Optional) At this point, you might prefer to save a copy of the protocol to another location (or under a modified name), to keep both the original and modified versions available.

2. On the **View** group of the ribbon, click **Properties**.
   This opens **Assay Properties** panel. If the tabs are not immediately visible, click **<< Show All Properties** to expand.

3. Explore the assay configuration and then click **Calculate** to generate a report.

4. Review the report then make changes to the assay configuration. Click **Calculate** again to generate the report with your updates.

You also can create your own assay protocols with the New Protocol wizard.

> MyAssays Desktop is available in multiple editions and configurations; certain functions are only available if your current license supports this feature.

Providing the Data

Each installed protocol contains **Overview**, **Measurements** and, after calculation, the **Results** tab. Also, most protocols apply a layout definition when calculating results. On the **Microplate** tab (**Rack (Layouts)** tab for Dual DPM protocol), you can select or create a layout that represents your data's configuration.

Additional tabs may be available depending on the functionality of the assay protocol. Here the most general tabs—**Standard Concentrations** and **Dilution Factors**—are described. The tabs specific to a particular protocol are documented under their topics.

Standard Concentrations

In the **Standard Concentrations** tab, you can provide concentration values for each **Standard** sample. The display and options depend on the way in which the standard concentration values are specified:

- A start concentration with a common dilution/concentration series

- Unique concentration values for each standard

Concentration Modes

Click the **Series** button to switch the concentration modes: one designed for serially diluted standards, and one for standards with independent values. In the right **Conc.** (concentration) column of the **Standard Concentrations** grid, specify concentrations using:

- **Series** – With **Series** turned on, provide a value for the first calibrator group and a factor to apply to all groups. Use this if all calibrators share a common concentration or dilution series. For example, here the editor displays a start concentration and series to multiply by 2 for each **Standard** sample:

- **Non-Serial** – With **Series** turned off, you can specify concentration values for each calibrator separately. Use this if known concentrations do not share a common dilution series or if they are not in a simple mathematical series. For example, here the editor displays a non-serial concentration value for each **Standard** sample:

Paste Option

You can copy and paste the clipboard contents to the **Concentrations** column. The content is pasted starting from the first row on a line by line basis. This is useful if you have your concentration values in another application (such as Excel or Notepad).

> ℹ️ If you click **Paste**, the mode automatically switches to **Non-Serial**.

Flashing Standard Samples

With **Serial** mode, all Standards on the layout flash on the Layout Preview pane. With **Non-Serial** mode, only the selected group in the Standard Concentrations grid flashes.

Dilution Factors

In the **Dilution Factors** tab, you can configure how the unknowns are diluted in your experiment. The dilution factors can be specified as:

- Serial dilution of all unknowns

- Serial dilutions repeated for subsets of any number of unknowns

- Unique dilution factors for any **Unknown** sample (for example, you can use this setting for samples that have been reassayed due to their original values falling outside the standard curve)

The two-column **Dilutions** table lists all unknowns as defined by the selected layout in the **Sample** column, and the applied dilution values in the **Factor** column. The available options will depend on the selected dilution mode.

Dilution Modes

Click the **Series** button to switch the mode. In the **Factor** column, provide dilution factors as:

- **Series** – Use this mode if the dilution-fold is the same in each step, or if the dilutions follow a mathematical series.

  With **Series** turned on, provide a factor for the **Unknown1** and a common series to apply to all of the following unknowns. To define a series, select addition, subtraction, multiplication, or division icon operator along with a specified factor. With this, each dilution uses the previous dilution as the input for the next dilution step. For example, here the dilution factor for the **Unknown1** is 1, all subsequent dilutions are multiplied by the factor of 2:

- **Repeated Series** – Use this mode if the same dilution steps are repeated for each subset of unknowns.

  With **Series** turned on and its options defined (as described above), click **Repeat** and enter a number of contiguous Unknown samples each serial dilution will apply to. It will then be repeated from the beginning to the next subset of Unknowns. For example, if you set **Repeat** steps to 3, the specified Series will apply to Unknowns from 1 to 3, and then be repeated for Unknowns from 4 to 6, etc. and sequentially to the last subset:

- **Non-Serial** – Use this mode to dilute only specific unknowns or if your dilutions do not follow a simple mathematical series.

  With **Series** turned off, you can assign different dilutions for any **Unknown** samples. For example, here the dilution is specified only to the **Unknown4** and **Unknown7** sample groups:

Paste Option

You can copy and paste the clipboard contents to the **Factor** column. The content is pasted starting from the first row on a line by line basis. This is useful if the dilution scheme for the assay is in another application (such as Excel or Notepad).

> ℹ️ If you click **Paste**, the mode automatically switches to **Non-Serial**.

Flashing Samples

With **Serial** mode, all **Unknowns** on the layout flash on the Layout Preview pane. With **Non-Serial** mode, only the selected **Unknown** flashes.

Results and Report

Most of the installed protocols provide quantitative analysis of samples, so they share a lot of typical report elements. These are described in the Quantitative Assay Report Contents topic.

The report content specific for particular protocols is listed under their respective topics.

Quantitative Assay Report Contents

This topic explains the contents of a typical report generated for a quantitative assay.

A quantitative assay uses a standard curve to calculate concentrations of samples. The report can contain a variety of report elements, including:

- Fit Chart – A graphic of the curve fit
- Sample Table – Showing the computed concentrations
- Calibrators Table – The points used in the fit

- Various Details about the Fit, including:

  - Coefficients – The computed parameters of the fit equation
  - Goodness Measures – Applicable measures to assess how good the fit models the data
  - Fit Equations – Representations of the curve equations using mathematical notation
  - Quantification Limits – Any computed limits of the quantification range

> If you are working with MyAssays Desktop Pro edition, then you can configure how and whether to include the following report elements and how they will appear. For information about configuring your report, see Report Content. For specific report elements of endpoint curve-fitting transforms, see Curve Fit Transforms Report Contents.

Fit Chart

The fit chart plots the standard data points as red dots with their average values shown as pink triangles. The chart displays the fit line and calibrators. The thick black line shows the curve calculated from these standards. It's also possible to display unknowns on the curve.
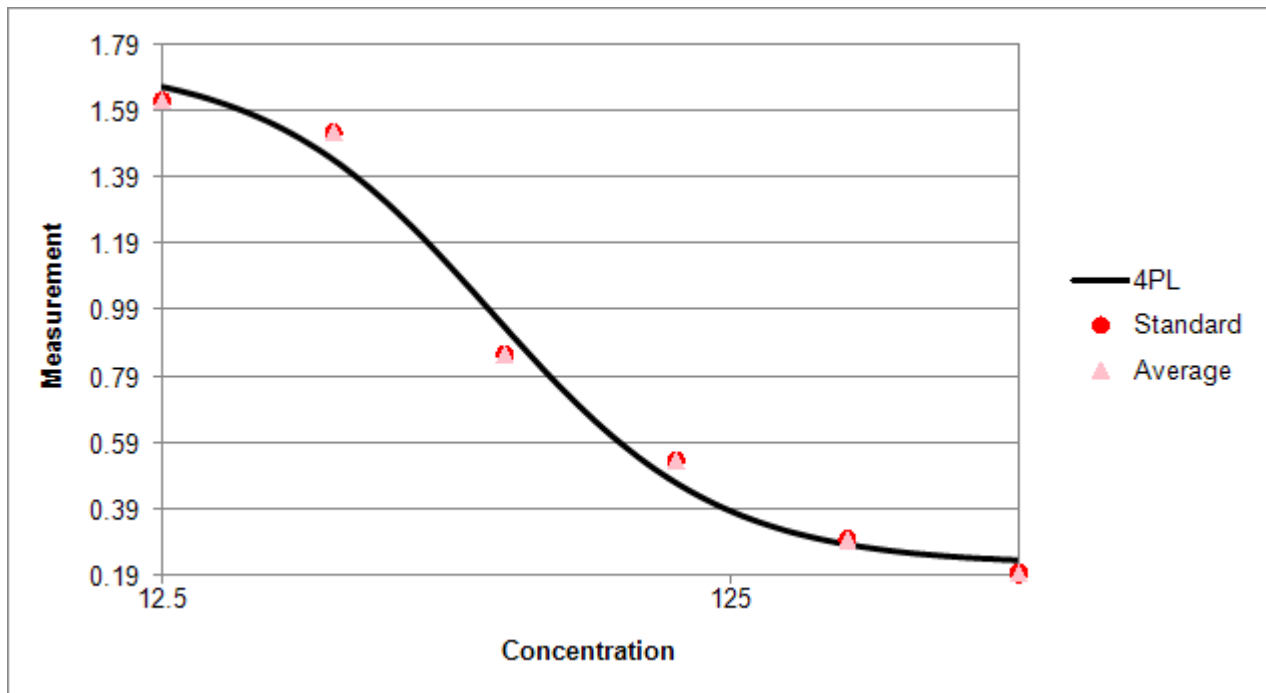
Sample Table

The Sample Table lists the calculation results for each sample by row. Columns can include the sample ID, positions along with the measurement and computed values. The available columns depend on the configured transforms. The included columns can be specified using

the [Matrices](#) tab under the Properties control, and clicking the **Include in Sample Tables** check box.

Relevant column titles can also include any specified output units. The output units can be specified under **Properties** | **Transforms**.

Here is the snippet of results for **Unknown1**:

Sample	Positions	Factor	Raw	Blank Corrected	Concentration	Concentration (x Dil. Factor)	%CV
● Unknown1	A3 A4	1	0.347 0.346	0.3455	142.103	142.103	0.280766

The following columns are typically included:

- **Sample** – The sample ID, e.g., **Unknown1**. For unknown samples the default name will be replaced by any provided sample ID (provided in the **Sample IDs** tab).

- **Positions** – The positions on the layout designated as containing the sample (as selected in the **Microplate** or **Layout (Racks)** tab).

- **Factor** – The dilution factor applied to any unknowns (in the **Dilution Factors** tab). If the sample is not diluted or its type is not **Unknown**, then "1" will be displayed.

- **Raw** – The raw measurements data (as provided in the **Measurements** tab).

- **Blank Corrected** – The mean of each sample minus the average of included **Blank** group(s). If you select layout with no blanks, this column (and calculations) will be omitted.

- **Concentration** – The average concentrations for each sample (**Raw** or **Blank Corrected**) determined from the fit.

- **Concentration (x Dil. Factor)** – If unknowns are diluted, this lists concentration of each sample with any specified **Factor** applied.

- **%CV** – If the samples are replicated (comprise more than 1 position), this column lists the percentage coefficient of variation between the replicates.

Samples outside the range of the standards (greater than the upper asymptote or below the lower asymptote) are highlighted in yellow. In this case, you might consider diluting these samples on the next assay run.

Curve Data Table

The Calibrators Table lists the measurement and calculation details for each calibrator used in the fit. Here is the snippet of calibrators table for **Standard1** and **Standard2**:

Calibrator	Positions	Conc. (Defined)	Blank Corrected	Blank Corrected (Average)	Conc. (Calc.)	%CV (Conc. Calc.)	% Accuracy
🔴Standard1	A1 A2	400	0.191 0.198	0.1945	(NA) (NA)	(NA)	(NA)
🔴Standard2	B1 B2	200	0.292 0.299	0.2955	186.523 178.336	3.17338	91.2147

Each row corresponds to the calibrator (typically a Standard) and typically includes the following columns:

- **Calibrator** – The sample IDs of the calibrator groups.

- **Positions** – The positions on the layout designated as containing standards.

- **Conc. (Defined)** – The known concentration value associated with the standard (as provided in the **Standard Concentrations** tab).

- **Blank Corrected** – The measurement values of each standard minus the average of included **Blank** group(s). If you select layout with no blanks, this column (and calculations) will be omitted.

- **Blank Corrected (Average)** – The average blank corrected concentration for each standard. If you select layout with no blanks, this column (and calculations) will be omitted.

- **Conc. (Calc.)** – The concentration values calculated from the curve for each standard.

- **%CV (Conc. Calc.)** – The percentage coefficient of variation between the calculated concentrations.

- **% Accuracy** – The ratio between the known concentration and the average of calculated concentration values.

Each row is highlighted based on whether it satisfies the precision and accuracy rules. The background colour is olive for rows that are within the defined thresholds and light red for those that are not. Calculated values that fall outside the range of the curve are reported with **(NA)** label.

Coefficients Table

The three-column table with coefficients of the fit, their calculated value, and +/- error in correspondent columns.

Goodness Measures Table

The two-column table with each calculated goodness measure followed by its value.

Fit Equations

The formulae and calculated results for equation and inverse equation (if available) of the fit method.

Quantification Limits

The two-column table that lists any additional values from the curve, such as lower and upper limits of quantification (LLOQ and ULOQ) or lower detection limit (LDL). It may also contain output units of the calculated values.

4PL (Constrained by B0 and NSB) Quantification

This protocol quantifies sample concentrations with constrained Four Parameter Logistic (4PL). With this analysis, the top and bottom asymptotes of the curve are constrained to non-specific and maximal binding as determined by the measurements of **B0** and **NSB** samples.

Assay Summary

This protocol is suitable for enzyme immunoassay (EIA) assays measured on 96-well (12x8) microplates. It includes:

1. **Background correction** – If a **Blank** sample group is included on the selected layout, first it subtracts the mean of the blank replicates from the raw data measurements (then uses the corrected values in the fit).

2. **B/B0% calculation** – Calculates percentage value of each sample ranging between the measured **B0** and **NSB** samples.

3. **Curve generation** – Fits Four Parameter Logistics (4PL) curve through the plotted standard data points (concentrations vs. B/B0% measurements) and constrains it so that upper and lower asymptotes equal **B0** (100% binding) and **NSB** (0% binding). Then calculates concentrations of the samples from the curve.

4. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

5. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch 4PL Quantification assay protocol or results file.

2. Supply your measurement data.

3. Select or create a layout that matches your assay design.

4. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.

5. Click **Calculate** to perform calculations and see the results.

Results

The 4PL (Constrained by B0 and NSB) Quantification protocol reports results in a sample table and also provides additional fit results.

For a general description of report content for this assay, see [Quantitative Assay Report Contents](). However, the report for this assay does not include curve equations.

4PL Quantification

This protocol quantifies sample concentrations using a Four Parameter Logistic (4PL) curve fit.

Assay Summary

This protocol is suitable for enzyme immunoassay (EIA) assays measured on 96-well (12x8) microplates. It includes:

1. **Background correction** – If a **Blank** sample group is included on the selected layout, first it subtracts the mean of the blank replicates from the raw data measurements (then uses the corrected values in the fit).

2. **B/B0% calculation** – Calculates the percentage value of each sample ranging between the measured **B0** (100% binding) and **NSB** (0% binding) or specified samples/values representative of 0% and 100% bound.

3. **Curve generation** – Fits Four Parameter Logistics (4PL) curve through the plotted standard data points (concentrations vs. B/B0% measurements). Then calculates concentrations of the samples from the curve.

4. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

5. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch 4PL Quantification assay protocol or results file.

2. Supply your measurement data.

3. Select or create a layout that matches your assay design.

4. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.

5. Click **Calculate** to perform calculations and see the results.

Results

The 4PL Quantification protocol reports results in a sample table and also provides additional fit results. The B/B0% calculations are listed under the column in the same name in the sample table.

For a complete description of report content for this assay, see Quantitative Assay Report Contents.

Alpha 384-well Screening

This protocol provides quantitative analysis of samples using a [Four Parameter Logistic (4PL)](#) curve fit with $1/y^2$ data weighting.

Assay Summary

This protocol is provided for 384-well (24x16) microplate layout. This assay:

1. **Curve generation** – Plots specified concentrations against the measurement data for each standard on log axes. Then fits [Four Parameter Logistics (4PL)](#) curve through the plotted standard data points using $1/y^2$ data weighting. After that calculates concentrations of the samples from the curve.

2. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

3. **LLOQ and ULOQ determination** – Computes upper and lower limits of quantification using precision and accuracy measures.

4. **LDL calculation** – Computes lower detection limit by interpolating the average background counts (blank wells without analyte) + 3 x standard deviation value on the standard curve.

Assay Protocol

To perform data analysis using this assay:

1. [Launch Alpha Screening assay protocol](#) or [results file](#).

2. Supply your measurement data.

3. [Select or create a layout](#) that matches your assay design.

4. In the **Standard Concentrations** tab, specify concentration values for Standards.

5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.

6. Click **Calculate** to perform calculations and see the results.

Results

The Alpha 384-well Screening protocol reports results in a sample table and also provides additional fit results.

For a complete description of report content for this assay, see [Quantitative Assays Report Contents](#).

ATP Lite Protocol

This assay protocol provides quantitative analysis of samples using a standard curve fit to calculate ATP concentrations.

Assay Summary

This protocol is suitable for ATP Lite 1-step luminescence assay system and is provided for 96-well (12x8) and 384-well (24x16) microplate layouts. It includes:

1. **Curve generation** – Fits the Linear Regression through the plotted standard data points (known concentrations vs. measurements). The concentrations of the samples are then calculated from the fit.

2. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

3. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch ATP Lite assay protocol or results file for your plate dimensions.
2. Supply your measurement data.
3. Select or create a layout that matches your assay design.
4. In the **Standard Concentrations** tab, specify concentration values for Standards.
5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.
6. Click **Calculate** to perform calculations and see the results.

Results

The ATP Lite protocol reports results in a sample table and also provides additional fit results.

For a general description of report content for this assay, see Quantitative Assays Report Contents.

Best-Fit Quantification

Play Video

This protocol performs multiple curve fits with different weighting models and automatically picks the Best Fit to quantify sample concentrations.

Assay Summary

This protocol is suitable for enzyme immunoassays (EIA) measured on 96-well (12x8) microplates. It includes:

1. **Background correction** – If a **Blank** sample group is included on the selected layout, first it subtracts the mean of the blank replicates from the raw data measurements (then uses the corrected values in the fit).

2. **B/B0% calculation** – Calculates the percentage value of each sample ranging betweenthe measured **B0** (100% binding) and **NSB** (0% binding) or specified samples/values representative of 0% and 100% bound.

3. **Curve generation** – Determines the Best Fit curve and fits it through the plotted standard data points (concentrations vs. B/B0% measurements). Then calculates concentrations of the samples from the curve.

4. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

5. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch 4PL Quantification assay protocol or results file.

2. Supply your measurement data.

3. Select or create a layout that matches your assay design.

4. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.

5. Click **Calculate** to perform calculations and see the results.

Results

The Best-Fit Quantification protocol reports results in a sample table and also provides additional fit results. It also contains best fit results table.

For a complete description of report content for this assay, see Quantitative Assays Report Contents.

Cell Confluency Assay Development

Assay Development protocol preconfigured to import EnSight data:

- Confluency [%]
- Foreground Roughness Mean
- Foreground Roughness SD
- Background Roughness Mean
- Background Roughness SD
- Total Roughness Mean
- Roughness Range Factor

This protocol is provided for 384-well (24x16) microplate layout.

Assay Protocol

To perform data analysis using this assay:

1. Launch Cell Confluency Assay Development assay protocol or results file.
2. Import your measurement data.
3. Select or create a layout that matches your assay design.
4. Click **Calculate** to perform calculations and see the results.

Results

This protocol imports data and automatically arranges it into 7 matrices. It does not perform any calculations on the data.

DNA 260nm

This assay protocol provides quantitative analysis of samples using a standard curve fit to calculate DNA concentrations.

Assay Summary

This protocol is suitable for assays measured on 96-well (12x8) and 384-well (24x16) microplates. It includes:

1. **Background correction** – If a **Blank** sample group is included on the selected layout, first it subtracts the mean of the blank replicates from the raw data measurements (then uses the corrected values in the fit).

2. **Curve generation** – Fits the Linear Regression through the plotted standard data points (known concentrations vs. measurements). Then calculates concentrations of the samples from the curve.

3. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

4. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch DNA 260 nm assay protocol or results file for your plate dimensions.
2. Supply your measurement data.
3. Select or create a layout that matches your assay design.
4. In the **Standard Concentrations** tab, specify concentration values for Standards.
5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.
6. Click **Calculate** to perform calculations and see the results.

Results

The DNA 260 nm protocol reports results in a sample table and also provides additional fit results.

For a complete description of report content for this assay, see Quantitative Assays Report Contents.

DNA Quantification

This assay protocol quantifies DNA in samples using a linear regression curve fit.

Assay Summary

This protocol is suitable for assays measured on 96-well (12x8) microplates. It includes:

1. **Curve generation** – Fits the Linear Regression model through the plotted standard data points (concentration vs. fluorescence). Then determines DNA concentrations of the samples from the linear model.

2. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch DNA Quantification assay protocol or results file for your plate dimensions.
2. Supply your measurement data.
3. Select or create a layout that matches your assay design.
4. In the **Standard Concentrations** tab, specify concentration values for Standards.
5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.
6. Click **Calculate** to perform calculations and see the results.

Results

The DNA Quantification protocol reports results in a sample table and also provides additional fit results.

For a general description of report content for this assay, see Quantitative Assays Report Contents.

Dose–Response Curves for EC50

Play Video

This assay protocol computes dose–response curves for each sample group using the Four Parameter Logistics (4PL) regression. The fitted curves are plotted and overlaid on a single chart for visual comparison, and the fit results values are reported.

Assay Summary

This protocol is provided for 96-well (12x8) and 384-well (24x16) microplate layouts. For each sample group, the measurement values are plotted against specified dose values. (This assumes that each sample group is dosed in the same way.)

Doses can be specified using:

- A start dose and a common dilution or concentration series
- Unique values for each dose

Assay Protocol

To perform data analysis using this assay:

1. Launch Dose–Response Curves for EC50 assay protocol or results file.
2. Provide your required measurement data for the assay.
3. Select or create a layout that matches your assay design.

> All sample groups are assumed to have the same number of positions defined on the layout (e.g., if **Unknown1** has 10 replicates, then all Unknowns on the layout must also have 10 replicates).

4. In the **Doses** tab, specify dose values (as described below).
5. Click **Calculate** to perform calculations and see the results.

Doses Configuration

The **Doses** editor specifies the doses (x values) to plot against the specified responses (measurements). The editor is displayed by clicking the **Doses** tab. Its display and options depend on the layout design and the mode in which the data has been specified.

Dose Replicates

Select the number of adjacent positions each dose value applies to. **Dose Replicates** are determined automatically and include all possible divisors (i.e., all divisors excluding itself) of the number of positions in each sample.

For example, for a 12x8 layout with 8 **Unknown** sample groups, each group contains 12 positions. Thus, **Dose Replicates** options include 1, 2, 3, 4, and 6.

Dose Concentrations

The left-hand **Doses** grid is used to select and indicate the dose value to edit. Select the dose to edit in a two-column grid.

The **Dose Group** column is numbered from 1 upwards, prefixed with "Dose". The number of rows is updated according to number of **Dose Replicates** selected.

In the **Dose** column, click the dose to edit its value. There are two modes for specifying dose values:

- **Series** – Provide a **Dose** value for the first dose group and common series to apply to all groups. Use this if all of the doses share a common dilution scheme or follow a simple mathematical series.

- **Non-Serial** – Provide a specific dose value for each dose group. Use this if your doses do not share a common concentration or dilution series or are not in a simple mathematical series.

Click **Series** to switch the **Series** and **Non-Serial** options.

Paste Option

You can copy and paste the clipboard contents to the **Dose** column. The content is pasted starting from the first row on a line by line basis. This is useful if you have your dose values in another application (such as Excel or notepad).

> When you click **Paste**, the mode automatically switches to **Non-Serial**.

Flashing Replicates

When a row is selected, the positions associated with the selection flash on the Layout Preview pane. With this, you can review to which replicates in each group a provided dose value is applied. For example, with the below layout:

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	2	3	4	5	6	7	8	9	10	11	12
B	1	2	3	4	5	6	7	8	9	10	11	12
C	1	2	3	4	5	6	7	8	9	10	11	12
D	1	2	3	4	5	6	7	8	9	10	11	12
E	1	2	3	4	5	6	7	8	9	10	11	12
F	1	2	3	4	5	6	7	8	9	10	11	12
G	1	2	3	4	5	6	7	8	9	10	11	12
H	1	2	3	4	5	6	7	8	9	10	11	12

⬤ Unknown

If **Dose Group** 1 is selected and **Dose Replicates** is 1, then all positions on row A flash. If **Dose Group** 1 is selected and **Dose Replicates** is 2, then all samples on rows A and B flash.

Results

This assay protocol fits a dose–response curve to each sample group of the **Unknown** type. It reports an overlaid chart, curve table that lists and a table with fit results values for each sample group.

Dose–Response Curve Chart

The chart contains a curve using [4PL](#) curve fitting plotted for each sample group, allowing you to review each fitting. For example, see the chart for example data plotted using the default layout:
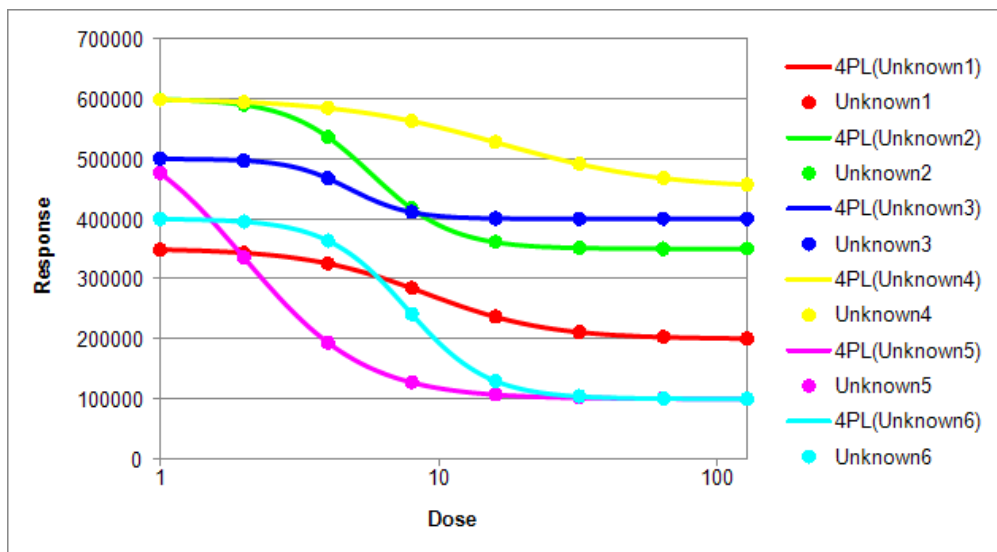
Dose–Response Fit Table

Here is a snippet that shows the Dose–Response Fit Table results for **Unknown1** (using the **Unknown1** data from the chart above):

Sample	Bottom	Top	Span	Hill Slope	EC50	Log(EC50)	R^2
●Unknown1	350370	199779	150591	1.98321	9.05295	0.95679	0.999978

Dose–Response Curves Data Tables

For each fitting, these tables list the measurement and calculation details for the calibration doses used in the fit. Here is a snippet of the Dose–Response Curves Data Table for Dose 1 and Dose 2 of **Unknown3** (using the data from the chart above):

Calibrator	Positions	Dose (Defined)	Raw	Dose (Calc.)	%CV (Dose Calc.)	% Accuracy
●Unknown3 (Dose 1)	A5 A6	1	499806 499550	(NA) 0.852352	(NA)	(NA)
●Unknown3 (Dose 2)	B5 B6	2	496982 496105	1.96526 2.11369	5.14615	101.974

Each row corresponds to the dose and includes the following columns:

- **Calibrator** – The sample ID followed by the dose group of the calibrator.

- **Positions** – The positions on the layout designated as containing this dose.

- **Dose (Defined)** – The specified dose (*x* value) associated with the calibrator (as provided in the **Doses** tab).

- **Raw** – The measurement data (response) associated with positions of the calibrator.

- **Dose (Calc.)** – The dose values (*y* values) calculated from the curve for each specified dose.

- **%CV (Conc. Calc.)** – The percentage coefficient of variation between the calculated dose values.

- **% Accuracy** – The ratio between the specified dose and the average of calculated dose values.

Each row is highlighted based on whether it satisfies the precision and accuracy rules. The background colour is olive for rows that are within the defined thresholds and light red for those that are not. Calculated values that fall outside the range of the curve are reported with **(NA)** label.

Dual DPM (10-vial rack)

This assay protocol computes disintegrations per minute from dual CPM measurements using the specified efficiency factor.

Assay Summary

This protocol is suitable for rack-based and RIA assays measured on racks with 10-vial width. It accepts dual spectrum data with common spectrum channel counts. For each data set, this protocol computes disintegrations per minute (DPM), counts, average counts per minute (CPM), and percentage error of CPM.

Assay Protocol

To perform data analysis using this assay:

1. Launch Dual DPM assay protocol or results file.

2. Supply your measurement data.

3. Select or create a layout that matches your assay design.

4. In the **Efficiency** tab, specify the efficiency factor.

5. Click **Calculate** to perform calculations and see the results.

Efficiency

In the **Efficiency** tab, provide the counting efficiency factor for use in calculating DPM.

Results

The Dual DPM (10-vial rack) protocol reports results in a sample table and includes the defined efficiency factor.

Here is a snippet showing the Sample Table results for **Unknown1** using the example data included in the protocol:

Sample	Number	Spectrum	I-129 Counts	I-129 CPM	I-129 Error CPM %	I-125 Counts	I-125 CPM	I-125 Error CPM %	I-129 DPM (0.65)	I-125 DPM (0.65)
Unknown1	1		17795	44551	0.47	19993	50058	0.45	28958.2	32537.7

ELISA (96 well) - Single Page Report

This assay protocol provides quantitative analysis of samples using a Four Parameter Logistics (4PL) curve fit to calculate concentrations. The page-based report is designed for printing on a single page.

Assay Summary

This protocol is suitable for enzyme-linked immunosorbent assays measured on 96-well (12x8) microplates where samples are measured in replicate groups. It includes:

1. **Background correction** – If a **Blank** sample group is included on the selected layout, first it subtracts the mean of the blank replicates from the raw data measurements (then uses the corrected values in the fit).

2. **Curve generation** – Fits Four Parameter Logistics (4PL) curve through the plotted standard data points (known concentrations vs. measurements). Then calculates concentrations of the samples from the curve.

3. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

4. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch ELISA - Single Page Report assay protocol or results file.

2. Supply your measurement data.

3. Select or create a layout that matches your assay design.

4. In the **Standard Concentrations** tab, specify concentration values for Standards.

5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.

6. Click **Calculate** to perform calculations and see the results.

Results

The report lists the computed concentrations and %CV values for unknown and control sample groups. Calculated data points for **Unknowns** are plotted on the curve. Validation tests check for a good R² value (greater than 0.9) and that all samples meet the acceptable precision threshold (%CV is less than 15).

Page-based report is designed to be printed on a single page.

ELISA

This assay protocol provides quantitative analysis of samples using a Four Parameter Logistics (4PL) curve fit to calculate concentrations.

Assay Summary

This protocol is suitable for enzyme-linked immunosorbent assays and is provided for 96-well (12x8) and 384-well (24x16) microplate layouts. It includes:

1. **Background correction** – If a **Blank** sample group is included on the selected layout, first it subtracts the mean of the blank replicates from the raw data measurements (then uses the corrected values in the fit).

2. **Curve generation** – Fits Four Parameter Logistics (4PL) curve through the plotted standard data points (known concentrations vs. measurements). Then calculates concentrations of the samples from the curve.

3. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

4. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch ELISA assay protocol or results file for your plate dimensions.
2. Supply your measurement data.
3. Select or create a layout that matches your assay design.
4. In the **Standard Concentrations** tab, specify concentration values for Standards.
5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.
6. Click **Calculate** to perform calculations and see the results.

Results

The ELISA protocol reports results in a sample table and also provides additional fit results.

For a complete description of report content for this assay, see Quantitative Assay Report Contents.

LANCE cAMP

This assay protocol provides quantitative analysis of samples using a standard curve fit to calculate concentrations for a LANCE assay.

Assay Summary

This protocol is suitable for LANCE assays and is provided for 96-well (12x8) and 384-well (24x16) microplate layouts. It includes:

1. **Ratio calculation** – Calculates the ratios of the 615nm and 665nm channels for each sample.

2. **Curve generation** – Fits the selected curve (Four Parameter Logistics (4PL) by default) through the plotted standard data points (concentration vs. ratio). Then calculates concentrations of the samples from the curve.

3. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

4. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch LANCE cAMP assay protocol or results file for your plate dimensions.

2. Supply your measurement data.

3. Select or create a layout that matches your assay design.

4. In the **Standard Concentrations** tab, specify concentration values for Standards.

5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.

6. Click **Calculate** to perform calculations and see the results.

Results

The LANCE cAMP protocol reports results in a sample table and also provides additional fit results.

For a general description of report content for this assay, see Quantitative Assay Report Contents.

Linearized (Logit-Log) Quantification

This assay protocol quantifies sample concentrations with the linearized (Logit-Log) method that plots logit B/B0 versus log concentration using a linear fit.

> This protocol is provided to support legacy requirements and methods. In general, the 4PL or 5PL methods are better suited for dose-response curves. The main weakness of Logit(B/B0) is that the accuracy reduces towards the upper and lower limits.

Assay Summary

This protocol is suitable for enzyme immunoassays (EIA) and is provided for 96-well (12x8) microplate layouts. It includes:

1. **Background correction** – If a **Blank** sample group is included on the selected layout, first it subtracts the mean of the blank replicates from the raw data measurements (then uses the corrected values in the fit).

2. **B/B0 calculation** – Calculates the value of each sample with respect to the measured **B0** (100% binding) and **NSB** (0% binding) or specified samples/values representative of 0% and 100% bound; then multiplies the calculated values by 100.

3. **Curve generation** – Fits the Linear Regression through the plotted standard data points (concentration vs. Logit B/B0 with log transform). Then calculates the concentrations of the samples from the fit.

4. **Dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

5. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch Linearized (Logit-Log) Quantification assay protocol or results file.
2. Supply your measurement data.
3. Select or create a layout that matches your assay design.
4. In the **Standard Concentrations** tab, specify concentration values for Standards.
5. In the **Dilution Factors** tab, optionally provide the dilution factors for your Unknowns.
6. Click **Calculate** to perform calculations and see the results.

Results

The Linearized (Logit-Log) Quantification protocol reports results in a sample table and also provides additional fit results.

For a complete description of report content for this assay, see [Quantitative Assay Report Contents](#).

Liquid Handling QC

This protocol provides quantitative precision results (%CV), and qualitative analysis of the results to determine if the measurements are within specified precision limits.

Assay Summary

This protocol is suitable for assays measured on 96-well (12x8) microplates. It includes:

1. **Calculation of the mean and %CV** – Calculates the average and percentage coefficient of variation for all measurements by-plate, by-row, and by-column.

2. **Comparison against limits** – Compares the %CV of the plate, each row, and each column against the %CV limit. The % difference of each position's measurements and the plate mean is compared against the specified ±% limit.

Assay Protocol

To perform data analysis using this assay:

1. Launch Liquid Handling QC assay protocol or results file.

2. Supply your measurement data.

3. In the **Threshold** tab, provide **Plate/Row/Column %CV** and **Each measurement's difference with plate mean (±%)** values as described below.

4. Click **Calculate** to perform calculations and see the results.

Threshold

In the **Threshold** tab, provide acceptable limits for:

- **Plate/Row/Column %CV** – The imprecision between positions in each row, column, and across the entire plate.

- **Each measurement's difference with plate mean (±%)** – The percentage difference between value of each position related to average value for the plate.

Results

This report shows the quality control analysis of measurements from a 96-well microplate. The results are arranged in tables:

- **Thresholds** – The limits provided in the **Threshold** tab.

In each of the following tables, the results are reported with pass (✔) or fail (✖) icons in the **Success** column to indicate if they are within the acceptable limits.

- **Plate Analysis** – The calculated mean and %CV of all measurements on the plate.

- **Position Analysis** – The position ID, value and % difference between each position's measurement and the plate mean.

- **Row Analysis** – The mean and %CV of all measurements in each row.

- **Column Analysis** – The mean and %CV of all measurements in each column.

Also, the report contains the heatmap-based graphical representation of the measurements.

For more information about heatmap view, see Heatmap.

For further details about this report element, see Matrix View.

Multiplex

Play Video

This assay protocol fits a standard curve and calculates concentrations, lower and upper limits of quantification (LLOQ and ULOQ), and limit of detection (LOD) for each analyte. It also applies specified dilutions and calculates %CV between replicates.

Assay Summary

This protocol is suitable for multiplex analysis on any number of analytes and is provided for 96-well (12x8) microplate layouts. For each analyte:

1. **Curve generation** – Fits the Four Parameter Logistics (4PL) curve through the plotted standard data points. Calculates concentrations of the samples from the standard curve and computes with LLOQ, ULOQ and LOD.

2. **Plate dilution factor application** – Applies specified Plate Dilution Factor to the calculated concentrations and limits.

3. **Sample dilution factors application** – Applies any specified dilution factors to **Unknown** samples.

4. **%CV calculation** – If **Unknowns** on the selected layout are replicated, computes the percentage coefficient of variation for final concentration between the replicate values.

Assay Protocol

To perform data analysis using this assay:

1. Launch Multiplex assay protocol or results file.

2. Supply your measurement data.

3. Select or create a layout that matches your assay design.

4. In the **Plate Dilution Factor** tab, specify dilution to apply to calculated concentrations and limits.

5. In the **Sample Dilution Factors** tab, provide the dilution factors for your Unknowns.

6. Click **Calculate** to perform calculations and see the results.

Plate Dilution Factor

In the **Plate Dilution Factor** tab, enter or paste a factor to multiply all samples by.

Sample Dilution Factors

In the **Sample Dilution Factors** tab, specify dilution factors for your **Unknown** samples.

See Dilution Factors for a detailed description.

Results

The Multiplex protocol reports results per analyte in a sample table and also provides additional fit results. For a description of report content for each analyte, see Quantitative Assay Report Contents. Additionally, Quantification Limits table features calculated LOD, and all three values are multiplied by the specified Plate Dilution Factor (PDF).

OQ Absorbance

This assay protocol provides operational qualification (OQ) analysis of an absorbance test.

Assay Summary

This protocol operates on XY data and is suitable for absorbance assays measured on 96-well (12x8) microplates. In this case, a special test plate with two calibrated filters is used. The nominal Optical Density (OD) of these filters is different for each plate. It includes:

- **Data reduction** – Calculates the average, maximum, and minimum absorbance values for each position.

- **OQ calculation** – Calculates precision and accuracy for each sample.

Assay Protocol

To perform data analysis using this assay:

1. Launch OQ Absorbance assay protocol or results file.

2. Supply your measurement data for **B2** (negative control) and **G2** (positive control) positions.

3. In the **Parameters** tab, provide **High** and **Low** values.

4. Click **Calculate** to perform calculations and see the results.

Parameters

In the **Parameters** tab, specify the nominal optical density values for your plate:

- **Low** – This is low absorbance value.

- **High** – This is low absorbance value.

Results

This assay protocol plots average and peak (maximum and minimum) XY analysis charts and reports results for each sample in a sample table. Here is the snippet of sample table for **Control1** (**B2** position on the layout):

The following details are reported in the columns from left to right:

- **Sample** – The sample ID, e.g., **Unknown1**. For unknown samples, the default name will be replaced by any provided sample ID (provided in the **Sample IDs** tab).

- **Positions** – The positions on the layout designated as containing the sample (as selected in the **Microplate** or **Layout (Racks)** tab).
- **Absorbance** – The XY plot for each position (in plate scale).
- **Average Abs.** – The average absorbance value for each position.
- **Max Abs.** – The minimum absorbance value for each position.
- **Min Abs.** – The maximum absorbance value for each position.
- **Precision %** – The precision of the absorbance test in this position.
- **Accuracy %** – The accuracy of the absorbance test in this position.

Standards Curve with Titres and Parallelism Plots (Dual)

This protocol calculates difference between measurement and reference data, quantifies sample concentrations using a Four Parameter Logistic (4PL) curve fit, and then plots the fitted curves on an overlaid chart for line analysis.

Assay Summary

This protocol is provided for dual endpoint data measured on 96-well (12x8) microplates. It includes:

1. **Dual matrix background correction** – Corrects measurement data (Matrix 1) by subtracting reference data (Matrix 2) point-by-point.

2. **Curve generation** – Fits Four Parameter Logistics (4PL) standards curve (specified concentrations vs. corrected measurements). The concentrations of the samples are then calculated from the curve.

3. **Mean, SD and %CV calculation** – Computes average, standard deviation and percentage coefficient of variation for all standards.

4. **Titres calculation** – Calculates titre values for each sample (calculated concentration x specified dilution).

5. **Curves comparison** – Plots overlaid 4PL curves of each sample group for parallel line analysis (specified dilution vs. measurement).

Assay Protocol

To perform data analysis using this assay:

1. Launch Standards Curve with Titres and Parallelism Plots (Dual) assay protocol or results file.

2. Supply your measurements in the **Matrix 1** and reference data in **Matrix 2**.

3. Select or create a layout that matches your assay design.

   > 📝 The layout must contain at least one **Blank** and two **Standard** sample groups.

4. In the **Standard Concentrations** tab, specify concentration values for Standards.

5. In the **Sample Dilutions** tab, provide the dilution factors for your Unknowns, Standards, and Controls.

6. Click **Calculate** to perform calculations and see the results.

Sample Dilutions

In the **Sample Dilutions** tab, you can provide different dilutions for each replicate of **Standard**, **Control**, and **Unknown** samples. This tab displays grid-based view of the dilutions for the input data. The configuration of the grid depends on the selected layout, thus each position's background is coloured to match its sample type.

Within **Sample Dilutions** grid, you can select and specify dilution for:

- A single position
- Multiple positions to set to a same dilution

Multiple positions can be selected by:

- Dragging the mouse (for rectangular selection)
- Using **Ctrl** to select random positions
- Using **Shift** to select the end position (rectangular selection)

> ⓘ **Copy** and **Paste** keyboard commands are supported.

Results

The Standards Curve with Titres and Parallelism Plots (Dual) protocol results in:

- Sample results for **Standards**, **Controls** and each **Unknown** sample separately. These are presented as tables that list all calculation results for each sample.
- Standards Chart and Fit results for **Standards** that include goodness of fit measures and ± errors.
- Parallelism curve chart that contains a curve using 4PL curve fitting plotted for **Standards**, **Controls**, and each **Unknown** sample group, allowing you to review each fitting. Under the chart, the goodness measures are included in the table for comparison.

Z-Factor

Calculates Z-Factor in accordance with *Zhang JH, Chung TD, Oldenburg KR, A Simple Statistical Parameter for Use in Evaluation and Validation of High Throughput Screening Assays. J Biomol Screen. 1999;4(2):67-73*.

Assay Protocol

To perform data analysis using this assay:

1. Launch Z-Factor assay protocol or results file.

2. Provide your required measurement data for the assay.

3. Select or create a layout that matches your assay design.

> 📓 This assays requires a layout with at least one **Pos Control** and **Neg Control** groups.

4. Click **Calculate** to perform calculations and see the results.

Results

This protocol calculates the Z-Factor for the given measurements. It also reports:

Control Results table

The two-column table that lists evaluation results for positive and negative controls. For each control, the average (AVG), standard deviation (SD), and percentage coefficient of variation (%CV) are reported.

Heatmapped Raw Data

The heatmap-based graphical representation of the raw measurements data.

For more information about heatmap view, see Heatmap.

For further details about this report element, see Matrix View.

Metadata

The MyAssays Desktop version, file names of the protocol and results files, current user and date/time stamp are also included in the report.

Common Tasks

Data Storage

Storing Data

The default path for saving your data files lies in your **Documents** folder, under the MyAssays subfolder. You can open it in MyAssays Desktop Explorer, Windows Explorer, or any other content-managing application.

You may want to change the way your data files are stored. For example, you may prefer your data to be stored in a network location or in a shared folder that is shared with other users of the system.

How to Set an Assay Data Folder Root

1. Click the **File** tab to open MyAssays Backstage view and then click **Data**.

2. Click **Select Folder Root** and choose the preferable folder.

> Uninstalling MyAssays Desktop will not remove your data files.

Backing Up Data

Periodical backing up of your assets is beneficial so you will always have a copy of all important data, and is a part of responsible PC administration. To facilitate your backup process, all data files are stored under a single parent data folder that should be backed up.

To determine which folder to backup, launch MyAssays Desktop Explorer and select **File | Data** to obtain the current parent directory. All relevant data is stored in the MyAssays subdirectory of this folder.

Data Import

Overview

MyAssays Desktop supports the import of many different types of data, including:

- Measurement Data (endpoint, kinetic, spectral, multiplex, multiple plate, etc.)
- Measurement Meta Data (this is data associated with your readings, such as date/time, plate ID, operator ID, etc.)
- Worklist (sample IDs, dilution factors, standard concentrations, etc.).
- Protocol Configuration (such as sample layout, fit method, and other data analysis parameters using tweak files)

These settings can be built into an assay protocol so that each time the protocol is launched data is automatically imported from various sources.

The Folder Poll tool can be used to automatically launch an assay protocol as soon as a new file is detected. In this way your data collection, analysis, and report/export process can be fully automated and streamlined so no user-intervention is required for the processes of data for routine assays.

For more advanced scenarios, MyAssays Desktop can be automated from the command line for complete control over the data import and analysis process. The provided Analysis Launcher tool can help with configuring and writing the command line arguments.

Measurement Data

MyAssays Desktop provides several methods for getting your data into the system for analysis. Video Walkthrough...

- Entering or pasting data from the clipboard

- Importing measurements data from one or more files

- Creating a custom import method

- Importing worklist data (Sample IDs, Standard Concentrations, etc.)

- Advanced options for importing data

> If you are using the Enhanced Security features of MyAssays Desktop, some of these functions might not be available. For example, when working under GxP or 21CFR11, the editing of raw data might be blocked.

Entering or Pasting Measurements from the Clipboard

To enter your data quickly and easily into MyAssays Desktop, type or paste measurement data from the Windows clipboard. On the **Measurements** tab, you will see:

Where to enter or paste measurements

How MyAssays Desktop organizes numerical data

Typical reasons why measurements data cannot be resolved.

How to Enter or Paste Measurements

1. Launch an assay protocol.

2. Select the **Measurements** tab.

3. Select the **Pad** subtab.

4. Enter or paste your data into the **Pad** edit box.

Preparing Your Data Set

You can provide, review, and edit all types of data directly in the **Pad** edit box. Here are the basics of data structuring used by MyAssays. To allow MyAssays Desktop to recognize and process your measurements correctly, format your data set according to these formatting principles.

Measurements Type

MyAssays Desktop protocols can be designed to process endpoint, kinetics, or spectral data. The data type defines the number of data points included for each position.

With endpoint data, each position contains a single numerical value (data point). Use **spaces**, **tab**, or **new lines** to separate each data point.

Example

For example, raw data for a single endpoint microplate assay could be formatted in a 12x8 (96-well) arrangement:

0.344 0.344 2.115 2.115 1.220 1.220 1.175 1.175 0.113 0.113 1.472 1.472

0.448 0.448 1.879 1.879 1.211 1.211 1.193 1.193 0.131 0.131 0.777 0.777

0.581 0.581 0.494 0.494 1.223 1.223 1.207 1.207 0.115 0.115 0.620 0.620

0.790 0.790 0.371 0.371 1.177 1.177 1.226 1.226 0.104 0.104 0.490 0.490

1.085 1.085 0.323 0.323 1.220 1.220 1.248 1.248 0.113 0.113 1.564 1.564

1.435 1.435 0.395 0.395 1.201 1.201 1.213 1.213 0.109 0.109 0.784 0.784

1.797 1.797 0.579 0.579 1.217 1.217 1.307 1.307 0.127 0.127 0.656 0.656

0.262 0.262 0.467 0.467 1.238 1.238 0.116 0.116 0.115 0.115 0.484 0.484

Alternatively, the data can be separated by tabs or spaces:

2.33 2.32 0.347 0.346 0.325 0.321 0.803 0.797 1.589 1.593 0.241 0.246 1.68 1.7 0.586 0.584 0.8 0.793 0.402 0.401 0.839 0.837 0.562 0.564 1.35 1.34 0.549 0.547 0.878 0.875 0.471 0.471 0.759 0.756 1.039 1.043 1.234 1.2 0.32 0.325 0.531 0.53 1.552 1.551 0.429 0.427 0.424 0.424 0.878 0.876 0.486 0.49 1.289 1.283 1.43 1.438 1.494 1.501 1.427 1.429 0.63 0.63 0.621 0.626 0.667 0.663 1.35 1.347 0.631 0.634 1.695 1.694 0.47 0.48 0.356 0.352 0.418 0.412 1.172 1.174 1.572 1.57 0.595 0.59 0.006 0.005 0.796 0.801 1.517 1.515 0.96 0.965 0.534 0.527 0.585 0.584

For kinetics or spectral assays, each position contains 2-dimensional data set of measurement data values. Provide data for each position on a new line preceded with the position identifier **position ID** (e.g., **A1**, **B6**, **H12**) in any order as:

○ Indexed XY – A list of *y* numerical values where *x* values are assumed to be 1-based continuous and thus omitted.

○ XY – A list of *x;y* numerical value pairs separated with semicolon (;) where *x* values represent time stamps, wavelength values, scan distance, etc.

> ℹ The *x* values between positions, matrices, and containers may or may not be related.

Example

Indexed:

A1 1.061 0.914 0.905 0.961 1.004 0.999 0.932 1.016 1.058 0.951

A3 0.128 0.149 0.248 0.249 0.33 0.209 0.279 0.277 0.488 0.639

XY:

A3 1.000;0.309 1.200;0.457 1.300;0.488

A1 0.000;0.363 1.000;0.374 2.000;0.353

Pad Format

The pad format represents numerical data set used by MyAssays Analysis as a text. It is designed to easily provide, review, and edit all types of data directly in the **Pad** edit box.

The format for entering of pad data depends on the following factors:

- **Type** – Type of measurements data: endpoint, kinetics, or spectral. This defines the number of data points in each position.

- **Container** – The type of a scientific instrumentation on which data is measured.

- **Arrangement** – How the numerical data is stored. This includes:

  - Number of Containers – Defines if the data is measured on one microplate/rack or across multiple containers.

  - Number of Matrices – This is the number of matrices in each container.

The actual format depends on and must be compatible with the type of assay you are working with. For example, with a 12x8 microplate endpoint assay, 96 data points should be provided.

> Use **Import Wizard** to import the relevant data directly from files.

Measurements Type

The data is provided as a string of numerical values. The key types of data are:

- **Endpoint**

  With endpoint measurements, each position contains a single numerical value (data point). The positions are separated by **spaces**, **tab**, or **new line** and are treated as a row-wise list.

  Regardless of formatting of the data set in the edit box (list of values, each value on a separate row, etc.), the Container Layout defines which numerical value belongs to which position. The first data value in the edit box corresponds to the first used well on the plate/analyte or the first vial or tube on the rack. In other words, the data is read starting from the top-left used position progressing rightwards along the first row. Each subsequent row also being read from left-to-right.

  ### Example

  For example, raw data for a single endpoint microplate assay could be formatted in a 12x8 (96-well) arrangement.

0.344 0.344 2.115 2.115 1.220 1.220 1.175 1.175 0.113 0.113 1.472 1.472

0.448 0.448 1.879 1.879 1.211 1.211 1.193 1.193 0.131 0.131 0.777 0.777

0.581 0.581 0.494 0.494 1.223 1.223 1.207 1.207 0.115 0.115 0.620 0.620

0.790 0.790 0.371 0.371 1.177 1.177 1.226 1.226 0.104 0.104 0.490 0.490

1.085 1.085 0.323 0.323 1.220 1.220 1.248 1.248 0.113 0.113 1.564 1.564

1.435 1.435 0.395 0.395 1.201 1.201 1.213 1.213 0.109 0.109 0.784 0.784

1.797 1.797 0.579 0.579 1.217 1.217 1.307 1.307 0.127 0.127 0.656 0.656

0.262 0.262 0.467 0.467 1.238 1.238 0.116 0.116 0.115 0.115 0.484 0.484

Alternatively, the data can be separated by tabs or spaces:

2.33 2.32 0.347 0.346 0.325 0.321 0.803 0.797 1.589 1.593 0.241 0.246 1.68 1.7 0.586 0.584 0.8 0.793 0.402 0.401 0.839 0.837 0.562 0.564 1.35 1.34 0.549 0.547 0.878 0.875 0.471 0.471 0.759 0.756 1.039 1.043 1.234 1.2 0.32 0.325 0.531 0.53 1.552 1.551 0.429 0.427 0.424 0.424 0.878 0.876 0.486 0.49 1.289 1.283 1.43 1.438 1.494 1.501 1.427 1.429 0.63 0.63 0.621 0.626 0.667 0.663 1.35 1.347 0.631 0.634 1.695 1.694 0.47 0.48 0.356 0.352 0.418 0.412 1.172 1.174 1.572 1.57 0.595 0.59 0.006 0.005 0.796 0.801 1.517 1.515 0.96 0.965 0.534 0.527 0.585 0.584

- **XY (Kinetic, Spectral or Scan)**

  With kinetic/spectral data, each position contains 2-dimensional data set of measurement data values. The data is provided for each position on a new line and each line starts with the position identifier **position ID** (e.g., **A1**, **B6**, **H12**).

  Positions in the **Pad** edit box can be entered in any order, because the **position IDs** are used to arrange the data on the Container Layout.

  XY data can be entered as:

  - Indexed XY – A list of *y* numerical values where *x* values are assumed to be 1-based continuous and thus omitted.

  - XY – A list of *x;y* numerical value pairs separated with semicolon (;) where *x* values represent time stamps, wavelength values, scan distance, etc.

  > The *x* values between positions, matrices, and containers may or may not be related.

Example

Indexed:

A1 1.061 0.914 0.905 0.961 1.004 0.999 0.932 1.016 1.058 0.951

A3 0.128 0.149 0.248 0.249 0.33 0.209 0.279 0.277 0.488 0.639

XY:

A3 1.000;0.309 1.200;0.457 1.300;0.488

A1 0.000;0.363 1.000;0.374 2.000;0.353

> ℹ️ All examples above use period decimal (.) separator. When actually entering your data in the pad, you can switch it to comma(,) decimal separator.

Container Layout

MyAssays arranges data sets in accordance with dimensions of the scientific measurement device on which the data was measured:

- **Microplate** – A container with fixed dimensions (width and height) and number of positions that are measured on a plate or analyte. All containers in a data set must use the same dimensions.
  If the entire plate was not read and you have values for specific positions only, you can list and obtain results for those values that were measured.

  > 📝 Use the Plate Layout Editor to define the assay layout.

- **Rack** – A container with fixed width (number of tubes or vials) of each rack of data and floating height. Data values correspond sequentially to the next used position on the dynamic layout.

  > 📝 Use the Rack Layout Editor to define the assay layout.

The assay layout defines how your samples are arranged (on a microplate or rack) and can be reused for different assays. For more information about layout abstraction, see Layout section.

Data Arrangement

MyAssays supports processing data sets that span on multiple containers, such as:

- **Multiple Plate** – For microplate assays with data measured across separate plates, select the **Multiple Plates** check box (above the **Pad** data edit box).

  > ℹ️ You can select or create multiple plate layout with different arrangement of samples on each plate.

- **Multiplex** – For multiplex assays, the measurement data is provided by <u>analyte</u>.

  🗒️ For multiplex assays, only single plate layouts can be applied.

- **Rack** – For rack assays, the data is provided by <u>batch</u> of racks.

To identify the next container of data, precede each container's data with a separate row that starts with the <u>Container ID</u> and a number:

- **Plate {N}** – Fur multiple plate assays
- **Analyte {N}** – For multiplex assays
- **Batch {N}** – For rack assays

Where **{N}** is the number of the container in the containers sequence.

For each container, provide the numerical data with each measurement separated by a space or new line.

ℹ️ If your data is measured on a single container, the container identifier can be omitted.

Each container may contain 1 or more matrices (as configured in the <u>New Protocol Wizard</u>), providing that:

- All containers have the same number of matrices
- For multiple matrices, a single line is used to contain the name of the matrix (no keyword is required)
- The <u>Data Type</u> and name of each matrix are consistent across containers
- All matrices have the same number of positions

For example, if Container 1 has 2 matrices, then all other containers in the data set must also provide 2 matrices of data. If Container 1's matrix data types are as follows:

Matrix 1: Type Endpoint

Matrix 2: Type Kinetics

Then all other containers matrices must be defined in this way – otherwise the data is invalid and cannot not be resolved. In this case, a warning message appears beneath the **Pad** edit box in red.

Decimal Separator Options

Your measurements data can use a period decimal separator(.) or a comma decimal separator
(,). To change the decimal separator option, click the **Data Format** button in the lower right
corner of **Pad** subtab and select an option from a drop-down list:

- **System Default** – The settings used by your operational system

- **Period (.)** – Use period (.) as decimal separator

- **Comma (,)** – Use comma(,) as decimal separator

> The **Data Format** settings are persisted across sessions.

File Import

MyAssays Desktop supports import of measurements from a wide variety of text, excel, proprietary and instrument-specific file formats.

Which Data Types Are Supported?

MyAssays Desktop can import measurement data and metadata from a wide variety of file formats. The software can identify and import readings from a wide range of proprietary instrument file formats. Data can be stored in a single measurement data file, or in multiple files.

- Pad Format – Text files with measurements data organized in the pad format structure.
- 3rd Party Proprietary File Formats – Data stored in over 100 formats used by major instrument manufacturers by built-in extensive Import Script library.
- Excel (XLS/XLSX) – Even if the Excel is not installed on your system, you can select and import the cells with your data. Video Walkthrough...

> With MyAssays Desktop Pro, you can also create a new assay protocol around imported measurement data file(s).

Importing Data with Import Wizard

Within the MyAssays Desktop protocol, the Import Wizard simplifies the process of importing measurement data, as well as sample IDs, plate IDs, and dilution factors. Video Walkthrough...

How to: Import Measurements with Import Wizard

1. Launch an assay protocol or open a results file.
2. On the **Home** tab, in the **Data** group, click **Import**.
3. In the **Import Wizard** dialog box, select **Measurements**.
4. Configure the import as required.

> To perform calculations with the new data and to see the results instantly after the wizard is finished, select **Calculate results**.

5. Click **Finish**.

The selected import method will be used each time data is imported into the protocol, however the import method can be changed by importing a data file in a new format to the protocol.

Importing Data with New Protocol Wizard

With MyAssays Desktop Pro, the ability to create a new custom data analysis protocol is included. By providing your measurement data file within the New Protocol Wizard, the data format and type can be automatically inferred.

Importing Data with New Protocol Wizard

1. Launch MADE.

2. In the upper-left corner of **Welcome** screen, click **New Protocol** to launch New Protocol Wizard.

3. Select **My data is in file or spread across multiple files**.

    > To create process readings from multiple analytes in a single assay, select **Create multiplex assay**.

4. Browse for and select the measurement data file.

5. Configure the data import as required.

6. Proceed through the remaining steps of the New Protocol Wizard to create and launch the new protocol file.

Additional Import Wizard Settings

MyAssays Desktop can automatically recognize and import data from a variety of instrumentation sources. With **Automatically import measurement data** selected, data from recognized file formats will automatically be imported and displayed in a layout-based preview.

Alternatively (or if the format is not recognized), you can define the delimiter characters that are used in both delimited and .csv text files. Click **Advanced** to specify further import options. For more information please view the topic Creating a Custom Import Method.

Import from Multiple Files

Using the Import Wizard (or New Protocol Wizard) it is possible to import data from multiple files into a single analysis. With this configuration, each measurement file should contain the data for a separate plate.

Select the **My data is spread across multiple files (one plate per file)** option in either Import Wizard or New Protocol Wizard. Use **Plus** button to add files and **Cross** button to remove them from the list. Select a file and use **Up** and **Down** arrows to change its positioning on the list.

Import Wizard　　　　　　　　　　　　　　　　　　　　─　□　✕

○ My measurement data is contained in one single file

◉ My data is spread across multiple files (one plate per file)

1 C:\Users\taylo\OneDrive\Desktop\desktop items 081121\FP Test\raw data plate 1.xlsx
2 C:\Users\taylo\OneDrive\Desktop\desktop items 081121\FP Test\raw data plate 2.xlsx
3 C:\Users\taylo\OneDrive\Desktop\desktop items 081121\FP Test\raw data plate 3.xlsx

☑ Automatically import measurement data

Back　　　　　　　　　　　　　　　　　　　　Next

> ℹ The order of the files in the measurement data pane corresponds to the plate number. For example, the first file will be imported as Plate 1, the second file as Plate 2, etc.

> ℹ All data files must be of the same format.

Automating the Importing Process (with Folder Poll)

By using the Folder Poll tool, importing and analyzing data can be performed automatically as soon as new measurement files are detected in a specified folder. Video Walkthrough...

To configure your protocol to perform automatic import and analysis:

1. Open the **Import Wizard**.

2. Select **Measurements**.

3. Browse for and select your data file.

4. Select **Automatically launch this protocol when a new measurement file is detected (via Folder Poll)**.

5. Allow Folder Poll to make changes

6. Specify the Folder, and any applicable file filters.

> ℹ️ File filters will allow you to restrict which files will be processed by Folder Poll. For example, if your measurement data is always contained in .xlsx files, a file filter of ***.xlsx** will only process files with an .xlsx extension added to the folder.

7. Use the dropdown box to specify what should happen when a new file is detected in the folder.

8. Review the Folder Poll configuration summary and press finish to save changes.

Creating a Custom Import Method

Overview

MyAssays Desktop supports the import of many different reader export file formats, however in the event your endpoint data is not automatically recognized by MyAssays Desktop, a custom import method can be created to automatically import data in the same format.

Defining How to Import Data

1. Open the Import Wizard

2. Select the **My data is in a file or spread across multiple files** option

3. Browse for and select the measurement data file

4. Select the location of the endpoint values

Please select endpoint values to import and then press Next.

	A	B	C	D	E	F	G	H	I	J	K	L
1	Instrument	SNP56712										
2	Date	8/1/2018										
3	Time	1:00PM										
4	Assay	Cortisol										
5	Tech	tpl										
6												
7	0.187	0.199	0.347	0.346	0.325	0.321	0.803	0.797	1.589	1.593	0.241	0.246
8	0.28	0.3	0.586	0.584	0.8	0.793	0.402	0.401	0.839	0.837	0.562	0.564
9	0.537	0.422	0.549	0.547	0.878	0.875	0.471	0.471	0.759	0.756	1.039	1.043
10	0.858	0.855	0.32	0.325	0.531	0.53	1.552	1.551	0.429	0.427	0.424	0.424
11	1.54	1.527	0.486	0.49	1.289	1.283	1.43	1.438	1.494	1.501	1.427	1.429
12	1.622	1.621	0.621	0.626	0.667	0.663	1.35	1.347	0.631	0.634	1.695	1.694
13	0.001	0.001	0.356	0.352	0.418	0.412	1.172	1.174	1.572	1.57	0.595	0.59
14	0.297	0.297	0.796	0.801	1.517	1.515	0.96	0.965	0.534	0.527	0.585	0.584
15												
16												
17												
18												

Selection:

[raw data plate 1.xlsx]Sheet1!$A$7:$L$14

☐ Configure metadata import

[Back]   [Next]

5. Optionally select to configure metadata import

6. Review the imported data

7. Press **Finish**

With the import method now configured, when using this protocol in future analyses data in this format will be automatically imported.

Defining Data Ranges

Data ranges can be defined as finite or unbounded ranges. The example above demonstrates a finite range, $A$7:$L$14. With this selection applied, the protocol file will recognize files in the same format and always look to cells $A$7:$L$14 for measurement data.

In the event your measurement data files may contain a variable number of measurement values (for example in a Rack Layout configuration), it may be helpful to define an unbounded range. By defining an unbounded range such as Column C ($C:$C), all data contained in that column will be included and imported as measurement data, whether you are importing 10 measurements or 200. Video Walkthrough...

Additional Settings

When defining an unbounded range, it is recommended to use the **Trim whitespace at end of file** Advanced option. This will support scenarios where files contain whitespace at the end of the measurement data that could otherwise result in an empty line.

The **Decimal Separator Symbol** will default to the current system setting, however if your data file uses a different decimal separator symbol, select the appropriate option: **Period (.)** or **Comma (,)**.

Worklist Import

Video Walkthrough...

This feature allows table based data contained in text files of any format to be imported into the software as:

- Sample IDs
- Plate IDs
- Dilution Factors
- Standard Concentrations

The Import Wizard may contain further worklist options for providing data specific to certain preconfigured assays or those included with the MyAssays Desktop installation. For example, you can supply Dose configurations for the Dose–Response Curves for EC50 assay.

You can easily import data specific to a run. For example, you can import data from a fixed file or from a file dynamically created alongside a run (such as LIMS). Video Walkthrough...

Adding Field Data Alongside Measurements

Using the Field Data feature, you can include additional details for each sample position in your assays alongside numerical measurements and calculated results. Field data can be imported from the same file as your measurement data or from a data file separate to the file containing measurement data.

What Is the Field Data?

Field data is any textual or numerical data associated with a particular sample position on a field matrix. Field data matrices can be either:

- String (text)
- or Numerical

Textual field data matrices are not included in data analysis; they are imported into the protocol and reported in Sample Tables and Matrix Tables alongside measurements and calculation results. Typically, textual field data can include information such as label name, measurement time, detection parameters, and other background measurement data.

Numerical field data values are available for further data analysis, they can be used as transform inputs and can be referred to from expressions (such as in selected transform parameters, evaluations and validations).

Field data might be automatically imported alongside your measurement data for your instrumentation (e.g. WIZARD^2 counters with the **All** data import option), or you can add field data matrices to your assay protocol configuration as needed.

How to Include Field Data in Your Assay?

To include field data in your assay, first create and configure an assay protocol that includes the number of field data matrices you need.

1. Launch MADE.

2. In the upper-left corner of **Welcome** screen, click **New Protocol** to launch the New Protocol Wizard.

3. Supply your measurements data and:

   - For RIA assays with measurements imported from WIZARD^2 instrument readers, select **My measurement data is in a file or spread across multiple files** option. Click **Next** and select the **Automatically import measurement data** check box on the next step.

- When importing measurements from other instrumentation sources, select **I will enter/paste in my data** or **I don't have any data yet** option.

   1. When selecting type of your measurements data, select the **Other/Combination** option and click **Next**.

   2. On the next step, under the **Data** pane, click **Add Data**, select **Field Data** and select the **Field Type** (either **String** or **Numeric**). For Numeric field data also specify numerical formatting and precision.

      To rename the matrix, select it and edit its **Name** on the **Configuration** pane.

      > 📝 Add at least one measurement data matrix to proceed.

4. Click **Next** to continue.

> ℹ️ When creating an assay protocol with more than 5 field data matrices, for conciseness, these matrices will be excluded from the report by default. To learn how to include field data in the report, see Handling a Large Number of Raw and Field Matrices.

Field Data with Multiple Plate Assays

With multiple plate assays, each plate will contain the configured number of field data matrices. In this case, the **Field Data** sub tab features the **Plate** drop-down selector, where you can choose the plate to view.

Field Data with Multiplex Assays

With multiplex data, the field data is common for all analytes.

How to View and Edit Field Data?

You can view the field data on the **Field Data** sub-tab of the **Measurements** tab. It presents all field data matrices in a table structure, where each column corresponds to a matrix.

- For microplate assays, each row is preceded with a position ID (e.g., **A1**, **B6**, etc.) coloured according to its sample type.

- For rack assays, each row is preceded with the 1-based position number for each sample and coloured according to its sample type.

You have several options when adding, editing, or removing data. You can paste data into a field data matrix, enter it into a single cell, or into several cells.

Paste Data in a Matrix

1. Right-click the field data matrix header.

2. Click **Paste**.

> To remove values from all cells in the matrix, click **Clear**.

Enter or Paste Data in a Cell

- To enter data manually, click a cell.
  Type the text or numbers and then press **Enter**.

- To paste data from clipboard, right-click a cell and click **Paste**.

Paste the Same Data into Multiple Cells

1. Select the cells to paste data into. These cells do not have to be adjacent.
   To select adjacent cells, select the first cell, press **Shift** and select the last cell in the range. Or click the first cell, then hold and drag the pointer to the last cell in the range. To select cells that are not adjacent, press and hold **Ctrl** and select the cells to paste into.

2. Right-click an active cell, and then on the drop-down menu click **Paste**.

What Can I Do with Field Data?

Apart from viewing and editing field data in your assay, you can:

- Configure how Field matrices are reported

- Label the Field data that matches specified word, phrase, or number

With Numerical field data matrices, the field data values can be used in the analysis. Numerical field data matrices are available as inputs to transforms (in the same way as endpoint measurement matrices)

Referencing Numerical Field Data Values in Expressions

Numerical Field Data values can be referenced in expressions by specifying the field data matrix letter as part of the reference. The field data matrix lettering starts from A. View the **Matrices** tab to see the lettering of any field data matrices.

For example, the expression **Unknown1.A** refers to the value of the Unknown1 sample group for field data matrix with letter A (the first field data matrix). Similarly, the expression **A1.B** refers to the numerical field data value at position A1 of the second field data matrix (lettered B).

For more information see [numerical field data operands](#).

Visualizing Data

Heatmap Plate View

The **Heatmap View** displays a plate or rack layout coloured in accordance with the measurement data numerical values. For example, data with smaller numerical values is depicted in dark green and data with larger numerical values is shown in red.

How to: Access the Heatmap View

1. In MAA, select the **Measurements** or **Microplate** (**Layout (Racks)** for rack assays) tab.

2. Check the **Heatmap View** option in the lower left corner of the **Layout Preview** pane.

> ℹ️   Heatmap view is relevant for endpoint data only.

Structure

Heatmap View comprises:

- Plate preview with the colour of each position based on its numerical value converted to a colour within a given scale

> 📝   Data for **Unused** positions is not displayed; the wells appear white and empty.

- A heatmap scale (located under plate preview) with clickable minimum and maximum controls
- A scale function menu that determines the heatmap scale type (linear or Log10)
- The auto scale option
- 2D/3D view buttons

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.3640	0.3230	2.1050	2.1240	1.2130	1.2260	1.1590	1.1900	0.1100	0.1160	1.4630	1.4810
B	0.4550	0.4410	1.8690	1.8880	1.2030	1.2180	1.1800	1.2060	0.1320	0.1300	0.7860	0.7680
C	0.5870	0.5750	0.4740	0.5140	1.2060	1.2390	1.2030	1.2100	0.1130	0.1160	0.6130	0.6260
D	0.8060	0.7740	0.3640	0.3780	1.1670	1.1870	1.2110	1.2410	0.1010	0.1060	0.4890	0.4900
E	1.1050	1.0650	0.2790	0.3670	1.2150	1.2250	1.2330	1.2620	0.1110	0.1140	1.5790	1.5490
F	1.4250	1.4450	0.3780	0.4110	1.1960	1.2060	1.2260	1.1990	0.1090	0.1080	0.7920	0.7750
G	1.7910	1.8030	0.5600	0.5970	1.2050	1.2280	1.3080	1.3060	0.1260	0.1270	0.6520	0.6590
H	0.2530	0.2700	0.4630	0.4700	1.2140	1.2610	0.1150	0.1160	0.1150	0.1150	0.4900	0.4770

Heatmap View Settings

Minimum and Maximum Controls

These settings allow you to set the colour scheme range displayed on the heatmap plate preview. Each position on the layout is coloured according to its numerical value and the colour scale (using the colour range min/max values). Values outside the range are rounded to the nearest min or max colour.

How to: Change the Minimum Value

1. Hover to and click the minimum value on the left side of the colour bar to edit the heatmap minimum value.

2. Type in a minimum value for the heatmap (e.g., 0.05).

3. Click the check icon to save your changes or the cross icon to cancel them.

> If you type in a minimum value that is greater than the maximum value, an error message will be displayed.

How to: Change the Maximum Value

1. Hover to and click the maximum value (right side of the colour bar) to edit the maximum value.

2. Type in a maximum value for the heatmap (e.g., 2.00).

3. Click the check icon to save your changes or the cross icon to cancel them.

> For multiple plate multiplex assays, consider all used positions before you type in minimum and maximum values for the heatmap.

Scale Function

With the Heatmap View, you can use one of the following scale settings for heatmap generation:

- **Log 10 scale** – Minimum and maximum control values change based on a logarithmic function

- **Linear scale** – Minimum and maximum control values change with a constant speed

How to: Switch Between the Log10 and the Linear Scales

1. With the Heatmap View turned on, click on the **Scale function** button (from the

righthand side of the heatmap maximum control) to display the scale settings.

2. Select the scale you want the Heatmap View to display with:

- **Log10 scale** – Click the **Log10 scale button** (right one). The heatmap is refreshed to display a Log10 colour scale.

- **Linear scale** – Click the **Linear scale button** (left one). The heatmap is refreshed to display a linear colour scale.

Auto Scale

The **Auto Scale** setting allows you to automatically scale the plate preview if the minimum and maximum values are changed for a set of measurement data. For example, if you type a custom maximum value in the heatmap maximum control and then change the measurement data, the Heatmap View will be updated with the original scale.

If you select the Auto Scale and there is a change in the measurement data, the Heatmap View is updated using the new scale. In this case, if the edited measurement data has a new min/max, then the heatmap scale is updated accordingly.

How to: Access the Auto Scale

1. With the Heatmap View turned on, click the **Auto Scale** button (on the right side of the heatmap maximum control).

> You can switch the Auto Scale setting on and off by clicking the **Auto Scale** button.

2D/3D View

Similar to the Layout View, you can view the heatmap in a 2D or a 3D format.

How to: View the Heatmap in a 3D Format

1. In MAA, select the **Measurements** or **Microplate** tab.

2. Select the **Heatmap View** option in the lower left corner of right pane.

3. Click the **3D** button.

> You can switch between the 2D and 3D view using the corresponding buttons.

3D View

The 3D view projects single endpoint measurement data layout in three dimensions for a convenient visual comparison. The 3D view can use Layout or Heatmap colours.

How to: View Endpoint Measurement Data in 3D

1. Launch an assay protocol or open a results file.

2. Select the **Measurements**, **Microplate** (**Layout (Racks)** for rack assays), or **Sample IDs** tab.

3. For assays that contain multiple matrices and/or containers, select the matrix you want to view from the drop-down list.

4. In the lower left corner of the Layout Preview pane, click **3D**.

> ℹ️ Switch between 2D and 3D view using the corresponding buttons.

The 3D view is based on the default 2D view comprising of rows and columns corresponding to the x-axis and y-axis of the 3D model; the z-axis represents the measurement at each position.

All other actions applicable to 2D layout are also applicable to the 3D view.

Change 3D View

To manipulate the 3D view:

- Rotate: Hold the mouse button down and drag in the required direction.

- Zoom In/Out: Use the mouse scroll wheel or hold down left and right mouse button and move up and down.

- Reset: Press the **r** key.

Move

You can move the layout model by pressing the wheel mouse button and moving the mouse.

Enable or Disable 3D View

The 3D view is available for layouts up to 384 positions. This setting can be modified under the **3D View** subsection of **View** tab in the MAA's File backstage area.

Fit Chart

When using assays with endpoint measurement data, the Fit Chart allows you to inspect your sample data alongside the fitted curve. Also, you can flag standard points directly from the chart; this is useful for excluding outliers from the curve fit.

> The Fit Chart is included in the report as one of Transform Content report elements.
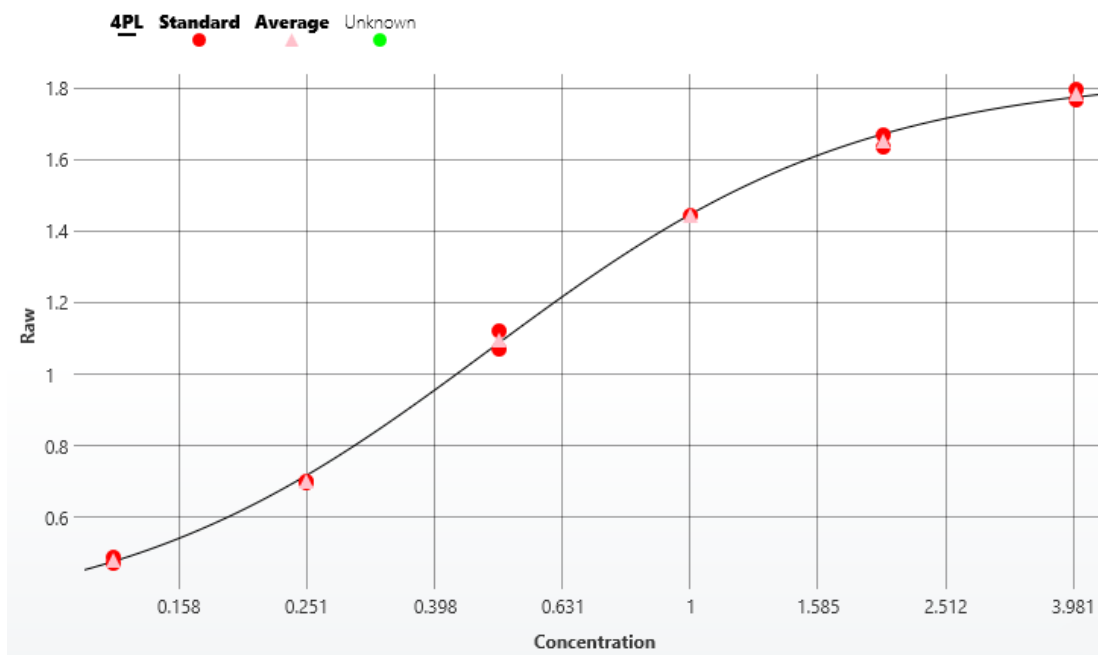
Displaying Samples

Click the sample name legend above the chart to show or hide the sample groups. For example, here the **Unknown** legend has been clicked to show where the **Unknowns** fall on the curve.

> To plot non-calibrator sample types on the fit line in the report, you can use **Points on Curve** setting.
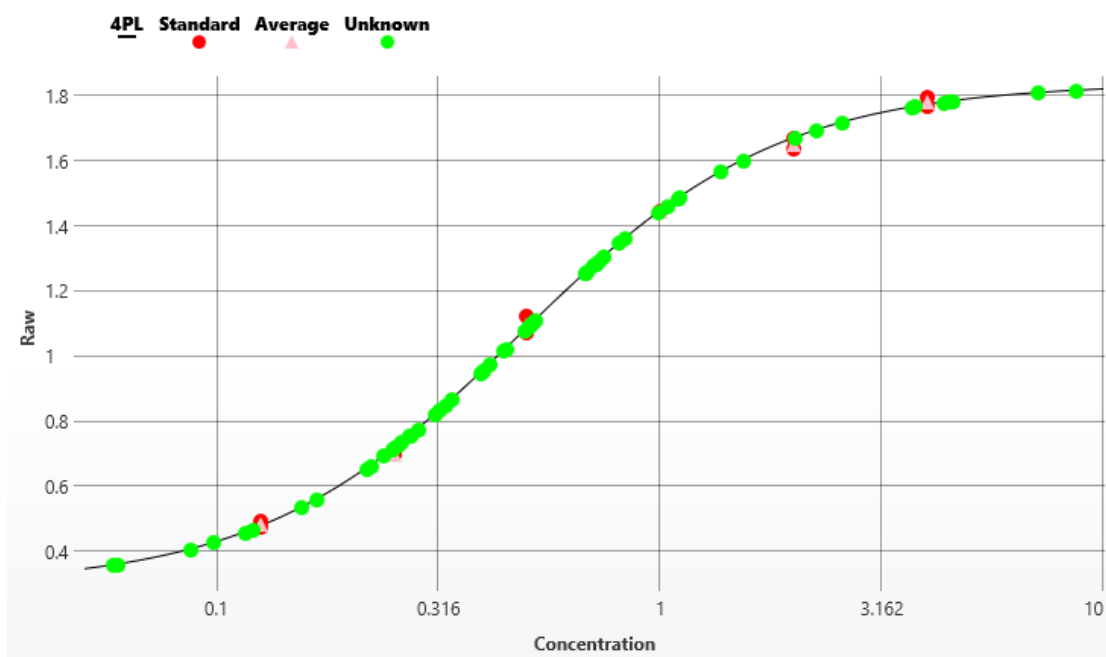
Flag Outliers

Outlier standard points can be removed by simply clicking on the point. After marking the point or points to remove, click **Calculate** to generate a new report with the new data set. The flagged points are excluded from the calculations (i.e., not used in the curve fit).
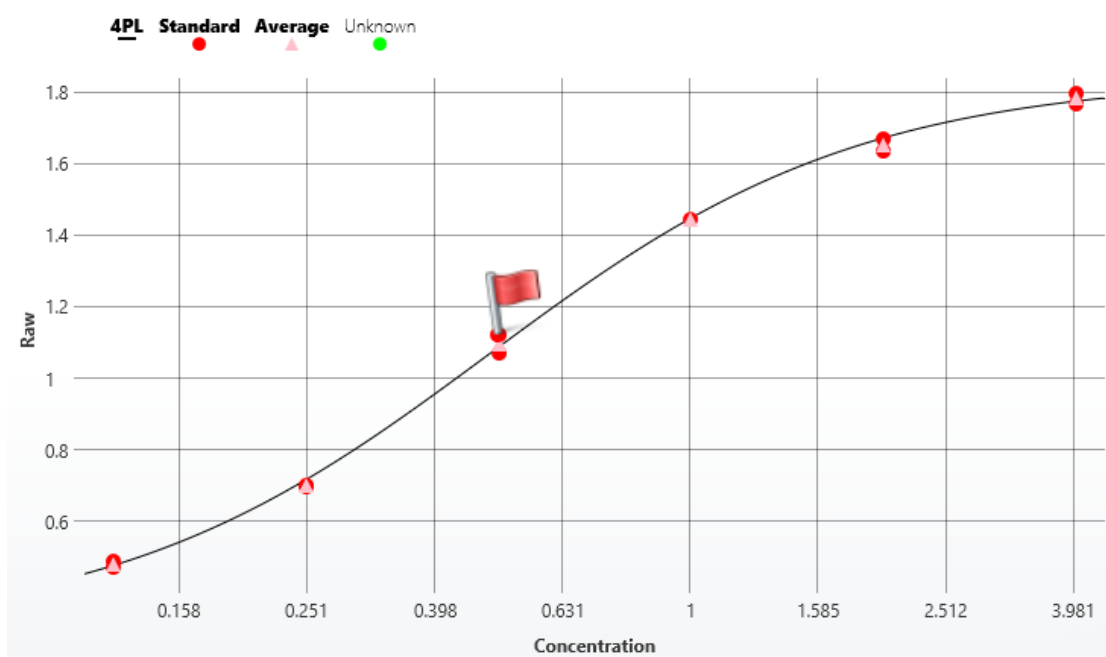
> When viewing a Fit Chart for Standard Curve Fit (From Library) or Dose–Response Curves transform, flagging **Library Standards** and **Library Average** points in not available.

Chart Zoom

For a closer look at your data points, you can zoom in on the chart by clicking and holding the mouse whilst dragging an area to zoom. Release the mouse button to zoom the chart area. Click the **Reset Zoom** button or double-click the chart to return to the full view.

Point Details

Hover the mouse over a point to view further information about that point. In the image below, the mouse has been positioned over the point of the third standard to display the point details.
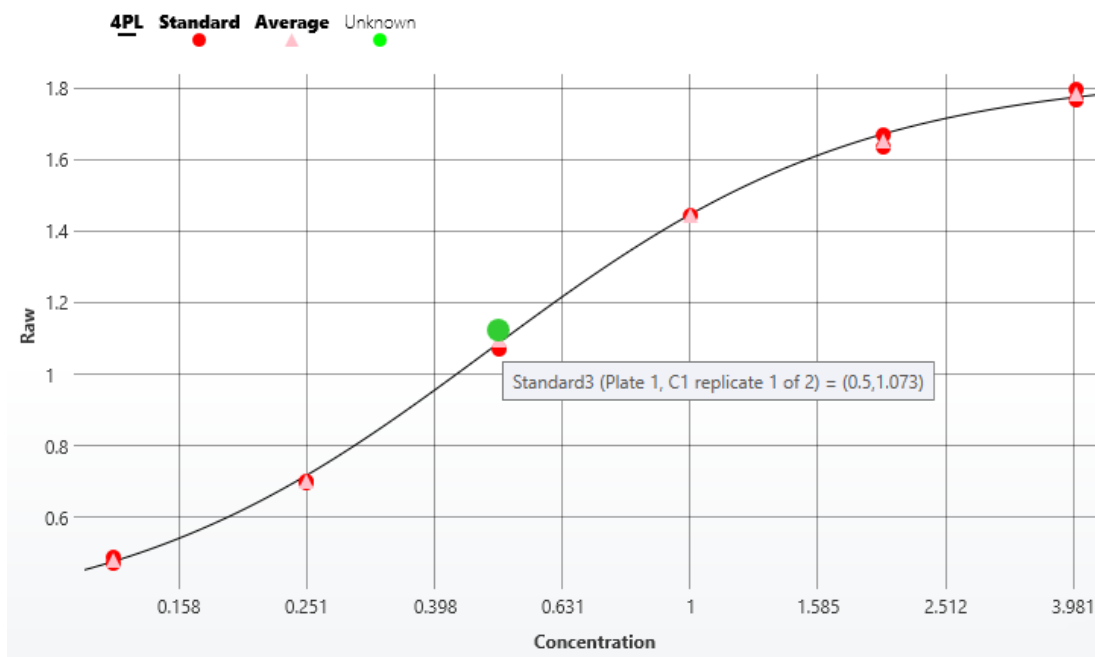
Curve Overlay Chart

When working with multiple fitted curves, it can be useful to overlay each curve on to a single chart for visual inspection and curve comparison. The Curve Overlay feature allows curves from different sources to be overlaid to a single chart. Also, points of interest can be interpolated and plotted on the curves. This topic explains how to work with a curve overlay chart.

> To learn how to configure curve overlay charts in your assay protocol, see Curve Overlay report element topic.

The Curve Overlay chart shows the fitted curves together in a single chart. For example,
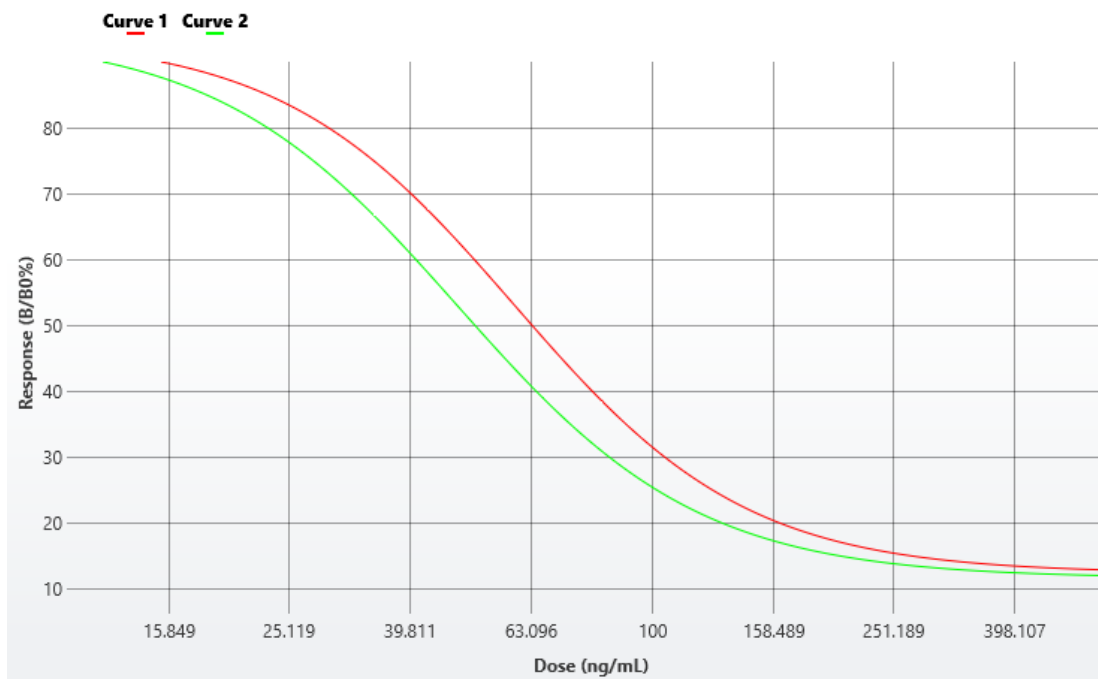
Displaying Curves

Click the curve name legend above the chart to show/hide the curves. For example, here the **Curve 1** legend has been clicked to hide this curve.
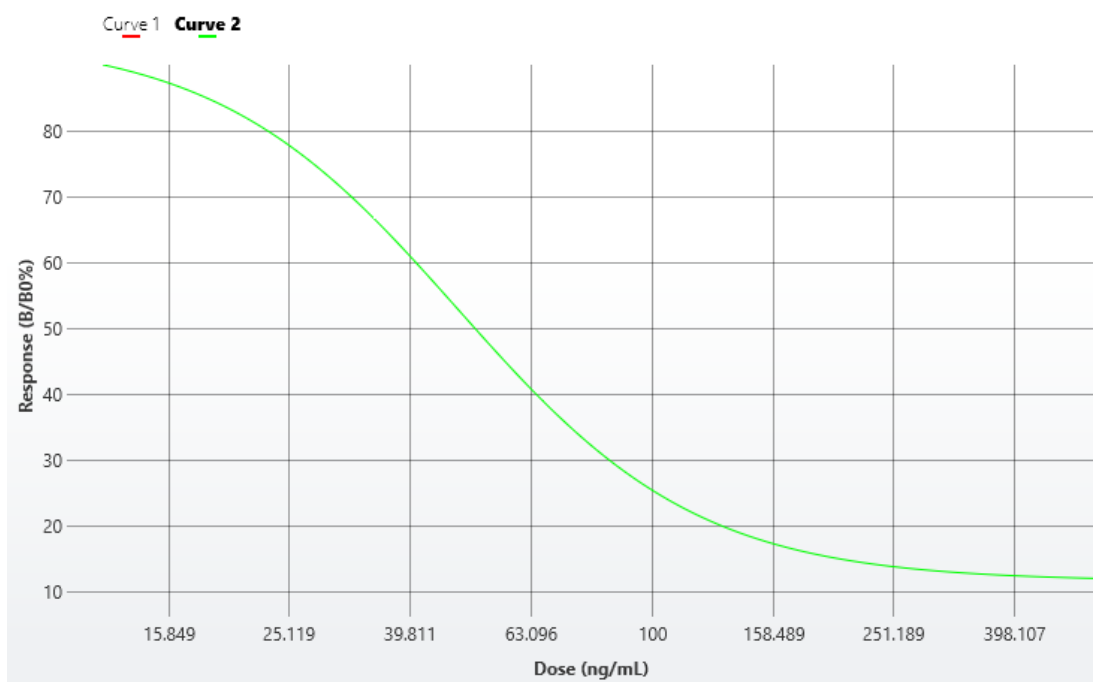
Chart Zoom

For a closer look at a specific area of the chart, zoom in by clicking and holding the mouse whilst dragging an area to zoom. Release the mouse button to zoom the chart area. Click the **Reset Zoom** button or double-click the chart to return to the full view.

Curve Overlay Chart Evaluations

A curve overlay chart might include evaluations to indicate where certain values fall on each of the chart. See Curve Overlay Evaluations for the configuration steps.
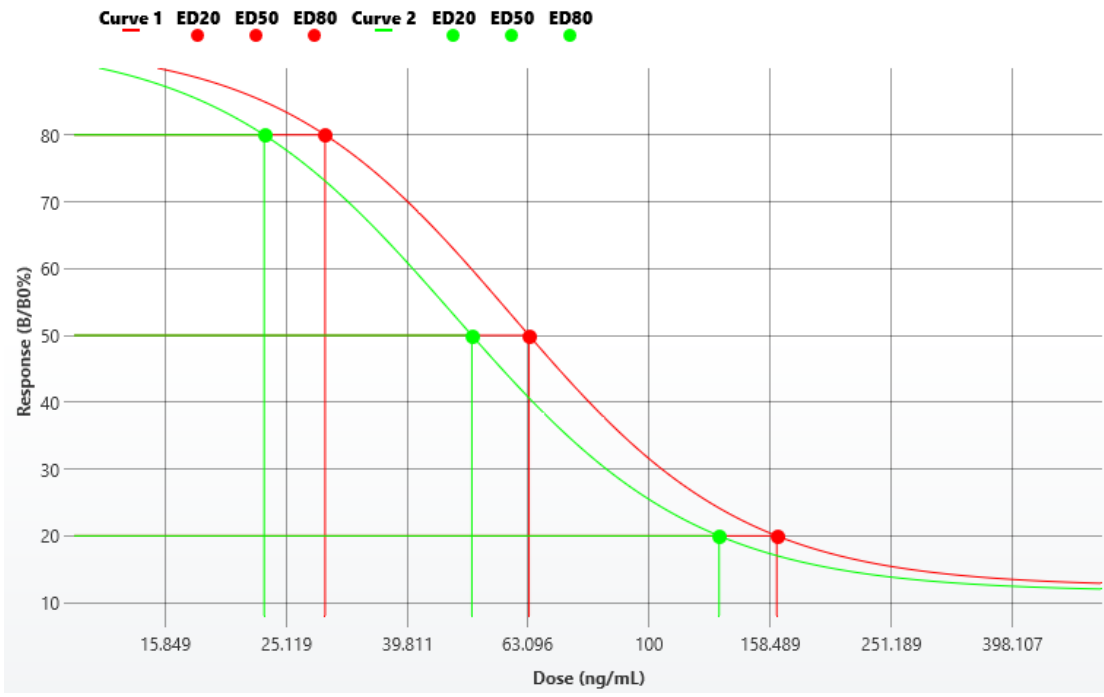
Kinetic/Spectral Overlay

When working with kinetic or spectral data, the Kinetic/Spectral Overlay Chart gives you a clear view of measurements at the position(s) or group(s). The y-axis of the chart corresponds to measurement values; the x-axis represents (depending on the assay) cycle, time, or wavelength values.
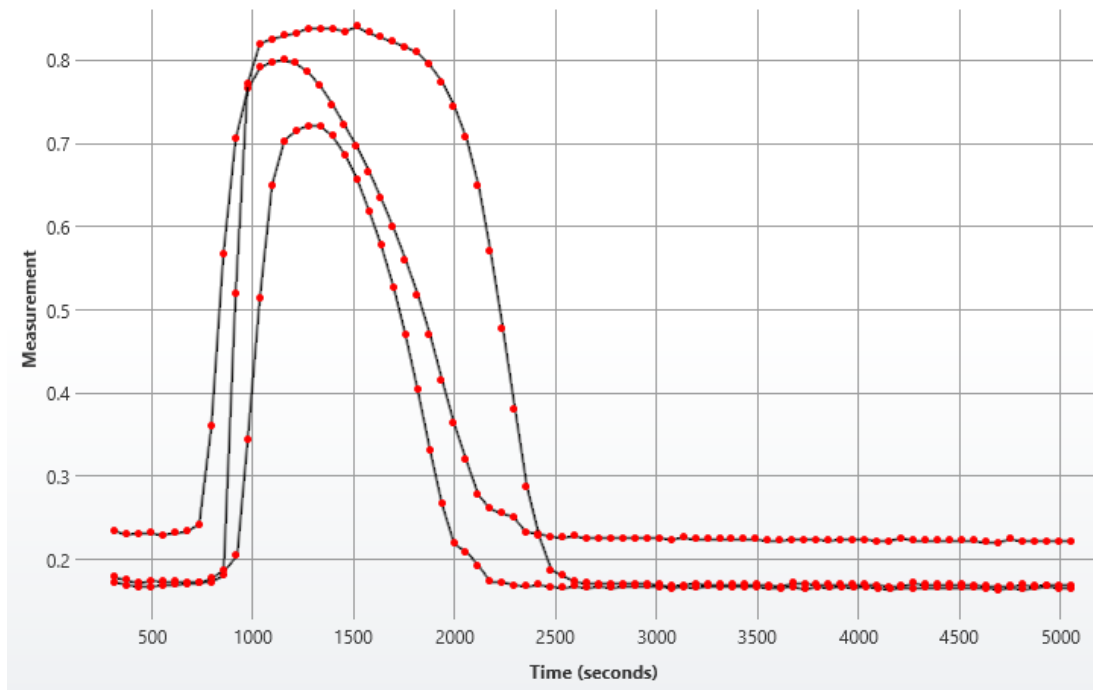
View Selection Modes

Depending on the view selection, you can explore data ranging from a plot that belongs to a single position to the overall plate/analyte values.

How to: View XY Overlay Chart

1. In MAA, select the **Measurements** tab.

2. Select the **Chart** subtab.

3. Use the **Select Group**/**Select Position** controls to select the view mode.

There are two modes for Kinetic/Spectral Overlay:

- Position
- Group

For kinetic or spectral data, any specific position can be selected and viewed on a Kinetic/Spectral Overlay chart.
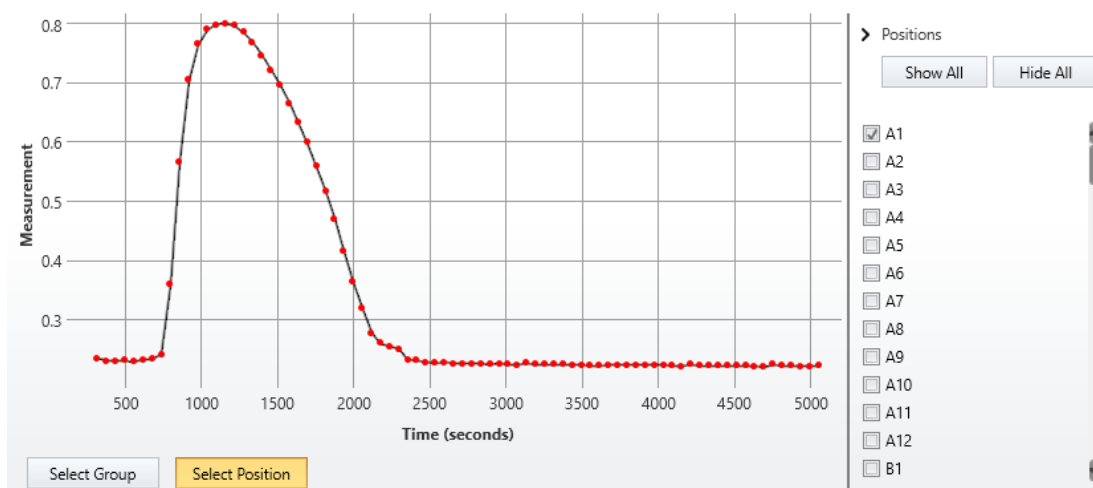
Moreover, any number of positions in any combination can be selected from the right-most View Selection pane. Select the check boxes corresponding to positions you want to view.

Alternatively, any sample group can be also viewed on the Kinetic/Spectral Overlay chart with the same actions as described above.
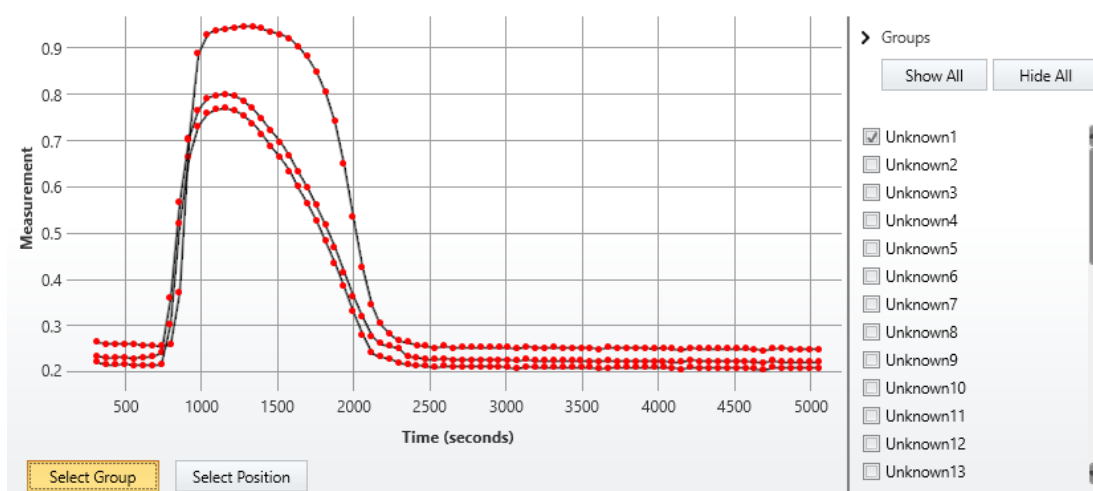
Additionally, you can click **Show All** or **Hide All** to display plots for all plate/analyte positions or for none, respectively.

Zoom In/Out

Position the mouse pointer on the area you want to enlarge, press and hold **Ctrl** button, and scroll the middle mouse button up or down to zoom in or out. Alternatively, hold down left mouse button and drag a rectangular area to zoom in.

Double-click or click **Reset zoom** on the upper left of the enlarged area to reset the zoom.

Flagging Outliers

Any data point can be flagged and unflagged interactively on this view. The chart will update accordingly.
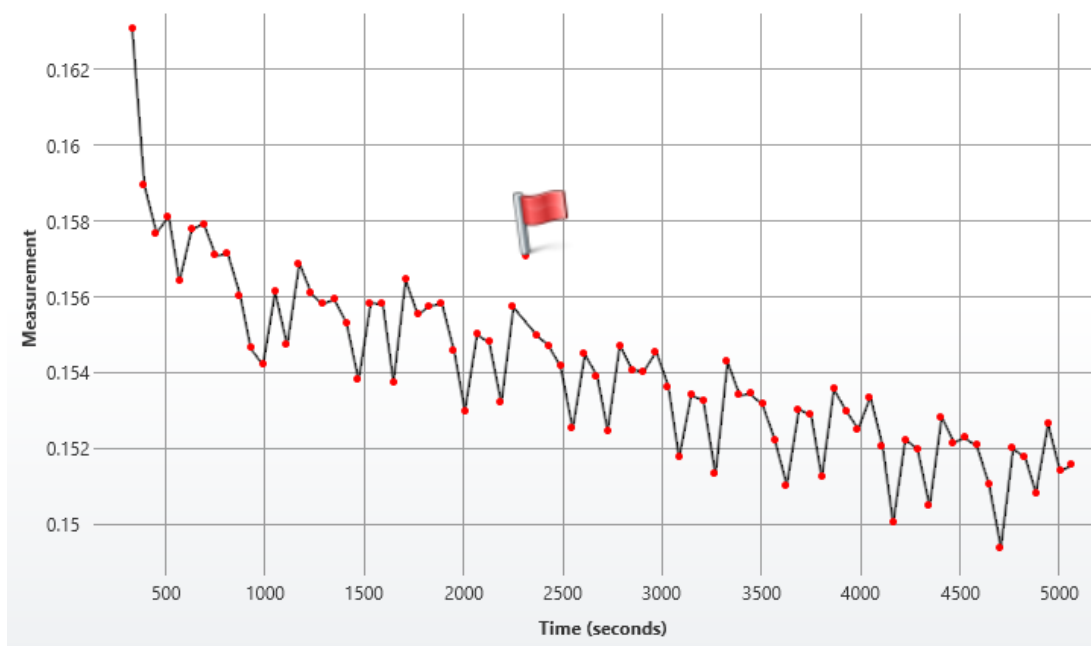
Multiple Plate View

If your measurement data is spread across multiple containers, you can choose which plate/analyte to be displayed. Select the required container from the drop-down list in the left upper corner of the Kinetic/Spectral Overlay Chart.

Kinetic/Spectral Analysis Chart

For kinetic/spectral assays, you can inspect the data analysis results on a Kinetic/Spectral Analysis Chart with respect to the configured XY data settings. Moreover, you can flag points and define subset of data points to consider directly on the chart.
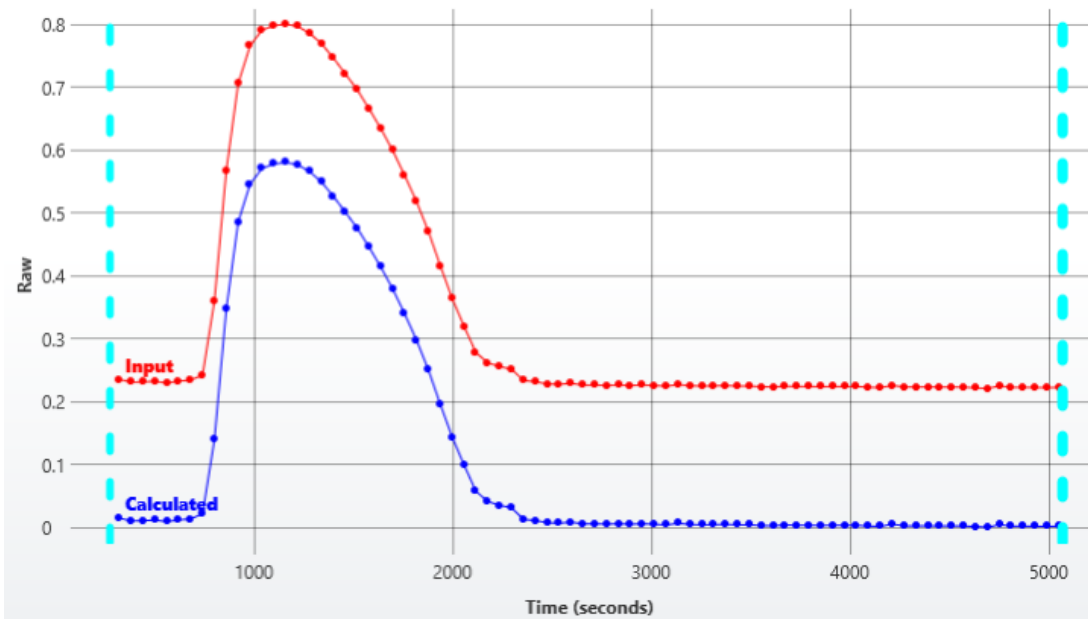
The y-axis of the chart corresponds to the measurement values; the x-axis represents (depending on the assay) cycle, time, or wavelength values.

Displaying Data Plots

In most cases, the results are presented in terms of each position and contain input data plot in red colour and calculated result represented in blue.

> ℹ️ For XY Replicates Average and XY Replicates Function, the results are presented for each sample group.

> 📝 For XY Blank Correction transform results, the chart is not produced.

Flagging Outliers

To flag an outlier data point, click it. After marking the point or points to remove, click **Calculate** to generate a new report with the new data set. The flagged points are excluded from the calculations.
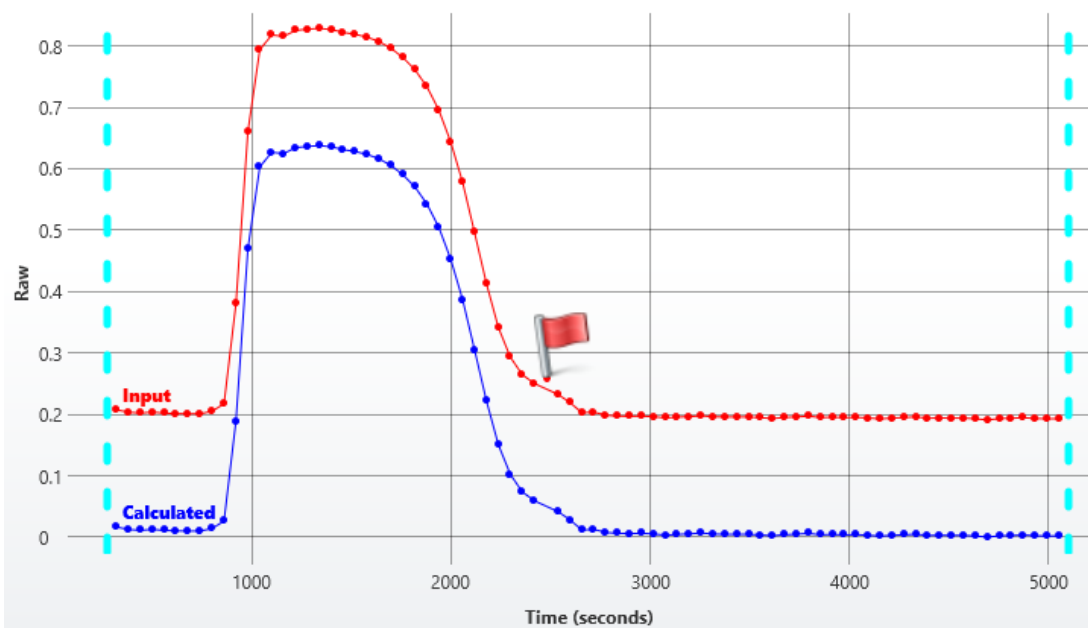
Specifying XY Data Subset

For any position, you can define a subset of kinetic/spectral data points to include in calculations via the positioning of vertical dashed range selectors. The points outside the selected range are displayed as greyed out with no lines between them and are exlcluded from further calculations.

Recalculate to generate a new report with the new data set.
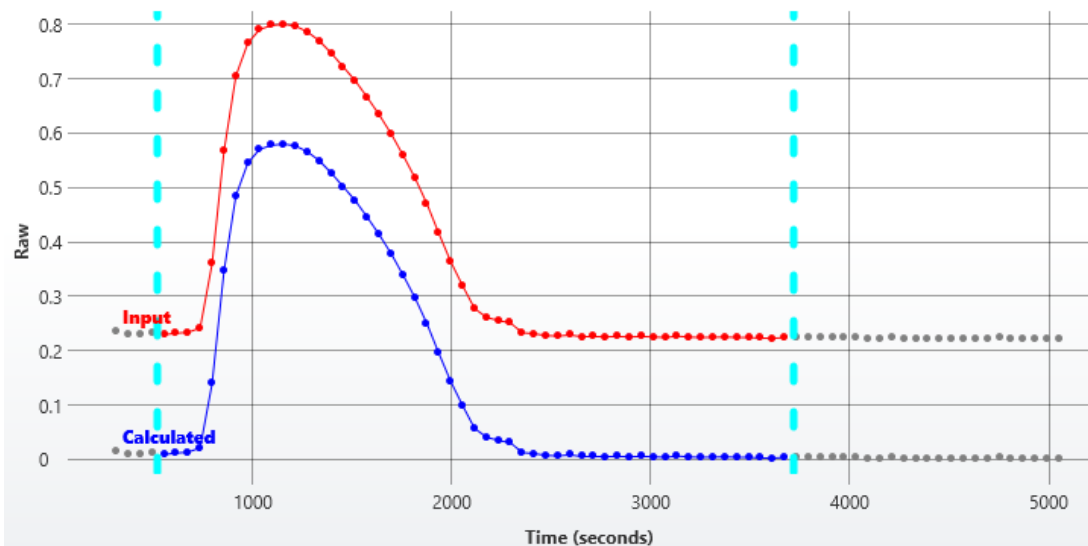
Analysis Description

Also, for all XY Reduction transforms, XY Baseline Correction, XY Fit, and XY Outlier Removal, the description of analysis performed and any non-matrix data for each plot is displayed immediately below the chart.

Fit Parameter

$y = 5.36915x + 0.440824$

Coefficient	Value	+/- Error
m	5.36915	0.221636
c	0.440824	0.118321

| Goodness Measure	Value
R^2	0.986551
aR^2	0.98487
P	0.00000000899332
SE	0.201311
F	586.856
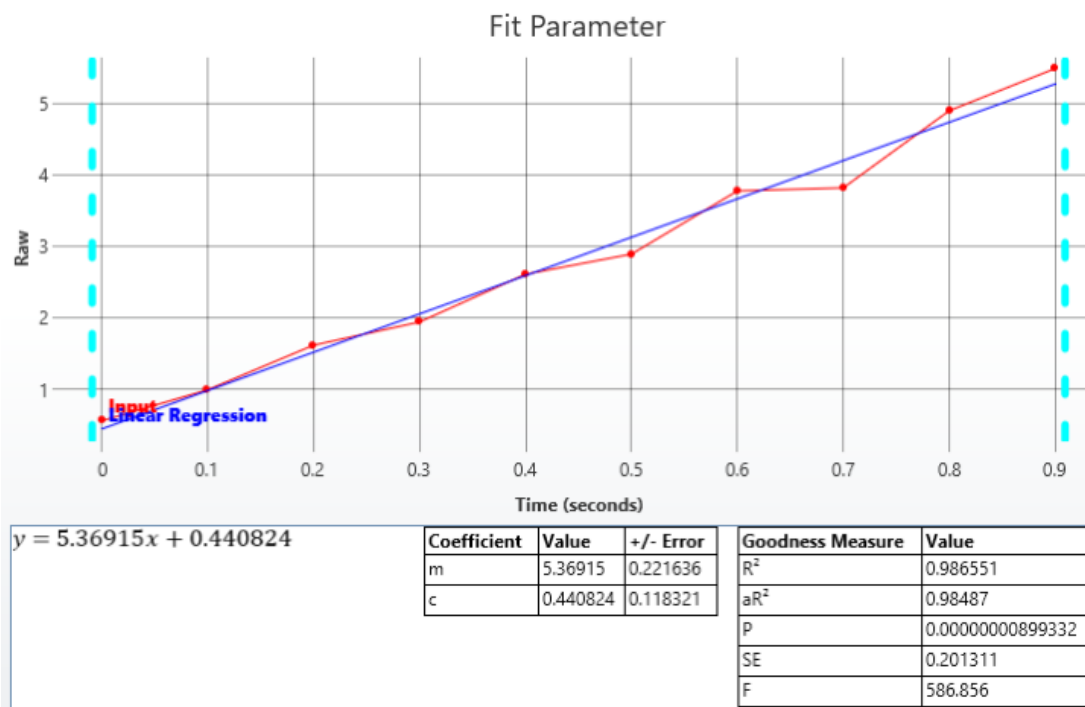
Zoom Options

Position the mouse pointer on the area you want to enlarge, press and hold **Ctrl** button, and scroll the wheel mouse button up or down to zoom in or out. Alternatively, hold down left mouse button and drag a rectangular area to zoom in.

Double-click or click **Reset zoom** on the upper left of the enlarged area to reset the zoom.

Multiple Plate View

If your measurement data is spread across multiple containers, each plate/analyte is displayed in a separate Kinetic/Spectral Analysis Chart tab.

Flagging/Outlier Exclusion

Overview

Flagging is used to mark and indicate data to exclude from further analysis. This can be used to identify outliers to ignore issues such as poor measurements or data for incorrectly prepared or contaminated samples.

There are two types of data that can be flagged:

- Position
- Point

For all measurements types, any position can be marked as flagged (e.g., position **A1**). When the data at a position is flagged, any reference to the sample contained at that position will not include the flagged position's data.

For example, if **Standard1** comprises of 3 replicates measured at position **A1**, **A2**, and **A3**, if position **A1** is flagged, **Standard1** would refer to only the non-flagged values (i.e., the average of the data at positions **A2** and **A3**).

For kinetic or spectral data, any specific data point can be marked as flagged too (e.g., the data point for cycle 1 of position **A1**). Any flagged data points are not included in any further analysis. If all points of a position are flagged, then the position is considered to be flagged.

For example, if the kinetic measurement data at position **A1** comprises of 10 cycles, if point 1 is flagged, then a kinetic reduction operation is performed (such as computing the average of kinetic cycles in XY Reduction Average) and the calculations would ignore the data of the flagged point.

Data can be flagged interactively or by calculations. Any flagged data will be indicated in the report and export accordingly. It is also possible to customize the labels for flagged data in the report.

Interactive Flagging

Position or point data can be flagged (and "unflagged") interactively by left-clicking the mouse on the position or data point to flag. This is possible in:

- Measurements View (in the **Measurements** tab)
- Standards Chart (in the **Results** tab when working with Standard Curve Fit transform)
- Kinetic/Spectral Measurements Chart (in the **Measurements** tab | **Charts** subtab when working with kinetic/spectral data)

- Kinetic/Spectral Analysis Chart (in the **Results** tab when working with Kinetic/Spectral transforms)

How to: Flag Data Position with Measurements View

1. In MAA, select the **Measurements**, **Microplate**, or **Sample IDs** tab.

2. Hover to the Plate Preview pane on the right of the selected tab.

3. Position the mouse pointer over the point to flag and left-click.

> ℹ️ A flagged position appears on the Measurements View with a cross through it.

How to: Flag Data Position with Standards Chart

1. Add the Standard Curve Fit Transform:
   1. Launch an assay protocol or open a results file.
   2. If you cannot see the **Assay Properties** panel, click the **Properties** button to open it.
   3. Click the **Add** button.
   4. Select the Standard Curve Fit transform.
   5. Click the **Create** button.
   6. Review or edit the transform's input matrix and output matrix name as required.

7. Provide your required settings for the transform (see the **Properties** section above).

8. Click **Calculate**.

2. Select the **Standard Curve Fit** tab of the **Results** tab. If your assay comprises multiple plates, select the one that contains the analysis view for your data.

3. Select the sample type on the legend to view how the points are spread on the curve.

4. Position the mouse pointer over the point to flag and left-click.

5. Click **Calculate** to perform the calculations with the new settings and to see the results.

> ℹ️ Any flagged item can be "unflagged" by left-clicking on the flagged item.
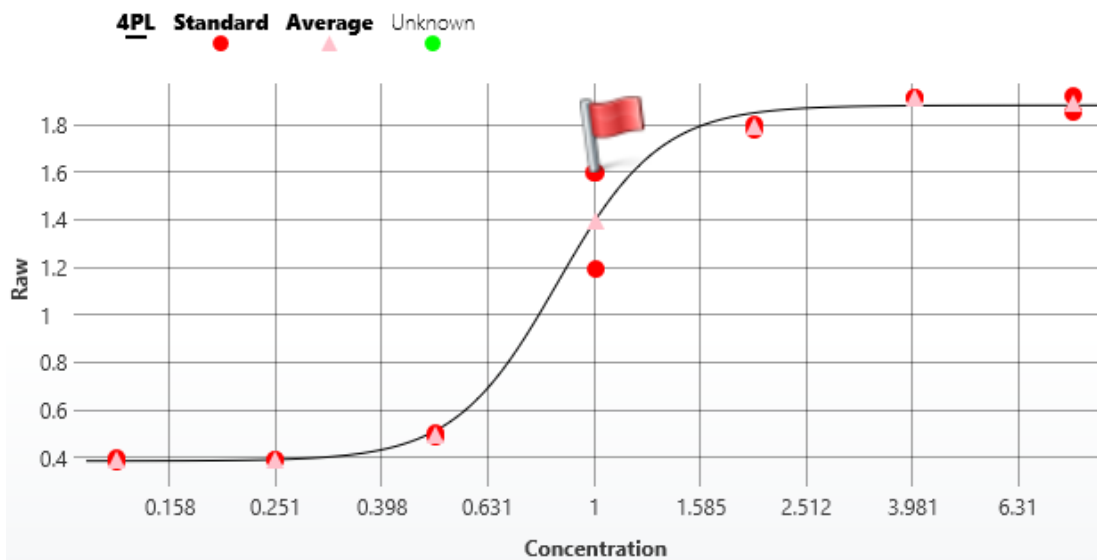
How to: Flag Kinetic/Spectral Data Point with Kinetic/Spectral Measurements Chart

1. In MAA, select the **Measurements** tab.

2. Select the **Chart** tab.

3. Use the **Select Group/Select Position** controls to select the required data.

4. Position the mouse pointer over the point to flag and left-click.
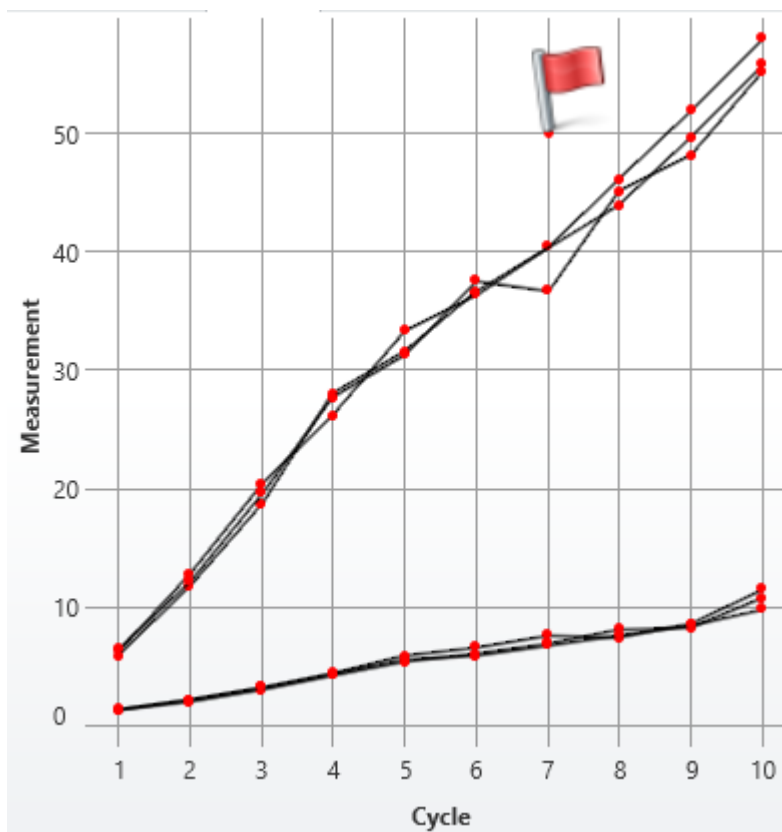
How to: Flag Kinetic/Spectral Data Point with Kinetic/Spectral Analysis Chart

If your data analysis includes an Analysis View (used to display further information about the performed data analysis), then you can flag XY points directly from this view.

1. In MAA, select the **Results** tab.

2. Select the tab that contains the analysis view for your data.

3. Position the mouse pointer over the point to flag and left-click.

> ℹ️ Any flagged item can be "unflagged" by left-clicking on the flagged item.

XY Maximum Slope

Maximum slope is 9.279
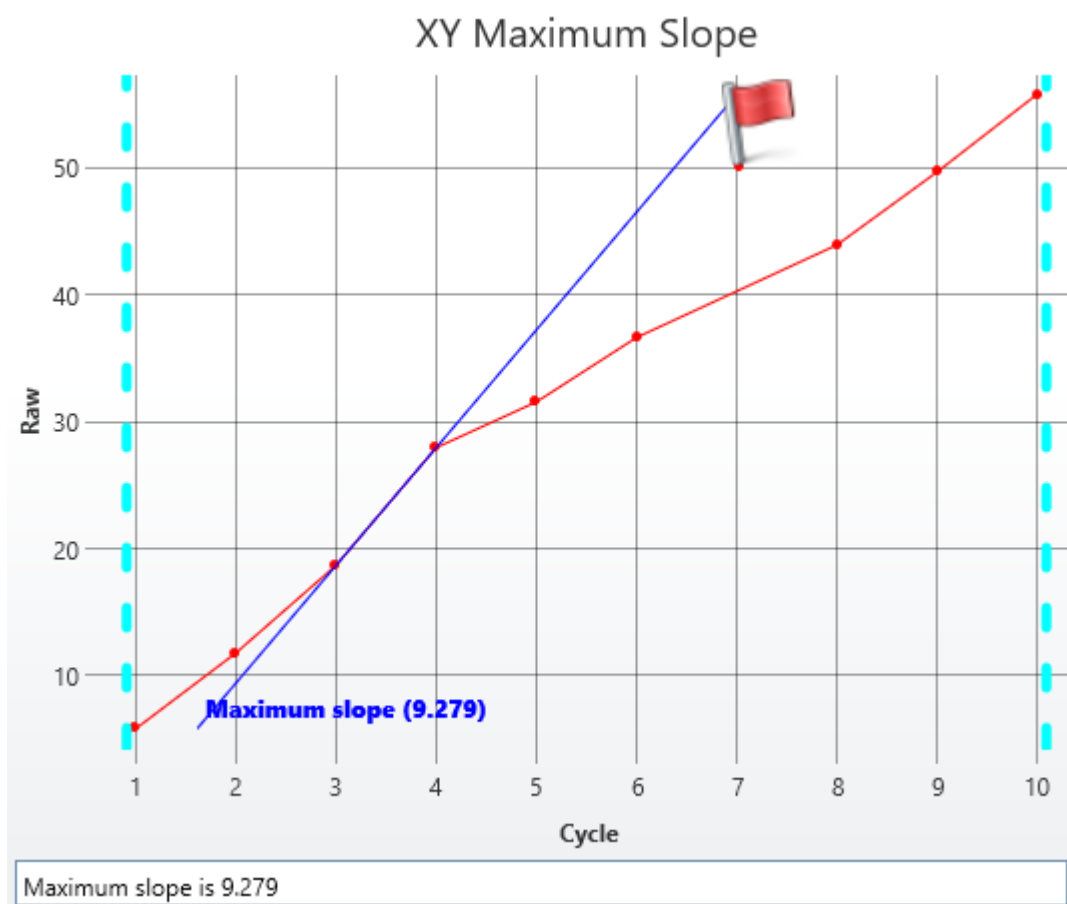
Flags View

If there is any flagged data, then the **Flags** option will appear in the **View** group of the **Home** ribbon tab. The **Flags** view control will display a list of the currently flagged items (including both positions and point data if relevant).

Status	Type	Position	Point	Plate	Matrix
☑	Point	A5	7	Plate 1	Raw
☑	Point	A5	6	Plate 1	Raw
☑	Point	A5	5	Plate 1	Raw
☑	Position	A1	-	Plate 1	Raw
☑	Position	A2	-	Plate 1	Raw
☑	Position	A3	-	Plate 1	Raw

Select or clear the status of an entry to change its flagged status.

Calculated Flagging

In addition to manually selecting which data to flag, calculations may result in flagged results.

For example, the [Replicate Outlier Removal](#) transform can be used to automatically flag sample replicates that are outside a definable expected range. For more flexibility, the [Auto Flag](#) transform enables you to define conditions to flag endpoint values.

When working with kinetic or spectral data, the [XY Outlier Removal](#) transform can be used to automatically detect specific data points that deviate from an expected pattern beyond an expected threshold.

Also, for certain calculations there might not be a valid result for the calculation. In those cases the result will be marked as flagged (as no further calculation is possible).

Advanced

All transforms include a setting under the **Advanced** properties group for selecting which sample types the transform should calculate results for. For those samples that are not to be calculated, the results can be set to be flagged as either:

- **Flagged with Value**
- **Flagged no Value**

Flagged Data in the Report

The report will indicate flagged data as strikethrough text (such as **1.23** or **Flagged**). Where data has been flagged and there is a value associated with it, the original value appears in strikethrough.

Where there is no value associated, the text Flagged appears (also in strikethrough).

For example,

Sample	Positions	Raw	Concentration
🟢 Unknown1	A3	~~1.599~~	1.53791
	A4	1.665	

Here, position **A3** has been flagged. In this case the calculation of the concentration will use only the value from position **A4**.

Here the **Raw** values in positions **A3** and **A4** have been flagged. This means that there is no result for the **Concentration**.

Sample	Positions	Raw	Concentration
🟢 Unknown1	A3	~~1.599~~	~~Flagged~~
	A4	~~1.665~~	

Flagged Data in Text-Based Exports

For text-based export (such as CSV, TXT) where strikethrough is not available, flagged data is identified by asterisk symbols surrounding each flagged data item, for example:

1.23

Flagged

For example, the following export text shows three data values flagged:

```
Sample,Positions,Raw,Concentration
Unknown1,A3 A4,*1.599* *1.665*,*Flagged*
```

Custom Flag Label

If the default strikethrough text "**Flagged**" is not suitable, you can specify your own text to use instead. For example, here the text **No result** is used instead of Flagged.

Sample	Positions	Raw	Concentration
🟢 Unknown1	A3	1.599	No result
	A4	1.665	

This is an advanced setting that can only be configured through the XML editor. For more information please refer to Custom Flag Label configuration.

Custom Flag Label Configuration

The Custom Flag Label feature enables specific labels to be defined and used to indicate flagged results instead of the default strikethrough flagged text (such as ~~1.23~~ or ~~Flagged~~).

The settings are available at different levels of the Matrix-Transform Analysis configuration; this provides a fine degree of control over how flagged results are reported. For example, you may prefer to label flagged raw data differently than flagged concentration results.

Additionally, the Standard Curve Fit transform supports conditional flagging and applying labels. This enables the definition of rules to apply that define how to flag and label results in accordance with calculations from the curve. For example, you may want to flag or use a custom label for samples that fall outside a defined concentration range. This is described further in Standard Curve Fit Custom Flag Labels.

> About label sample results that satisfy specified conditions without flagging them, see Applying Labels to Endpoint Data.

Custom Flag Label Levels

Flag labels can be set at the following levels:

1. By Transform Calculations
2. By Output Matrix
3. General

If there is a combination of custom flag labels defined, then they are handled in the order given above. Custom labels higher in the list take precedence over those further down the list (e.g., any specified in the transform implementation override any defined at both the output matrix and general level).

To apply a custom label to Flagged data using the **Properties | Matrices | Sample Labels** settings, see IsFlagged Sample Label.

XML Configuration

These advanced settings are only available through the XML editor. To access the XML editor, select the **XML** tab in the **Assay Properties** panel.

Custom Flag Label: General

The general custom flag label is the label to use in place of the default ~~Flagged~~ label. Note, when specifying custom flag text, strikethrough is not applied.

You can set the general custom flag label at the **Transforms** root level. All flagged data positions on any matrix (raw or calculated) will then use this setting. Enter the flag label with the following syntax:

<Transforms FlagLabel="No result" >

With this setting, the flagged data will appear as follows:

Sample	Positions	Raw	Concentration
⬤ Unknown1	A3	~~1.599~~	No result
	A4	~~1.665~~	

How to: Set General Custom Flag Label

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Locate the **Transforms** element.

3. Add the **FlagLabel** element to the **Transforms** element.

Custom Flag Label: By Output Matrix

A custom flag label can be set on any output matrix of any transform. This defines a common flag label to use for all data positions flagged by the transform.

Provide the label with the following syntax (editable label highlighted in yellow):

<Matrix Id="Calc1" Name="Calc1" FlagLabel="Outlier Removed" />

> 📝 This setting only applies to data points flagged by the transform.

How to: Set Custom Flag Label for an Output Matrix

1. Select the **XML** tab in the **Assay Properties** panel.
   If the **XML** tab is not immediately visible, click the **<< Show All Properties** button to expand.

2. Locate the **Transforms** element.

3. Locate **Output** element.

4. Add the **FlagLabel** element to the **Matrix** element.

Custom Flag Label: By Transform Calculations

The Standard Curve Fit and General Curve Fit transforms provide custom flag settings by calculation. For more details, see Custom Flag Labels by Fit Transform Calculations.

Custom Flag Label Reporting

The specified custom flag labels will be used in the report and export; however, the **Sample Table Replicates** setting of [matrices configuration](#) also impacts which labels are displayed. This is explained as follows:

- **List**

  For any flagged position that has a custom flag label associated with it, that custom flag label is displayed.

- **Average**

  In this case the flag label is displayed only if all positions in a sample group are flagged; otherwise, average of non-flagged data points is calculated. For the former, the following scenarios apply:

  1. If all positions have no custom flag label then the default flagging settings are used.

  2. If all positions have the same custom flag label, associated with them, then that custom label is displayed.

  3. If positions of a sample group have different flag labels associated with them, then the list of flag labels (custom and/or default) are displayed in the order of the positions. **Example**: If there are 3 positions in a group and they are all flagged (the first has no custom label, the second has custom label "Label A," and the third has custom label "Label B"), then "Flagged, Label A, Label B" will be displayed.

- **First**

  Any custom flag label associated with the first position is displayed.

Quick Protocol Editor

The Quick Protocol Editor allows users to edit custom protocol parameters like the **Standard Concentrations** or any configured **Macros** through a convenient editor without opening the protocol.

> ▶ Play Video

Launching the Quick Protocol Editor

1. Open the **MyAssays Desktop Explorer** and select **File | View** and **Show Quick Protocol Editor Button**
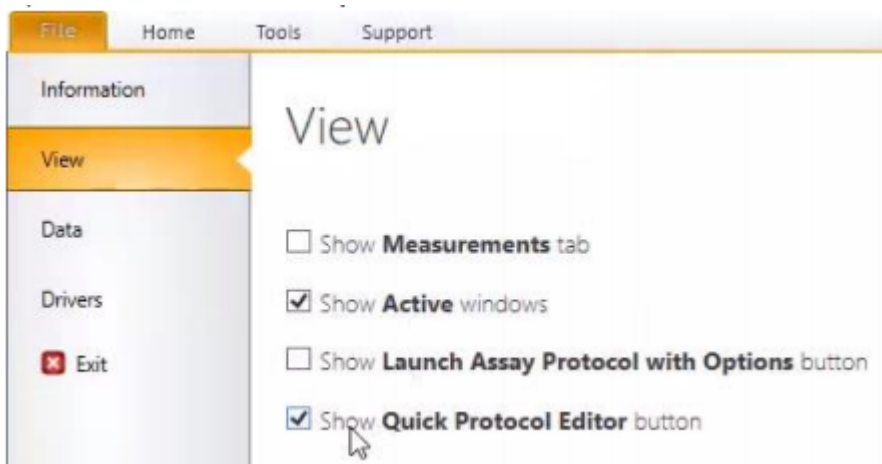
2. Under the **Protocols** tab, either select the **Quick Edit** button

Alternatively, right click on a protocol name and select **Open with MyAssays Desktop Quick Protocol Editor**.
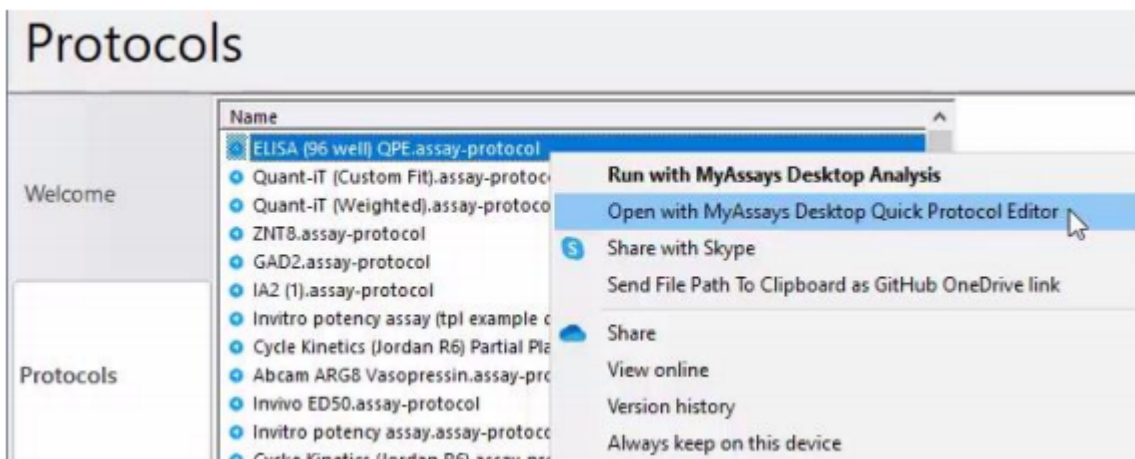
Using the Quick Protocol Editor

The Quick Protocol Editor can be used to edit common parameters. For example, if your protocol contains a Standard Curve Fit (or multiple standard curve fits), the standard concentrations values will be available for editing, as well as any parameters defined using Macros (Video Walkthrough...).

When the Quick Protocol Editor opens with a selected protocol, you can make changes to the applicable parameters, e.g.
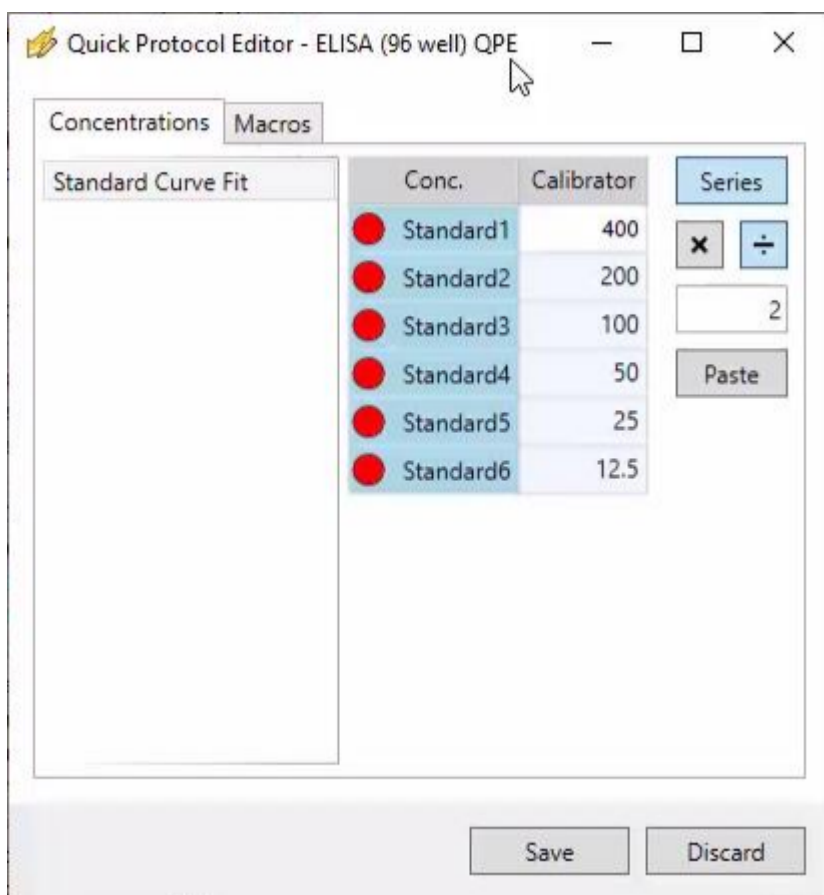
Make the necessary changes, and press **Save** to update the protocol.

Discard will exist without any changes being saved.

Editing Protocol Overview

The contents appearing in the **Overview** tab can be modified to include any useful information about the assay; this might include how to perform or use the assay or a description of the data analysis performed. Also, the assay name appearing in the tab can be modified.

> The provided **Name** applies only to the name appearing in the **Overview** tab (it does not change the file name of the assay protocol file).

Style Tags

The bold, italics and sub-script HTML style tags are available for use in the Overview **Name** and **Description**. For example:

Your text – displays as: **Your text**.

<i>Your text</i> – displays as: *Your text*.

H_{Your text}0 – displays as: $H_2 0$.

Resource References

In addition to specifying the assay name and overview text, use the Resource Reference feature to provide links to related content that might be useful to users of the assay. This might include SOPs or troubleshooting note; in fact links to any internal or external resources can be provided.

Editing Assay Protocol Name and Description

In the **Overview** pane, you can edit assay protocol's name and description by:

1. Launch an assay protocol file.

2. Right-click anywhere on **Overview** pane.

3. Click **Edit Overview**.

   This opens an **Edit Overview** dialog.

4. Enter or paste **Name** and **Description**.

5. To save changes, click **OK**.
   This updates the contents of the **Overview** pane accordingly.

Referencing External Resources in Protocol Overview

You can include links to any external resources associated with a protocol in the assay overview. For example, you could use this feature to link the assay-specific standard operating procedure (SOP) directly to the protocol.

 Play Video

The included resource references appear under the **Resources** section of the **Overview** tab. The reference can be applied to a single protocol or to all protocols produced by your MyAssays Desktop application. If both reference types are specified for the protocol, then protocol-specific links are displayed first.

> If you are using Enhanced Security edition, assign the users of your system to an authorization group where the **Analysis** | **Edit References** authorization is enabled. For more details about authorization settings, see Authorizations.

Link External Resources in the Overview

1. Launch an assay protocol file.

2. Right-click anywhere on **Overview** pane.

3. Click **Edit Resource References**.

   This opens **Resource Reference Manager**.

4. Depending on where you want to add links to, select:

   - **This Assay** tab to apply the references to the current assay protocol only.

   - **All Assays** tab to apply the references to all assay protocols.

   > Only Windows administrator account can make changes that apply to all users.

5. Click **Add Resource**.

6. For each added resource, configure **Text** and **Link**.
   To learn how the reference will appear in the Overview, see **How References Appear in Overview** below.

   To remove a reference, click the **Remove Reference** icon (✖) on the right of the Resource link field.

7. To save changes, click **Save**.
   This updates the contents of the **Overview** pane accordingly.

What Resources Can Be Referenced?

Using **Resource References Manager**, in the **Link** field, you can include references to:

- **Websites**. **Example**: www.myassays.com.

- **External Folder (Local or Domain)**. **Example**: **Local**: c:\MyInstrumentOutput\ **Domain**: \\server\MyInstrumentOutput.

- **External File (Local or Domain)**. **Example**: **Local**: c:\Conventions\SOP.docx **Domain**: \\server\Conventions\SOP.docx.

When the reference is clicked, the contents will be opened in the default associated application.

> If you reference a domain resource, make sure that users can log in to that resource. Otherwise, they will not be able to see the associated contents.

How References Appear in Overview

Each reference can be configured with Text, Link, or both. If you specify:

- Both **Text** and **Link**, the reference will include named hyperlink:

  Resources

  MyAssays Desktop Home Page

- Only **Link**, the reference will include exposed hyperlink:

  Resources

  https://www.myassays.com/myassays-desktop.html

- Only **Text**, the reference will include plain text:

  Resources

  MyAssays Desktop Home Page

Viewing Available Matrices and Configuring Their Settings

MyAssays Desktop stores all data sets in matrices. Each matrix can contain one or more samples, and for each matrix relevant transforms can be applied. You can configure the settings for each matrix in your assay through the **Matrices Tab**.

View Matrices Tab

1. Launch an assay protocol or open a results file.

2. In the **Assay Properties** panel, select the **Matrices** tab.
   If you cannot see **Assay Properties** panel, click **Properties** to open it.
   If the **Matrices** tab is not immediately visible, click **<< Show All Properties** to expand.

Selecting a Matrix to Configure

On the left-hand **Matrix Selection** pane, you can view a tree list with available matrices branched by their type:

Raw

These matrices contain the input data that is stored in the **Measurements Tab**. The quantity and type of **Raw** data matrices will depend on the assay type and configuration.

Calculated

All new matrices created and added by transforms are included in this branch.

Field

This branch lists all text matrices that are stored in the **Measurements Tab**. The presence, quantity, and type of **Field** data matrices will depend on the assay configuration.

Select a matrix for the list to see its configuration and applicable settings.

Applying Settings to the Matrix

Each input and output matrix of a newly added transform is automatically included in both Sample and Matrix Tables. With the following settings, you can configure what matrices will be displayed and how they will appear.

General

Name	A title for a matrix in the Sample Table and Matrix Table headers.
	If it is not specified, then the default title is used.

Numerical Formatting

Precision	The number of digits to be displayed for a numerical value. The interpretation of **Precision** depends on the **Type** setting.
Type	Specifies how a numerical value is formatted with regard to precision and rounding options: • **Significant Figures** – The value is reported to the specified number of significant figures. This accepts **Precision** values in range 1 through 14. • **All Significant Digits of Precision** – This setting displays all stored significant digits of precision using fixed-point notation or scientific notation. The result contains a decimal point if required, and trailing zeros after the decimal point are omitted. Fixed-point notation is used if the exponent that would result from expressing the number in scientific notation is greater than -5 and less than 15 digits of precision; otherwise, scientific notation is used. (MyAssays Desktop uses IEEE 754-2008-compliant double-precision floating-point numbers; providing up to 17 significant digits of precision.) • **Decimal Places** – The number of digits to display to the right of the decimal point. This accepts **Precision** values in range 0 through 14.

Report Contents

Include in Matrix Tables	Defines if the associated matrix will be included in the Matrix Tables.
Include in Sample Tables	Defines if the associated matrix will be included in the Sample Tables.
Matrix Table Ids	Defines in which Matrix Tables the associated matrix should be included.
Sample Table Ids	Defines in which Sample Tables the associated matrix should be included.

	Determines how replicates of each sample group are included in the Sample Table:
Sample Table Replicates	• **Average** – The average value of all replicates is displayed. This applies to **Endpoint** data only. • **List** – All replicate values are included in the table. This does not apply to **Field** matrices. • **First** – Only the first value is displayed. This simplifies the view of transforms that result in the same values for all replicates of each sample group (e.g., Average, XY Replicates Average).

Additional Settings for Endpoint Matrices

You can also apply the following settings to Raw and Calculated endpoint matrices.

Sample Labels

If a Label is specified, the **Condition** is evaluated for each position of the associated matrix and the **Label** is displayed in place of the value for the position. For additional details on this feature, see Applying Labels to Endpoint Data.

Value Bars

Within this category you can configure if and how to fill replicate values with colour for any **Raw** or **Calculated** endpoint matrix. The value bars are created using the minimum and maximum data values of the matrix. These are treated as 0% and 100%, respectively, and filled in accordingly.

Display Value Bars	Defines whether this feature is used in the Sample Tables.
Fill	Defines how to fill in the value bars: • **Solid** – Self-coloured with **Fill Colour**. • **Gradient** – Gradation from **Fill Colour** in the left to white on the right.
Fill Colour	Click the drop-down to open a colour picker and select the colour to fill the bars with.
Border	It defines how to fill in the value bar borders: • **Solid** – Self-coloured with **Fill Colour**. • **None** – Don't display the **Border**.

Value Colour Scales

For more flexibility in formatting your data analysis results, you can apply preset colour-scaling schemes for any **Raw** or **Calculated** endpoint matrix in the Sample Table, Matrix Table, or both. Using this functionality can simplify comparing value variance and distribution within a matrix.

When the colour scheme is applied, the values are shaded with gradations that correspond to minimum (smaller), midpoint (middle), and maximum (larger) values.

	Click the drop-down to select the colour scale scheme:
Value Colour Scales	**None** **Green-Yellow-Red** **Red-Yellow-Green** **Green-White-Red** **Red-White-Green**

Handling a Large Number of Raw and Field Matrices

When creating a new protocol via New Protocol Wizard, some readings may contain a large amount of input data including both raw matrices of data and field data matrices that accompany the measurements. Including all of these matrices will make the report excessively large and hard to manage. To avoid such complications, if the number of imported matrices exceeds the default matrix limit, MyAssays Desktop will notify you accordingly about their default exclusion.

All other matrices will be available for analysis, processing and reporting. This topic explains how to select and include additional matrices to your reports, and how the limit is applied.

Including Additional Matrices in the Report

For including any matrix in the report's Sample Table, Matrix Table, or both, follow these steps:

1. Launch an assay protocol or open a results file.

2. In the **Assay Properties** panel, select the **Matrices** tab.
   If you cannot see **Assay Properties** panel, click **Properties** to open it.
   If the **Matrices** tab is not immediately visible, click **<< Show All Properties** to expand.

3. From the **Matrix Selection** pane, select the matrix you want to include.
   The measurements and the field data matrices are stored under the **Raw** and **Field** branches, respectively.

4. In the **Matrix Configuration** pane, locate the **Report Contents** settings and select the **Include in Sample Tables** or **Include in Matrix Tables** check boxes to add the matrix to the associated report element.

5. Review or edit other data analysis settings.

6. Click **Calculate** to perform the calculations with the new settings and to see the results.

Refer to Viewing Available Matrices and Configuring Their Settings to learn more about configuration of the matrices.

How the Matrix Limit Is Applied

When importing data into a new protocol, the matrix limit restricts reporting the measurements and field data as follows:

- For raw data that contain more than 10 matrices, only the first matrix is included.

- For field data that contain more than 5 matrices, these matrices will all be excluded.
  See Adding Field Data Alongside Measurements to learn more about field matrices.

All of the imported data is stored inside the protocol's configuration and you can add the necessary data to your reports in the MAA.

> For advanced users, it is possible to change the number of matrices restricted by the limit. See Changing the Default Matrix Limit for Including Raw and Field Matrices for reference.

Applying Labels to Endpoint Data

Applying labels to data quickly draws attention to particular data analysis results. This section covers how, where, and what data you can apply a label to.

For example, for a qualitative assay you could label samples as "Positive" or "Negative" based on their relationship to control values.

For drawing attention to samples close or outside expected ranges, samples can be highlighted or labelled to clearly indicate possible issues. For example, you can label samples that:

- Are outside an acceptable threshold
- Close to the curve asymptotes
- Out of the within-run accuracy range

Any number of labels can be configured using a conditional expression. It's also possible to include graphical symbols as part of the label.

- About Labels
- Applying Sample Labels to Matrices
- Applying Evaluation Labels to Evaluation Results
- Configuring Labels
- Advanced (XML) Labels
- Reporting Matrix and Sample Table with Labels
- Reporting Evaluations Table with Labels
- Examples of Label Conditions

About Labels

Labels can contain text, numbers, symbols, and icons in place of or alongside the resulting value. Applying label, unlike flagging, does not exclude data from calculations, nor does it change the actual value used in subsequent calculations. It simply replaces the reported values with a specified label and applies any colouring to the text or background. This feature is useful for detecting and reporting samples that are outside expected ranges. For example, you might want to highlight or label samples whose concentration, response, or %CV is outside a specific range.

> Labels are not applicable to XY data matrices. To label XY data, use an XY Reduction transform and label the endpoint result.

The **Labels** editor is used to configure the labels for your assay. Depending on what you label, the title of the setting expands to:

- **Sample Labels** – For samples or replicates of raw, calculated, or field data matrices. The results with labels appear in associated matrix's Sample Table and Matrix Table.
- **Evaluation Labels** – For single evaluation result or all results in an evaluations table. The results with labels appear in Evaluations Table.

If sample values are outside the calculable limits of the transform and result in "**Flagged**", a custom label can be applied using **IsFlagged(x)**. For more information see IsFlagged Sample Label.

It is also possible to mark other data with labels. For more information, see Advanced (XML) Labels.

Apply Sample Labels to a Matrix

1. Launch an assay protocol or open a results file.

2. In the **Assay Properties** panel, select the **Matrices** tab.
   If you cannot see **Assay Properties** panel, click **Properties** to open it.
   If the **Matrices** tab is not immediately visible, click **<< Show All Properties** to expand.

3. Select one of the numbered matrices from under **Raw** or **Calculated** branch, which contains the data to label.
   If your assay contains field data, you can also select a matrix under the **Field** branch.

4. Click the **Sample Labels** drop-down of the Matrix Configuration pane.

5. Enter the condition (in terms of *x*) along with the label and any highlight or text colouring to apply.

6. Click **Add** to add further rules. Click outside the editor when you finish.

7. Click **Calculate** to perform calculations with the new settings and to see the results.

Apply Evaluation Labels to Evaluations Table or Evaluation

1. Launch an assay protocol or open a results file.

2. In the **Assay Properties** panel, select the **Evaluation** tab.

   If you cannot see **Assay Properties** panel, click **Properties** to open it.

   If the **Evaluation** tab is not immediately visible, click **<< Show All Properties** to expand.

3. Select **Evaluations Table** or **Evaluation**, which contains the data to label, and then click the **Evaluation Labels** drop-down.

4. Enter the condition (in terms of *x*) along with the label and any highlight or text colouring to apply.

5. Click **Add** to add further rules. Click outside the editor when you finish.

6. Click **Calculate** to perform calculations with the new settings and to see the results.

Label Settings

Label, colouring, or both are applied in accordance with the rules that you specify. You can define as many rules as you need. If a value satisfies multiple label conditions, then all corresponding labels are displayed in the report.

Condition	Label	Symbol	Highlight	Text
x < 0.05	{x} < 0.05	(None)	Yellow	(Default)

Add   Remove   More >>

ⓘ Use {x} in your label to refer to the original value.

You can add and remove any number of conditions and move them up or down with the corresponding arrow buttons. The rules are specified with the following editable text box properties:

Condition	A Boolean condition to evaluate (typically a conditional expression) in terms of *x*. The *x* value specified in the expression refers to: • A sample or replicate of the selected raw or calculated matrix. A different matrix can be specified using a Sample Label Matrix Modifier • A result of a single evaluation or all results in an evaluations table If the **Condition** is satisfied, the value is reported with the corresponding **Label** in place of its value.

Match	For **Field** data matrices, enter any text, numbers, or both to find and replace with the **Label**.
Label	Enter or paste text, numbers, symbols, or their combination to display if the **Condition** is satisfied or **Match** found. ⓘ Use **{x}** to refer to the original data value that is used in the condition.
Symbol	Select a graphical icon to display to the left of the **Label**: ○ **None** – Display no icon ○ **Pass** – Display a ✔ icon ○ **Fail** – Display a ✖ icon ○ **Question** – Display a ❔ icon
Highlight	Set the background colour for the cell when **Condition** is satisfied. Where there are multiple **Conditions** satisfied, the colour of the first satisfied **Condition** is applied.
Text	Set the text colour for the cell when **Condition** is satisfied. Where there are multiple **Conditions** satisfied, the colour of the first satisfied **Condition** is applied.

Additional Settings

Click **More>>** to expand editor with more configuration settings:

Sample Types	When configuring the labels for matrices, select the sample types to include when evaluating a **Condition**. By default, label applies to all sample types.
Highlight Row	Select this to apply a **Highlight** to the whole row and not just the cell. ⓘ Where there are multiple rules satisfied with **Highlight Row**, the colour of the first satisfied rule is applied. This applies to rules satisfied in the associated matrix or evaluation and rules satisfied in other matrices or evaluations (in case a label applies to the evaluations table).

Advanced (XML) Labels

In addition to the Sample and Evaluations Labels, you can also label other elements in the XML editor:

- Flagged replicates or sample groups. For more information, see Custom Flag Labels.

- Values flagged by Standard Curve Fit or General Curve Fit transform. For more information, see Custom Flag Labels by Fit Transform Calculations.

- Fit Table results of Dose–Response Curves transform. For more information, see Advanced Dose–Response Curves Evaluations.

Reporting Data with Sample Labels in Matrix Tables and Sample Tables

Conditions for sample labels are applied to the corresponding data included in the report:

- In the Matrix Table report element, the label or colouring applies to each position.

Example

Here is a Matrix Table output highlighting all sample measurements **>1.5** in yellow.

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.586	1.575	1.590	1.556	1.575	1.517	1.741	1.671	1.668	1.778	1.669	1.718
B	0.179	0.186	0.174	0.176	0.181	0.175	2.153	2.067	2.239	2.084	2.177	2.054
C	2.372	2.394	2.306	2.483	2.447	2.267	1.771	1.691	1.711	1.731	1.735	1.843
D	1.408	1.397	1.440	1.424	1.470	1.411	0.589	0.566	0.560	0.565	0.595	0.587
E	1.019	1.047	1.005	0.974	1.014	0.997	2.347	2.336	2.423	2.344	2.315	2.426
F	2.115	2.163	2.069	2.015	2.010	2.017	0.522	0.537	0.528	0.513	0.536	0.505
G	1.377	1.342	1.330	1.360	1.439	1.379	0.082	0.085	0.086	0.084	0.083	0.079
H	1.734	1.760	1.753	1.800	1.705	1.793	0.209	0.201	0.200	0.218	0.215	0.204

- In the Sample Table report element, you can configure each matrix to display the average of the sample group or list each replicate. (This can be set with the Sample Table Replicates setting in the Matrix configuration.)

Example

The following Sample Table has been configured with the Raw data listing all replicate values. In this case, the label is applied to each replicate that satisfies the rule.

Sample	Positions	Raw
🟢 Unknown1	A1	1.586 > 1.5
	A2	1.575 > 1.5
	A3	1.590 > 1.5
	A4	1.556 > 1.5
	A5	1.575 > 1.5
	A6	1.517 > 1.5

In the following example, the Sample Table has been configured with the Raw data listing the <u>average</u> of the replicates values. In this case, the label is applied to the computed average.

Sample	Positions	Raw
🟢 Unknown1	A1	1.566 > 1.5
	A2	
	A3	
	A4	
	A5	
	A6	

Example with {x} Reference

Here the Condition **x>1** and Label **>1** are specified for **Concentration** matrix. In this case, the calculation of the concentration for positions **A3** and **A4** is reported as **>1**.

Sample	Positions	Raw	Concentration
🟢 Unknown1	A3	1.694	>1
	A4	1.766	>1

Where label has been applied on the data and there is a **{x}** reference associated with the Label, the numeric value appears in the **Label**. For example, with the Condition **x>1** and Label **{x}>1**, the calculation results are reported as:

Sample	Positions	Raw	Concentration
🟢 Unknown1	A3	1.694	2.153>1
	A4	1.766	3.857>1

Reporting Evaluations Tables with Labels

Depending on what a label applies to, the report displays:

- A specific evaluation result with a label.

Example

Here the Condition **x**, Label **SSC={x}**, Highlight (**Orange**), and Highlight Row selected for SSC evaluation.

Description	Expression	Results
SSR	tov4.ssr	0.0220295
SSC	tov4.ssc	SSC = 0.00335946
Residual SumSquares	eval1.SSR+eval1.SSC	0.025389

- All associated evaluation results that satisfy the condition are reported with label.

Example

Here the Condition **x < 0.05**, Label **{x}<0.05** and Highlight (**Yellow**) are specified for Evaluations Table.

Description	Expression	Results
SSR	tov4.ssr	0.0220295 < 0.05
SSC	tov4.ssc	0.00335946 < 0.05
Residual SumSquares	eval1.SSR+eval1.SSC	0.025389 < 0.05

- Different labels are applied to both the evaluations table and a specific evaluation, both are reported but the label specified for evaluation takes precedence.

Example

Here the table is configured with Condition **x<0.05**, Label **{x}<0.05** and Highlight (**Yellow**), and SSC evaluation result contains label with Condition **x**, Label **SSC={x}**, Highlight (**Orange**), and Highlight Row selected:

Description	Expression	Results
SSR	tov4.ssr	0.0220295 < 0.05
SSC	tov4.ssc	SSC = 0.00335946
Residual SumSquares	eval1.SSR+eval1.SSC	0.025389 < 0.05

Examples of Label Conditions

Condition	Label Applied If
x<1	The value is less than 1.
and(x>0, x<1)	The value is in the 0–1 range.
x<Control1	The value is less than mean of **Control1** sample group.
x<eval1.ssr	The value is less than the result of the first evaluation (assuming that the 1st is assigned with a **ssr** name). See Named Evaluation Variables for more details of how to refer to such results.
x>TOV1.d	The value is greater than the d coefficient of the 4PL curve fit (assuming that the 1st transform is a Standard Curve Fit transform using the 4PL curve fit). See Transform Output Variables for more details of how to refer to such results.
x.2>x	The value of the sample on Matrix 2 is greater than the value of the sample on

Condition	Label Applied If
	the current matrix.
IsFlagged (x)	The value is Flagged

IsFlagged(x) Sample Label

The IsFlagged(x) function enables specific labels to be defined and used to indicate flagged results instead of the default strikethrough flagged text (such as **~~1.23~~** or **~~Flagged~~**).

How to: Use IsFlagged(x) Sample Label

1. In the **Assay Properties** panel, select the **Matrices** tab.
   If you cannot see **Assay Properties** panel, click **Properties** to open it.
   If the **Matrices** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Select one of the numbered matrices from under **Raw** or **Calculated** branch, which contains the data to label.

3. Click the **Sample Labels** drop-down of the Matrix Configuration pane.

4. Enter the condition **IsFlagged(x)** along with the label and any highlight or text colouring to apply.

5. Click **Add** to add further rules. Click outside the editor when you finish.

6. Click **Calculate** to perform calculations with the new settings and to see the results.

For example:

Specifying the condition **IsFlagged(x)** and the label **No Result** to the Concentration matrix:

Condition	Label	Symbol	Highlight	Text
IsFlagged(x)	No Result	(None) ▼	☐ (None) ▼	■ (Default) ▼

The flagged results appear in the Sample Table as follows:

Sample	Positions	Factor	Raw	Blank Corrected	Concentration
🟢 Unknown1	A3 A4	1	2.347 2.346	2.34550	No Result

IsFlagged(x) can also be used in more advanced expressions to identify certain conditions. For example, to label samples as > or < Curve.

Adding a label to the Concentration matrix specifying the condition **and(IsFlagged(x), x.2<min(tov2.a,tov2.d))** and the label **< Curve**, and a subsequent label with the

condition **and(IsFlagged(x), x.2>max(tov2.a,tov2.d))** with the label **> Curve** will identify samples that have flagged concentration values, and blank corrected values outside the limits of the a and d parameters of the curve.

Sample	Positions	Factor	Raw	Blank Corrected	Concentration
🟢 Unknown1	A3	1	2.347	2.34550	> Curve
	A4		2.346		

For more information on using Sample Label Matrix Modifiers, and TOVs, please see the associated topics.

IsFlagged(x) Reporting Scenarios

The specified custom flag labels will be used in the report and export; however, the **Sample Table Replicates** setting of matrices configuration also impacts which labels are displayed. This is explained as follows:

- **List**

  For any flagged position, the custom flag label is displayed.

- **Average**

  In this case the flag label is displayed only if all positions in a sample group are flagged; otherwise, average of non-flagged data points is calculated.

- **First**

  In this case, the flag label is displayed only if all positions in the sample group are flagged; otherwise, the first non-flagged data point is displayed.

Sample Label Matrix Modifiers

Sample Label Matrix Modifiers refer to a specific matrix within the Sample Report Label condition.

Syntax

The syntax for adding a sample label matrix modifier is **x.{N}** where N refers to the matrix number. Matrix numbering is 1-based, with the raw measurement data being matrix 1.

Examples

By adding the following expression to the Concentration matrix as a sample label:

and(x.1>tov2.a, x<Standard6)

Samples with raw values (located on matrix 1) greater than the a parameter of the standard curve, and concentration values less than Standard 6 will be labeled:

Sample	Positions	Factor	Raw	Blank Corrected	Concentration	Concentration (x Dil. Factor)	%
🟢 Unknown1	A3 A4	1	1.687 1.666	1.67550	11.3179	11.3179	11.
🟢 Unknown2	B3 B4	1	0.586 0.584	0.584000	80.3020	80.3020	0.2

Validation

You can automatically check that measurements and results are within expected ranges by using validations. Any configured validation tests are performed as a part of each assay run with the results (pass or fail) being clearly presented in the report. For example, you can test that the %CV of the replicates of all sample groups is less than 15.

- About Validations and Validations Tables
- Adding Validation to an Assay
- Changing the Sequence of Validations in a Table
- Deleting Validations Tables and Validations
- Configuring Validation Rules (with Examples)
- Validating Non-Matrix Data
- Validation Results

About Validations and Validations Tables

A validation is a rule defined using a Boolean condition. This condition is specified as an expression along with a matrix reference and type. If the condition evaluates to true, then the result for the validation is **Pass**. If the condition evaluates to false, the validation result is **Fail**.

For example, the validation condition expression

x<15

when associated with the %CV matrix and evaluated on all groups, checks that the %CV of all sample groups is <15.

Validation rules are arranged by Validations Tables in the **Validation** tab. It consists of two panes:

- **Tables** – For defining the tables that are available for inclusion in the report. You can create as many validations tables as you need and group related validations into tables accordingly. For example, you might want each validations table to appear on a different sheet in the report.
  For configuring the order, settings, and inclusion of each Validations Table, see Report contents.
- **Condition Configuration** – For specifying a condition for a validation rule.
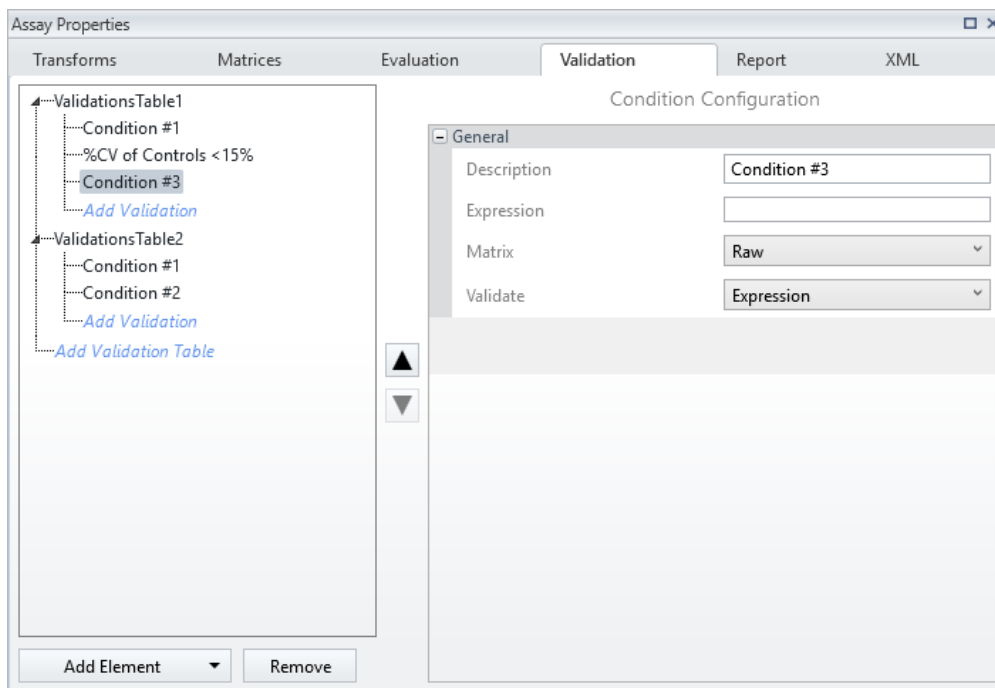
Add Validations Tables and Validations

1. Launch an assay protocol or open a results file.

2. In the **Assay Properties** panel, select the **Validation** tab.
   If you cannot see **Assay Properties** panel, click **Properties** to open it.
   If the **Validation** tab is not immediately visible, click **<< Show All Properties** to expand.

3. Add validation table for your assay with one of the following:

   - In the **Validations** pane, click **Add Validation Table**.

   - Below the pane, click **Add Element** button, and then select **Validation Table**.

   Each table is given a unique identifier (e.g., **ValidationsTable1**) and is automatically populated with a single validation element.

   Each element is given a description (e.g., **Condition #1**). You can change it immediately after adding or do so later, after you configure its settings. To change the description, right-click the **Condition** and select **Edit** from the drop-down list or, on the **Condition Configuration** pane, edit the **Description** setting.

4. Add more validations to this table with one of the following:

   - Under the validation element, click **Add Validation**.

- Below the pane, click **Add Element** button, and then select **Validation**.

> You may prefer to include all validations in a single table or arrange them between multiple tables. To add another table and populate it with validation conditions, repeat the steps **3** and **4**.

Change the Sequence of Validations

You can set the order in which the validation conditions appear in the selected validations table. To do this, select the evaluation you want to move and click **Up** or **Down** arrow button on the right of the **Validations** pane.

> The validations cannot be moved between the tables.

Delete Validations Tables or Validations

To delete a table or condition from your assay, do one of the following:

- Right-click on the item and select **Remove** from the drop-down menu.
- Select the item and click **Remove** button below the pane.

> If you delete a **Validations Table**, all associated conditions are also deleted.

Configure Validation Rules

The **Condition Configuration** pane is used to specify the selected validation's condition.

Condition Configuration Settings

To set up a condition to a validation rule, define the following settings:

Description	Use this to provide a clear textual description; this is used in the report to convey what has been validated. The other way to change description is to right-click on the condition in the Conditions pane's tree view and select **Edit**.

Expression	The **Expression** setting is used to define the validation expression Boolean condition. This is typically an expression with a [logical operator](#) and perhaps a [conditional function](#). The interpretation of the expression depends on the **Validate** setting. For a complete description of available expression functionality, see [Expressions](#).
Matrix	Select the matrix the **Condition** applies to from the drop-down list. For example, if you plan to validate measurement data (i.e., a **Raw** matrix), select the **Raw** matrix to validate. Any of the raw or calculated matrices that contain endpoint data can be validated. If there are no available matrices, then the (NA) label appears. In this case, validation conditions can still be created that do not refer to endpoint matrix data. Validation conditions are not applicable to XY data matrices. To validate XY data, use an [XY Reduction transform](#) and validate the endpoint result.

Validate	Click on the drop-down and select how to evaluate the **Expression**:
	Expression – The expression is evaluated once on the specified matrix of each container (useful for checking specific sample groups). **Example**: **Standard1<Standard2** validates that the average of **Standard1** replicates is less than those of **Standard2** on the specified matrix (for multiple plate assays, this condition is evaluated on every plate).
	Expression with Every Sample Group (x) – The expression is evaluated in terms of *x* for every sample group on the matrix of every container. A sample group reference *x* refers to the average of the replicates that belong to the group that are not flagged. **Example**: to check that the average value of each group in a matrix is less than 3, use the **Expression with Every Sample Group (x)** setting with the expression **x<3**. In this case, the average of every sample group (on the selected matrix) is validated.
	Expression with Every Sample Replicate (x) – The expression is evaluated in terms of *x* for every sample replicate on the matrix of every container. The *x* reference here is expanded to value at each position. **Example**: to check that the value at every measured position in a matrix is greater than 0.5, then use the **Expression with Every Sample Replicate (x)** setting with the expression: **x>0.5**. In this case, every data point (on the selected matrix) is validated.
Sample Types	Specify which sample types to evaluate an **Expression with Every Sample Replicate (x)** or **Expression with Every Sample Group (x)** expressions on. By default, these validation expressions are evaluated for all sample types. If you only want to test specific sample types, then use this setting.

Examples of Condition Expressions

Here are examples of validations along with descriptions of their behavior. They apply the validation on the selected data matrix.

Type	Condition	Validates
Expression with Every Sample Replicate (x)	*x*<2.5	All positions (that are not flagged) have a value less than 2.5.
Expression with Every Sample Replicate (x)	and(*x*>0,*x*<2.5)	All positions (that are not flagged) have a value greater than zero and less than 2.5.
Expression with Every Sample Group (x)	*x*<2.5	The average of the replicates (that are not flagged) of all sample groups is less than 2.5.

Type	Condition	Validates
Expression with Every Sample Group (x)	and(*x*>0,*x*<2.5)	The average of the replicates (that are not flagged) of all sample groups is greater than 0 and less than 2.5.
Expression	Control1<1.5	The average of Control1 replicates (that are not flagged) is less than 1.5.
Expression	sd(Control1)<10	The standard deviation of the Control1 replicates (that are not flagged) is less than 10.
Expression	pcv(Control1)<15	The %CV of the Control1 replicates (that are not flagged) is less than 15.
Expression	median (Control1)>0.75	The median of the Control1 replicates (that are not flagged) is greater than 0.75.
Expression	TOV1.R2>0.9	The R^2 value of the curve fit (as used in the first transform) is greater than 0.9. (The R^2 value is referenced using a Transform Output Variable).

Validate Non-Matrix Data

In addition to validating matrix data, it is also possible to validate other types of numerical data. For example, you may want to verify that the R^2 value of a curve fit is greater than a specific threshold. These types of validations can be defined using the **Expression** type and referring to the data to validate within the expression. This is typically using a Transform Output Variable (TOV). The TOVs that are available depend on your configured transforms.

For example, the expression **TOV1.R2 > 0.9** checks that the R^2 value of the curve fit (as used in the first transform) is greater than 0.9.

Validation Results

Validation conditions are checked when the data analysis is performed (after all transform calculations). All validations are evaluated irrespective of whether they are included in the report. In any case, the results of each validation test are listed in the Calculation log.

Each validation test verifies the result in terms of the specified Boolean condition.

The results appear in the associated Validations Table in the report and are marked as **Pass**, **Fail**, or **Inconclusive** accordingly:

✔ **Pass**

If the validation condition is true (the numerical result ≠ 0).

> For **Expression with Every Sample Replicate (x)** and **Expression with Every Sample Group (x)** validations, the result is **Pass** only if all positions or groups evaluate to true.

❌ Fail

If the validation condition is false (the numerical result = 0). For **Fail**, the whole validation table row is highlighted with yellow background.

❓ Inconclusive

If the validation expression could not be evaluated (e.g., a syntax error in the expression), the result is treated as **Inconclusive** with the error message shown in **Results** column (in red text).

If you apply any new or modified settings to validation rules, click **Calculate** and inspect the report to see the results.

Evaluation

To calculate and present specific quantities of interest in the report, you can use MyAssays Desktop's Evaluation feature. For example, you can compute and report the limits of detection of an assay using an evaluation. The topics in this section cover how to add, define, label, and format evaluations.

- About Evaluations and Evaluations Tables
- Adding Evaluations to an Assay
- Changing the Sequence of Evaluations in the Table
- Deleting Evaluations Tables or Evaluations
- Configuring Evaluation Settings (with Examples)
- Named Evaluation Variables
- Evaluation Results

About Evaluations and Evaluations Tables

Evaluations are expression-based calculations that result in a single numerical value and can be referenced in other calculations.

Evaluations are arranged and reported as Evaluations Tables. Any value that can be referenced or computed can be included in an Evaluations table. Each evaluation can be given a description to accompany the result. If there is an error in evaluating the expression, then the error message is reported (in red) as the result.

It is useful to group related evaluations into Evaluations Tables accordingly. You can add as many evaluations as you need to each Evaluations Table. You can create as many tables as you need and configure how and if they are reported.
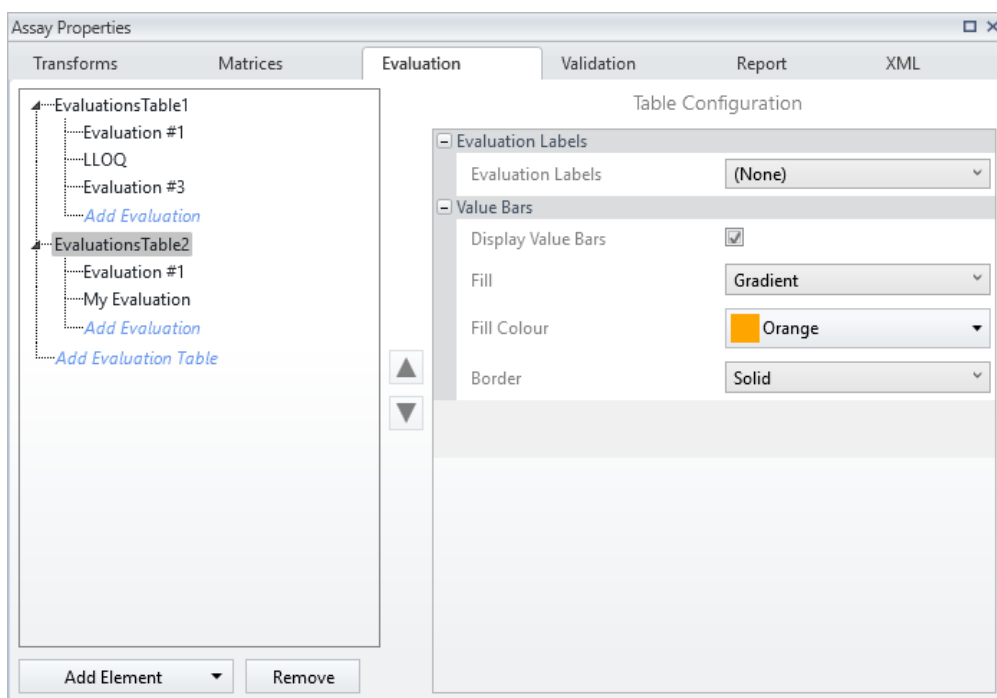
Add Evaluations Tables and Evaluations

1. Launch an assay protocol or open a results file.

2. In the **Assay Properties** panel, select the **Evaluation** tab.
   If you cannot see **Assay Properties** panel, click **Properties** to open it.
   If the **Evaluation** tab is not immediately visible, click **<< Show All Properties** to expand.

3. Add evaluation table for your assay with one of the following:

   - In the **Evaluations** pane, click **Add Evaluation Table**.

   - Below the pane, click **Add Element** button, and then select **Evaluation Table**.

   Each table is given a unique identifier (e.g., **EvaluationsTable1**) and is automatically populated with a single evaluation element.

4. Add more evaluations to this table with one of the following:

   - Under the evaluation element, click **Add Evaluation**.

   - Below the pane, click **Add Element** button, and then select **Evaluation**.

Each element is given a description (e.g., **Evaluation #1**). You can change it immediately after adding or do so later, after you configure its settings. To change the description, right-

click the **Evaluation** and select **Edit** from the drop-down list or, on the **Expression Configuration** pane, edit the **Description** setting.

> You may prefer to include all evaluations in a single table or arrange evaluations between multiple tables. To add another table and populate it with evaluations, repeat the steps **3** and **4**.

Change the Sequence of Evaluations

You can set the order in which the evaluations will appear in the selected Evaluation Table. To do this, select the evaluation you want to move and click **Up** or **Down** arrow button on the right of the **Evaluations** pane.

> The evaluations cannot be moved between the tables.

Delete Evaluations Tables or Evaluations

To delete a table or evaluation from your assay, do one of the following:

- Right-click on the item and select **Remove** from the drop-down menu.

- Select the item and click **Remove** button below the pane.

> If you delete an **Evaluations Table**, all associated **Evaluations** are also deleted.

Configure Evaluations and Evaluations Tables

Depending on what you are configuring, the right pane expands to:

- **Table Configuration** – For configuring settings of the selected Evaluations Table. This includes filling the results with colour and value bars, and applying labels on all results in this table.

Evaluations Tables Settings

On this pane you can define how the table will appear. In addition to the settings described here, you can configure the Evaluations Table report element settings.

> Each evaluation table is a separate report element and can be configured separately. For example, you might want each evaluation table to appear on a different sheet.

Evaluation Labels

Evaluation Labels	Use this to replace the results of any evaluations included in this table with a label you specify. Label is applied if the results meet the condition and can contain text, numbers, symbols, and icons in place of or alongside the resulting values. ⓘ A label applied here is overriden by any defined for the associated Evaluation. To learn more about how to configure and use this feature, see Applying Labels to Endpoint Data.

Value Bars

The value bars are created using the minimum and maximum values of the evaluated results in the table. These are treated as 0% and 100%, respectively, and filled in accordingly.

Display Value Bars	Select to fill evaluation result values with colour in the report.
Fill	Click the drop-down and choose how to fill in the value bar: • **Solid** – To fill value bars self-coloured with **Fill Colour**. • **Gradient** – To fill value bars with the gradation from **Fill Colour** in the left to white on the right.
Fill Colour	Click the drop-down to open a colour picker.
Border	Click the drop-down and choose how to fill in the value bar's border: • **Solid** – To fill value bars self-coloured with **Fill Colour**. • **None** – To not display the **Border**.

- **Expression Configuration** – For setting up the selected **Evaluation**. Here you specify an expression to evaluate, how to format the result, and assign a name for the result to reference it in further calculations. Formatting settings and naming the result are optional. Also, you can specify a label to report instead of the resulting value.

Evaluation Expressions and Settings

Each Evaluation is defined with the following settings.

Evaluation Labels

Evaluation Labels	Use this to replace the evaluation result with a label you specify. Label is applied if the result meets the condition and can contain text, numbers, symbols and icons in place of or alongside the resulting value.
	ℹ️ A label applied here overrides any defined for the associated Evaluations Table.
	To learn more about how to configure and use this feature, see Applying Labels to Endpoint Data.

General

Expression	Defines the expression to evaluate. This might reference a specific sample group or position on the selected matrix. It may also perform a calculation or function. The evaluation applies on the non-flagged samples of the selected endpoint **Matrix** or on non-matrix data.
	For a complete description of available expression functionality, see Expressions.
Description	Use this to provide a clear textual description; this will be used in the report to convey what has been evaluated.
	The other way to change this is to right-click on the evaluation in the Evaluations pane's tree view and select **Edit**.
Matrix	Select the matrix the **Expression** applies to from the drop-down list. For example, if you plan to evaluate a quantity using measurement data (i.e., a **Raw** matrix), select the **Raw** matrix. Any of the raw or calculated matrices that contain endpoint data can be referenced in an evaluation. Also, it is possible to evaluate non-matrix data (such as Transform Output Variables).
	ℹ️ If there are no available matrices, then the (NA) label appears. In this case, you can still create evaluations that do not refer to endpoint matrix data.
	📝 Evaluations are not applicable to XY data matrices. To perform an evaluation on XY data, first use an XY Reduction transform and evaluate the endpoint result.

Name	Designates a name to the evaluation result. The named evaluation can be referenced in other calculation as a variable. See Named Evaluation Variables for more details.

Numerical Formatting

Precision	The number of digits to be displayed for a numerical value. The interpretation of **Precision** depends on the **Type** setting.
Type	Specifies how a numerical value is formatted with regard to precision and rounding options: • **Significant Figures** – The value is reported to the specified number of significant figures. This accepts **Precision** values in range 1 through 14. • **All Significant Digits of Precision** – This setting displays all stored significant digits of precision using fixed-point notation or scientific notation. The result contains a decimal point if required, and trailing zeros after the decimal point are omitted. Fixed-point notation is used if the exponent that would result from expressing the number in scientific notation is greater than -5 and less than 15 digits of precision; otherwise, scientific notation is used. (MyAssays Desktop uses IEEE 754-2008-compliant double-precision floating-point numbers; providing up to 17 significant digits of precision.) • **Decimal Places** – The number of digits to display to the right of the decimal point. This accepts **Precision** values in range 0 through 14.

Examples of Evaluation Expressions

Here are examples of expressions along with descriptions of their behavior.

For a complete description of the expressions available, see Expressions section.

Evaluates	Computes
Control1	The average of all Control1 replicates
Control1/Control2	The ratio of Control1 and Control2
sd(Control1)	The standard deviation of the Control1 replicates
pcv(Unknown1)	The percentage coefficient of variation of **Unknown1**.
Blank1+(3*sd(Blank1))	The average of the sum of **Blank1** plus 3 times the standard deviation of **Blank1** (this is often used to

Evaluates	Computes
	compute LLD).
pcv ([Unknown1,Unknown2])	The percentage coefficient of variation of all **Unknown1** and **Unknown2** replicates.
median(Unknown.2.All)	The median of all Unknowns on the 2nd matrix across all containers.

Named Evaluation Variables

When evaluating non-matrix results for an assay, it is useful to refer to the evaluation results from other calculations. A Named Evaluation Variable (NEV) is simply an evaluation result that has been assigned a name. The NEV can be referenced using expressions in:

- Evaluation expressions (that follow its definition)
- Validation conditions
- Label conditions

Referencing Named Evaluation Variables

The syntax for referencing NEVs in expressions is as follows:

eval{N}.{Name}

Where:

{N} – 1-based Evaluations Table index

{Name} – The name assigned to the evaluation

> All calculations are computed in the order they are defined in the Report Elements pane, therefore ensure that Evaluations Tables appear earlier in the sequence of the included elements to where they are referenced. (To change the actual report content ordering, use a Report Template.)

For example, to refer to a NEV in the Sample Label configuration, the Evaluations Table must be above the Sample Table and, if included, Matrix Table in the report elements order.

Evaluation Results

Unlike the Sample Table or Matrix Table report elements (which display the results of a calculation performed on each sample), an Evaluations Table reports calculations that return a single numerical result.

All evaluations are performed irrespective of whether they are included in the report. You can configure how and if the Evaluations Tables are reported. In any case, the results of each evaluation are listed in the Calculation log.

Evaluations are computed when the data analysis is performed (after all transform calculations). To apply any new or modified settings, click **Calculate** and inspect the report to see the results.

> To calculate a result for every sample, use a transform with the results for each sample displayed in the Sample Table or Matrix Table.

Specifying the Report Content

The report is the primary output of the data analysis process. You can use MyAssays Desktop's comprehensive functionality to specify:

- **Content** – What elements of the performed data analysis will be featured in your report.

- **Presentation** – The order and inclusion of elements, and any additional styling specified.

- **Export** – The format in which your report will be output.

By using these options, you can customize your report to display the data exactly as you require.

Within the MyAssays Desktop Application, the report can be displayed as **Sheet View** or **Page View**; these settings are available in the **Report** ribbon tab. When getting started, we suggest using the Sheet View so that your outputs are not confined by the limitations of a printed page. Use the Page View only if and when the layout of the printed page is important. You can also define a report template to apply to your MyAssays Desktop output.

About Report Content

The content available for inclusion in the report depends on the configuration of each of the following settings (these each correspond to a tab in the **Assay Properties** pane):

- **Transforms** – Any configured transforms will result in calculated elements (such as numerical results or charts).

- **Matrices** – The settings of each matrix (raw measurement data and any calculated) can be configured. This includes how numerical data is presented (numerical formatting settings), if it is included, how replicate values are reported, and any optional coloured value bars.

- **Evaluation** – Any configured evaluation settings will result in one or more evaluations tables, each listing the results of the computed evaluations.

- **Validation** – Any configured validation settings will result in one or more validations tables, each listing the results (pass or fail) of the computed validations.

Various report elements are available depending on these settings. For example, if a curve-fitting transform such as the Standard Curve Fit is configured, you can include the calculated concentrations in a Sample Table and/or Matrix Table, along with the transform-specific elements such as fit chart and equations. Each of the included elements can be configured further.

> ℹ️ All MyAssays Desktop reports are generated using **Tahoma 10pt** font by default.

Report Element Configuration

The ordering and basic configuration of each report element is defined in the **Report** tab.

View Report Tab

1. Launch an assay protocol or open a results file.

2. If you cannot see the **Assay Properties** panel, click **Properties** to open it.

3. Select the **Report** tab.
   If the **Report** tab is not immediately visible, click **<< Show All Properties** to expand.

4. Review and edit the report elements as required.

The **Report** tab consists of two panes:

- **Report Elements** – This pane manages the report elements and their ordering.

- **Report Configuration** – This displays the available settings for the selected report element.

Report Elements Pane

The **Report Elements** pane lists the elements that will be included in the report. Their ordering reflects the order in which they will be added to the report.

Click **Add Element** to add a new report element. A list of available report elements will appear. The selected item will be added to the end of the list.

Click **Remove** to remove the selected report element.

To change the ordering of report elements, select an item and use the **Up** or **Down** arrow buttons on the right of this pane.

Report Configuration Pane

The **Report Configuration** pane displays the properties of the selected report element. The actual settings depend on the element; however, there are a number of common settings:

General

Id	Each report element is automatically given a unique identifier (Id). This identifier is used to identify the report element when configuring custom report templates (It is also used for advanced settings such as custom export and XML configuration). 📝 For general use, it should not be necessary to change the name of the identifier.
Include	This check box can be used to exclude the report element (without deleting the settings).
Title	Optionally provided title for the report element. When specified, the title appears immediately before the element. This property can refer to report macros (such as **{PlateNum}**, **{PlateID}** and **{AnalyteName}**) to automatically refer to the associated data. If a title is not specified, then the element is displayed without any title.

Sheet

Sheet Name	This setting defines the name of a sheet to contain the report elements. This is only applicable to sheet-based content such as Excel output or data in the **Sheet View**. Each report element can be included on its own separate sheet or elements can be added together on the same sheet. Where a common sheet name is used across report elements, the elements are added in the order as defined in the **Report Elements** pane. A custom sheet order can be defined using the **Sheet Name (CSV)** setting This property can refer to report macros (such as **{PlateNum}**, **{PlateID}** and **{AnalyteName}**) to automatically group associated content into a sheet of the same name. Note, if **Sheet Name** is defined for one report element, then the report content is exported on one sheet with provided **Name**.

📝 When viewing report content in **Sheet View**, the sheet names appear in the bottom left of the **Report** tab (in the **Results** tab). If there is only one named sheet, then this sheet name will not appear.

Report Elements and Multiple Plate or Multiplex Analyses

If your assay is comprised of measurements across multiple plates or measurements for multiple analytes (multiplex assay), then the report will contain an element for each plate or analyte.

To help arrange this type of content into an easy-to-navigate report, we recommend using the **Sheet Name** setting to arrange content into separate sheets.

For example, with a multiple plate assay, set the **Sheet Name** setting to:

Plate {PlateNum}

With this setting applied to a Sample Table element, the results for each plate will appear in a separate worksheet named by the plate number (such as Plate 1, Plate 2, Plate 3, etc.).

Using **Plate {PlateID}** for multiple plate and **Analyte {AnalyteName}** for multiplex assays, you can arrange the results from each plate/analyte into separate worksheets titled by their provided IDs (as configured in **Measurements** | **Plate IDs**/**Analytes**).

Report Macros

The following table lists the macros that are available for use in the **Title** and **Sheet Name** properties.

Macro	Expands To
{PlateNum}	1-based plate number
{ContainerNum}	1-based container number (for a multiple plate assay, this is the plate number; for multiplex, this is the analyte number)
{PlateID} {PlateName}	The plate ID as it appears under the **Measurements**	**Plate IDs**
{AnalyteName}	The analyte name as it appears under the **Measurements**	**Analytes**
{ContainerName}	For a multiple plate assay, this is the plate name; for multiplex, this is the analyte name

> You can combine these macros with other text. For example, **Plate {PlateNum}** will be expanded to **Plate 1** for the first plate.

Report Elements

To simplify configuration, various report elements are automatically added to the report and configured with default settings as you add new steps to your analysis:

- The Sample Table is the most widely used report element, so it is included by default in all configurations. The Sample Table displays the results of each defined sample group (in accordance with the defined layout).

- If any Evaluation or Validations are configured, an Evaluation or Validation report element will be added automatically.

- If any transform generates additional content, a Transform Content element will automatically be added. For example, the Standard Curve Fit transform produces a standards chart, concentrations table, and equations; this content is automatically added to the report as a Transform Content report element.

You will see these elements appear automatically in the **Report Elements** pane of the **Report** tab. You are free to edit or delete this default content as you require. If analysis steps are removed, then the associated report element will also be automatically removed.

Beyond the automatically added report elements, you can further add your own elements to the report:

How to: Add a Report Element to the Report

1. Select the **Report** tab.

   If the **Report** tab is not immediately visible, click **<< Show All Properties** to expand.

2. In the **Report Elements** pane, select the required report element from the **Add Element** drop-down list.

3. Review and edit the element's settings as required.

4. Click **Calculate** to perform calculations with the new settings.

The following table summarises each available report element. Further details and settings are included in the provided linked topics.

Report Element	Description
Curve Overlay	An overlaid chart displaying two or more curves for visual comparison. This is an advanced report element that is configured and included in the report through XML.
Evaluations Table	The details and results of any configured evaluations arranged in a table.
Histogram	The Histogram represents the data by displaying the average of each sample in vertical columns. Each sample is denoted by a bar matching the colour of its sample type. In addition, to indicate the error or uncertainty in a reported measurement or calculated data, the variability of data can be

Report Element	Description
	represented with optional error bars.
Layout	A graphical representation of the sample layout.
Matrix Table	The results displayed in a matrix-table structure. For endpoint data, a numerical value is reported. For XY data, a thumbnail plot is displayed. Each raw or calculated matrix can be marked for inclusion or exclusion in a matrix table using the **Report Contents** section of the Matrices tab.
Matrix View	A layout-based representation of the matrix data. For endpoint data, a numerical value will appear at each position. For XY data, a plot will appear at each position. The colour of each position can be determined using the layout colour or with a heatmap to represent the endpoint value intensity.
Measurement Meta Data	A table listing the measurements meta data (reported as name value pairs). This corresponds to the data as it appears under the **Measurements** | **Meta** tab.
Notes	Any notes associated with the assay run. Notes can be entered using the **Notes** button in the **View** section of the **Home** tab.
QC Results	Inter-assay quality control results (as defined by Quality Control settings). This could include Observation Table, Levey-Jennings, CUSUM, or Control Charts reporting the latest results along with historical results.
Sample Table	A table reporting the results of each defined sample group (in accordance with the defined layout). Each row contains the data for a specific sample group. For endpoint data, a numerical value is reported. For XY data, a thumbnail plot is displayed. Each raw or calculated matrix can be marked for inclusion or exclusion in a sample table using the **Report Contents** section of the Matrices tab.
Text	A textual information element allowing the optional inclusion of macros.
Transform Content	Various report elements generated as a consequence of a specific transform.

Report Element	Description
	For example, a Standard Curve Fit transform adds a concentration table, a chart, and equations to the report as Transform Content report elements.
Validations Table	The details and results of any configured validations arranged in a table. Each validation result is reported as a pass or fail.
XY Plot	A chart that includes position plots for one or more XY positions. 📝 This is an advanced report element that is configured and included in the report through XML.

Selecting the Data to Include in a Sample Table/Matrix Table

The data to include in a Sample Table or Matrix Table can be configured on a matrix-by-matrix basis. For example, you may want to include only certain matrices in your tables, perhaps excluding the results of intermediary data analysis steps.

The easiest way to specify which data to include in your Sample Tables or Matrix Tables is to use the matrix options: **Include in Matrix Tables** and **Include in Sample Tables**. These settings are available for each matrix. To access these settings, select the **Matrices** tab and select the matrix to edit. These settings apply to all of the Sample Tables or Matrix Tables in your report.

📝 For each matrix, the **Sample Table Replicates** setting can be used to specify how to report the values for replicates in the Sample Table on a matrix-by-matrix basis.

Working with Multiple Sample Tables or Multiple Matrix Tables

You may want to include multiple Sample Tables or Matrix Tables in your report with each reporting different aspects of the data.

When working with multiple tables, you might require control over which data to include in which Sample Tables or Matrix Tables. The **Sample Table IDs** and **Matrix Table IDs** settings can be used to select which tables each matrix should be included in. The table Ids correspond to the report element Ids of the Sample Table or Matrix Table (as defined in the **Report** tab).

📝 Each table could be configured to report data for different sample types using the Sample Table's **Type** setting.

Report Elements

Curve Overlay Chart Configuration

> 📝 This is an advanced feature that can only be configured through the XML editor.

A Curve Overlay Chart can be used to plot curves from different sources to compare them on a single chart. It's possible to include a chart from the current analysis or a chart made on a previous run. The overlaid charts can originate from analyses computed by the Standard Curve Fit, Standard Curve Fit (from Library) or General Curve Fit transforms.

For example:
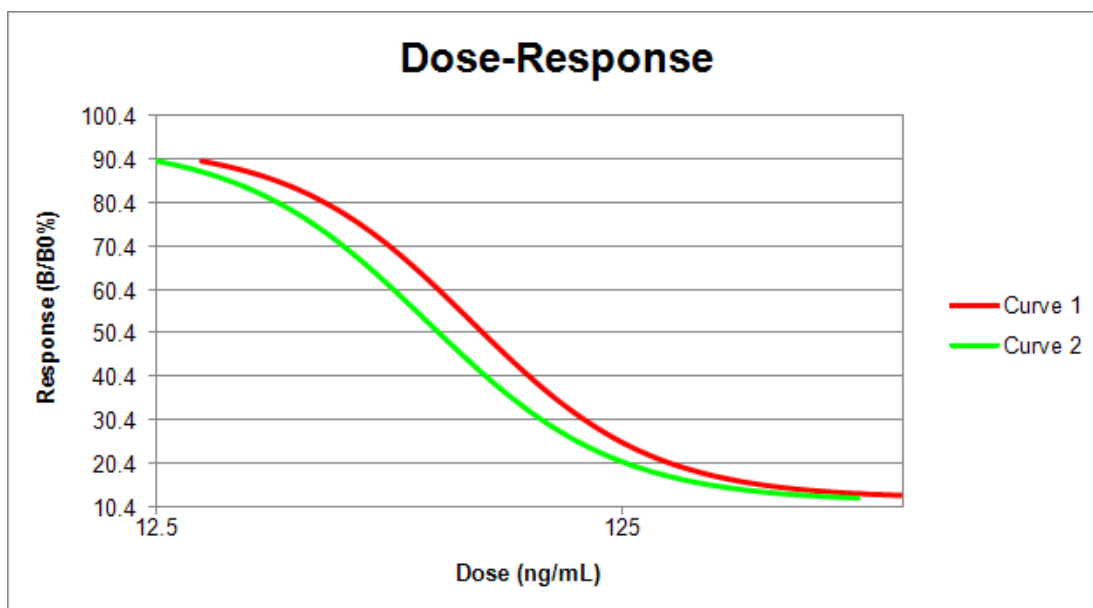
Here, the Curve Overlay chart is titled **Dose-Response**. It contains two overlaid curves named **Curve 1** and **Curve 2**. Also, the axes titles and types are defined.

It's also possible to compute values from each curve using the Curve Overlay Evaluations feature:

Dose-Response
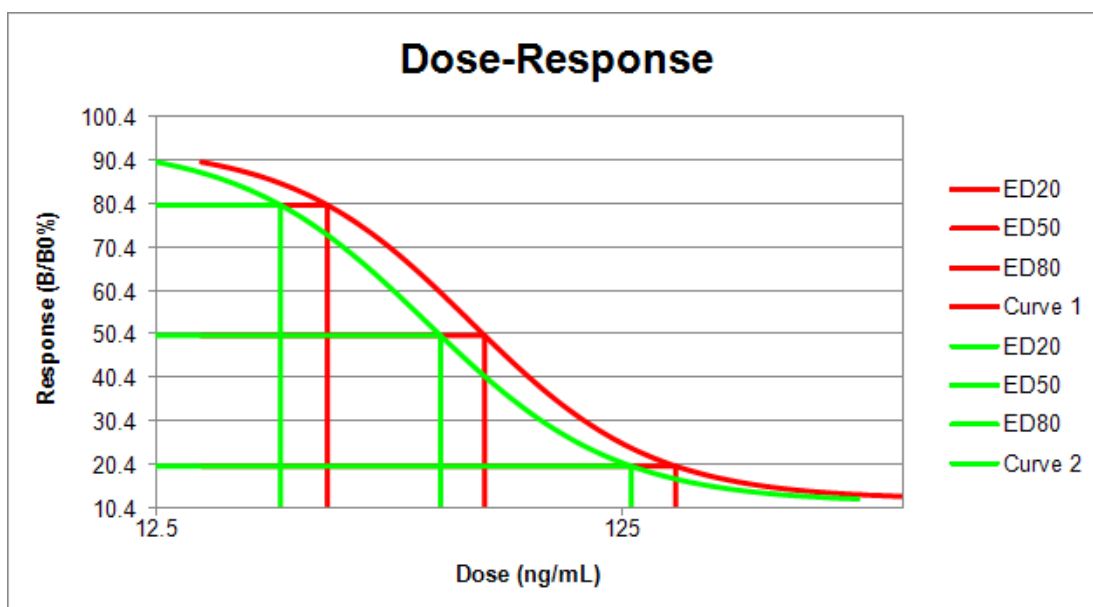
Settings and Configuration

You can configure one or more Curve Overlay charts to include in your report. Specify their attributes and syntax in the XML Editor as described below.

How to: Add Curve Overlay Configuration to Report

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Locate the **Report** element and add the **CurveOverlay** child element and then specify its settings as described below.

3. Add a child element **Curves** and for each curve add a child element **Curve** and define its attributes.

4. Click **Apply** to save changes to the protocol and then **Calculate** to generate new report.

CurveOverlay Attributes

On this level, specify general settings that apply to a Curve Overlay chart.

General

Id	A unique identifier that is used to identify the report element in the Report Elements pane and when configuring custom report templates.
SheetName	If defined, inserts curve overlay chart to a sheet with the specified SheetName. For more details, see Sheet Name in the Report content section.

Title	An optional title for a curve overlay chart that can refer to <u>Report Macros</u>. If not specified, then a default "Curve Overlay" title is displayed.
Include	Boolean setting that defines whether the curve overlay chart is included in the report.

You can also optionally specify axes settings. If any of them is not specified, then the setting from the first defined curve is used.

Axes

XAxisTitle	The name of the x-axis on the chart.
XAxisType	The scale type to be used for the x-axis: • **Logarithmic** • **Linear**
XAxisPrecision	The precision to plot the x-axis with.
YAxisTitle	The name of the y-axis on the chart.
YAxisType	The scale type to be used for the y-axis: • **Logarithmic** When y-axis is logged, negative (or zero) *y* values are not included in the plot. • **Linear**
YAxisPrecision	The precision to plot the y-axis with.

This is specified in the XML editor inside the **CurveOverlay** element with following syntax:

<CurveOverlay Id="*Id*" SheetName="*Name*" XAxisTitle="*Title*" YAxisType="*Type*" YAxisTitle="*Title*" XAxisType="*Type*" Title="*Title*">

Curve Attributes

Specify each curve to include in the chart with the following attributes:

TransformNum	This refers to 1-based number of the transform in the sequence. The references transforms must be <u>Standard Curve Fit</u>, <u>Standard Curve Fit (from Library)</u>, or <u>General Curve Fit</u>.

FilePath	When referencing a Library Curve file: • For files stored in the **Curves** folder of your MyAssays root folder, enter or paste curve.xml filename without the folder. • For files stored in other locations, provide a full file path to an existing curve.xml file.
Name	A title for a curve on the chart.

> The **TransformNum** and **FilePath** settings are mutually exclusive.

This is specified in the XML editor as a child of the **CurveOverlay** element with following syntax:

<Curves>

    <Curve TransformNum="*Number*" Name="*Name*"/>

    <Curve FilePath="*Full path to a Library Curve file*" Name="*Name*"/>

</Curves>

XML Example Configuration

The following XML snippet shows a complete configuration of the Curve Overlay chart for the example image (without evaluations) above:

    <CurveOverlay Id="CurveOverlay1" SheetName="Curves" XAxisTitle="Dose (ng/mL)" YAxisType="Linear" YAxisTitle="Response (B/B0%)" XAxisType="Logarithmic" Title="Dose-Response">

        <Curves>

            <Curve TransformNum="2" />

            <Curve FilePath="4PL.curve.xml" />

        </Curves>

    </CurveOverlay>

Curve Overlay Evaluations

For each Curve Overlay, you can additionally evaluate expressions that:

• Result in a single numerical value for each curve featured on the chart

• Plot the evaluation result on each curve

• Are included in the report in a table

The Curve Overlay Evaluations are added as a child of CurveOverlay element. These are configured and displayed in the report in the same way as the Standard Curve Fit Evaluations.

For example, the Curve Overlay configuration for the example chart image (with evaluations) above:

```
<Evaluations>
        <Evaluation Type="CalcX" Expression="20" Description="ED20" Name="ED20"/>
        <Evaluation Type="CalcX" Expression="50" Description="ED50" Name=ED50"/>
        <Evaluation Type="CalcX" Expression="80" Description="ED80" Name="ED80"/>
</Evaluations>
```

In addition to the chart, the computed results are displayed in the report as a simple three-column table:

Curve 1	ED20	162.67
Curve 1	ED50	63.3061
Curve 1	ED80	29.1162
Curve 2	ED20	130.595
Curve 2	ED50	1.55167
Curve 2	ED80	0.998171

The columns contain curve name in bold, **Description** if specified or **Expression** if it was not, and the numerical value of the evaluated result or any syntax or computation error in red (in same way as the Evaluation feature).

Evaluations Table

The Evaluations Table report element includes in the report details and results of any configured evaluations arranged in a table, which typically consists of three columns. For example,

Description	Expression	Results
Evaluation #1	Unknown	0.826
Evaluation #2	median(Unknown)	0.649
Median of all Unknown	median(Unknown)	0.649

Here, the **Description** column contains **Expression #{index}** in the first and the second rows and the specified description in the third. The **Expression** column contains the evaluated expression and the **Results** display the computed result of each configured Evaluation.

Settings

Depending on the configuration of the Evaluation settings, the results are arranged in one or more Evaluations Tables. The number of rows in each table corresponds to the number of configured Evaluations.

Evaluations Table

While the **Results** are definitely included, you might prefer to hide other columns by clearing corresponding check boxes.

Include Description	Include the description column.
Include Expression	Include the expression column.
Include Header	Determines whether to include the table header.

The Evaluation Table is also configured with common report settings that are covered in the Report Content section.

Histogram

The Histogram report element includes in the report a chart that graphically presents the spread of measurements or results. This can be useful for spotting outliers.

For example,
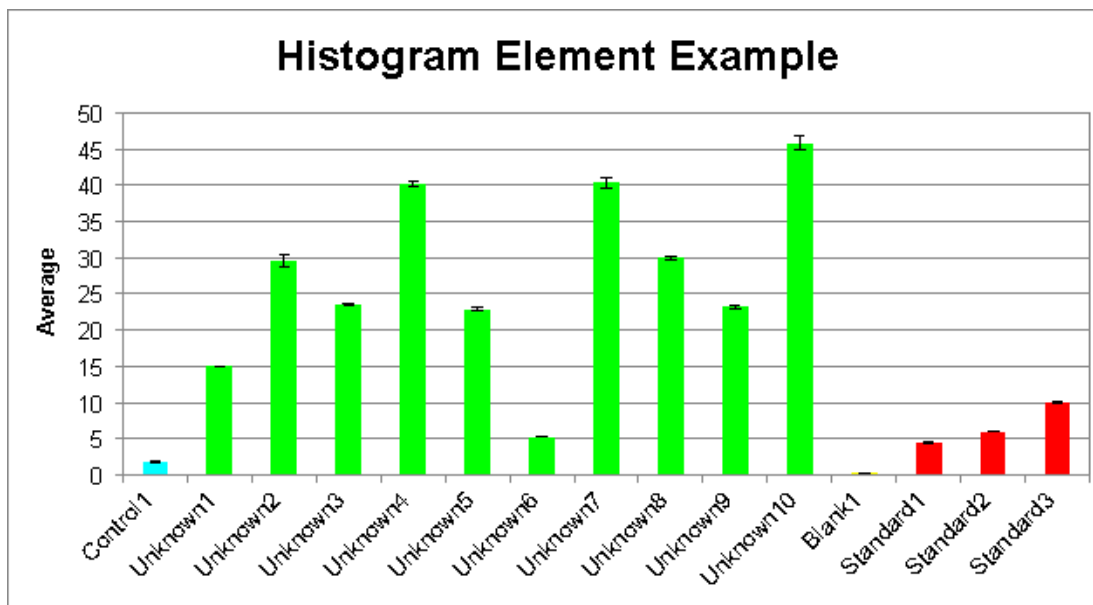
Here the Histogram was generated using a configuration to plot the Average values of **Control**, **Unknowns**, **Blank** and **Standards** samples with error bars indicating the standard deviation and a custom title.

Settings

The Histogram is configured with the common report settings covered in the Report Content section plus the Histogram specific settings described below.

Axes (Advanced)

Use these additional settings to adapt the chart's appearance to your needs.

X Axis Major Units	The numeric interval between numbers on the x-axis. Starting from the minimum value, a major unit is displayed at every increment.
X Axis Minor Units	The numeric interval between supplementary tickmarks on the x-axis. The minor units are not displayed unless this attribute is specified.
X Axis Numerical Formatting	The formatting for the **X Axis Major Units** values. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.

X Crosses Y At	Select where the x-axis will cross the y-axis from the drop-down: • **Automatic** – Determine the location that makes the most sense for your data automatically. • **Axis Value** – Cross y-axis at specified **X Crosses Y at Value**. • **Maximum Axis Value** – Cross y-axis at the maximum *y* value of the chart. • **Minimum Axis Value** – Cross y-axis at the minimum *y* value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
X Crosses Y at Value	The numerical value at which the x-axis will cross the y-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.
Y Axis Major Units	The numeric interval between the gridlines on the y-axis. Starting from the minimum value, a major unit is displayed at every increment.
Y Axis Minor Units	The numeric interval between supplementary tickmarks on the y-axis. The minor units are not displayed unless this attribute is specified.
Y Axis Numerical Formatting	The formatting for the **Y Axis Major Units** values. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.
Y Crosses X At	Select where the y-axis will cross the x-axis from the drop-down: • **Automatic** – Determine the location that makes the most sense for your data automatically. • **Axis Value** – Cross x-axis at specified **Y Crosses X at Value**. • **Maximum Axis Value** – Cross x-axis at the maximum *x* value of the chart. • **Minimum Axis Value** – Cross x-axis at the minimum *x* value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
Y Crosses X at Value	The numerical value at which the y-axis will cross the x-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.

These settings can be also applied to other charts as an advanced configuration. To learn more, see Change the Units and Number Format of the Charts and Customize X and Y Axes Positions for Curve Charts topics.

General

Matrix	The matrix of data to plot. Select the relevant matrix name from a drop-down list.

Each histogram can be configured to plot samples of one or more types (e.g., Standards, Unknowns, etc.). The values of each sample group is plotted as a coloured bar on the x-axis. The colour of each sample bar matches its sample type with a label to indicate the sample group name (or any applied Sample ID).

Histogram

Error Bars	Use this setting to select the type of error bars to use (or none). Error bars can display the **Standard Error**, **%CV**, or **Standard Deviation** of the (non-flagged) replicates of the group. If the **Replicates** option is selected the error bars reflect the minimum and maximum value of the replicates of the sample. With the **None** selection, the error bars are not shown.
Title	The title for a histogram chart.
Sample Types	Which sample types to include in the histogram.

Layout

The Layout report element includes in the report an image of the sample layout used in the assay. This includes a layout itself and a legend with the sample types that are included in the layout. For example:

Here is the layout for a 96-well microplate with 6 **Standard**, 1 **Blank**, 1 **Control**, and 40 **Unknown** samples in duplicate. Under the layout image, a sample types collection of the assay is displayed.

Settings

Layout report element includes the following configurable setting:

General

Size	Small, Medium, or Large (medium size will fit on an A4 page-width).

> ⓘ If multiple layouts are defined in the assay protocol, then all of them will be included in the report.

As with other Report Elements, you can configure how it appears in the report using common report settings.

Matrix Table

The Matrix Table report element includes in the report the results of the performed analysis in a matrix-table structure. This is a table matching the layout dimensions with the data reported in each cell corresponding to the associated position on the matrix. Flagged data is displayed as defined by the associated transform and matrix configuration. Each cell in the table corresponds to the associated position on the matrix.
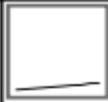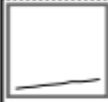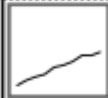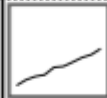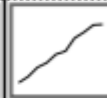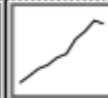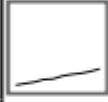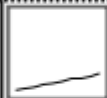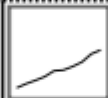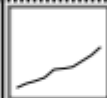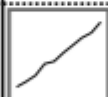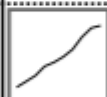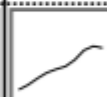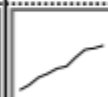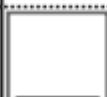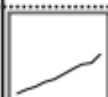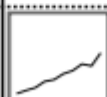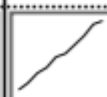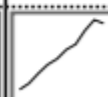
For example,

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Here is the Matrix Table is reported for an endpoint matrix. In each cell, the value for a corresponding position is displayed. For XY data, each position would contain a thumbnail plot.

All matrices could be reported separately (i.e., a separate Matrix Table for each included matrix) or in a combined arrangement.

For example,

	1	2	3	4	5	6
A	4.318	4.460	15.053	15.003	29.063	30.118
B	6.045	6.003	23.532	23.636	40.364	39.902
C	9.923	10.092	22.744	23.132	5.246	5.273
D	1.809	1.840	40.937	39.919	29.764	30.177
E	0.057	0.057	23.440	22.989	45.226	46.526
Key:	Raw					
	Average					

Here is a snippet of a Matrix Table for the XY Reduction Average raw and calculated data, where each cell contains the thumbnail plot for corresponding input XY position and the calculated numerical result. The last row features the key explaining the arrangement in each position.

Matrix Table with Multiple Plate/Multiplex

If the assay defines multiple plates then matrix tables are included for each of them. Each set of matrices for each plate is prefixed with the plate name and number (e.g., "Plate 1"), then the matrices are included for that matrix.

> With **Combined**, there will be one matrix table for each plate.

> With **Separate**, there might be more than one matrix table for each plate.

Settings

The Matrix Table is configured with specific to this report element and with general report configuration settings.

Matrix Table

The matrix table has 2 configurations that define how the results will be displayed.

Arrangement	Select **Combined** for each cell in the table to list the values of all included matrices (per plate/analyte). In this case, the final row of the table will contain a key that explains ordering of the matrices. Or select **Separate** for a separate table for each included matrix.
Field Data	If your assay contains field data, this indicates where it appears in the table: • **Before** – On rows before the numerical data. • **After** – On rows after the numerical data.

For XY data, there are additional settings for configuring how the thumbnail plots are displayed in the report.

Thumb Plot

For XY data, various options for defining the inclusion and sizing of XY thumb plot charts are available.

Include Thumb Plots	Defines whether thumb plots are included in the report.
Thumb Plot Height	Specifies the height for all thumbs in the report.
Thumb Plot Width	Specifies the width for all thumbs in the report.

For XY data, various options are included for defining how XY thumb plot charts are scaled. These can be fixed values or determined for each position. The plot lines will be plotted within the defined scale.

Thumb Scale

Thumb Auto Scale Max X	Specifies whether the maximum *x* scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Max X** value. • **Plot** – The scale limit of each thumb plot is automatically determined by the maximum *x* data in each plot (i.e., each plot may have a different maximum *x* limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the maximum *x* data point from all plots in the table.

Thumb Auto Scale Max Y	Specifies whether the maximum *y* scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Max Y** value; • **Plot** – The scale limit of each thumb plot is automatically determined by the maximum *y* data in each plot (i.e., each plot may have a different maximum *y* limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the maximum *y* data point from all plots in the table.
Thumb Auto Scale Min X	Specifies whether the minimum *x* scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Min X** value. • **Plot** – The scale limit of each thumb plot is automatically determined by the minimum *x* data in each plot (i.e., each plot may have a different minimum *x* limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the minimum *x* data point from all the plots in the table.
Thumb Auto Scale Min Y	Specifies whether the minimum *y* scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Min Y** value. • **Plot** – The scale limit of each thumb plot is automatically determined by the minimum *y* data in each plot (i.e., each plot may have a different minimum *y* limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the minimum *y* data point from all the plots in the table.
Thumb Scale Max X	Determines custom maximum *x* scale for thumb plots if **Thumb Auto Scale Max X** is **Fixed**.
Thumb Scale Max Y	Determines custom maximum *y* scale for thumb plots if **Thumb Auto Scale Max Y** is **Fixed**.

Thumb Scale Min X	Determines custom minimum *x* scale for thumb plots if **Thumb Auto Scale Min X** is **Fixed**.
Thumb Scale Min Y	Determines custom minimum *y* scale for thumb plots if **Thumb Auto Scale Min Y** is **Fixed**.

Matrix View

The Matrix View report element includes in the report a layout-based graphical representation of the matrix data. All corresponding settings of the associated matrix are applied to the view too. Flagged positions are indicated and displayed with a cross-through it.

Matrix view can be output with colouring of:

- **Layout** – Each position shows the numeric value in endpoint matrices or a thumb in XY data according to its sample type. Also, the sample type legend is included.

  For example,
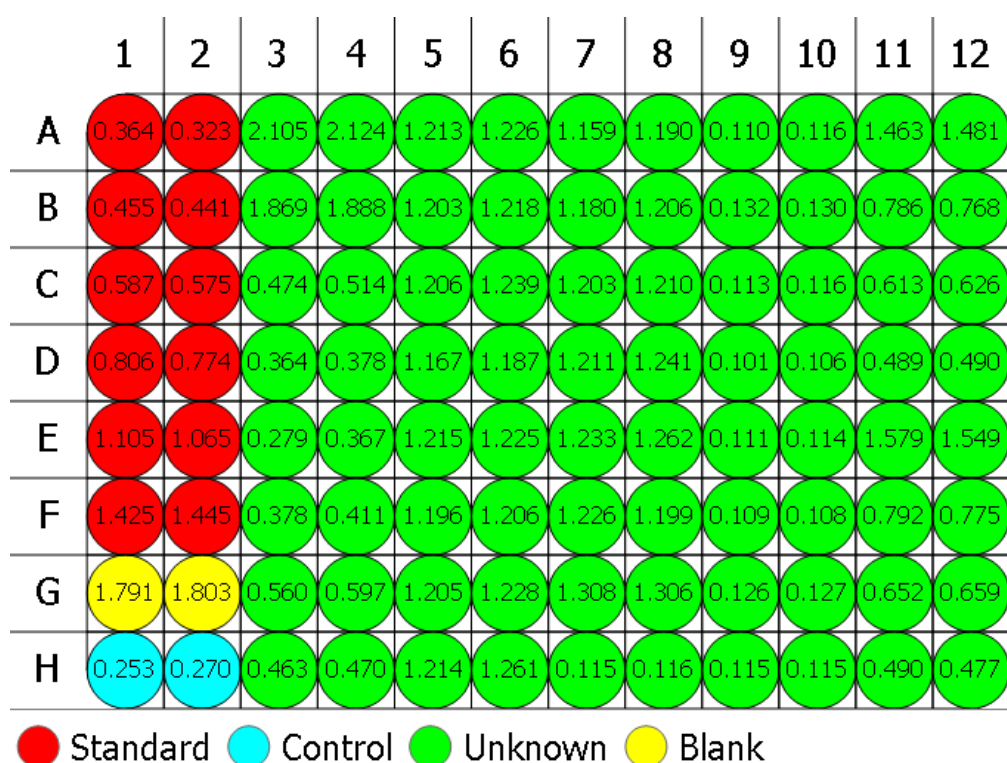
- **Heatmap** – Each position displays the numeric value with respect to the default or custom heatmap scale. The scale legend is also included.

  > (i) This setting is relevant for endpoint data only.

For example,

Settings

Matrix View includes the following configurable settings:

General

Matrix	The matrix of data to plot. Select the relevant matrix name from a drop-down list.
Size	**Small**, **Medium**, or **Large** (medium size will fit on an A4 page-width).

Matrix View

Colouring	**Layout** or **Heatmap** (Heatmap setting does not apply to XY data).

The Matrix View is also configured with common report settings that are covered in the Report Content section.

Measurement Meta Data

The Measurement Meta Data report element includes in the report a table listing the measurements metadata (reported as name-value pairs). This corresponds to the data as it appears under the **Measurements** tab, in **Meta** tab.

This data is reported in a two-column table with the name of each entry and its value. For example,

Data Filename	C:\...\Documents\MyAssays\Measurements\ELISA Absorbance.xlsx
Data Main Filename	ELISA Absorbance
Data File Created	7/10/2017
Data File Last Modified	7/10/2017
MEASUREMENT START DATE	Tue Jun 13 2017 13:02:29 GMT+0100 (GMT Summer Time)
MEASUREMENT COMMENT	Comment On Multiple Lines
User interface program version	3.1.1.9
Instrument interface version	0
Instrument serial number	0
PROTOCOL NAME	ELISA Absorbance
PROTOCOL CREATOR DATE	FACTORY PROTOCOL
PLATE TYPE	PerkinElmer OptiPlate
PLATE FORMAT	96 wells (8X12)

Here the metadata table features details about the measurements data file and the details obtained from the VICTOR plate reader.

Settings

The Measurement Meta Data is configured with common report settings that are covered in the Report Content section.

Notes

Play Video

The Notes report element includes in the report any provided notes (e.g., preparation notes, Lot ID, etc.). Notes can be used to reference the peculiarities of this data analysis run.

How to: Add Notes to the Analysis

1. Launch an assay protocol or open a results file.

2. On the **Home** tab, in the **View** group, click **Notes**.

3. The **Notes** panel will appear down-most of the screen.

4. Enter or paste any Notes as required.

Entered Notes will appear under **Notes:** title. For example,

Notes:

An eyelash contaminated well B4.

Settings

Notes

Notes element includes the following check box setting:

Exclude If Empty	Exclude Notes from the results, if it contains no information.

The Notes element is also configured with common report settings that are covered in the Report Content section.

QC Results

The QC Results report element includes in the report any inter-assay quality control results (as defined by Quality Control settings) defined for an assay. This could include Observation Table, Levey-Jennings, CUSUM, or Control charts, and QC summary reporting the latest results along with historical results.

For example,
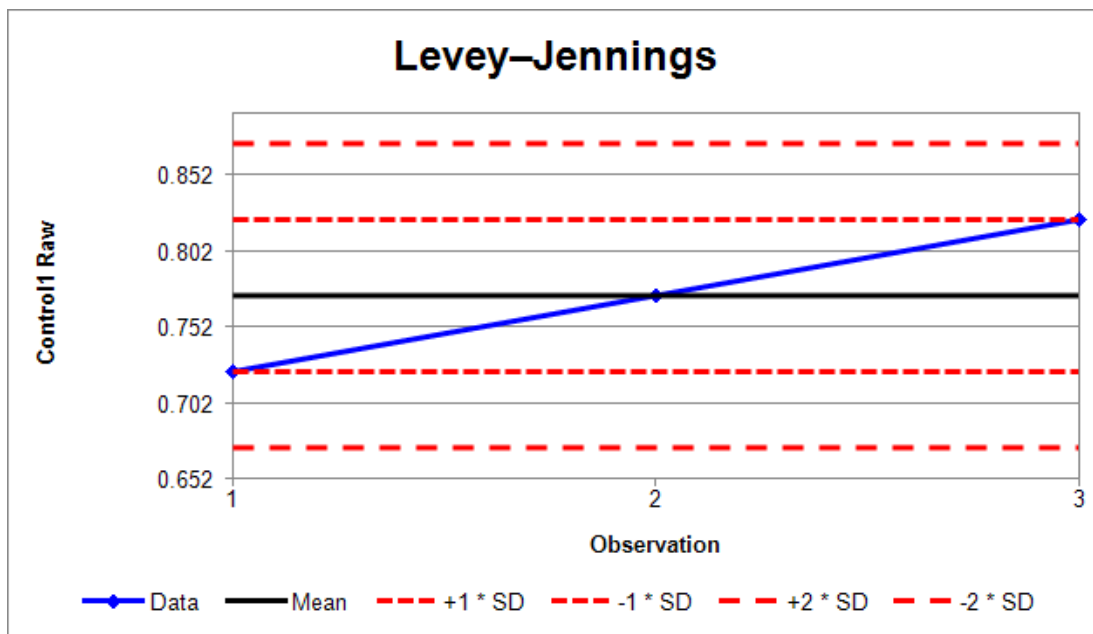
Observation	Control1 Raw	Date	File
3 (Current)	**0.823**	**2017-07-01 / 16:34:07**	**ELISA (3)**
2	0.733	2017-07-01 / 12:32:04	ELISA (2)
1	0.722	2017-07-01 / 11:54:02	ELISA (1)

✔ All observations are within the ±2SD range.

Here the Levey-Jennings chart, Observation Table and Observation summary are reported for current and two previous results of an ELISA assay protocol.

Settings

The QC Results element is configured with common report settings that are covered in the Report Content section.

Sample Table

The Sample Table report element lists the results of the performed data analysis by sample groups defined on the layout. Flagged data is displayed as defined by the associated transform and matrix configuration. Each row in the table corresponds to a sample.

Here is an example of a Sample Table:

Sample	Positions	My Raw Data	%CV
🔴 Standard1	A1	0.364	8.440
	A2	0.323	
🔴 Standard2	B1	0.455	2.210
	B2	0.441	
🔴 Standard3	C1	0.587	1.460
	C2	0.575	
🔴 Standard4	D1	0.806	2.864
	D2	0.774	
🔴 Standard5	E1	1.105	2.607
	E2	1.065	

It includes a snippet of five **Standard** samples and the positions they are assigned to. Also, the raw values (**My Raw Data** column) for each replicate and the calculated results from the Percentage Coefficient of Variation transform (**%CV** column) are included for each sample. Each row contains replicates of the corresponding sample in the **Vertical** orientation.

Use the Sample Data Processing options to further configure the results in the table by sample. Using these settings, you can:

- Order the results by specific values.
  For example, report from highest to lowest concentration values.

- Filter.
  Include only sample results of interest. It is possible to filter by text, numerical Boolean condition or regular expression. For example, configure a sample table that includes only **Positive** Sample Label results. Or, include only results that are above or below a threshold.

- Limit the number of included samples.
  Show only the first *n* samples; this is useful when combined with the ordering setting.

For XY data, the Sample Table contains **Thumb Plots** which are thumbnail graphical representations of each kinetic/spectral data set plotted for each position.

Here the replicates for each sample group, XY Raw data and calculated results for the XY Replicates Average transform are displayed in **Horizontal** orientation.

Settings

The Sample Table is configured with general report configuration settings. Element-specific settings are listed in the tables below:

Sample Table

Field Data	If your assay contains field data, this indicates where it appears in the table: • **Before** – On columns to the left of the numerical data. • **After** – On columns to the right of the numerical data.
Include Positions	Include the **Positions** column to report the sample positions where the data was measured. For plate assays, this is selected by default (with **Include Sample Numbers** setting cleared).
Include Sample Icons	Include coloured circle icons to the left of each sample.

Include Sample Numbers	Include a column titled **Number** to report the 1-based position number for each sample. For rack assays, this is selected by default (with **Include Positions** setting cleared). ⓘ If both **Include Positions** and **Include Sample Numbers** are selected, the latter appears to the right of the former.
Replicate Orientation	How the replicates appear in the table: • **Vertical** – Each position is listed in a new line of the column. • **Horizontal** – All positions are listed in the same line.
Sample Types	Which sample types to include in the sample table.

Sample Data Processing

Using these settings, you can shape the appearance of the Sample Table to report exactly the data you need. Initially, the editor includes three check box options that expand with associated settings when selected:

- **Filter**

  You can filter your data analysis results to include only samples that satisfy specific conditions. For example, you could filter a sample table so that it only includes samples marked with a specific label (such as "Positive"), or you could include only results that are associated with a specified field data value (such as "Male"). It's also possible to filter by numeric conditions (such as x < 1 or x > Control 1) so that the sample table includes only values of interest.

  > 📝 Use this feature in conjunction with Sample Labels to filter samples by their associated label.

Sample Filtering Settings

Configure the sample table to include only the values of interest. Use the **Filter Rows By Column** setting to specify which column is used for filtering. Then define one or more filter rules. Each specified filter rule is used to test each sample's value (in the selected column); only sample values that satisfy any of the filter rule(s) are included.

There are 3 filter rules options:

- By Text

- By Regular Expression

- By Numeric Expression

A sample is included if a filter rule is satisfied for the sample's value. A sample's value comprises of any text, numbers, symbols, or their combination as they appear in the report. If the sample result is reported using Sample Labels, then any applied label will be considered as the sample's value (this makes it easy to filter by sample labels).

The three filter options can be used in conjunction with each other; all samples which satisfy any of the specified filter rules will be included in the sample table.

> ℹ️ With Sample Table Filter, when the matrix has Sample Table Replicates set to **List**, all replicates must match the filter to be included.

Filter Rows By Column	Select a column to filter the rows by from the drop-down list. In addition to the available matrices, you can also filter the table by Samples and Positions included in Sample Table. > ℹ️ In general, this feature will be used where there is a single value or result appearing in each row of the sample table (i.e. **Average** or **First** setting of Sample Table Replicates). If the selected column is selected to display **List** of Sample Table Replicates, the value of the first replicate will be used to filter each row by.
Filter By Text	Filter using a simple text match. Any value that contains a case-sensitive match will be included. For example, if Positive and Negative labels are used, use the setting **Positive** to show only Positive results. To show only flagged results enter **Flagged**.

Filter By Regular Expression	Filter using a text string comparison defined using a regular expression. This offers more flexibility in text matching than the **Filter By Text** option but does require knowledge of regular expressions to work with. For example, to include values that are either **Positive** or **Negative**, use the regular expression: **Positive|Negative** To include only values that are not marked as **Flagged**, use the regular expression: **^(?!Flagged).*$**
Filter By Numeric Expression	Filter using a numeric Boolean expression. The expression is defined terms of x and is evaluated for each numeric sample value. Only results that evaluate to true (equal to 1) will be included. (Sample values that are not numeric will not be tested and not included.) The expression should be written in terms of **x** where **x** refers to the sample value being tested. The expression may refer to all operands (such as sample groups), operators and functions available in MyAssays Desktop expressions. For example, to include only values less than 1: **x < 1** To include only values greater than the value of Control1: **x > Control1**

Example

In this example, we will create a Sample Table that only reports values with a concentration over 100. To do this, we use the Sample Label feature to assign the Positive label to any sample with a concentration over 100 and then use the filter feature to only include samples assigned with the Positive label. This is achieved as follows:

1. In the Matrices tab, select **Concentration** matrix and apply Sample Label with Condition **x>=100** and Label **Positive**. With this, the Sample Table looks like:

Sample	Positions	Raw	Blank Corrected	Concentration	%CV
● Unknown1	A3 A4	0.347 0.346	0.3455	Positive	0.280776
● Unknown2	B3 B4	0.586 0.584	0.584	80.302	0.232345
● Unknown3	C3 C4	0.549 0.547	0.547	85.5316	0.250679
● Unknown4	D3 D4	0.320 0.325	0.3215	Positive	1.7101
● Unknown5	E3 E4	0.486 0.490	0.487	95.9167	0.584993

2. In the Report tab, add an additional Sample Table element, and specify Sheet Name as **Positive Results**. By default, it will be assigned the **SampleTable2** Id.

3. In the **SampleTable2** element, from the **Sample Data Processing**, select **Filter**. The editor will expand with applicable settings.

4. In **Filter Rows By Column**, select the **Concentration** from the drop-down.

5. Enter or paste **Filter By Text** as **Positive**.

6. Click **Calculate** to generate a new report with the updated settings.

On calculation, the results with Positive label are additionally reported on a separate Positive Results spreadsheet (in the Sheet View) as follows:

Sample	Positions	Raw	Blank Corrected	Concentration	%CV
● Control1	H1 H2	0.297 0.297	0.296	Positive	0
● Unknown1	A3 A4	0.347 0.346	0.3455	Positive	0.280776
● Unknown4	D3 D4	0.320 0.325	0.3215	Positive	1.7101
● Unknown7	G3 G4	0.356 0.352	0.353	Positive	1.06505
● Unknown9	A5 A6	0.325 0.321	0.322	Positive	1.36171

- **Limit**

When only the highest or lowest data analysis results matter, you can limit the number of rows to include in the table. With this setting you can review or print only those results that are in the range of interest.

> ℹ️ Use this setting to include only the first *n* rows which satisfy any filtering rules and/or the ordering of any defined sequence.

Sample Limiting Settings

To limit the number of rows in the Sample Table:

Limit To Maximum Count	Enter a 1-based number of rows to include.

Example

In this example, we'll include only the three highest results of the Average transform to the sample table. We'll also use Sample Ordering Settings to rank the results. Here is a snippet of how the Sample Table looks before setting the row limitation:

Sample	Positions	My Raw Data	Average
🟢 Unknown1	A1	0.364	0.3435
	A2	0.323	
🟢 Unknown2	A3	2.105	2.1145
	A4	2.124	
🟢 Unknown3	A5	1.213	1.2195
	A6	1.226	
🟢 Unknown4	A7	1.159	1.1745
	A8	1.19	
🟢 Unknown5	A9	0.11	0.113
	A10	0.116	

To limit the number of samples included, follow these steps:

1. In the **Report** tab, select **SampleTable** element.
   If your report features more than one Sample Table, select the element with appropriate ID such as **SampleTable2**.

2. In the **SampleTable** element, from the **Sample Data Processing**, select **Limit** and **Order** check boxes.
   The editor will expand with applicable settings.

3. In the **Order Column**, select the **Average** from the drop-down.

4. In the **Order Sequence**, select **Descending**.

5. In **Limit To Maximum Count**, enter 3.

6. Click **Calculate** to generate a new report with the updated settings.

Here is the Sample Table that lists the highest three results of the Average transform:

Sample	Positions	My Raw Data	Average
⬤ Unknown2	A3	2.105	2.115
	A4	2.124	
⬤ Unknown8	B3	1.869	1.879
	B4	1.888	
⬤ Unknown37	G1	1.791	1.797
	G2	1.803	

- **Order**

By default, samples are arranged by sample type and group number, but you might prefer to display your samples in a different order. For example, it might be useful to present your results in concentration order with the highest first.

Sample Ordering Settings

The ordering of rows is defined with the following settings:

Order Column	Select the column to sort the rows by from the drop-down list. In addition to the available matrices, you can also sort the table by Samples and Positions included in your Sample Table. If the specified column contains a **List** of Sample Table Replicates, then the value of the first replicate is used to sort the rows.
Order Sequence	Specify the order sequence, based on the selected **Order Column** setting: - **Ascending** – For numerical values, the results are listed from the lowest to the highest value. For textual content, the results are listed in alphabetical order. - **Descending** – For numerical values, the results are listed from the highest to the lowest value. For textual content, the results are listed in reverse alphabetical order.

Example

In this example, we'll sort samples by Standard Curve Fit (Concentration) results from highest to lowest values. By default, the Sample Table presents data consequently for all included **Sample Types**:

Sample	Positions	Raw	Concentration
⬤ Unknown1	A3	0.347	142.103
	A4	0.346	
⬤ Unknown2	B3	0.586	80.302
	B4	0.584	
⬤ Unknown3	C3	0.549	85.5316
	C4	0.547	
⬤ Unknown4	D3	0.320	157.858
	D4	0.325	
⬤ Unknown5	E3	0.486	95.9167
	E4	0.490	

To change how samples are ordered, follow these steps:

1. In the **Report** tab, select **SampleTable** element.
   If your report features more than one Sample Table, select the element with appropriate ID such as **SampleTable2**.

2. In the **SampleTable** element, from the **Sample Data Processing**, select **Order**. The editor will expand with applicable settings.

3. In the **Order Column**, select **Concentration** from the drop-down.

4. In the **Order Sequence**, select **Descending**.

5. Click **Calculate** to generate a new report with the updated settings.

With the example configuration provided above, the samples will be ordered as follows:

Sample	Positions	Raw	Concentration
⬤ Unknown33	A11	0.241	327.389
	A12	0.246	
⬤ Unknown4	D3	0.320	157.858
	D4	0.325	
⬤ Unknown9	A5	0.325	157.465
	A6	0.321	
⬤ Unknown1	A3	0.347	142.103
	A4	0.346	
⬤ Unknown7	G3	0.356	138.052
	G4	0.352	

Thumb Plot, Scale, and Data Format Settings for XY Data

For XY data, there are additional settings for configuring how the thumbnail plots are displayed in the report.

Thumb Plot

For XY data, various options for defining the inclusion and sizing of XY thumb plot charts are available.

Include Thumb Plots	Defines whether thumb plots are included in the report.
Thumb Plot Height	Specifies the height for all thumbs in the report.
Thumb Plot Width	Specifies the width for all thumbs in the report.

For XY data, various options are included for defining how XY thumb plot charts are scaled. These can be fixed values or determined for each position. The plot lines will be plotted within the defined scale.

Thumb Scale

Thumb Auto Scale Max X	Specifies whether the maximum x scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Max X** value. • **Plot** – The scale limit of each thumb plot is automatically determined by the maximum x data in each plot (i.e., each plot may have a different maximum x limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the maximum x data point from all plots in the table.

Thumb Auto Scale Max Y	Specifies whether the maximum *y* scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Max Y** value; • **Plot** – The scale limit of each thumb plot is automatically determined by the maximum *y* data in each plot (i.e., each plot may have a different maximum *y* limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the maximum *y* data point from all plots in the table.
Thumb Auto Scale Min X	Specifies whether the minimum *x* scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Min X** value. • **Plot** – The scale limit of each thumb plot is automatically determined by the minimum *x* data in each plot (i.e., each plot may have a different minimum *x* limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the minimum *x* data point from all the plots in the table.
Thumb Auto Scale Min Y	Specifies whether the minimum *y* scale of each plot is: • **Fixed** – The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Min Y** value. • **Plot** – The scale limit of each thumb plot is automatically determined by the minimum *y* data in each plot (i.e., each plot may have a different minimum *y* limit). • **Table** – The scale limit of every thumb plot in the table is the same. This is determined from the minimum *y* data point from all the plots in the table.
Thumb Scale Max X	Determines custom maximum *x* scale for thumb plots if **Thumb Auto Scale Max X** is **Fixed**.
Thumb Scale Max Y	Determines custom maximum *y* scale for thumb plots if **Thumb Auto Scale Max Y** is **Fixed**.

Thumb Scale Min X	Determines custom minimum *x* scale for thumb plots if **Thumb Auto Scale Min X** is **Fixed**.
Thumb Scale Min Y	Determines custom minimum *y* scale for thumb plots if **Thumb Auto Scale Min Y** is **Fixed**.

XY

Data Format	Specifies how XY data is included in the report: • **Thumb** – If **Include Thumb Plots** is selected, a thumb plot is reported for each plot. This is the default option. • **Y Values** – A list of *y* data point values is reported for each plot. • **X and Y Values** – A list of *x* and *y* data point values is reported for each plot. • **Index and Y Values** – For each plot, this reports a list where *x* are displayed as 1-based continuous data point numbers and *y* as data point values.

Sample Table (Custom Columns)

This topic describes the properties and configuration of the Sample Table (Custom Columns) Report Element.

Overview Video Walkthrough...

Multiplex Video Walkthrough...

XY and Well Scan Video Walkthrough...

Some settings are only available through the XML tab, for more information on those settings please see the topic at Sample Table Custom Columns XML Settings.

Overview

The Sample Table (Custom Columns) report element offers the following features:

- Custom column ordering
- Custom column titles
- Reporting specific containers in report columns (for example, from multiple plates or analytes)
- Adding qualifications

- Duplicating columns without the need to add a dummy Expression by Matrix transform
- Different output types for XY and Scan Data in the same sample table

Report Element Settings

General

- Id - The Report Element ID
- Include - Toggling this checkbox will include or exclude the sample table from the report
- Title - Allows for the addition of a title to the sample table

Sample Data Processing

- Filter - Configure the sample table to only contain values of interest
- Limit - Limit the number of rows included in the sample table
- Order - Order the sample table based on the results contained in a selected column

Sample Table

- Replicate Orientation - Display the replicates vertically or horizontally
- Sample Types - Specify which sample types should be included in the table

Sheet

- Sheet Name - Specify the sheet name that will contain the sample table

Column Configuration

Once the Sample Table (Custom Columns) report element has been added, select **Edit** beside the **Columns** field to open the **Sample Table Columns Editor**.
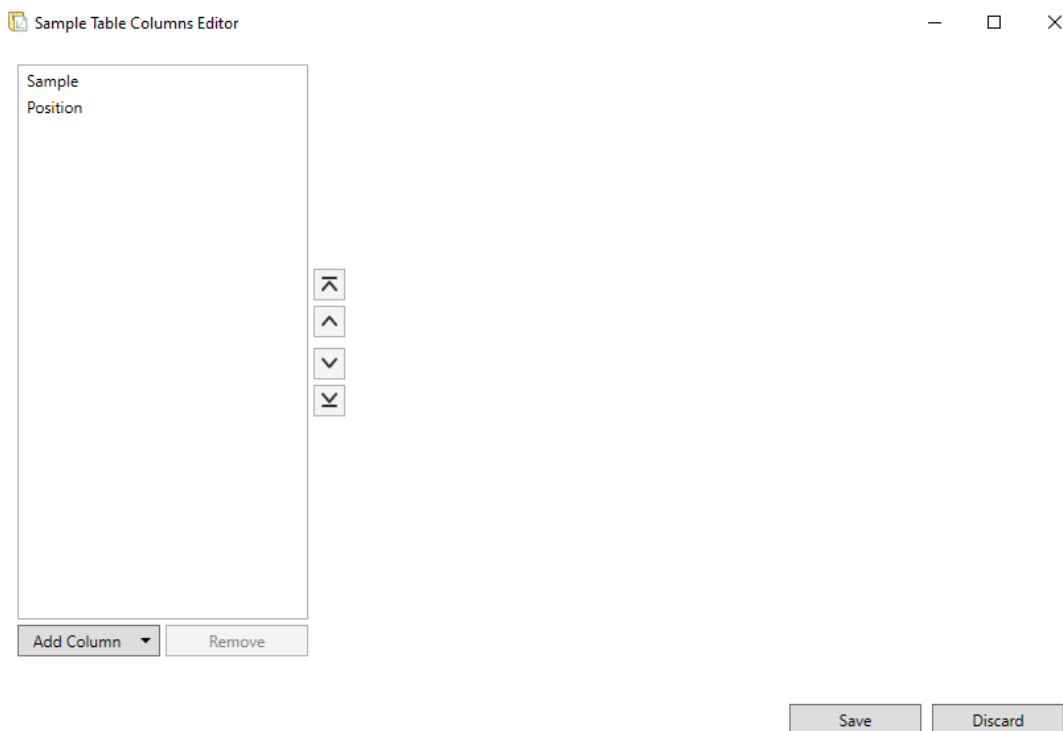
Column Types

To add columns to the sample table, select the **Add Column** dropdown box and select the type of column to add:

- Sample - Reports the Sample ID.
- Position - Reports the sample position, either as Reference or Number.
- Matrix - Reports the data contained in a specified matrix.
- Qualification - Allows the addition of custom rule conditions and labels.
- Transform Content - Reports data contained in transforms, such as Dilution Factors.

Preconfigured Columns

With the addition of the Sample Table Custom Columns report element, Sample and Position columns are automatically added to the table.

Sample

The Sample column reports the Sample IDs, and allows you to specify a custom name, whether the Sample Icons (coloured dots) are included, and whether to include the Group Numbers.

Position

The Position column reports the sample positions with a custom column name either as Reference (alpha numerical, i.e. "A1") or Number (numerical only, i.e. "1").

Adding Matrix Columns

To add a Matrix column to the sample table, select the **Add Column** dropdown box and select **Matrix**.

Specify the settings:

- Custom Name - The name displayed at the top of the column.

- Matrix - The matrix containing the data to be displayed.

- Plate - The plate containing the data.

The below example shows the addition of a Matrix column displaying the Concentration data in a column with the custom name **Conc.**

Adding Qualification Columns

Qualification columns are columns that reference existing data matrices that allow for the addition of sample labels based on specified conditions. To add a Matrix column to the sample table, select the **Add Column** dropdown box and select **Qualification**. Specify the settings:

- Custom Name - The name displayed at the top of the column

- Replicates - A drop-down box selection for either Average (displaying the results for the average of the replicates) or Replicates (displaying the results for each replicate).

- References - The data to used for the reference

- Rule Condition - Using the Reference Id, the conditions for the sample label

- Label - The label to display when the rule condition is met

The below example specifies a new qualification column named Concentration > 50, with two sample labels reporting pass or fail designations based on the concentration matrix:

Flagged Sample Handling

For qualification columns referencing data matrices with flagged samples, it may be helpful to use the **IsFlagged** function to assign a label for flagged samples. The below configuration demonstrates how to specify a label for flagged samples:

Sample Table Columns Editor — □ ✕

| Sample |
| Position |
| Matrix - Concentration (Conc.) |
| Qualification (Concentration > 50) |

Custom Name: Concentration > 50

Replicates: Average

References

Name	Matrix	Plate	
a	Concentration	<Current>	

Add   Remove

Rules

Condition	Label	Highlight	Highlight Row	Text	Symbol
IsFlagged(a)	Flagged Conc.		☐		(None)
a >= 50	Pass		☐		(None)
a < 50	Fail		☐		(None)

Add   Remove

Add Column ▼   Remove

Save   Discard

Using References in Labels

To reference the input matrix value in qualification labels, enter the reference name surrounded by curly brackets, i.e. **{a}**. A label reference enclosed in curly brackets can refer to the associated matrix value. In this case, the evaluated label reference is formatted using the numerical formatting setting of the associated reference.

A label reference can refer to a layout reference or a Transform Output Variable (TOV). For layout references, the container and matrix must be specified (i.e. A1.1 or A1.1.1). For these references, the evaluated value is displayed with 6 significant figures.

> ℹ The reference ID must be a valid variable, starting with a letter or underscore. The reference ID can contain letters, numbers, underscores, and dots only.

Default Sample Table Ordering

The default ordering of the Sample Table Custom Columns report element for both plate and rack layouts is: grouped by sample type, ordered by group number in ascending order. This can be changed using the Sample Data Processing | Order feature.

Sample Table (Custom Columns) XML Settings

This topic describes the XML-specific settings of the Sample Table (Custom Columns) Report Element.

This is an advanced topic, and these settings are currently only available through the XML tab. For general configuration of the Sample Table Custom Columns report element, please see the Sample Table Custom Columns topic.

XML Settings

Currently the following settings are available through the **Report | XML** tab.

Setting	Description
ThumbAutoScaleMaxX	Specified thumb plot X max scale type. Default value is Plot.
ThumbAutoScaleMaxY	Specified thumb plot Y max scale type. Default value is Table.
ThumbAutoScaleMaxZ	Specified thumb plot Z max scale type. Default value is Table.
ThumbAutoScaleMinX	Specified thumb plot X min scale type. Default value is Plot.
ThumbAutoScaleMinY	Specified thumb plot Y min scale type. Default value is Table.
ThumbAutoScaleMinZ	Specified thumb plot Z min scale type. Default value is Table.
ThumbPlotHeight	Specified thumb plot height. Default value is 40.
ThumbPlotWidth	Specified thumb plot width. Default value is 40.
ThumbScaleMaxX	Specified thumb plot X max scale if ThumbAutoScaleMaxX is fixed.
ThumbScaleMaxY	Specified thumb plot Y max scale if ThumbAutoScaleMaxY is fixed.
ThumbScaleMaxZ	Specified thumb plot Z max scale if ThumbAutoScaleMaxZ is fixed.
ThumbScaleMinX	Specified thumb plot X min scale if ThumbAutoScaleMinX is fixed.
ThumbScaleMinY	Specified thumb plot Y min scale if ThumbAutoScaleMinY is fixed.
ThumbScaleMinZ	Specified thumb plot Z min scale if ThumbAutoScaleMinZ is fixed.

Text

The **Text** report element includes any specified text and/or the evaluation of any available text macros.

This element is useful to include custom wording in the report. Also, text macros can be used to include data that may change from run-to-run of the assay. Available text macros include:

- Any imported meta-data
- Filenames (protocol, results, imported data file)
- Current date/time
- Calculation version number
- User name
- PC name

For example, with the following **Text** configuration:

> Protocol: <ProtocolName>
>
> Imported Data: <DataMainFilename>
>
> Results: <ResultsName>
>
> Date: <CurrentDateLong>

In the report, the macros will convert to:

> Protocol: ELISA (96 well)
>
> Imported Data: 96 wells_20170613_152121
>
> Results: ELISA (96 well) (21)
>
> Date: 30 April 2022

Settings

Text

Text	Click the drop-down to expand the text editor. The editor consists of: • A multiline edit box where you can enter or paste any required information. • A full list of all available macros and their current value. To insert a macro at current cursor position, double-click it in the list.

The Text element is also configured with common report settings that are covered in the Report Content section.

Transform Content

The Transform Content report element includes additional report content to illustrate settings or results of a specific transform. If the transform applied to the assay possesses any kind of optional items, they are added to the report automatically. Certain transforms comprise a number of optional content.

The additional report elements are:

- **Additional Sample Table Column** – This is an optional additional column that can be included in the sample table. For example,

Sample	Positions	Factor	My Raw Data	Concentration (x Dil. Factor)
⬤ Unknown1	A3	2	2.105	4.210
	A4		2.124	4.248
⬤ Unknown2	B3	5	1.869	9.345
	B4		1.888	9.440
⬤ Unknown3	C3	2	0.474	0.948
	C4		0.514	1.028
⬤ Unknown4	D3	5	0.364	1.820
	D4		0.378	1.890
⬤ Unknown5	E3	2	0.279	0.558
	E4		0.367	0.734

  Here is the Dilution Factors transform outputs optional report content named Factor Column.

- **Fit Chart** – The visual representation of a plotted curve that is included in a report by default. E.g.:
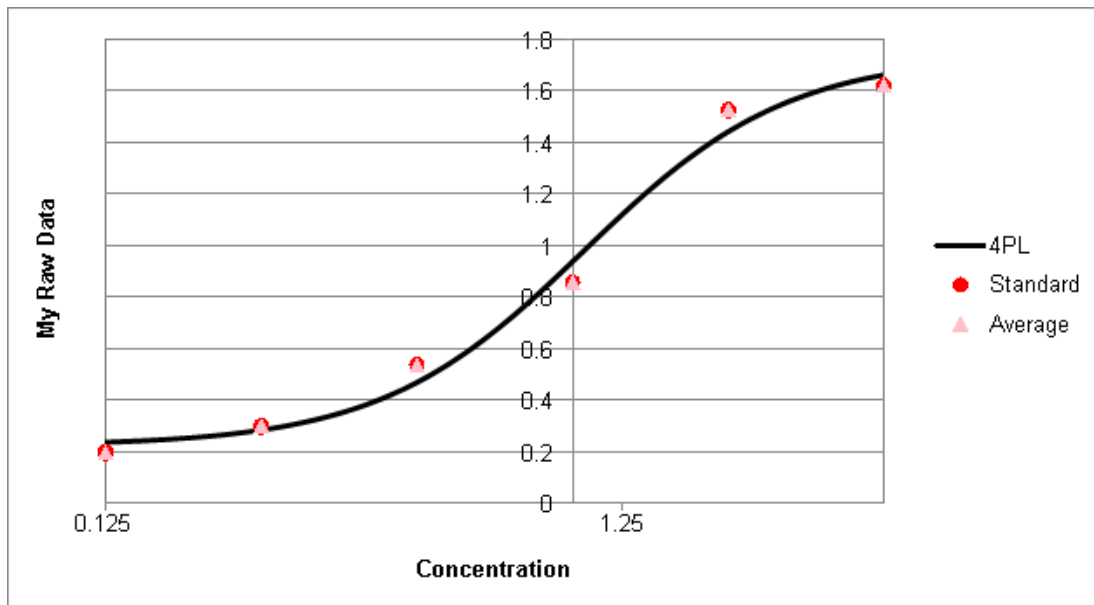
  Here is a chart for Standard Curve Fit transform example.

- **Table** – The table containing additional values computed from a transform. For example, this might refer to Goodness Measures Table, Dose–Response Curves Table, Curve Data Table, etc.

- **Equation** – The formula of a fit method that was used to plot a curve. E.g.:

$$y = mx + c$$

Here is the formula for Linear Regression.

Settings

A report can contain one or more **Transform Content** subelements.

The Transform Content is configured with common report settings that are covered in the Report Content section and the setting described below.

Content

Content	Use this drop-down to specify which subelements to include (or exclude) and their ordering. The available subelements depend on the associated transform. Select the subelement, move in to the **Included** or **Excluded** pane with right and left arrow buttons, or change its' positioning with the **Up** and **Down** icon buttons on the right of the **Included** pane. To include or exclude all transform content from the report, click the **Add All** or **Remove All** buttons, respectively.

Page Settings

Chart Size	If the transform content includes chart, here you can select **Small**, **Medium**, or **Large** option.

How to: Configure Transform Content in the Report

1. In the **Assay Properties** panel, select the **Report** tab.

   If the **Report** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Select Transform Content element that contains transform name, e.g., **TransformContentDoseResponseCurvesTable1**.

3. On the **Report Configuration** pane, click **Content** drop-down.

4. Review and edit content items as required.

5. Click **Calculate** to perform calculations with the new settings.

Curve Fit Transforms Report Contents

Curve-fitting endpoint transforms produce a number of additional report items under their Transform Content report element. This topic covers the items available for Standard Curve Fit, Standard Curve Fit (from Library) and General Curve Fit transforms, their content, and the way they will be included in the report. Some of the elements also contain additional advanced settings can be used to customize the report.

About Curve Fit Transforms Report Contents

The content for a specific transform is named as **TransformContent{TransformName}#**, where:

- **{TransformName}** is the title of the transform

- **#** indicates the number of the transform

If your assay is comprised of two Standard Curve Fit transforms (for example the unrestricted and the restricted curve fits), the transform content will be titled as TransformContentStandardCurveFit**1** for the first transform in the sequence, and TransformContentStandardCurveFit**2** for the second.

> When configuring the report using the report template, the Id of each specific item is appended to the general transform content Id. For example, **{TransformContentStandardCurveFit1GoodnessMeasuresTable1}** will expand to the goodness of the fit measures calculated for the first defined Standard Curve Fit.

Best Fit Results Table

This table displays the results of Best Fit search ordered by rank (the fit with the highest score is listed first). It includes the following columns:

- **Rank** – The ranking of the fit (1 is the best).

- **Score** – The computed result of the Scoring Method for the fit.

- **Fit Method** – The curve-fitting method used for the search.

- **Weight Method** – The weighting method applied to the fit.

Coefficients Table

This table lists the calculated coefficients of the selected **Fit Method**, their value, and ± error.

> For customizing the numerical formatting option for the result and error, see Setting Numerical Formatting for Goodness Measures and Coefficients of the Fit.

Curve Data Table

This table reports the curve-fitting data used for the fit (for the Best Fit method the results of the best performing fit are displayed).

- For Standard Curve Fit and Standard Curve Fit (from Library), the table lists sample groups of the specified **Standard Type**, the defined concentrations, the responses, the calculated concentrations, and the computed % Accuracy and Precision (%CV).
  To clearly indicate whether each calibrator is within the acceptable range or not, each row is highlighted based on whether it satisfies the precision and accuracy rules (rows in light-red fail the test). Any flagged samples are indicated using the same convention as in the Sample Table.
  For advanced configuration settings, see Configure Contents of Curve Data Tables.

- For General Curve Fit, the table includes defined and calculated x and y values used in the curve fitting.

Goodness Measures Table

The table listing each calculated goodness measure.

> To define the numerical formatting for the results, see Setting Numerical Formatting for Goodness Measures and Coefficients of the Fit.

> Only curve-fit methods with a single equation are reported. For fit methods computed from multiple segments (**Point-to-Point** and the **Cubic Spline** methods) equations are not reported.

Fit Equation

Id: **{FitEquation#}**

The equation of the curve fit using mathematical notation.

Fit Equation with Values

Id: **{FitEquationWithValues#}**

The equation with the coefficients replaced by the values determined from the fit.
For example, the linear regression equation is:

y=mx+c

With linear regression, a value for **m** and **c** are computed. For example, if **m**=1.23 and **c**=4.56, then the equation would be:

y=1.23x+4.56

Inverse Fit Equation

Id: **{FitEquationInverse#}**

The equation of the curve fit in terms of *y* presented in mathematical notation.

Inverse Fit Equation with Values

Id: **{FitEquationInverseWithValues#}**

The equation in terms of *y* with the coefficients replaced by the values determined from the fit. For example, the inverse linear regression equation is:

x=(y-c)/m

With linear regression, a value for **m** and **c** are computed. For example, if **m**=1.23 and **c**=4.56, then the equation would be:

x=(y-4.56)/1.23

Fit Evaluation Table

Id: **{FitEvaluationTable#}**

This table lists results of fit evaluations in a table. For adding and configuring custom evaluations, see Advanced Curve Fit Evaluations.

For Standard Curve Fit and Standard Curve Fit (from Library), the first entries are the determined LLOQ and ULOQ that match one of the specified concentration values.

   LLOQ is the first concentration value (*x*) where:

- **% Accuracy** value (from the Curve Data Table) is within 100 +/- **Accuracy (±%)**
- **%CV** value (from the Curve Data Table) is less than **Precision (%CV)** limit

   ULOQ is the highest concentration value (starting from the highest value and going backward) where:

- **% Accuracy** value (from the Curve Data Table) is within 100 +/- **Accuracy (±%)**

- **%CV** value (from the Curve Data Table) is less than **Precision (%CV)** limit

Fit Chart

Id: **{Chart#}**

The Fit Chart plots the calibrator data points on axes with the response values (typically measured, corrected, or normalized values) versus the specified concentrations. The chart includes the fit line and calibrators. The calibrator replicates are plotted with dots. Flagged points are not included in the chart.

> When using Standard Curve Fit with **Fit To Standard** set to **Average**, then the average values are also plotted (in addition to the replicates) using a triangle (pink).

The chart's axes types are set in accordance with **X Axis Type** and **Y Axis Type**. The thick black line shows the curve calculated from these standards.

> To plot non-calibrator sample types on the fit line in the report, you can use **Points on Curve** setting.

You can adjust the chart's appearance in the report. Refer to the Change the Units and Number Format of the Charts and Customize X and Y Axes Positions for Curve Charts topics to learn more.

Validations Table

The Validations Table report element includes the details and results of any configured validations arranged in a table. This table indicates whether each validation has passed or failed and, when validations are defined, is added to the report automatically.

The Validation Table typically consists of three columns. For example,

Results	Expression	Description
❌ Fail	x < 2.5	All non-flagged positions have a value less than 2.5 (**Expression with Every Sample Replicate (x)** type)
✔ Pass	x < 2.5	The average of the replicates (that are not flagged) of all sample groups is less than 2.5 (**Expression with Every Sample Group (x)** type)
✔ Pass	Unknown1 > 1.5	Condition #3
❓Syntax Error	Control1 !< 1.5	Condition #4

Here, the **Results** column displays the evaluated result of each configured Validation. For the Fail and Inconclusive (i.e., Syntax Error), the row is highlighted with yellow and red background colour, respectively. The **Expression** column contains the verified condition. Note, that the expression for the first and the second validation is the same, but the type of validations is different, as stated in the Description. Finally, the **Description** column contains the description if specified (e.g., on third row) or **Condition#{index}** if it is not.

Settings

Depending on the configuration of the Validation settings, the results are arranged in one or more Validations Tables. By default, the Validation table is displayed as three-column table with the number of rows corresponding to the number of **Conditions** added.

While the **Results** column is definitely included to the report, you might prefer to hide former columns by clearing corresponding check boxes.

Description Header	A title for a Validation Table in the report.
Include Description	When selected, the column contains **Description** if specified or **Condition#{index}** if it was not.
Include Expression	If included, this outputs the **Condition** defined for each **Validation**.

Include Header	Determines whether to include the table header.
Results Column	This specifies whether **Results** column appears left-most or right-most in the table.
Results Header	A title for the **Results** column in the report.

The Validation Table is also configured with common report settings that are covered in the Report Content section.

XY Plot

XY Plot report element can be used to display plots from different positions on a single overlaid chart similar to the Position Mode of Kinetic/Spectral Overlay chart. The y-axis of the chart corresponds to measurement values; the x-axis represents (depending on the assay) cycle, time, or wavelength values. The data points for different positions are denoted with different colours. The flagged positions or data points are not included in the chart.

For example:
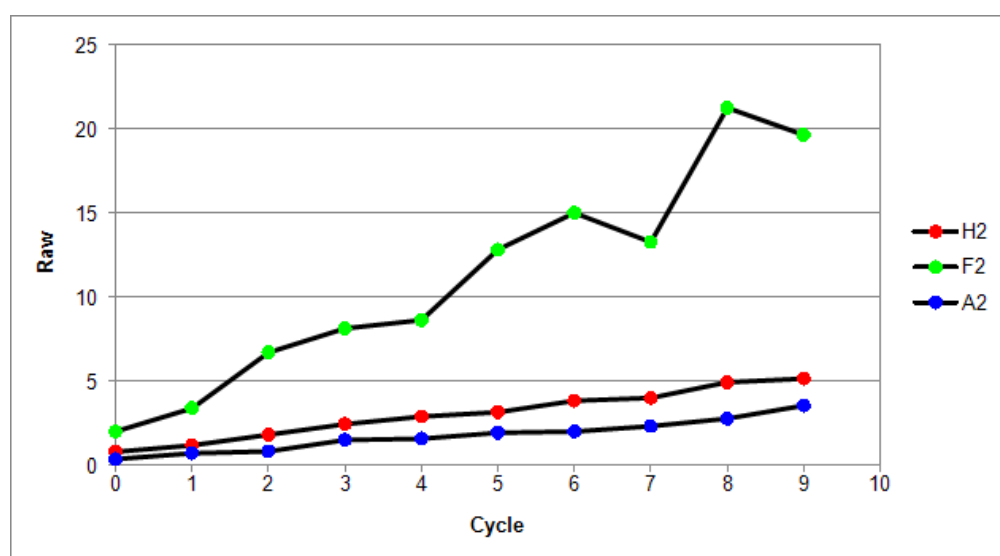
Here, the XY Plot chart contains three overlaid plots from positions **A2**, **F2**, and **H2**. The position plots can originate from any number of positions of any raw or calculated XY matrix.

You can configure one or more XY Plot charts to include in your report.

XY Plot Settings

Chart

Title	An optional title for an XY Plot chart that can refer to Report Macros. If not specified, then no title is displayed.
X Axis Title	The name of the x-axis on the chart.
Y Axis Title	The name of the y-axis on the chart.

Data

Matrix	The data matrix to be plotted on the y-axis.
Positions	The positions to overlay on the chart.
X Axis	The data to be displayed on the x-axis.

General

Id	A unique identifier that is used to identify the report element in the Report Elements pane and when configuring custom report templates.
Include	Boolean setting that defines whether XY Plot chart is included in the report. If not specified, then the chart is included.

Sheet

SheetName	If defined, inserts the chart to a sheet with the specified SheetName. For more details, see Sheet Name in the Report Content section.

Report Settings

Report Settings

The report parent settings available at **Properties | Report** allow you to specify the following settings:

- **Font** – What font will be used as the primary font on your report. Note: different report elements can use different fonts by using a report template.
- **Ordering (Sheet Name CSV)** – The order in which the sheet names should be presented in the **Sheet View**.
- **Print Scaling** – How the content should be automatically arranged for Page-Based reports.

By using these options, you can quickly apply formatting to your report without creating a report template.

Font

The font style and size can be edited using the **Font** setting under **Properties | Report**.

The **Font** setting displays a text field, and clicking on the adjacent button opens the font selector menu.

- **Text Field** – This displays the currently selected font style and size.
- **Font Selector Button** – This displays the available font styles and sizes to choose from.

Selecting a font style and size will apply the selected settings to all report elements, unless otherwise specified using a report template.

Ordering Sheet Name CSV

The order of the Sheets displayed in the **Sheet View** report can be updated by entering them in the order they should appear on the report, separated by commas. This reorders the sheets without changing the order of the report elements.

For example, with Sheets named **Results** and **Fit Details**, the order can be specified: **Results,Fit Details**

> Sheet Ordering can also be specified using Regular Expressions for more <u>advanced configurations</u>

Print Scaling

To simplify configuration, the **Print Scaling** settings specify how the content should be arranged with respect to the page width and height, without creating a report template. The settings available from the **Print Scaling** dropdown box are:

- **None** – This applies no print scaling settings to the page-based report.

- **Fit Sheet on One Page** – This fits each **Sheet** (as defined by the Sheet Name settings) on a single printed page.

- **Fit All Columns on One Page** – This fits all columns of the **Sample Table** or **Curve Data Table** on a single printed page.

- **Fit All Rows on One Page** – This fits all rows of the **Sample Table** on a single printed page.

Sheet Ordering

A custom sheet order can be specified in a CSV list format on the **Properties | Report** tab.
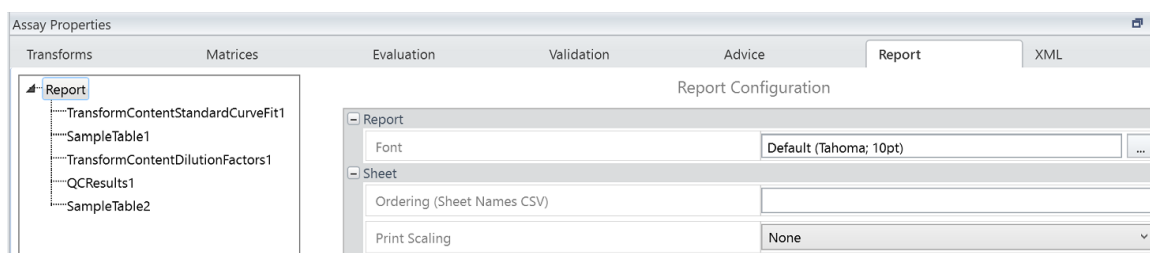
How to: Specify a Custom Sheet Order

1. Select the **Report** tab.

   If the **Report** tab is not immediately visible, click **<< Show All Properties** to expand.

2. In the **Report Elements** pane, select the **Report** header of the **Report Tree**.

3. Within the **Sheet** settings, enter the **Sheet Names** as CSV (each name separated by a comma)

4. Click **Calculate** to perform calculations with the new settings.

Sheet Ordering Example:

A protocol has three sheets: Assay Details, Results, and Fit.

The desired sheet order is: Results, Fit, Assay Details.

To reorder the sheets, enter the Sheet Order CSV list as: **Results,Fit,Assay Details**
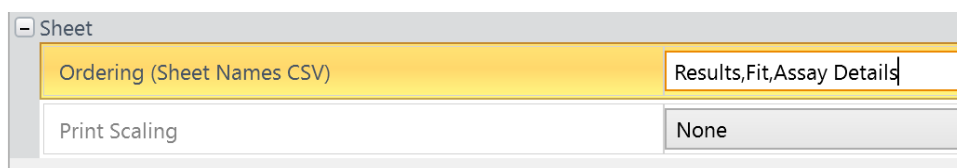
Recalculating the results displays the new sheet order.

Sheet Ordering Advanced Settings

For **Sheet Names** that are defined using **Macros**, i.e. **{AnalyteName}** for a Multiplex assay, or **{PlateNum}** for a Multiple Plate assay, **Regular Expressions** can be used to specify a custom Sheet Order.

About Regular Expressions

Regular Expressions or Regex is a string of text that allows you to create patterns to match and sort text. This functionality can be used to specify the sheet order for sheet names using Macros.

Regex Expression Components

The table below describes basic Regex Syntax.

Characters

^	Matches the beginning of a line
$	Matches the end of a line
.	Matches any character
*	Refers to a "greedy" match, which matches anything in the place of *
{Separator}	Custom macro used to support more complex sheet ordering scenarios

How to: Use Sheet Ordering Advanced Settings

1. Select the **Report** tab.

   If the **Report** tab is not immediately visible, click **<< Show All Properties** to expand.

2. In the **Report Elements** pane, select the **Report** parent element.

3. Add the Regex String to the **Ordering Sheet Name CSV** field.

4. Click **Calculate** to perform calculations with the new settings.

The following table summarises each available report element. Further details and settings are included in the provided linked topics.

Multiplex Sheet Ordering Example

Often when running a Multiplex protocol it is ideal to separate the data analysis by analyte. This can be accomplished by using the **{AnalyteName}** macro. However, if you would also like to separate out the results and the curve details from each analyte, specifying the sheet ordering can become more complicated.

In a Multiplex protocol with three analytes: Total Pro, Insul, and cPep, the sample table sheets are organized by analyte using **{AnalyteName}**:

The details of the curve fit are also organized by analyte, using **{AnalyteName} Curve Details**:

To organize the sheets as **Analyte1, Analyte1 Curve Details, Analyte2, Analyte2 Curve Details,** etc. we will use a regex to identify and apply the appropriate pattern.

{AnalyteName}{Separator}^{AnalyteName}.*$

{AnalyteName} refers to the Sheet Name for the sheet containing the sample table.

{Separator} is used here in place of a comma for the CSV format, this allows the sample table and curve details for each analyte to be displayed in tandem.

^{AnalyteName}.*$ will display the matching AnalyteName sheet, followed by additional text strings (for example, Curve Details).

Entering this expression into the **Ordering Sheet Name CSV** field returns sheets ordered:

Sheet	
Ordering (Sheet Names CSV)	{AnalyteName}{Separator}^{AnalyteName}.*$

| Total Pro | Total Pro Curve Details | Insul | Insul Curve Details | cPep | cPep Curve Details |

Configuring Template for Page-Based Report

Play Video

The report template enables presenting your analysis results tailored to your laboratory's standards and requirements. This feature merges together report elements with a configured template. Use the full power of MS Word or WordPad features to customize page-based reporting of the results.

For example, you can define a custom sequence of selected report elements, insert relevant images or textual descriptions for a printed document. Simply apply styling settings and include the results required.

> Report template affects Page View and page-based outputs (DOC, DOCX, PDF) of the analysis results only.

Add New Report Template for Page-Based Reporting

1. Launch an assay protocol or open a results file.

2. On the **Report** ribbon tab, in the **Views** group, select the **Page View** of the results.

3. Navigate to the **Template** group and click **New**.
   This launches the Template.DOCX file with a default application (typically MS Word or WordPad).

4. Review and edit the reporting template content as required.

5. After making and saving changes to the report template, click **Calculate** to generate a report with the new settings.

The application displays a Template.DOCX file for editing – this is the template file. Initially, it contains the MyAssays report element identifiers (**Ids**) in curly brackets. In addition to report element identifiers, meta data values and any macros configured in the protocol can also be referenced in the report template. To reference meta data values or macros in the report template, use the following reference syntax: **{<MacroName>}** or **{<MetaDataName>}**.

> All meta data macros can be seen by adding a report text element, and using the Text control. The table below demonstrates the reference syntax appropriate for each condition:

Reference Syntax	Description	Example
{ReportElementId}	Includes the specified report element	**{SampleTable1}** This refers to the first sample table report

Reference Syntax	Description	Example
		element, Sample Table 1
{<MacroName>}	Includes the specified macro as con-figured on the XML tab of the MyAs-says Desktop Protocol.	**{<Factor>}** This refers to the Factor macro configured on the XML tab of the MyAssays Desktop Protocol. Including this in the report will display the value of the macro.
{<MetaDataName>}	Includes the specified meta data macro.	**{<CurrentDateShort>}** This refers to the current date short macro. Including this in the report will display the current date.

Report templates have no restrictions regarding the specific information they contain. You can make any changes to the template and save them. For example, reposition, remove or duplicate Ids, change their font, style, and other properties, add textual information, macros etc. In fact, any change is possible if it is supported in the editor.

Add Report Element Id to the Report Template

1. Launch an assay protocol or open a results file.

2. Select the **Report** tab.

3. Select the Report Element from the list.

4. Copy the element's **Id** and insert it in the appropriate place of the template in curly brackets and press the spacebar to insert a space (e.g., **{SampleTable1}**).
If there is no space after the element's **Id**, table elements such as Sample Table will be merged together in the report.

5. Save changes to the report template and click **Calculate** to generate a report with the new settings.

After modifying the template file, you can switch back to MAA and generate an updated report while keeping the editor open. This way you can review modified report in Page View and make additional changes if needed.

The defined template will be applied to all page-based reports of this assay-results file.

> Only one template can be defined for the assay-results file at a time. If the previously defined template is no longer useful, edit or delete it.

Edit/Remove Existing Template

After you have created **New** template file, the **Template** group expands with two new options:

- **Edit** – Modifies the template file's content according to newly added report elements or updated formatting. This option will launch your default .DOCX editor with the existing template file.

- **Delete** – Removes the existing template file (a warning message will prompt for confirmation before this action is completed).

Print Settings and Print Preview

You can print your generated results directly from MAA with MyAssays Desktop printing functions. These include printing the generated report with the default or a selected printer, and previewing results before printing them. You can also configure automatic printing of the first results version if the data analysis is performed from an assay-protocol (this is useful when a protocol is launched automatically, perhaps by Folder Poll or from the command line).

Before Printing

To make sure that your report meets your specifications, preview your report before sending it to the printer. This can avoid wasting paper and verify that all the information is presented appropriately.

To Preview Report Before Printing

1. Launch an assay protocol or open a results file.
   If you launch a protocol, click **Calculate** to generate results.

2. Do one of the following:

   - On the **Report** tab of the ribbon, click **Print Preview**.

   - On the **File** backstage view, select **Print** tab, and then click **Print Preview**.

This launches the **Preview** window, where you can preview your report before printing it. To print your report and check or change the settings for your printer, click the **Print** icon in the upper-left corner of the window.

Set Up Report Layout and Content

MyAssays Desktop provides great flexibility in how your report content is presented. For maximum flexibility, consider using a page-based report template; with this feature you can change the font properties, page orientation and margins, and add any additional content needed. To learn about custom page-based layout for your report, see Configuring Template for Page-Based Report.

> After you create or edit a template, click **Calculate** to apply changes and update the report.

Automatically Print Report on First Calculation

When setting up the data analysis for a protocol, you can configure it to automatically print the report once the first set of results are calculated (using the default printer).

To Automatically Print Report on First Calculation

1. Launch an assay protocol.

2. On the **File** backstage view, select **Print** tab, and then select **Print report on first calculation** check box.

3. Save the updates to the protocol.

4. Click **Calculate**.
   On calculation, MAA switches to results mode, saves the results to .assay-results file and prints the report automatically. If you launch this protocol again (maybe importing a new set of measurements) and click **Calculate**, the results will be saved to another .assay-results file and printed automatically.
   For more information, see Save Options and Versioned Analysis.

Print Report with Default Printer

By default, all report content is printed as you see it in the **Page View** and in the **Preview** window with the default printer. If there is no printer available, you will be able to preview but not print generated reports.

To Print Report with Default Printer

1. Launch an assay protocol or open a results file.
   If you launch a protocol, click **Calculate** to generate results.

2. Do one of the following:

   - On the **Report** tab of the ribbon, click **Print**.

   - On the **File** backstage view, select **Print** tab, and then click **Print**.

Change Printer or Set Up Print Settings

If there are several printers connected to your PC, you can select the one you'd like to print to. You can also set up printing settings such as number of copies, printing preferences and page range.

To Print with Custom Printer or Set Up Print Settings

1. Launch an assay protocol or open a results file.
   If you launch a protocol, click **Calculate** to generate results.

2. On the **File** backstage view, select **Print** tab, and then click **Custom Print**.

3. Review or edit your printer settings, then click **Print**.

Avoiding Horizontal Page Splitting in Page-Based Reports

If the report contains content wider than the print area, the elements may be split horizontally between pages in the **Page View** and the page-based reporting. In this case, MyAssays Desktop will notify you and suggest rearranging the content to avoid undesirable formatting. This topic covers suggestions on how to resolve split tables or cropped images in your reports.

Why Page Splitting Occurs

MyAssays Desktop presents the calculated results in **Sheet View** and **Page View**. The page-based reporting is configured using the Page View and is limited by A4 page dimensions. Contents are fit to the page width. Therefore, if elements exceeding the width limitation are cropped horizontally and split between pages.

This is typically the case if your report contains a Sample Table with a lot of columns or image elements such as layouts or charts that are set to **Large** size.

Tips for Avoiding Horizontal Splitting over Two Pages

Here are some ways to prevent the content of your report from splitting (with the easiest being **Fit Sheet on One Page**):

Fit Each Sheet on One Page

The easiest way to eliminate horizontal page splitting is to use the report's **Print Scaling** setting; this can automatically resize the content to fit each sheet on one page by setting to **Fit Sheet on One Page**.

Assuming you have the assay to modified already opened, follow these steps:

1. In the **Assay Properties** panel, select the **Report** tab. If you cannot see the **Assay Properties** panel, click **Properties** to open it. If the Report tab is not immediately visible, click **<< Show All Properties** to expand.

2. From the **Report** header in the Report Tree, select the **Sheet | Print Scaling** dropdown box.

3. Select from the options the most appropriate setting for your assay:

   1. **Fit Sheet on One Page** – with this setting, all report elements contained on a single sheet will be fit to one page

   2. **Fit All Columns on One Page** – with this setting, all columns in the sample table will be scaled to fit on one page

3. **Fit All Rows on One Page** – with this setting, all rows in the sample table will be scaled to fit on one page

4. Click **Calculate** to perform the calculations with the new settings and to view the report.

Exclude Redundant Columns from the Sample Table

If your Sample Table contains a lot of columns, you can consider excluding some matrices from the table. For example, you could choose to exclude intermediate transform results that are not essential for your experiment. Assuming you have the assay results already launched, follow these steps:

1. In the **Assay Properties** panel, select the **Matrices** tab.
   If you cannot see **Assay Properties** panel, click **Properties** to open it.
   If the **Matrices** tab is not immediately visible, click **<< Show All Properties** to expand.

2. From the **Matrix Selection** pane, select the matrix you want to exclude.

3. In the **Matrix Configuration** pane, locate the **Report Contents** settings and select the **Include in Sample Tables** or **Include in Matrix Tables** check boxes to add the matrix to the associated report element.

4. Review or edit other data analysis settings.

5. Click **Calculate** to perform the calculations with the new settings and to view the report.

Split the Results between Sample Tables

If all the transform results should be reported but the Sample Table is split inconveniently, you can divide the content between several Sample Tables. Assuming you have the assay results already launched, follow these steps:

1. Add additional Sample Table element to the report.
   By default, it will be assigned with the **SampleTable2** Id.

2. In the **Matrices** tab, from the **Matrix Selection** pane, select the matrix for including in the second Sample Table.

3. In the **Matrix Configuration** pane, under the **Report Contents**, click **Sample Table Ids** drop-down, and remove selection from **SampleTable1**. This will include the matrix in the **SampleTable2** only.

   In the same way, select the matrices to include in **SampleTable1** only.

4. Review or edit other data analysis settings.

5. Click **Calculate** to perform the calculations with the new settings and to view the report.

Define Template for Page-Based Reports

Using the report template, you can configure the report to appear as desired. Refer to the [Configuring Template for Page-Based Report](#) to learn about setting up the template.

Below are some settings you can use to avoid cropping and splitting the contents between pages:

- Use smaller font for Sample Tables, Matrix Tables, or both

- Narrow the margins

- Change the page orientation to Landscape

Enhanced Security

Introduction

MyAssays Desktop Pro's Enhanced Security edition provides features compatible with working in GxP and 21 CFR Part 11 environments. This includes protected and tracked access to MyAssays Desktop Pro's features and data from inside a secured environment. The system can securely import, process, and output secure and protected content.

> This edition is only available to users with a MyAssays Desktop Pro Enhanced Security license.

Key features include:

- Access control – Authentication and authorization are used to permit or deny access to MyAssays Desktop functions.

- Operating-system-level security data storage protection – Only authorized users can make changes to MyAssays Desktop Pro data and configuration files.

- Secure hand-off of data – To ensure integrity of imported measurement data.

- Electronic Signatures - approve and sign protocols and results files electronically in accordance with 21CFR11 rules.

- Secured file protection – To ensure that data files are only accessible by authorized users.

- Audit trail and Login log – All activity is logged with date and time stamp against the logged in user.

- Excel and Word report protection – Changes to all Excel outputs can be protected with a password.

- Autologin account – To automate working with third-party software in an efficient and secure manner.

The Enhanced Security system shares user management and system security policies with Windows to simplify user management and to eliminate redundant administrator tasks. For example, if your users are already configured on a domain, it is easy to provide those domain users with secured access to MyAssays Desktop Pro.

The Enhanced Security system provides a number of configuration options to support different workflows, system configurations, and data handling methods.

> Use of the Enhanced Security mode alone does not provide compliancy with 21 CFR

Part 11. Any facility that requires compliance with 21 CFR Part 11 rules must implement the necessary procedures and controls specified by the regulation throughout the workplace.

The US FDA does not preapprove or certify systems with respect to 21 CFR Part 11. (It is misleading for any vendor to claim that a system, whether it be an instrument or standalone software, is Part 11 compliant.)

Full compliancy is always a combination of both technological and procedural controls. The compliancy assessment is always made on-site by the FDA.

Training Course

The restricted-access online training course has been designed to equip users in regulatory environments with training to configure and operate the secured system. Assessments and participant certification is available to verify that your team are up-to-speed.

The course covers all topics for installation, configuration, usage. The course is arranged into multiple tracks to cater for different user types:

- Security Administrators
- User Managers
- Analysts
- Operators

Features:

- Video content with interactive links
- Assessments
- Tracked Attempts/Score Results
- Multi-track course
- Participation/Results certification

Available at https://www.myassays.com/myassays-desktop-es-training-course.html

Authentication and Authorization

Throughout this documentation, the terms **authentication** and **authorization** are used; it is important that these terms be clearly defined and understood:

Authentication – The process by which users are identified by their username and password

Authorization – The actions that an authenticated user is allowed to perform

For example, when a user logs in to Windows by providing her username and password, she is authenticated. An authenticated user is authorized to perform certain operations. For example, an administrator is authorized to perform administrator operations whereas a standard user is not.

Authentication Options

With MyAssays Desktop Pro's Enhanced Security, there are two different authentication systems available:

- **Windows Log In**
- **MyAssays Desktop Log In**

The key difference is how the user must log in, either through the standard Windows Log In method or through a MyAssays Desktop Log In.

With **Windows Log In**, users will log in to Windows as they would do normally. The MyAssays Desktop application can be used without requiring an additional log in prompt.

With **MyAssays Desktop Log In**, when the MyAssays Desktop application is launched, the user must log in to the application to authenticate.

In both cases, user accounts are managed (e.g., adding/creating/disabling/locking user accounts) by the administrator using the standard Windows user management tools (see General User Administration). The user authorizations that are specific to MyAssays Desktop are managed using the MyAssays Desktop Pro **Security Management** tool.

> For Windows Login Authentication, the **Check Names** feature can be used to verify the existence of the user account within the specified context.

Authentication Context

MyAssays Desktop Pro's Enhanced Security supports these authentication contexts:

- **Local Machine**
- **Domain**

This means that user accounts can be managed either locally (on the local machine itself) or via a domain controller.

Which Authentication Method?

Deciding on the correct authentication method depends on how the workstation will be accessed:

- If each user will log in to Windows using their own Windows account, then use **Windows Log In**.

- If the workstation is configured to use a single common login that is shared by multiple users for general access, then use **MyAssays Desktop Log In**.

In many ways, the **Windows Log In** method is the simplest to work with and administer. End users have a single familiar login method to work with.

However, if you are working with third-party software (such as instrument control software), you may find that it imposes certain requirements on the Windows log in that must be followed. For example, it may be necessary for that software to be operated under a specific restricted Windows login to ensure it is correctly secured. In these cases, it may not be feasible to allow system users' their own Windows log in session; it is for this reason that the MyAssays Desktop Log In authentication option is available.

Windows Log In	MyAssays Desktop Log In
The workstation can only be accessed by a user providing their own personal credentials via the Windows Log In. The credentials provided when the user logs in to Windows are used by MyAssays Desktop. This means that the user does not need to log in to both Windows and MyAssays Desktop separately.	The workstation is routinely used through a single Windows log shared by multiple users. To secure MyAssays Desktop data and features by user, each user has their own user account that MyAssays Desktop uses to authenticate. This means that when MyAssays Desktop is used, the user must log in to the application directly.

Authorization

Any authenticated user will be able to launch the software; however, the operations that they can perform depend on the authorization settings that have been assigned to them.

> ℹ For a complete list of available authorization settings, see Authorizations.

Each user is assigned to a single authorization group. The system administrator can assign authorizations to users with the MyAssays Desktop Pro Security Management tool.

For example, a user assigned to the **Run and Review Only** authorization group would only be able to run protocols and review results (he would not be able edit protocol settings), whereas a user assigned to the **Unrestricted** authorization would be able to perform any permitted operation.

If a user successfully logs in to MyAssays Desktop Pro Enhanced Security and that user has not yet been added to the system, the user will be treated as a **Guest** user with no permitted authorizations. (The system advises guest users to contact the administrator to gain access to the software).

With MyAssays Desktop Pro Enhanced Security, any attempt to perform a protected operation is stored in the audit trail (including whether the operation was permitted or denied in accordance with the user's authorization).

Secure Data Hand-Off

When working with measurement data originating from instrumentation (such as microplate readers or gamma counters), it is important to ensure the integrity of the imported data.

In many systems, the hand-off of data between one system and another provides an opportunity for users to tamper with and modify the data either unscrupulously or in error. Such a vulnerable workflow is unlikely to pass regulatory validation or stand up to scrutiny.

For example, after the readings are completed the measurement data is written to a file. This data must then be transferred or imported into the analysis software (MyAssays Desktop Pro). It is at this point that the data could be intentionally (or unintentionally) falsified. MyAssays Desktop Pro Enhanced Security can detect and block such insecure actions.

In addition, in certain scenarios, it is important to ensure that a data file originates from a particular source. For example, in a laboratory with multiple plate readers, it may be important to ensure that measurement data is collected from a specific reader and not transferred to the system from another unexpected or untracked source.

It is for these reasons that MyAssays Desktop Pro Enhanced Security supports restricting the import of measurement in a number of different ways including:

- Requiring a valid data certificate
- Blocking files that were modified after creation
- Restricting data import from only a specific location

These methods can be used alone or in combination to ensure that the data imported into the system meets regulatory requirements for authenticity and traceability.

In addition to the above restrictions, for some laboratory workflows, the data to be processed is stored in restricted folders. This can be useful where third party software such as instrument control software can write secure content to a protected folder. In such a scenario, for security reasons and to ensure data integrity, standard users are not authorized to access the folder and make changes.

With Import Impersonation, the system administrator can configure MyAssays Desktop to access the folder by providing the secret credentials MyAssays Desktop should use to access the folder using impersonation. The credentials are stored privately within MyAssays Desktop's configuration, allowing the software to securely import the data from the protected folder without any loss of data integrity. Video Walkthrough...

Data Certification

The most reliable method to secure the hand-off of data is to configure the system so that a valid data certificate is required for all measurement data to import.

A MyAssays data certificate file is generated by the instrument control software. The certificate file includes the information necessary for MyAssays Desktop to validate the authenticity and source of the measurement data file.

If the certificate file is missing, or if the data file has been modified since the measurement data file was certified, then MyAssays Desktop Pro Enhanced Security will block the import (and log the attempt).

The certificate file also stores the origin of the file; this makes it possible for MyAssays Desktop to reject data files that are transferred from another system.

Data Certification with PerkinElmer EnVision

PerkinElmer's EnVision microplate reader supports MyAssays data certification.

To export certified measurement from the EnVision:

1. Ensure that you are using v14.xxx or later of the manager software.

2. Configure or perform the export function.

3. Select Export format option as CSV for MyAssays Desktop option:
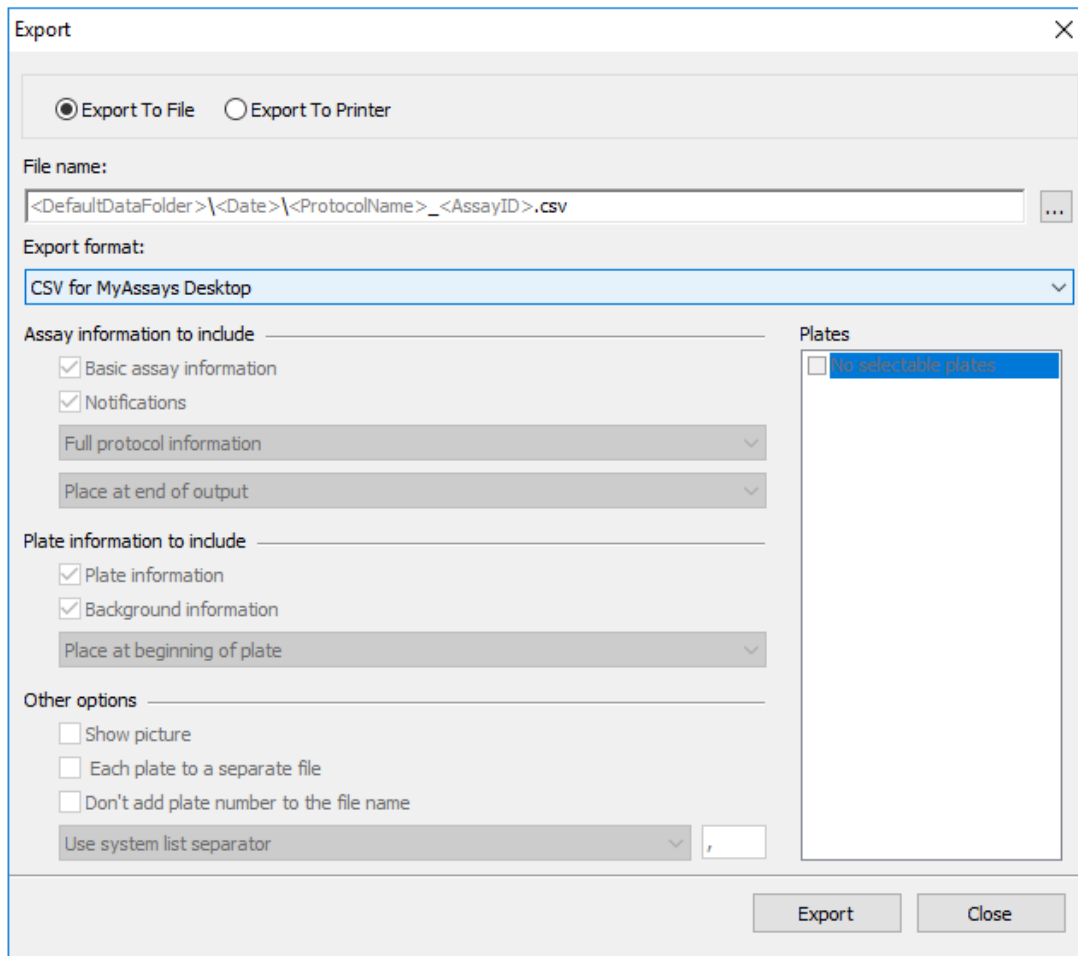
The generated data certificate files are stored alongside the exported file. Data certificate files are hidden by default (so they would not appear in Windows Explorer unless it is configured to show hidden files).

Data Certification with PerkinElmer VICTOR Nivo (GxP)

PerkinElmer's VICTOR Nivo GxP microplate reader produces MD5 files. The generated MD5 files are stored alongside the exported file. MyAssays Desktop can use the MD5 file as a certificate file to validate that the exported file has not been modified since its creation.

To configure MyAssays Desktop Enhanced Security for VICTOR Nivo certification:

1. Log into the MyAssays Desktop Explorer using an Administrator account

2. Open the Security Configuration Wizard under **Tools | Security Configuration**

3. Proceed through the steps of the Wizard to reach the **Data Certification Method** step.

4. Select the **MD5 Hash Code (Nivo)** Setting
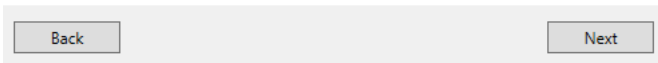
Data Certification with Other Instrumentation

If you are working with other instrumentation, please contact support@myassays.com for advice how to secure the hand-off of data.

MyAssays Ltd. offers solutions for retrofitting secure data certification to legacy systems (without requiring any modification to the third-party software).

Import Impersonation

Import Impersonation

Import impersonation can be used to provide secure access to protected data folders, granting MyAssays Desktop access to the content in a protected folder, even though end-users cannot access the content directly outside of MyAssays Desktop.

In some laboratory workflows, the data to be processed is stored in restricted folders. This can be useful where third party software such as instrument control software can write secure content to a protected folder. In such a scenario, for security reasons and to ensure data integrity, standard users are not authorized to access the folder and make changes. With Import Impersonation, the system administrator can configure MyAssays Desktop to access the folder by providing the secret credentials MyAssays Desktop should use to access the folder using impersonation. The credentials are stored privately within MyAssays Desktop's configuration, allowing the software to securely import the data from the protected folder without any loss of data integrity.

To enable Import Impersonation:

1. Log into MyAssays Desktop Enhanced Security with an administrator account.

2. Open the Security Configuration Wizard and continue through the steps to **Define Approved Import Folder**. Browse for and select the protected folder.
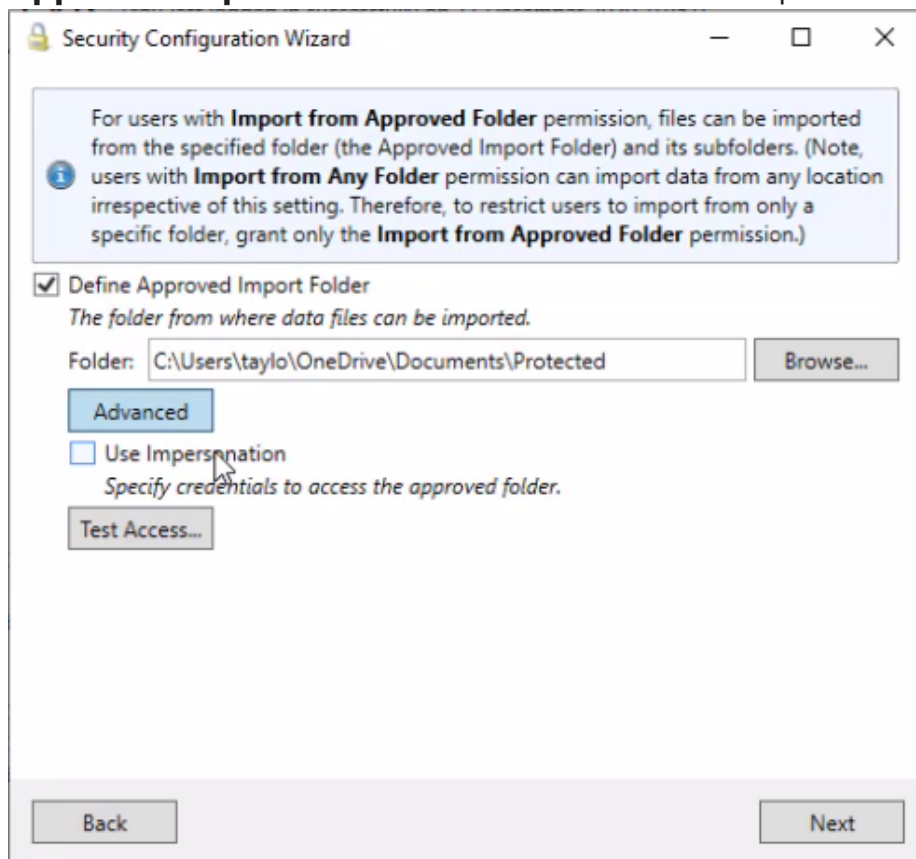
3. Open the **Advanced** options and select to **Use Impersonation**. Enter the Credentials required to access the protected folder.
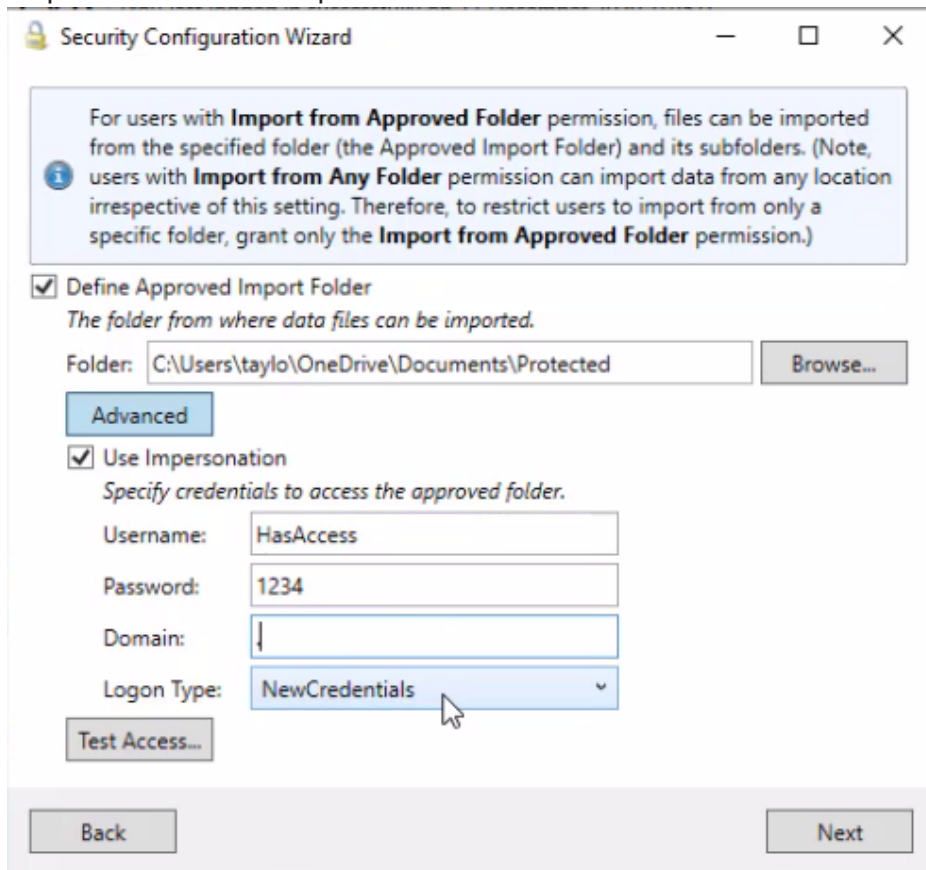
4. Specify the Logon Type. Logon Type provides different impersonation logon options. For most cases, **NewCredentials** should be used. However, other Logon Types are available for us in other impersonation scenarios. For a complete description of all Logon Types for impersonation, please see https://msdn.microsoft.com/en-us/library/windows/desktop/aa378184(v=vs.85).aspx

5. Select **Test Access** to ensure the provided credentials are configured correctly.

6. Ensure Users belong to an authorization group that includes **Import from Approved Folder** and does *not* include **Import from Any Folder**.
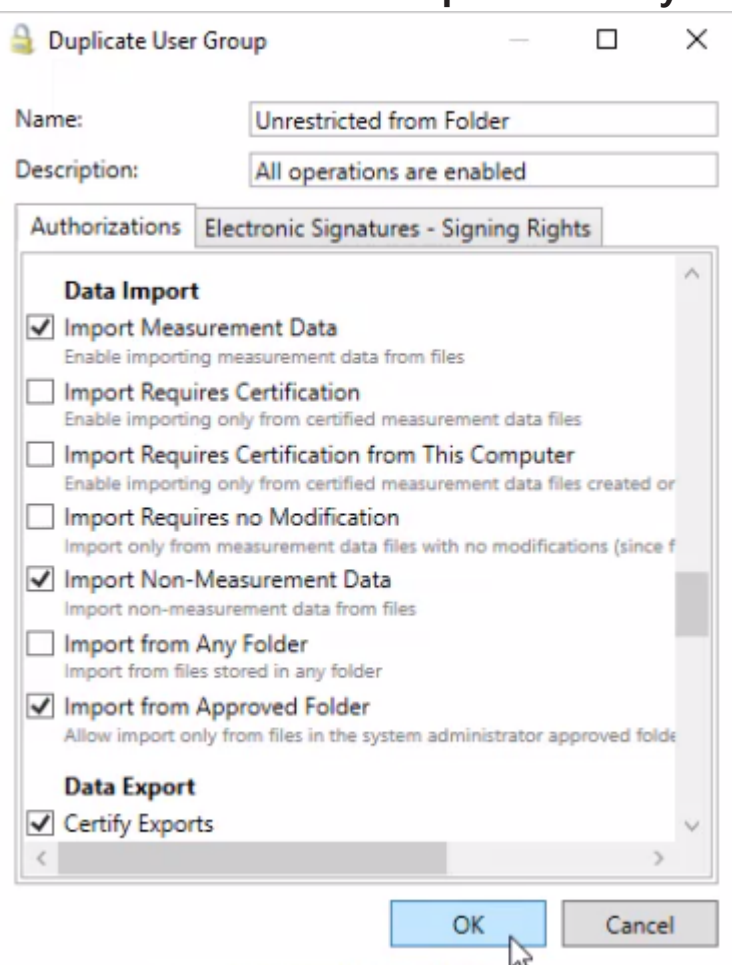
Data Protection

One of the advantages of MyAssays Desktop Pro is that it does not require a database to administer. All assay data is stored in standard files, making it easy to manage and transfer data files between users and systems. The Enhanced Security features enable you to configure and restrict access to MyAssays Desktop data files and folders, and to restrict the operations that can be performed on those files.

> For a complete list of available authorization settings, see Authorizations.

MyAssays Desktop Pro's Enhanced Security provides various features and options for securely protecting files. The configuration you choose will depend on how your organization prefers to arrange data. For example, you can:

- Partition files by users (**Windows Log In** authentication only)
- Share files between users

What Are the Assay Data Files?

The term **assay data files** refers to all the types of files used by MyAssays Desktop to configure, manage, and store details about the operations that it performs. This includes files for:

- Protocol
- Results
- Layout
- Export method
- Library curves
- Quality control settings
- User preferences
- Export reports (only those exported to the default **Reports** folder)

What about Measurement Data Files?

Measurement data files are generated by instrument manager software and therefore cannot be managed or controlled directly by MyAssays Desktop Pro Enhanced Security. It is the function and responsibility of the instrument manager software to ensure the integrity and security of the measurement data files it generates. To ensure that you have a fully secured system, you will need to ensure that the instrument manager software is sufficiently secured to meet your regulatory requirements.

Where MyAssays Desktop Pro Enhanced Security can help is in the secure hand-off of measurement data from the instrument manager through to data analysis in MyAssays Desktop Pro. In this way, a secure workflow from instrument to exported results can be achieved.

> If you can configure the location of where your instrument manager software outputs measurement data files, then it is suggested that you use the **Measurements** subfolder as the default location of the **Assay Data Folder**. In this case, the administrator will need to configure appropriate permissions for the instrument manager software to be able to write to this folder.

Where Are the Assay Data Files Stored?

With MyAssays Desktop, data file management is simplified using the **Assay Data Folder Root**. All assay data is stored under this parent folder (data is arranged under subfolders). Using a single parent folder for all assay data simplifies management of users' assets.

A typical scenario (and the default scenario when Enhanced Security is not used) is for the **Assay Data Folder Root** to be the **MyAssays** folder under each user's **My Documents** folder. Each user has their own protected folder for storing their own data files. Each user's data is kept separate from one another. In this case, the operating system provides secure functions for restricting access and permissions to resources.

A common requirement is to share all assay data between users of the system. In this case, the **Assay Data Folder Root** is the same path for all users. This could be a local file path or a network location. This is easy to configure by changing the **Assay Data Folder Root**. However, securing data shared in this way can be a challenge, and it is for this reason that MyAssays Desktop Pro Enhanced Security provides functions to simplify and manage this process.

Traditionally, managing shared access to common assets is difficult in Windows with various authorization settings being spread across different management tools. MyAssays Desktop Pro Enhanced Security simplifies this file management using easy-to-use authorization groups.

For example, if a user should not be permitted to delete or edit files, he can be assigned to the restricted **Run and Review** authorization group. This group does not include the permissions necessary to delete data files.

How Are Files Protected?

Protected data is stored in secure folders protected at the operating-system level. This means that only programs and users with permission to access or modify data can access and make

changes to the protected data. Any attempts to manipulate data using tools outside MyAssays Desktop Pro will be denied by the operating system.

There are two types of data protected by MyAssays Desktop Pro's Enhanced Security mode:

Security Data

Only the security system itself has access to the Security Data folder (where all audit trail, login, and user details, and all authorization settings, are stored). In all cases, the security data is protected and cannot be accessed or modified by users without administrator privileges.

Assay Data

Where assay data is shared between more than one user, MyAssays Desktop can provide Secure File Protection. With this feature enabled, MyAssays Desktop Enhanced Security takes control over securing the assay data files between different users.

Only MyAssays Desktop Pro Enhanced Security (and an administrator account) has the ability to make changes to data stored in MyAssays Desktop Pro data folders; in this way, the assay data files are securely protected. Only operations approved by the system (in the form of an authenticated user with the required authorizations granted) can be performed. Also, secured operations on the data are logged in the audit trail.

Electronic Signatures

 Play Video

MyAssays Desktop Enhanced Security's Electronic Signatures permits authorized users to approve and sign protocols and results files electronically. Electronic signatures are:

- Protected from removal or tampering

- Stored as part of the protocol or results files

- Recorded in the audit-trail

> The Electronic Signatures feature of MyAssays Desktop Enhanced Security feature has been designed and implemented to satisfy 21 CFR Part 11 rules.

To sign a file two distinct identification components must be entered (username and password). Each stored signature contains the signer's unique User ID.

Each user can be assigned specific signing rights and actions. For each signing a reason for signing is provided, including:

- Approve and Lock

- Disapprove

- Lock

- Unlock

- Review

- Take Authorship

- Take Responsibility

- *(Plus, custom actions...)*

For example, users in the **analyst** role would typically be granted rights to create protocols as well as sign protocols as "approved and locked". Users in the **operator** role would not be able to create, edit or approve protocols and only be able to use protocols that have been approved.

In this way, electronic signature supports traceability and accountability as well as controlling access to approved functions.

To support typical workflows, MyAssays Desktop Enhanced Security provides a default configuration with authorizations and signing rights. Simply assign users to the appropriate authorization group.

Configuring Electronic Signatures

Play Video

Enable Electronic Signatures from the **Security Configuration Wizard**:
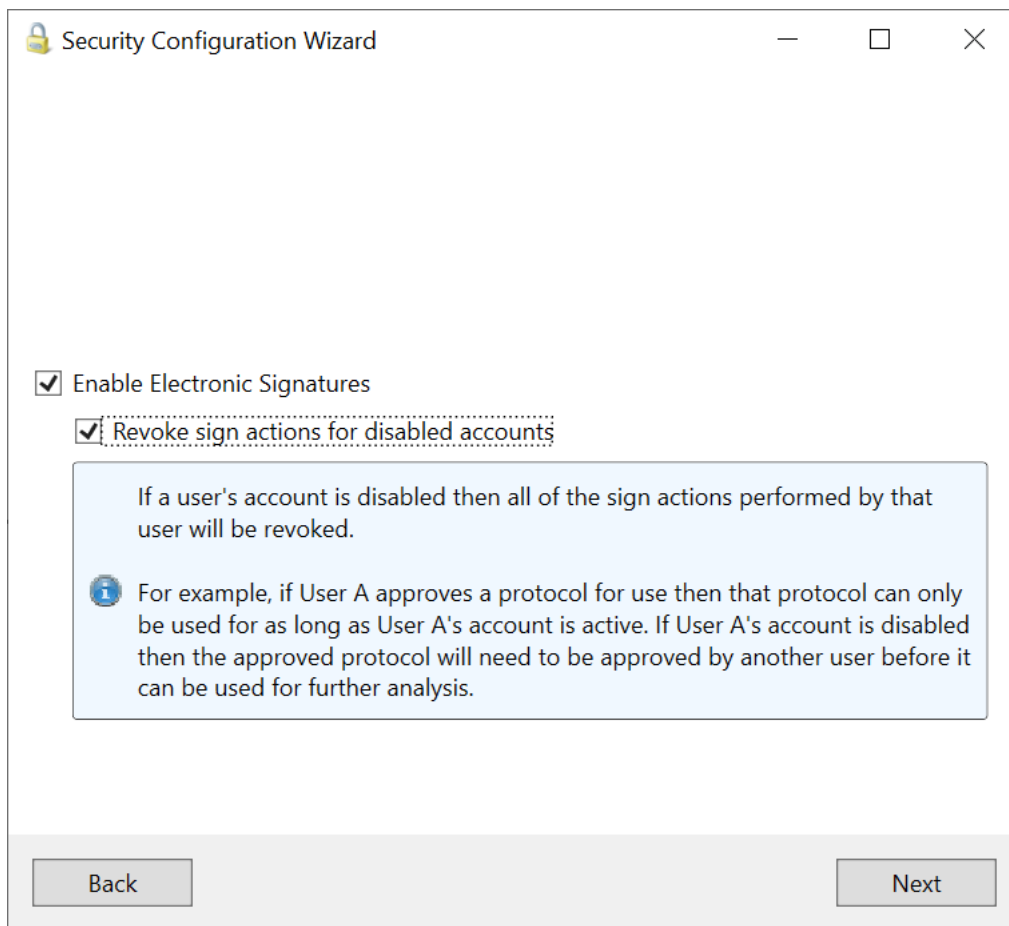
There is one sub-option: **Revoke signatures for disable accounts**. Set this option to revoke any signatures that belong to a disable account. With this setting, in any case where a user has electronically signed a file but that user account is disabled, any actions granted by the user's signing will be revoked. More...

Electronic Signatures Authorizations

The following electronic signature authorizations can be configured and assigned to each user:

Authorization	Operation
Protocols Requires Approval for Launch	Assay protocol files require approval for launch (i.e. a protocol must have been electronically signed with reason: approve).

Authorization	Operation
Results Requires Authorship for Exporting	Assay results files require authorship for exporting (i.e. a results file must have been signed with reason: authorship before it can be exported).
Results Requires Authorship for Printing	Assay results files require authorship for printing (i.e. a results file must have been signed with reason: authorship before it can be printed).
Results Requires Authorship for Saving	Assay results files require authorship for saving (i.e. a results file must have been signed with reason: authorship before it can be saved).

For example, if a user is assigned to a user authorization group with the **Protocols Require Approval for Launch** setting then the user can only launch protocols which have been approved.
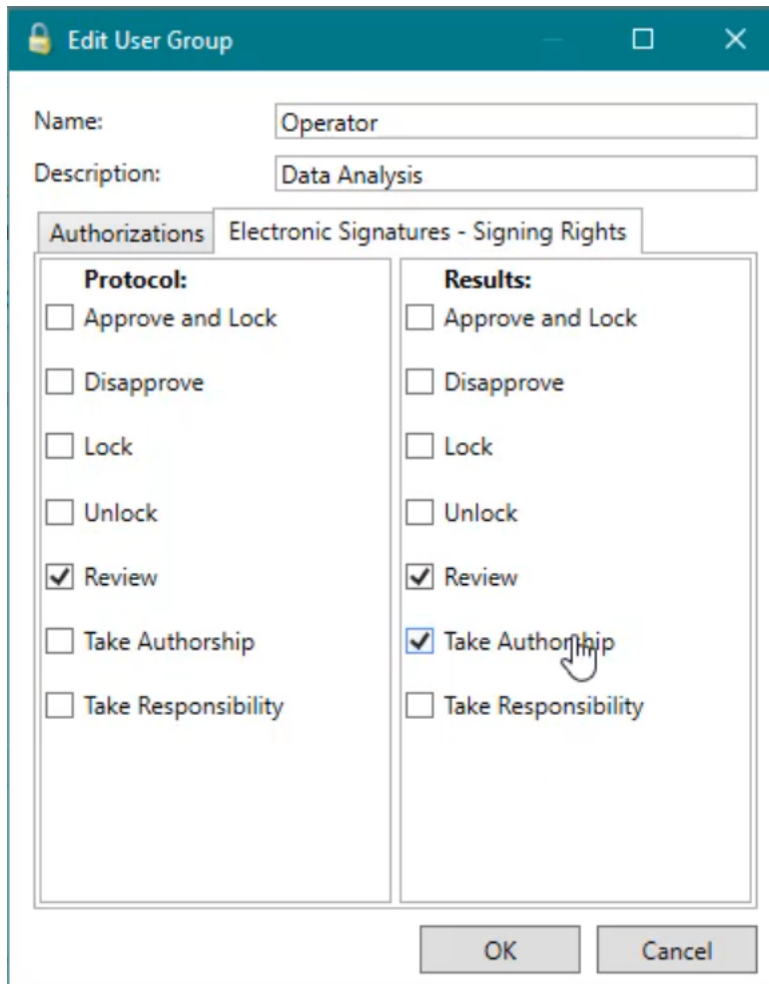
The **Security Management tool** can be used to define authorization groups including authorizations associated with Electronic Signatures:
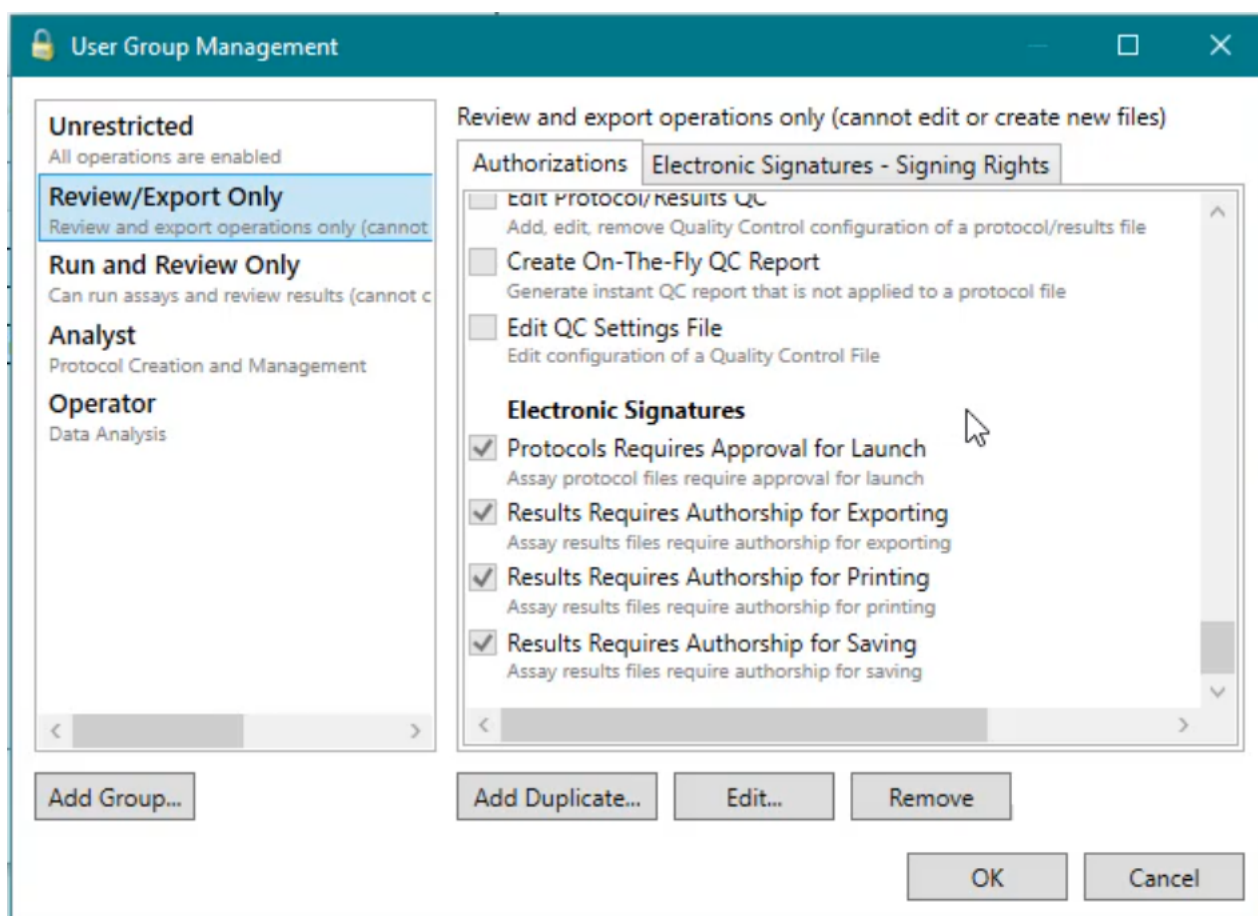
Signing Rights

Each authorization group can be assigned electronic signing rights. Each user will be able to sign in accordance with the authorization group assigned to.

Rights can be specified for Protocol and Results file separately:

Signing

When a user electronically signs a document, the user name and password must be entered. Also, a reason for signing should be specified. The available reasons will depend on the authorization group the user is assigned to.

Sign Actions

Each electronic signature is associated with a sign action as given by the signer as the reason for signing. The electronic signing of a document will perform the action on the document as described here:

Reason	Action
Approve and Lock	Approve the protocol for use and prevent further modifications.
Disapprove	Unlocks protocol for editing, prevents users from opening with "Protocol Requires Approval for Launch" authorization setting.
Lock	Locks protocol against further modification.
Unlock	Unlocks protocol allowing modification by users with appropriate authorizations.
Review	Indicates review of protocol/results.
Take Authorship	Marks the user as an author of the file (more than one user can be marked as the author).
Take Responsibility	Marks the user as responsible for the file (more than one user can be marked as responsible).

Electronic Signatures in Report

To include details of the signings in the report add the **Electronic Signature** report element to the report:

```
◢ Report
    TransformContentStandardCurveFit1
    SampleTable1
    TransformContentDilutionFactors1
    ElectronicSignature1
```
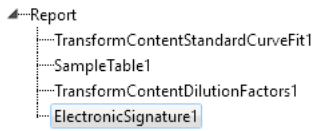
This will show details of all signings associated with the report. For example:

Electronic Signatures
Protocol Approved and Locked by *taylo*   14:05 20 January 2020

Revoking Electronic Signatures

When working with electronic signatures that are used to control access to the system, consideration must be given to the validity of signatures if a user's access to the system is removed.

For example, if an analyst's electronic signature is used to approve protocols for use by operators, if that analyst's access to the system is removed – then should those approvals still be valid and should those protocols still be usable?

MyAssays Desktop Enhanced Security provides an option to define what happens if a user's account is disabled. If an account is disabled, any signings by that account can be revoked automatically. This can be useful to prompt a review of the former user's signings.

Use the **Security Configuration Wizard** to specify if signatures should be revoked for disabled users.
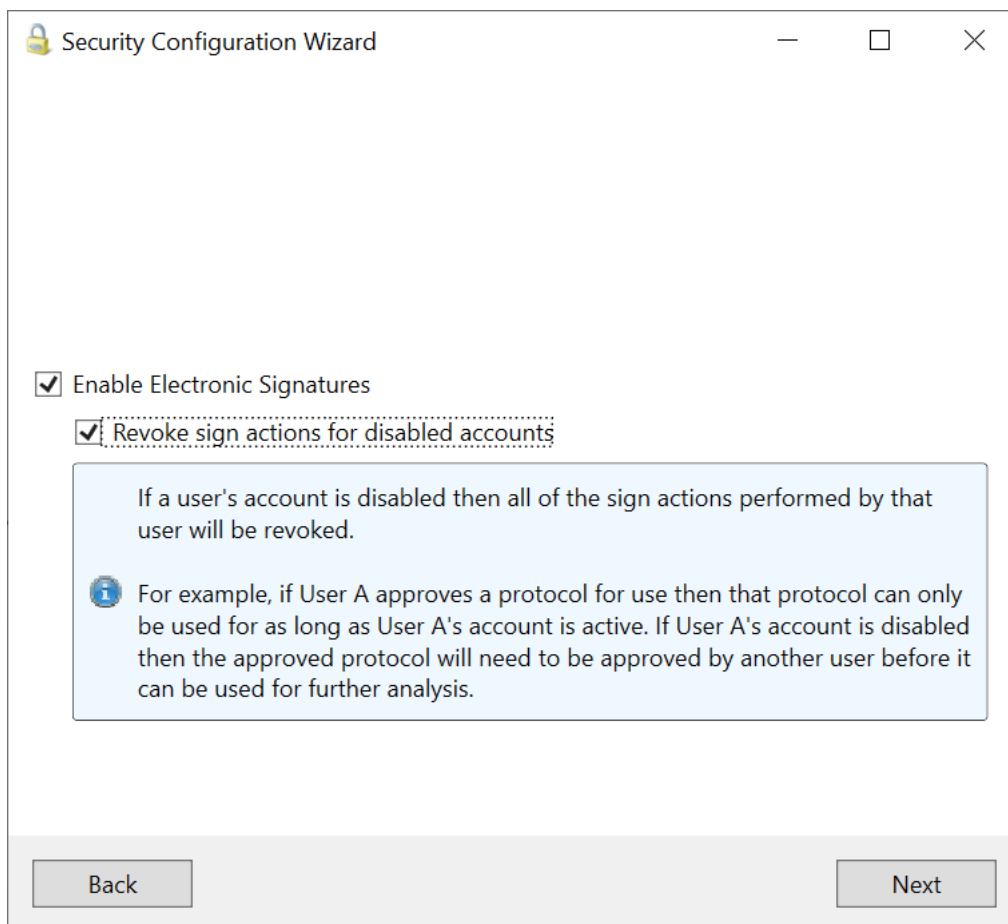
If the **Revoke sign actions for disabled accounts** is selected then signatures will be revoked automatically for any disabled user account.

Revoked signatures appear with a strike-through. For example, here the Operator's account has been disabled causing this signature to be revoked:

If a valid signature is required to permit operations (such as an approval signature is required for a protocol to be launched) then any impacted files will need to be signed by a user with the required signing rights.

Audit Trail and Login Log

The **Audit Trail** keeps track of user activity; user operations are logged by user with a date and time stamp. In addition, the **Login Log** keeps track of log in attempts.

The log data is stored in a protected folder, so it cannot be accessed or modified by standard users.

Log data can be exported to CSV or XML.

Autologin Account

When working with MyAssays Desktop authentication, the MyAssays Desktop Autologin account is available and provided for:

- Performing automated data analysis in a secured environment, such as under regulatory requirements
- Working with third-party systems, such as reader software

Typically, when you work under regulatory requirements, the third-party data collection or reader software provides their own user-management and security protections. Because users usually have to log in to each secured system separately, automating the workflow can become tedious.

To simplify this integration, MyAssays Desktop Enhanced Security enables performing the permitted data analysis under a protected and tracked Autologin account. This avoids the need to log in the software just to run data analysis.

The Autologin account is intended to be used solely for automatic operations where user intervention is not required.

With this approach, the users can benefit from a seamless secured solution. The workflow is simply a case of initiating measurements from the reader control software. Meaningful analyzed results and reports can be provided automatically be MyAssays Desktop along with necessary tracking information all securely protected.

> The Autologin account is not applicable for working with Windows Log In authentication. This configuration does not require a separate log in because all operations are performed using the logged in Windows user.

For information on how to enable Autologin account, see Configuring Autologin Account. To learn how to set up analysis with it, see Launching Analysis with the Autologin Account.

> By default, Autologin is only available for use under the specified shared Windows Log In Account. If Autologin is required for use from other standard Windows accounts then the feature can be enabled as described here.

Configuring Autologin Account

When working with MyAssays Desktop authentication, normally a log in prompt appears to perform the data analysis process. However, with the Autologin account, you do not need to log in to MyAssays Desktop. Instead, you can run permitted operations (such as data import, analysis, and export) automatically under this account.

Typically, the measurement data is collected from a reader with a separate third-party software. If such software provides their own user-management system to satisfy regulatory requirements, the users need to log in. And, rather than also logging in the MyAssays Desktop Enhanced Security system each time, use the Autologin account to fully automate the process in a secure and traceable manner.

How Is the Data and Workflow Secured?

The MyAssays Desktop Enhanced Security administrator can define which operations can be performed by the Autologin account. Routine day-to-day operations such as running particular protocols are limited to just that with full traceability.

To perform operations such as creating protocols and changing the analysis settings, a log in to MyAssays Desktop account with the necessary permissions is required.

> To satisfy regulatory requirements when working with separate systems, always ensure that there is a clear data trail from measurements to results.

> We advise including metadata that describes the origins of the imported data in the exported data or reports generated by MyAssays Desktop. This should include details such as date/time of measurements, instrument serial number, imported filenames and the operator details from the reader software. This content can be added to the MyAssays Desktop report using the report elements: Measurement Meta Data or Text (with macros) or both.
>
> The availability of such data depends on the reader software that is in use and the data that is being imported into MyAssays Desktop. MyAssays Desktop can be configured to import measurement and metadata from many sources and file formats. If you are working with a data format not already supported, please contact support@myassays.com for details of how to import the necessary metadata in a secure and traceable manner.

Setting Up the Autologin Account

1. Launch MADE.

2. On the **Tools** tab, click **Enable Security**, and then click **On**.

3. Select **MyAssays Desktop Log In**, and then specify the **Windows Log In** account that must be used by your reader control software (e.g., **LabUser**).

4. Select the authentication context.

   Typically this will be the **Local Machine**.

5. Enter or accept the **User Group Name**.

6. Enable the **Autologin Account**.

7. Select the authorization group that the Autologin account should belong to.

   This defines what operations can be performed by the Autologin account. Typically, this should be configured with only the operations necessary to perform the required data analysis.

   If you select **None**, then the Autologin account will not be able to perform any operations. The **Run and Review Only** option is preconfigured to permit operations typical for running and reviewing data analyses.

   > If you're not yet sure which operations should be permitted under the Autologin group, then select **None** for now. You can define your own authorization group to specify exactly what operations should be permitted under this account from the Security Management tool (available after completing the Security Configuration tool). From here you can assign the MyAssays Desktop Autologin account to the appropriate group.
   > For a complete list of available authorization settings, see Authorizations.

8. Complete the setup as required.

   > Because Autologin account is intended for automated workflow only, users cannot log in with it through the **Log In** dialog. The only way to use this account is to run MAA with **/autologin** command-line argument. See Launching Analysis with the Autologin Account.

Data Analysis Integration

When you have configured Autologin account and assigned it to an authorization group that satisfies your security requirements, then:

- Integrate a suitable existing protocol (e.g., download from MyAssays.com, use a installed protocol).
- Create assay protocols that perform the required data analysis.
- Copy or move the protocols from another source (e.g., obtained from colleagues) to the Protocols folder.

When you create new protocols or transfer them from another source, log in to MyAssays Desktop Enhanced Security with an account that has the necessary permissions. Then test that the protocols import measurements, run the data analysis, and export the results or report as required. Do not use the Autologin account to test these because the authorization group it belongs to should not have such permissions.

Once the data analysis operations performed by your MyAssays Desktop assay protocols are meeting your requirements, you can integrate the data analysis as part of an automated workflow with:

- Command Line – If your reader software supports launching an application after completing measurements and provides access to the new filename, then configure the reader software to launch MyAssays.Desktop.Analysis.exe using the command line. The Analysis Launcher can help you to build the command-line arguments.
- Folder Poll – If your reader software does not support launching an application when measurements are completed, then use the included Folder Poll tool to set this up. See https://www.myassays.com/folder-poll-with-myassays-desktop.video.

Autologin with the Shared Windows Log In Account

With MyAssays Desktop Log In authentication, the system will be routinely accessed through a shared single Windows log in. This is a standard Windows log in account that is shared between users of the system. This shared Windows Log In account is used to provide quick and easy access to the system to all users in the lab. This **Windows Log In Account** is specified in the Security Configuration Wizard, for example, here it is set to **LabUser**:
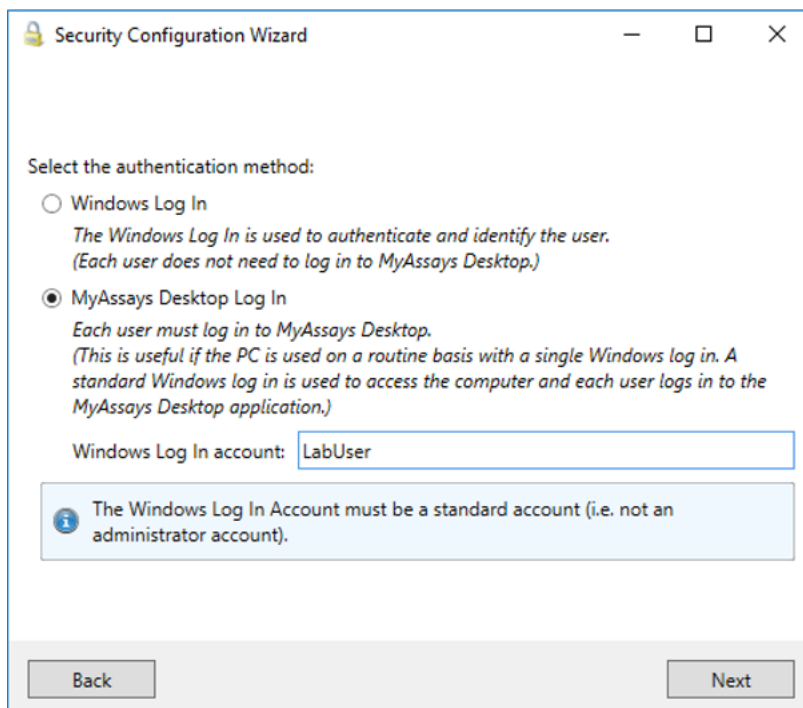
With this configuration, each user will log in to Windows using the **LabUser** account.

With MyAssays Desktop Log In authentication, each time a user works with MyAssays Desktop, the user will log in to the MyAssays Desktop software by providing their own private credentials.

With the Autologin feature enabled, permitted operations can be performed automatically without requiring authentication. This is useful to automate operations (such as performing data analysis as soon as measurement are completed).

By default, the system is configured to only allow these autologin operations if the current Windows session is either:

- The specified **Windows Log In Account** (e.g. LabUser)

- A local machine administrator

Or, the process is launched using local machine administrator privileges (e.g. elevated command line).

In cases where autologin function is used from standard Windows sessions, including:

- Local machine accounts

- Domain accounts

access to the autologin feature is blocked by default. This is to ensure that autologin operations are only available under the specified Shared Windows Log In Account.

Enable Autologin from Any Windows Account

Where autologin functionality is required under standard Windows accounts (in addition to the specified **Windows Log In Account**), an HKLM registry setting is available to permit autologin operations from standard user accounts. This can be enabled by creating a DWORD key:

AutologinAnyWindowsAccount at:

HKEY_LOCAL_MACHINE\Software\MyAssays\MyAssays Desktop\Security

Set this to **1** to enable autologin with any Windows account. Set this to **0** or remove the key to disable autologin for users other than those specified above.

Launching Analysis Using Autologin Account

When you use the command line to launch protocol with MyAssays.Desktop.Analysis.exe, include the **/autologin** command-line parameter. With this, the analysis will be performed under the Autologin account (without requiring to log in).

> When a command line is run with the **/autologin** parameter, any open MyAssays Desktop windows (running sessions with another user account) will be automatically closed.

To ensure that the MAA window is closed after calculations are completed and to prevent any user from being able to interact with the analysis application, use the **/exit** parameter.

If the **/exit** is not used, then the analysis window will remain open and allow the user to interact with the software anonymously. Please be aware that the user will be able to perform any operation that the Autologin account is authorized to do, although such operations will be logged against the Autologin account. For this reason, it is important that the Autologin account is restricted to only allow operations that are permitted for anonymous use (or use **/exit** if the user should not be able to interact anonymously).

> To help build and configure command line, use the Analysis Launcher.

If you are working with Folder Poll, you can add this setting via Folder Poll Manager:

1. Open Folder Poll Manager to review the changes.

2. Edit the Poll, select Operations and add **/autologin** to the Parameters.
   For example:
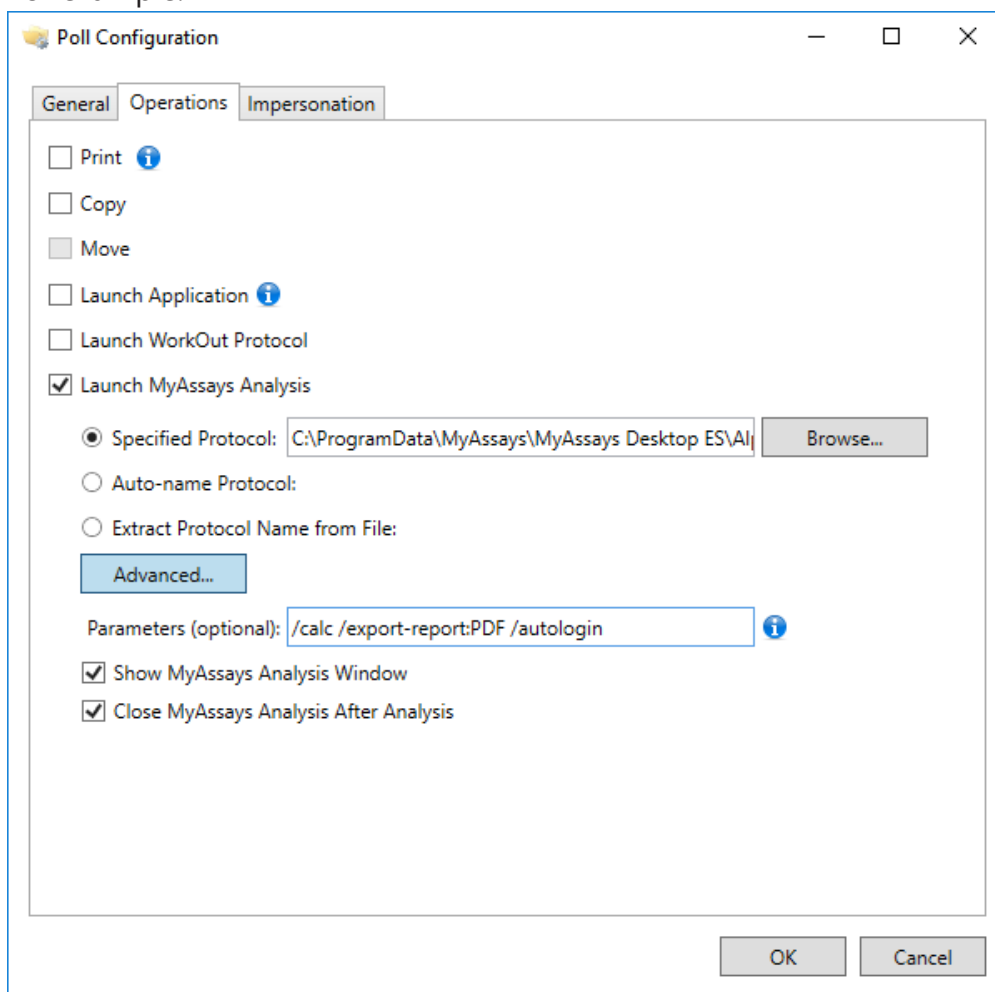
> ℹ **Close MyAssays Analysis after Analysis** check box here corresponds to the **/exit** parameter.

If you select **Automatically launch this protocol when a new measurements file is detected** from the Import Wizard, then you can configure the automated workflow for the protocol on the last step of the wizard.

Administrator Tasks

This section covers the system administrator tasks necessary to set up and maintain the system:

- Install MyAssays Desktop Pro
- Enable and Configure Enhanced Security
- Manage/Add/Authorize Users
- Monitor Usage

Installation

Installation tasks must be performed by a Windows user with local machine administrator privileges.

Please refer to release notes for latest installation instructions.

Enable and Set Up Enhanced Security

> **For security reasons, a local machine administrator account is required to enable Enhanced Security features. Once enabled, only the administrator account that enabled ES can make further changes to the ES configuration.**

After you have installed MyAssays Desktop and activated your license, the Enhanced Security system will not initially be enabled. To enable and initially configure Enhanced Security system with MyAssays Desktop Pro:

1. Launch **MyAssays Desktop Explorer**.

2. On the **Tools** tab, select **Enable Security**.
   This will launch the Security Configuration Wizard.

   > **Security Configuration Wizard** makes changes to the system and thus requires local administrator privileges. If the standard Windows **User Access Control** prompt appears, click **Yes** to start the wizard.

3. Select **On** to enable the Enhanced Security features.

4. Depending on how the users will log in to the application, select one of the following and follow the substeps:

   ### Each user works under their own Windows account (Windows Log In)

   a. Select **Windows Log In** and click **Next**.

   b. Select to authenticate **Local Machine Users**, **Domain Users**, or both.

      When selecting **Domain Users**, enter or paste the **AD Domain Name** of your domain.

      When specifying the AD Domain Name in the Security Configuration Wizard, use the Active Directory (NetBIOS) domain name, e.g., *CORP*.

      > Windows refers to two types of domain names: Active Directory (AD) and DNS. Windows will use the AD name when listing users, however the DNS domain is used to specify to the name of the network domain. For example:

c. Specify the path for saving your data files with one of the following:

- **User's Own Folder**
  Each user's assay data is stored under the logged in Windows users account's default **Documents** location. This is useful if you want to partition each user's data by their own account. In this case, Windows manages the partitioning of data (e.g., one standard user cannot access another user's data).

- **Shared Folder**
  All users of the system share the same folder. Select the **Secure File Protection** check box to secure the specified folder. With this, when running under a standard Windows account, authorized users can perform operations on files in that folder.
  For more information about this feature, see Secure File Protection.

All users of the system share a single Windows account (MyAssays Desktop Log In)

a. Select **MyAssays Desktop Log In**.

With this, each user will use their login and passwords to log in to MyAssays Desktop.

b. Specify a standard **Windows Log In** account and click **Next**.

This is a non-administrator account from which the system will be used routinely, with the account's access being shared between all users of the system. You can use default account name of **LabUser** or enter a different account name as required. In any case, please ensure that the account name is a valid local machine account.

c. Select authentication context.

When selecting **Domain Users**, enter or paste the **AD Domain Name** of your domain.

When specifying the AD Domain Name in the Security Configuration Wizard, use the Active Directory (NetBIOS) domain name, e.g., *CORP*.

> Windows refers to two types of domain names: Active Directory (AD) and DNS. Windows will use the AD name when listing users, however the DNS domain is used to specify to the name of the network domain. For example:
>
> **AD Domain name**: *CORP*
>
> **DNS name**: *corp.test*

d. Enter or accept the **User Group Name**.

   Only users that belong to the specified User Group (e.g., **MyAssaysDesktopUsers**) will be able to authenticate to access MyAssays Desktop Pro. In most cases, you can accept the default settings here to use the specified **User Group Name**.

e. Select the **Add the *Current user* to the user group (and set as an System Administrator)** check box and click **Next**.

   > For **Domain Users**, the *Current User* is always added as a system administrator.

f. To allow automating routine operations, select Enable Autologin Account and then select an Autologin group. For more details, see Configuring Autologin Account.

> For more information, see Authentication Options.

5. If you want to limit importing files only from the selected folder, keep **Define Approved Import Folder** check box selected, specify path to this folder and then click **Next**.

   For more information, see Approved Folder for Import.

6. To restrict editing of the reports, keep **Use Word/Excel Report Protection** check box selected and enter or paste password for allowing to modify the output files.

   With Word outputs, you can select to lock the whole document or only the results from editing.

   For more information about this feature, see Protecting Word and Excel Reports with Password.

7. Review the summary of your configuration, close any open MyAssays Desktop windows

and then click **Apply** if you are content with the settings.

8. Click **Finish** to close the wizard. Changes will be applied the next time MyAssays Desktop is launched.

> When working with a shared assay data folder, launch MyAssays Desktop Pro at least once with a successful authentication to install the preconfigured protocol and example files under the protected folder.

If you want to make changes to the initial configuration, run the Security Configuration Wizard again.

What's Next?

After you set up the general configuration of the Enhanced Security system, follow these steps:

- Add users of your Enhanced Security system

  For more information about adding, creating, disabling, and locking accounts, see General User Administration.

- Review and configure Groups
- Set up the authorizations for each group
- Configure each user

Secure File Protection

When all users of the system share the same Windows account or the same assay data folder, it is important to ensure the security and integrity of sensitive data. With Secure File Protection, the files stored in the secured **Shared Folder** are protected against unauthorized altering, deleting, copying, and moving.

How Secure File Protection Works

MyAssays Desktop Enhanced Security protects the assay data files stored under the **Shared Folder**. Only the application itself and a system administrator account have sufficient permission to make changes to the data stored in MyAssays Desktop Pro data folders. This prevents any unauthorized operations on data.

Secure File Protection requires that the system account has permission to take ownership of the specified resource. This is normally the case for the resources of a local machine (such as a local hard drive). If this is not the case (such as with a restricted network resource), then data can still be shared between users, however the protection of such files should be managed and configured by the resource's administrator.

Users can only perform operations approved by the system (in the form of an authenticated user with the required authorizations). Also, secured operations – Copy and Paste, and Delete – are logged in the audit trail.

For more information about how the operations are secured, see File Operations.

When Secure File Protection Is Applied

When you enable Enhanced Security on your system with:

- MyAssays Desktop Log In authentication, the same Windows account (e.g., LabUser) is typically logged in all day with different users in the lab using it. However, MyAssays Desktop authentication controls the access to MyAssays Desktop Pro and to a folder where all assay data is stored. With this, different users have different levels of access to the data as authorized for the group they belong to. In this case, data is already stored under a protected shared folder.

- Windows Log In Authentication, you can turn on **Secure File Protection** by selecting the check box if you select **Shared Folder** as the Assay Data Folder.

To change the initial settings, run Security Configuration wizard again.

> A shared data root folder that is protected during Security Configuration remains in the same state even if an administrator selects another folder to protect. The

administrator must acquire ownership and reconfigure the previously protected folder security permissions manually.

Where the Shared Folder Is

The default location of the shared assay data folder **is**

C:\ProgramData\MyAssays\MyAssays Desktop ES\Assay Data. For Windows Log In authentication, it can be changed to another location within the computer or on the network.

Active Directory (AD) Domain Name

When setting up Enhanced Security for domain accounts, you have to provide the AD Domain Name of the domain you are using.

What Is AD Domain Name?

The AD Domain Name is the short name of your Active Directory domain. It is also referred to as the NetBIOS name. The Active Directory Domain Name is not the full DNS domain name but typically the leftmost part of the DNS name. For example:
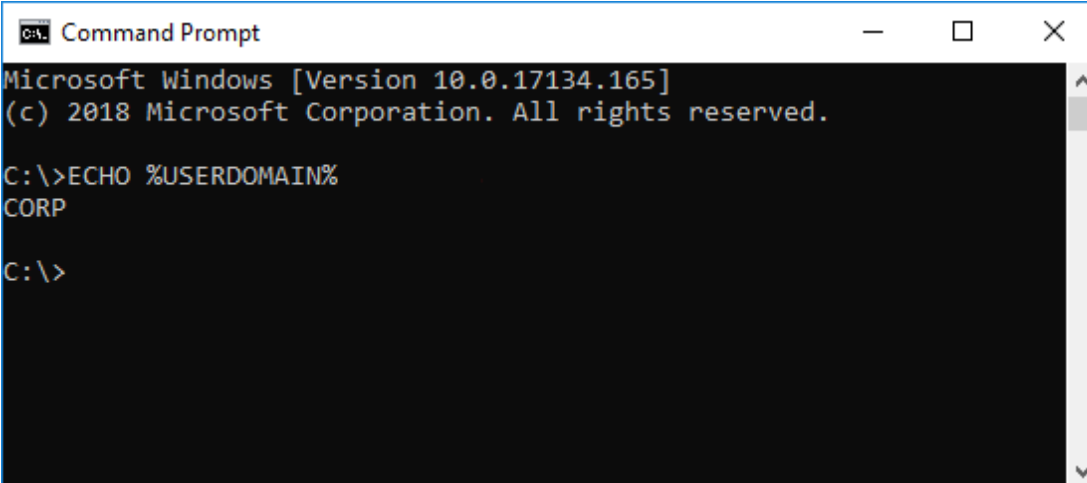
AD Domain name: *CORP*

DNS name: *corp.example.org*

How to Determine AD Domain Name?

1. Log in to Windows with a domain account.

2. Launch **Command Prompt**.

    a. Display **Run** menu by pressing **Windows** logo key + **R**.

    b. Type **cmd** and click **OK** or press **Enter** key.

3. At the command prompt, type **ECHO %USERDOMAIN%**.

4. Press **Enter** key.

This displays the AD Domain name (NetBIOS name) of your domain. For example:

Provide this name in the **AD Domain Name** field when setting up Enhanced Security or reconfiguring the system to include domain accounts.

Approved Folder for Import

To provide additional control surrounding data import, you can restrict the import of measurement data files to a specified approved folder and its subfolders. This is typically an instrument output folder. For example, the instrument control software might output measurement data to a specific folder. For additional security, the system could be configured so that only the instrument reader software can write to this folder.

How to Restrict Import to an Approved Folder

First, when enabling or reconfiguring Enhanced Security on your system:

1. In the Security Configuration Wizard, select **Define Approved Import Folder** check box.

2. Specify the existing folder where data files can be imported from.

3. Complete the wizard.

Second, assign the users of your system to an authorization group where the **Data Import | Import from Approved Folder** authorization is enabled and where the **Data Import | Import from Any Folder** is disabled.

For more details about authorization settings, see Authorizations.

> If an authorization group has **Import from Any Folder** permission, then users can import data from any location irrespective of this setting.

Therefore, to restrict which folders users can import from only a specific folder, grant only the **Import from Approved Folder** permission. Using this setting, files can only be imported from the specified folder (the Approved Import Folder) and its subfolders. If a user tries to import from other resources, the operation will be blocked by the system and corresponding entry will be added in the audit trail.

Protecting Word and Excel Reports

To ensure the integrity of data contained in exported reports, Word (.doc/.docx) and/or Excel (.xls/.xlsx) outputs can be protected, preventing any further modification after they have been generated. In this way, users will not be able to accidentally or deliberately change or delete data contained in MyAssays Desktop exported reports.

How the Reports Are Protected?

The administrator can specify to protect the exported outputs with a password. Only users with knowledge of this password will be able to edit the protected documents.

For Excel outputs, the password protects the entire workbook against any further changes.

For Word outputs, there are two additional options:

- **Whole Document** – Prevent users from making any changes to the document.
- **Only Results** – Restrict modifying the sections of the document containing results generated by MyAssays Desktop, but, make other parts of the file editable. In this way, you will maintain accuracy and consistency of MyAssays Desktop data analysis results but allow inclusion of additional content such as digital signatures or other additions a user might want to make.

How to Set Up Password for Outputs?

This is a two-level process:

First, when enabling Enhanced Security on your system, select and configure password protection:

1. In the **Security Configuration Wizard**, select **Use Word/Excel Report Protection** check box.

2. Enter or paste the password to apply for document protection.

> You can change this password by rerunning the wizard. This will apply to exports created after the change is made.

3. Select how to protect Word outputs from the drop-down list.

4. Complete the wizard.

Second, assign the users of your system to authorization group with the required **Data Export** operations selected. This is **Protect XLS/XLSX** for Excel and **Protect DOC/DOCX** for Word outputs. Users belonging to an authorization group with these authorizations set will only be able to export protected documents.

> ⓘ For a complete list of available authorization settings, see Authorizations.

Export Certification

The Export Certification feature is used to ensure integrity and authenticity of data exported from MyAssays Desktop. For example, if you are exporting results from MyAssays Desktop (perhaps PDF, DOCX, TXT) or any file for use in other system, for regulatory purposes you may need to validate or prove that content generated by MyAssays Desktop has not been modified since it was created.

 Play Video

How are the Reports Certified?

With the **Certify Export** authorization set, all exported data will also have a corresponding **myassayscert.xml** file.

This certification file will ensure the data has not bee modified since its creation.

How to Add the Certify Export Authorization

1. In the **Security Management Tool**, select to **Manage Groups**

2. Add the **Certify Export** authorization to the necessary User Groups

Data Export
☑ Certify Exports
  Create a data certification file with each exported file.
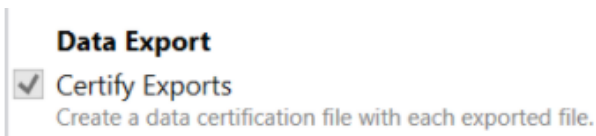
> ⓘ With MyAssays Desktop R8 and forward, all user groups are assigned the **Certify Export** authorization by default.

3. Apply the User Groups to the appropriate Users.

> ⓘ For a complete list of available authorization settings, see Authorizations.

How to Check File Certification

1. In the **MyAssays Desktop Explorer**, open the **Certificate Validator Tool**

 Play Video
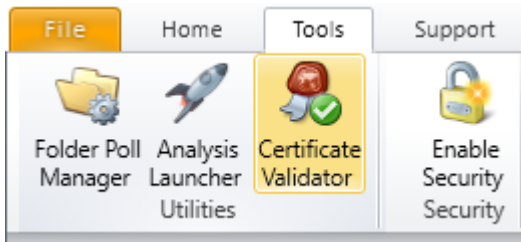
2. Browse for and select the desired file

3. Press **Validate**

4. The results of the validation will appear with additional details
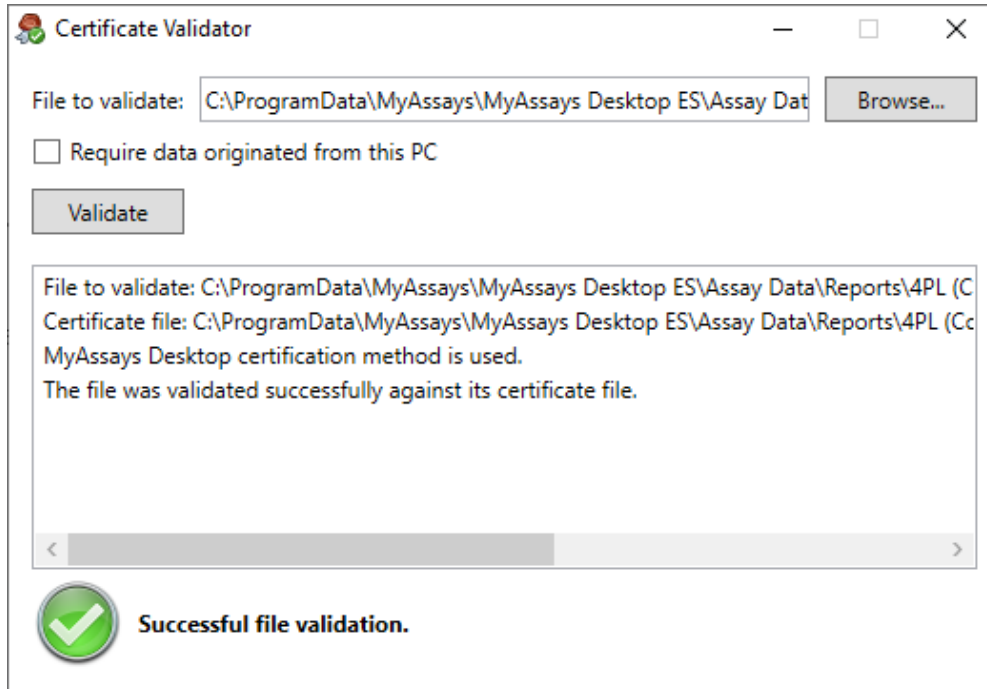
Security Configuration

To configure Enhanced Security system with MyAssays Desktop Pro, use **Security Configuration Wizard**. When you enable Enhanced Security, it guides you through setting up the initial configuration of the system.

To make changes to an existing configuration, run this wizard again and follow the steps as described below:

1. Launch **MyAssays Desktop Explorer**.

2. On the **Tools** tab, select **Security Configuration**.

   When you rerun the Security Configuration Wizard, it features all the configuration settings you initially set up when enabling Enhanced Security on your system. These are covered in the Enable and Set Up Enhanced Security.

3. However, it also contains an additional step that allows you to keep the existing user management and security data configuration or remove it.

4. Select **Use existing security data** check box to keep your administration settings, or clear it to delete the configuration from your system. Click **Next** to apply the changes and finish the wizard.

What is Security Data?

Security data includes all your configured user administration and security settings:

- Login log and audit trail
- User details
- Authorization settings
- Security options (for **MyAssays Desktop Log In** method)

User Administration

With Enhanced Security enabled and configured, initially the only user account that will be added to the Enhanced Security system is the user account that was used to perform the setup (i.e., the administrator account). This account is automatically added to the **Unrestricted** authorization group and assigned to the Enhanced Security account type **System Administrator**.

To grant other users permission to use MyAssays Desktop Pro, each user must be added to the Enhanced Security system and assigned to an appropriate authorization group and account type.

Guest Users

When working with **Windows Log In** authentication, users that are not added to the Enhanced Security system can launch MyAssays Desktop Pro but will be treated as a guest user. Guest users are advised to contact the system administrator for access to the software. Guest users cannot perform any operation.

User Accounts

The Enhanced Security system uses the Windows user management system for administering user accounts. This means that you do not need to create a whole new set of user accounts; you can use existing accounts that may already be defined on your system (both local or domain accounts).

Autologin Account

With **MyAssays Desktop Log In** authentication, if this account is enabled, it is added automatically alongside administrator account. Autologin account is useful if working with third-party software (such as instrument control software or LIMS) where operations should be performed independently of any specific user account with an automatic log in procedure.

For more information, see Autologin Account.

General User Administration

General user management (such as adding, creating, disabling, and locking accounts) can be administered using the standard Windows user management tools.

Configuring Local Machine Accounts

In Windows 10, if using local machine context:

1. Right-click **Start** and then click **Computer Management**.

2. Under **System Tools**, select **Local Users and Groups** and then select **Users**.

Password policy rules (password history, minimum length, etc.) can be set in Windows 10 from **Start** | **Run** | **secpol.msc** | **Security Settings** | **Account Policies** | **Password Policy** and **Account Lockout Policy**. These should be set in accordance with your 21 CFR Part 11 compliance requirements. For more information on configuring Windows password policy, please see https://docs.microsoft.com/en-us/windows/device-security/security-policy-settings/password-policy.

Configuring Domain Accounts

If your network is connected to a domain, then your password policy rules and user management will be administered by the domain controller. Contact your domain administrator for more information.

Domain Users

MyAssays Desktop Enhanced Security can work with your existing domain accounts.

For both **Windows Log In Authentication** and **MyAssays Desktop Log In Authentication**, it is not necessary for a domain administrator to configure the system. The system configuration requires only local administrator privileges. This local administrator can set up the system and assign users (including domain users) access to the software at various authorization levels.

> With **MyAssays Desktop Log In Authentication**, the process of adding a user to the MyAssays Desktop user group might require authentication of the domain account. In this case, the user account to add can be used.

Adding Users

To grant a user account permission to use MyAssays Desktop Pro, the account must be added to the Enhanced Security system. The steps to add a user depend on the authentication method in use.

How to Add Users (Windows Log In)

With **Windows Log In** authentication, the administrator must add each user that requires access using the **Security Management** tool. Users that attempt to access MyAssays Desktop Pro but have not been added to the Enhanced Security system will be automatically assigned to the **Guest** account type.

The administrator can add users to the Enhanced Security system as follows:

1. Launch **Security Management** and click **Add**.

2. Under the **Username**, enter the Windows user name (as the user would enter it when logging in).

   If the user is a domain user, then enter the AD domain name followed by backslash (****) and the username (e.g., for a domain "*CORP*" and username "*LabUser*" the **Username** should be: *CORP\LabUser*).

3. Provide a **Full Name** for the user. Click **Check Names** to verify the entry is correct, and click OK to confirm.

> If a domain user name is specified, Windows may prompt for the name and password of an account with permission to access the domain. The credentials of the user account to add can be used (or a domain administrator account can be used if it is available).

For information about logging in with domain account, see Log In Options and Password Management.

Please now proceed to the Configuring a User section.

How to Add Users (MyAssays Desktop Log In)

With **MyAssays Desktop Log In** authentication, the administrator must first add each user that requires access to MyAssays Desktop to the defined MyAssays Desktop user group. This is the group that was specified in the Security Configuration Wizard and defaults to **MyAssaysDesktopUsers**:

Users can be added to this local machine group using the standard Windows user management tools:

1. In Windows 10, right-click **Start** | **Computer Management** and expand **System Tools** | **Local Users and Groups** | **Groups**.

2. Locate the user group **MyAssaysDesktopUsers** (or any custom name provided in the configuration) and double-click.

3. Click **Add** and enter the name (or names, each separated by a semicolon) of the user account to add.

   To add domain users, enter the AD domain name followed by backslash (****) and the username (e.g., for a domain "*CORP*" and username "*LabUser*" the **Username** should be: *CORP\\LabUser*).

   For information about logging in with domain account, see Log In Options and Password Management.

Users added to this user group will now be able to authenticate themselves when launching MyAssays Desktop Pro; however, each user must also be assigned to an appropriate authorization group and account type as described in the following section.

Configuring a User

After adding users to the Enhanced Security system (using the method appropriate for the authentication method), each user should be configured as required. This involves setting an appropriate:

- Account type
- Authorization group

Each user's settings are specified through the **User Details** panel, which can be accessed as follows:

1. In MADE, on the **Tools** ribbon tab, in the **Security** group, launch the **Security Management** tool.
2. Double-click a user, or select and click **Modify** to modify the user's details.
3. Review or edit the settings as required.
4. Click **OK** to accept changes.

Disabled and Locked Users

There are two ways a user account's access to MyAssays Desktop can be blocked:

- Disabled
- Locked

Disabling User Accounts

Disabling an account blocks the user's Windows account completely. This can be accomplished at the operating system level through the User Management tools such as **lusrmgr.msc**.
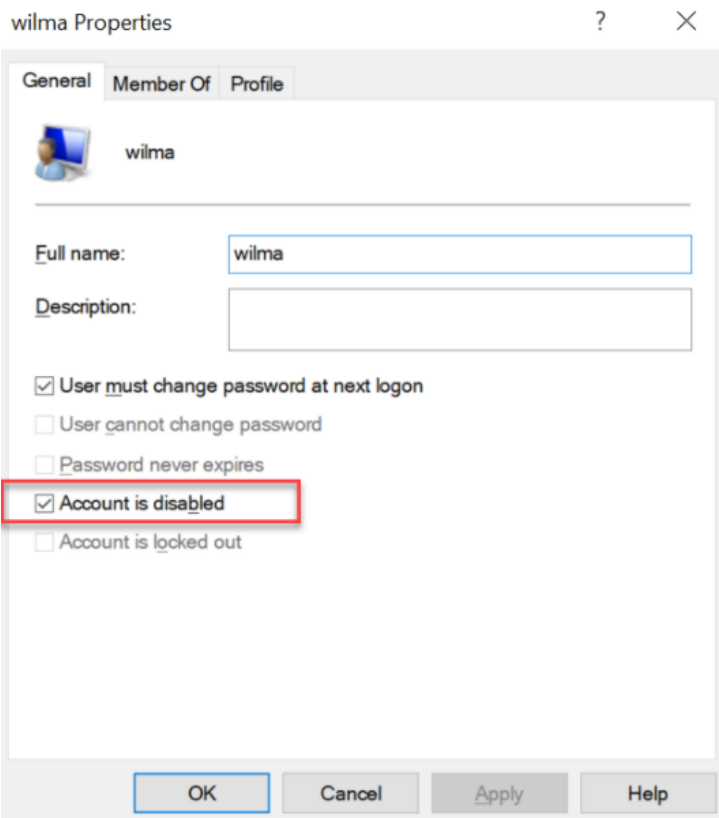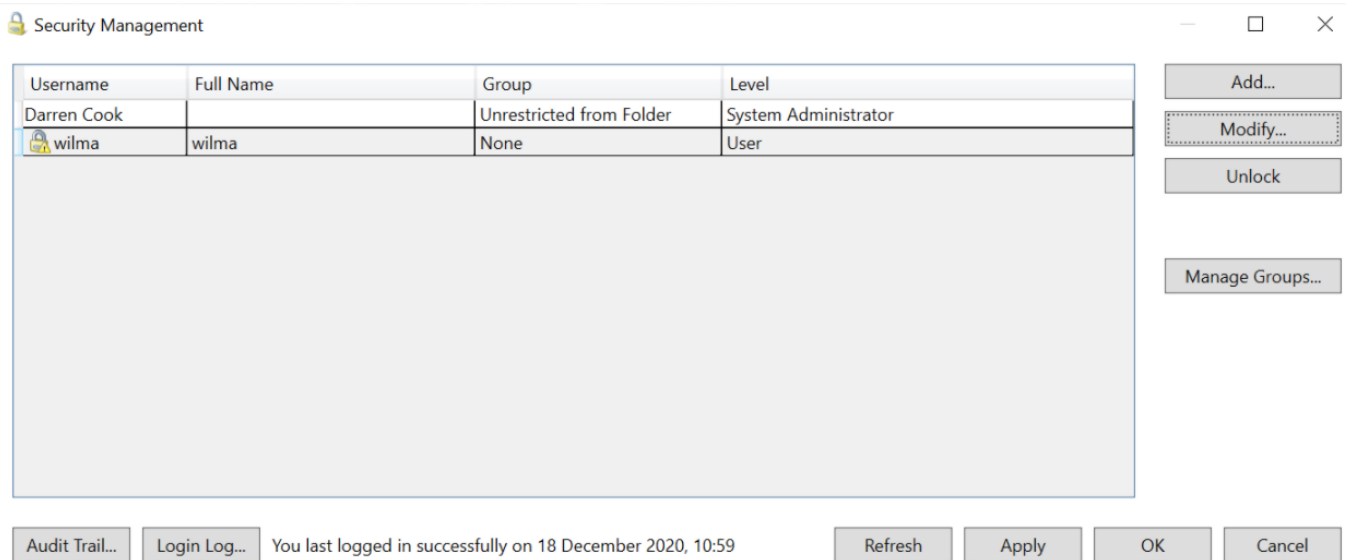
If an account is disabled, Windows blocks the use of that account completely, and as a result such user accounts will not have access to MyAssays Desktop. Disabled accounts will appear in the Security Management tool in red italics.
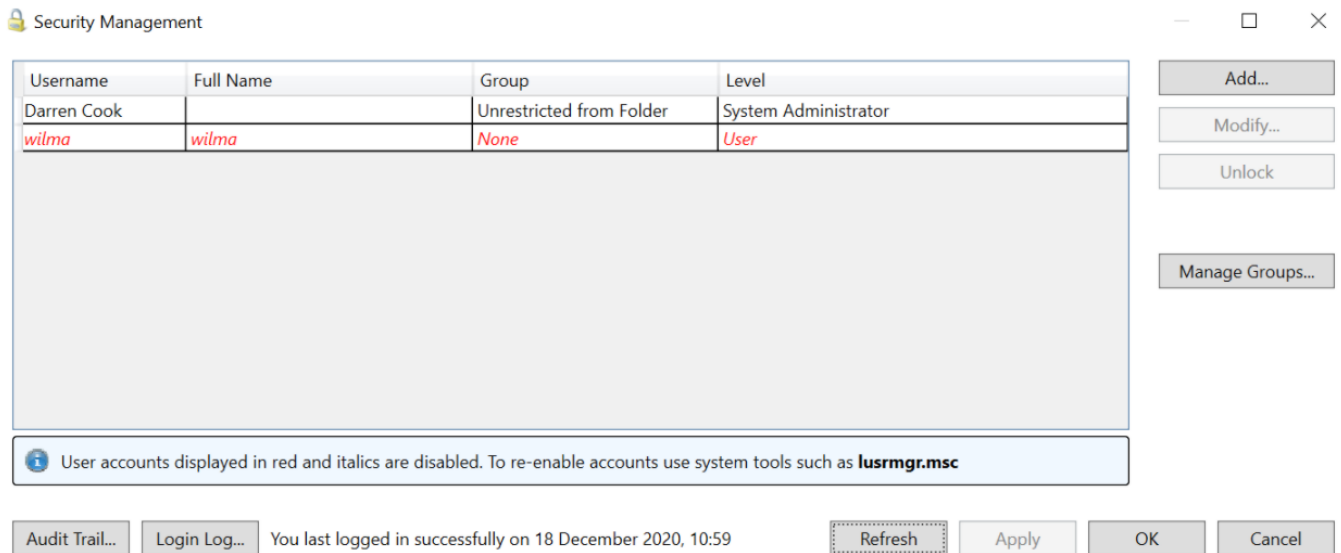
Disabled accounts cannot be re-enabled using MyAssays Desktop's Security Management tool. System tools such as **lusrmgr.msc** should be used to change user account disabled status.

Locking User Accounts

If a user account should not be disabled in Windows, however the user should no longer have access to MyAssays Desktop, the administrator can lock a user account using MyAssays Desktop's Security Management tool. A locked account will not be able to access MyAssays Desktop, but is still usable as a Windows account. Users can be locked and unlocked using MyAssays Desktop's Security Management tool. Locked users will be displayed in the Security Management tool with a padlock icon.

Account Types

The account type or **Level** can be one of the following settings:

- **User** – A standard user of the system. These users can perform operations permitted for their authorization group and cannot access the Security Management or Security Configuration tools.

- **User Administrator** – A Windows administrator account that has limited access the Security Management. This account can assign users to preexisting authorization groups and assign user levels to either User or User Administrator.

- **System Administrator** – The highest level administrator. A system administrator has all functions of the user administrator and can also:

    - Assign user levels to System Administrator.

    - Create and edit authorization groups (using **Manage Groups**).

    - With **MyAssays Desktop Log In** authentication, can change Security Options for the users.

    - Run Security Configuration Wizard to modify initial Enhanced Security configuration.

User Group

The user group (or **Group**) is an authorization group that defines which functions of the software the user can perform. MyAssays Desktop Enhanced Security provides various predefined authorization groups including:

- **None**
- **Unrestricted**
- **Review/Export Only**
- **Run and Review**

For example, users belonging to the **Run and Review** groups are restricted to running protocols and reviewing results. Conversely, an **Unrestricted** user can perform all operations in MyAssays Desktop Pro.

Authorization groups and permissions for each group can be configured by the system administrator as described in the following section.

Authorization Groups

System administrators can manage authorization groups.

Click **Manage Groups** in the Security Management tool to display the **User Group Management** dialog:
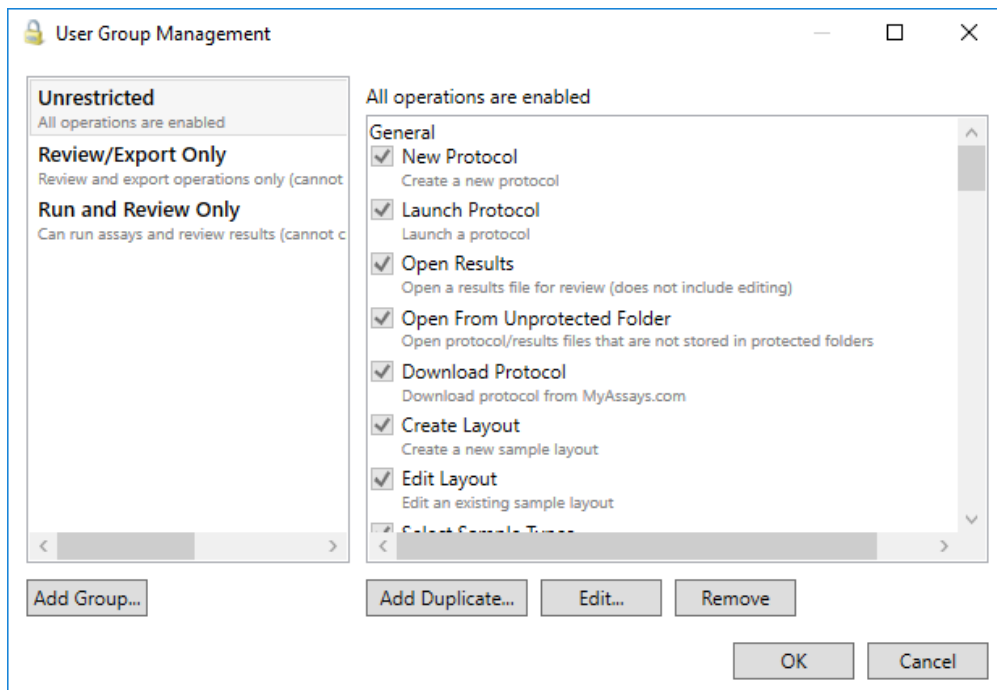
The list on the left shows the existing list of authorization groups. The controls allow a system administrator to edit operations and create new authorization groups. The **Add Duplicate** button can be used to create a new authorization group, which is a duplicate of the currently selected group. This is useful for quickly creating similar groups.

Adding Custom Authorization Group

To grant specific combination of authorizations, add a custom group and select the relevant permissions as follows:

1. Launch MADE.

2. On the **Tools** tab, click **Security Management**.

3. Click **Manage Groups**.

4. Click **Add Group**.

5. Specify a **Name** and, optionally, a **Description** for your group.

6. Select Authorizations for this group.

7. Click **OK**.

8. Assign users to this group.

Authorizations

With the Enhanced Security system enabled, users can only perform authorized operations. The tables below list all available authorizations (arranged by category), their operations, and any special preconditions.

> When a user attempts to perform any of these operations, an entry is recorded in the audit trail marking whether the operation was authorized or denied (alongside the username and date/time).

General

General authorizations relate to using MyAssays Desktop protocol and results files and working with sample layouts.

Authorization	Operation
New Protocol	Create new protocols in the New Protocol Wizard.
Launch Protocol	Launch and view existing .assay-protocol files in MAA.
Open Results	Open and view existing .assay-results files in MAA.
Open Files from Other Locations	Launch and view protocols, results, and layout files stored outside the Assay Data Folder Root. If this is not selected, user will be able to launch protocols, results, and layouts only from Assay Data Folder Root.
Download Protocol	Download preconfigured assay-protocol files from Search MyAssays.com.
Create Layout	Create a new assay layout in the New Protocol Wizard, and when running protocol or results in MAA.
Edit Layout	Change the existing .assay-layout files when running New Protocol Wizard, double-clicking on a file in MADE, or when running protocol or results in MAA.
Select Sample Types	Select existing sample types to use for layouts of the current assay. This refers to both the New Protocol Wizard and when running protocol or results in MAA.
Manage Sample Types	Create or edit sample types used in the assay when running protocol or results in MAA, and also remove sample types when creating a new protocol with New Protocol Wizard.

Parent Directory for Data Files

This authorization is applicable only for **Windows Log In** authentication method with **User's Own Folder** data arrangement setting. For more information about assay data, see Data Protection.

Authorization	Operation
Edit Assay Data Folder Root	Choose a custom root folder to store all assay data files in. By default, all file types used by MyAssays Desktop are stored in the default location. With this setting, you can allow or restrict changing the default root folder.

File Operations

For **Windows Log In** with **Shared Folder** and Secure File Protection feature enabled, files in the protected folder (Assay Data Folder Root) cannot be duplicated or removed. Authorizations in this category can be granted to allow users making such changes (either in MADE or in Windows Explorer). For more details, see File Operations.

Authorization	Operation
Delete Data File	Delete protocol, results, or layout files through Enhanced Security.
Copy + Paste Data File	Duplicate protocol, results, or layout files through Enhanced Security.

Analysis

Analysis authorizations relate to operations available when running protocols or viewing results in MAA.

> If a user has not been granted permission to perform an operation that is otherwise available through a button, then the button will not be displayed.

Authorization	Operation
Edit Measurements	Change measurements in the **Measurements** tab of MAA.
Edit Container IDs	Change Plate IDs, Analytes or Batch IDs in the **Measurements** tab of MAA.
Edit Field Data	Change the field data in the **Measurements** tab of MAA.
Edit Overview	Change protocol name and overview via the Overview Editor.
Edit References	Configure external references in the current or for all protocols in the Resource Reference Manager.
Calculate New Results	Click the **Calculate** button to perform calculations with new settings.
Purge	Remove all versions except the one currently selected if assay results contain more than one version.
Rollback	Remove all versions that follow the selected version if assay results contain more than one version.

Authorization	Operation
Manage Templates	Create new, make changes to or remove the existing report templates for page-based outputs (DOC, DOCX, and PDF).
Edit Header/Footer	Insert a custom header or footer for page-based outputs (DOC, DOCX, and PDF).
Edit Notes	Add, edit, or remove Notes associated with assay.
Save Results	Save changes to the current .assay-results file.
Save Protocol	Save changes to the current .assay-protocol file.
Results Save As	Save opened .assay-results file to a different location or with different name.
Protocol Save As	Save opened assay protocol file to a different location or with different name. This also allows the user to save results as a protocol. (This setting also applies to the Export Protocol operation)
Edit Results Naming	Change results file naming conventions and storage location for an assay protocol.
Add/Remove Transforms	Add or remove transforms in the data analysis configuration.
Edit Transforms	Make changes to the settings of a transform. For example, change the concentrations in Standard Curve Fit transform.
Edit Matrices	Edit the settings of a matrix in the Matrices tab of the **Assay Properties** panel.
Edit Evaluations	Add, configure, and remove Evaluations Tables and Evaluations in the Evaluations tab of the **Assay Properties** panel.
Edit Validations	Add or remove Validations Tables, configure Validations in the Validations tab of the **Assay Properties** panel.
Edit Report	Add, configure, and remove report content in the Report tab of the **Assay Properties** panel.
Edit XML	Make changes to the assay configuration in the **XML** tab of the **Assay Properties** panel.
Flag Sample/Point	Flag positions or data points to mark them as outliers to remove them from further analysis.
Edit with Quick Protocol Editor	Edit protocol parameters using the Quick Protocol Editor

Data Import

Data Import authorizations relate to importing data when:

- Creating new protocols (requires General **New Protocol** permission)

- Working with protocols or results in the MAA using the **Import** wizard (requires General **Launch Protocol**, **Open Results** permission, or both)

- Automating data analysis with Analysis Launcher or Folder Poll (including via the command line arguments)

Authorization	Operation
Import Measurement Data	Import measurements from a single or multiple files. This permission defines whether these files can be imported. Other **Import** authorizations can be used to restrict which files can be imported and from what locations.
Import Requires Certification	Restrict import of measurements only to the files that are validated against their signed certificates.
Import Requires Certification from This Computer	Restrict import of measurements only to files that are created on this computer and validated against their signed certificates. 📝 To enable this restriction, select **Import Requires Certification**.
Import Requires no Modification	Import only from measurement data files that have not been modified.
Import Non-Measurement Data	Import data such as sample IDs, container IDs, or any assay-specific non-measurement data from a file.
Import from Any Folder	Import data from files stored in any location. 📝 Overrides the **Import from Approved Folder**.
Import from Approved Folder	Restricts importing files from an approved folder (and its subfolders) only. ℹ️ To use this authorization, first define the approved folder for import in enabling Enhanced Security on your system or to use Security Configuration wizard to make changes to the current configuration. If the **Approved Folder** is not specified, the import will be denied. 📝 Do not use in conjunction with **Import from Any Folder**

Data Export

Data Export authorizations relate to export operations including an option to protect the exported content from further modification (available for Excel and Word outputs).

Authorization	Operation
Certify Exports	Create a data certification file with each exported file.
Export XLS	Export report in the Excel file with XLS extension.
Export XLSX	Export report in the Excel file with XLSX extension.
Protect XLS/XLSX	Restrict making changes to the Excel reports with a password. For more details, see Protecting Word and Excel Reports with Password. To use this authorization, first select **Use Word/Excel Report Protection** check box and provide a password when enabling Enhanced Security or use Security Configuration wizard to make changes to the current configuration.
Export PDF	Export report in the PDF file format.
Export DOC	Export report in a Word file with DOC extension.
Export DOCX	Export report in a Word file with DOCX extension.
Protect DOC/DOCX	Restrict making changes to the Word reports with a password. For more details, see Protecting Word and Excel Reports with Password. To use this authorization, you have to select **Use Word/Excel Report protection** check box and provide a password when enabling Enhanced Security on your system or to use Security Configuration wizard to make changes to the current configuration.
Export XML	Export the original XML report file.
Export with XSLT	Export the report with specific settings using XSLT transformations. For more details about these transformations, see How to Use XSLT for Custom Export.
Export with Plug-In	Export the report with specific export settings using Export Plug-In.
Export to Any Folder	Select a folder to export the reports to.

Quality Control

Quality Control authorizations are related to QC Add-On.

Authorization	Operation
Edit Protocol/Results QC	Add, edit, remove Quality Control configuration of a protocol or results file.
Create On-The-Fly QC Report	Generate instant QC report that is not applied to a protocol file.
Edit QC Settings File	Edit configuration of a QC Configuration File.

Electronic Signatures

Electronic Signatures authorizations are related to Electronic Signatures. If this feature is enabled then users can be granted or denied the following operations based on whether the document has been electronically signed with the specified reason. For example, if a user is assigned to an authorization group with the Protocols **Requires Approval for Launch** setting selected, then the suer can only use protocols which have been approved.

Authorization	Operation
Protocols Requires Approval for Launch	Assay protocol files require approval for launch (i.e. a protocol must have been electronically signed with reason: approve).
Results Requires Authorship for Exporting	Assay results files require authorship for exporting (i.e. a results file must have been signed with reason: authorship before it can be exported).
Results Requires Authorship for Printing	Assay results files require authorship for printing (i.e. a results file must have been signed with reason: authorship before it can be printed).
Results Requires Authorship for Saving	Assay results files require authorship for saving (i.e. a results file must have been signed with reason: authorship before it can be saved).

Automatic Logout

The Automatic Logout function suspends any open MyAssays Desktop windows after a defined period of inactivity. In this situation, the existing user must reenter their credentials to resume their session. If the correct credentials are not supplied, then the session is terminated (possibly with data loss).

> The Automatic Logout feature is applicable only when working with **MyAssays Desktop Log In** authentication. With **MyAssays Desktop Log In** authentication, multiple users share a single Windows session and the operating system cannot provide any automatic logout of the MyAssays Desktop users. (With **Windows Log In** authentication, automatic log out can be controlled by the system settings).

When Is User Logged Out?

System administrators can configure the period of inactivity after which the users need to log in again under **Security Options**. To do this:
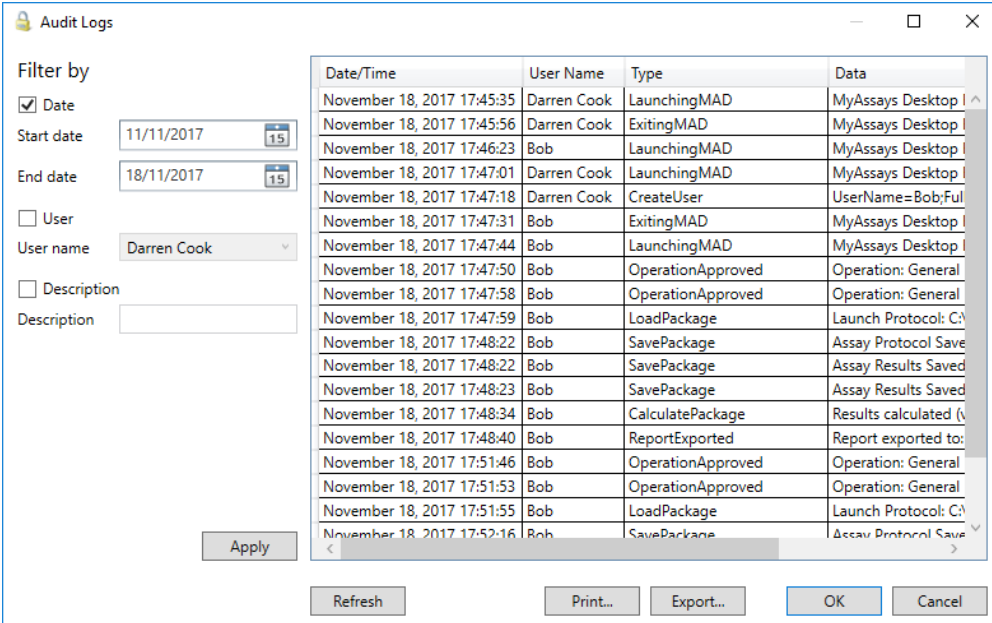
1. Launch MADE.

2. On the **Tools** tab, click **Security Management**.

3. Click **Security Options**.

4. Make sure that **Enable** check box is selected.

5. Review or edit **Log out after (seconds)**.

6. To accept changes, click **OK**.

> When configuring **Security Management** settings, log out and then back in for changes to take effect. Make sure you save your work and close all MyAssays Desktop windows.

Monitor Usage

User administrators and system administrators can use the **Audit Trail** and **Login Log** buttons to view the corresponding logs of information. For example:

Filter

Tools are provided to filter the log by date, user, and description. Select the appropriate controls, enter the parameters, and click **Apply** to filter the log.

Export

The **Export** button displays the Export log tool, which can be used to export the selected log information to an XML or a CSV file. Click **Export** to export the contents.

Enhanced Security Configuration Backup

The Enhanced Security Configuration Backup tool simplifies the back-up of Enhanced Security configuration data.

> This tool does not back-up assay data files; it only backs up the Enhanced Security configuration.

The back-up tool is available for administrators from MyAssays Desktop Explorer | **File** | **Data** | **Enhanced Security**:

Press **Config Backup** to create a backup.

This will create an encrypted and password protected backup ZIP of the ES configuration (stored in the Documents folder and named based on the current date and time).

By default, the ZIP file is protected with a default private password (known only to MyAssays Ltd.).

To set a custom password, create a registry string value named: **BackupPassword** at registry key: **HKEY_LOCAL_MACHINE\SOFTWARE\WOW6432Node\MyAssays\MyAssays Desktop\Security**

Working with MyAssays Desktop Pro and Enhanced Security

This section explains the functional differences when working with Enhanced Security enabled with MyAssays Desktop Pro; this section provides information for all users of the secured system.

MyAssays Desktop Explorer

The MyAssays Desktop Explorer Welcome screen displays a padlock icon to clearly identify that Enhanced Security is enabled.

Also, the Welcome screen displays the logged in user's Full Name and the details of the last log in attempt (this will include any failed login attempts).

The **File** | **User Accounts** section displays further details about the currently logged-in user including authorization group and account type.

Administrators can access the **Security** group under the **Tools** tab to find the various Enhanced Security configuration tools.

Administrator Security Tools

For administrator users, security tools are available from the **Security** group of the **Tools** tab. This includes the **Security Configuration** and **Security Management** options, i.e.:
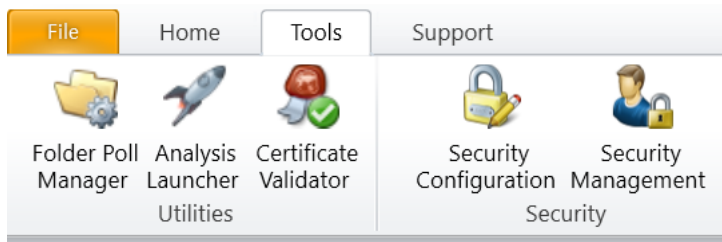
> These operations are only available for administrator users.

The Security Configuration Wizard can be used to modify the security setup (only available to system administrators).

The **Security Management** tool provides control over:

- Configuring users
- Assigning users to and setting up authorization groups
- Viewing and editing authorizations assigned to a group
- Viewing and exporting the Audit Trail and Login Log
- Automatic Logout settings

The **Security Management** tool is available for system administrators and user administrators.

File Operations

With Enhanced Security activated and the Secure File Protection feature enabled, destructive file operations on MyAssays Desktop Pro data stored inside the protected folders are prohibited. This means that the following Windows functions cannot be performed on protected MyAssays Desktop Pro assay data files:

- Delete
- Rename
- Create
- Move

However, authenticated users can be authorized to perform file deletion and file duplication through Enhanced Security by granting those users permission to:

- **Delete Data File**
- **Copy + Paste Data File**

in the File Operations section of Authorizations.

These operations are managed by the Enhanced Security system so they cannot be performed using the standard Windows commands (i.e., Windows delete and copy + paste will not work). Instead, the secure version of these operations can be accessed through the context menu (by right-clicking on a selected single file). These secure file operations are indicated with the security padlock icon.

For example, to duplicate an existing MyAssays Desktop Pro protocol file, right-click the file to duplicate and select the **Secure Copy + Paste** option:
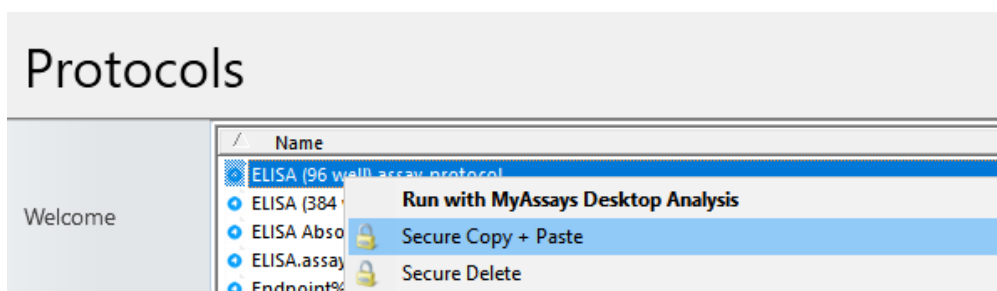
If the authenticated user is authorized to perform the secure file operation, then MyAssays Desktop Pro will prompt for a file name for the new file. Any performed secure file operation is logged in the audit trail alongside the authenticated user.

These secure file operations are available through the right-click context menu in MyAssays Desktop Explorer and in Windows Explorer. Note, the secure file operations can only be

performed on one file at a time (the secure file operations are not available when multiple files are selected).

Login Options and Password Management

The logging in options depend on the selected authentication method. The specifics of how each of them work are different and are described below.

Windows Log In Authentication

With **Windows Log In** authentication, the credentials used to log in to Windows are used to identify the current user; no additional log in step is required when launching any MyAssays Desktop window.
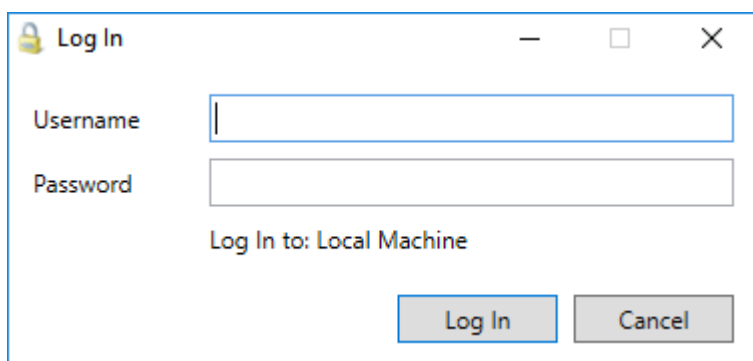
> For domain accounts, the user has to enter the AD domain name followed by backslash (****) and account name (as configured when adding users to the Enhanced Security system).

For logging out, the **File** menu includes the **Log Out + Exit** option. This command will exit MyAssays Desktop Explorer and log out of the current Windows session (closing any other open applications).

MyAssays Desktop Log In Authentication

With **MyAssays Desktop Log In** authentication, users will need to log in to the application with a **Log In** dialog:

The **Log In to:<context>** message shows to which authentication context (local machine or domain name) the user will log in.

Log In to Local Machine Account

In the **Username** and **Password** field, users need to enter or paste their provided credentials (as configured when adding users to the Enhanced Security system) and then click **Log In**.

Log In to Domain Account

In the **Username** field, the user has to enter the AD domain name followed by backslash (****) and account name (as configured when adding users to the Enhanced Security system). For example, for a domain "*CORP*" and account name "*LabUser*" the **Username** should be: *CORP\LabUser*. In the **Password** field, type in their password, and then click **Log In**.

> To log in to local system administrator account, in the **Username** field, enter dot (**.**) instead of the AD domain name. For example, **.***Admin*.

Logging Out

With **MyAssays Desktop Log In** authentication, users should log out when they have finished working with MyAssays Desktop Pro (otherwise other users can perform unauthorized changes on their behalf). Users can log out from the MyAssays Desktop Explorer under **File** | **Log Out + Exit**.

Automatic Logout

If the administrator has enabled the Automatic Logout feature, then the user session is kept active while there is any user activity. If the **Automatic Logout** period elapses without any user activity, then the user will be logged out of the system with any open windows closed. User can resume the session by entering the password again in the **Resume** dialog.

If the administrator has disabled **Automatic Logout**, then the user session is kept active while there are any MyAssays Desktop windows opened.

Password Management

For both authentication methods, password management is handled using the Windows security policy. If the security policy of the system dictates that the user must change his or her password, then after successful login, the user is advised to change the password. The new password must adhere to the system's password policy options (such as minimum length and password history).

Quality Control

This section describes the Quality Control (QC) feature of MyAssays Desktop.

> 📝 This feature is only available to users with the QC feature enabled on their license.

Overview

The Quality Control features enable the monitoring of measurements and analysis results across assays runs. This is known as "inter-assay analysis" and can be used to track whether assay performance remains in control by comparing current results with historical observations.

For example, a QC test can check whether the value of the **Control1** in all results files falls in the range of +/- 2*SD and indicate cases where results fall outside this range.

> ℹ️ For intra-assay monitoring you can use the Validation feature.

QC Observations

The general approach is to define specific observations of interest; these are collected and compared across assay runs.

Each observation results in a single numeric value for each assay run. An observation can be a measurement or calculated result (including TOVs). For example, the measurement or calculated results for the sample **Control1** is an observation that is commonly monitored.

The QC process will gather the values of each selected observation across runs of interest. The results can be presented in a table and/or plotted on a QC chart to monitor inter-assay change. If these observations deviate from the specified range, then the assay is "out-of-control" and is highlighted accordingly.

QC Configuration

QC is configured using the intuitive QC Wizard that can be launched from both MADE and MAA.

QC can be configured:

- On demand – Create a QC report as an when you need it
- As part an assay protocol – With the QC results included in each results' report.

Additionally, you can save the defined configuration to a QC settings file and reuse it for future QC operations.

QC Results

In the simplest case, the result for each observation can be displayed in a table reporting observation result for each included assay. More sophisticated outputs can be generated plotting the observation data over time as CUSUM, Levey-Jennings or Control Charts.

The following subsections explain how to add, define, and review inter-assay QC analyses.

QC Wizard

Introduction

Inter-assay quality control is configured through the QC Wizard.

> The QC features can be used in various scenarios to track inter-assay data for charting, analysis, and validation. The wizard provides a range of features and scenarios for convenient and simple inter-assay analysis tailored to your lab's needs and workflow.

The QC Wizard will walk you through the process of:

1. Selecting the files to consider

2. Specifying the observations to monitor

3. Selecting how the results should be presented

The QC Wizard can be launched in two different ways depending on the type of analysis you require:

QC On-Demand

QC On-Demand allows you to generate QC reports as and when you need to, selecting the files to consider. This is useful for the production of an occasional QC report.

To perform QC On-Demand, launch the QC Wizard from MADE.

How to: Launch the QC Wizard from MADE

1. Launch MADE.

2. Select the **Results** tab.

3. On the **Ribbon**, hover to the **Quality Control** group.

4. Click **Create** to launch QC Wizard or the **Edit** to launch it with an existing configuration file.

> Select two or more results files and then press **Create** to automatically populate the wizard with these files.

QC as Part of an Assay

QC can be built into an assay so that each time the assays is used the results are compared with historical results of the same protocol.

To add QC to an assay launch the QC Wizard from MAA.

How to: Launch the QC Wizard from MAA

1. Launch an assay protocol or open a results file.

2. On the **Ribbon**, click the **Add** drop-down button of the **Quality Control** group.

3. Click **New Configuration** to launch the QC Wizard or the **Existing Configuration** to specify the configuration file to launch the wizard with.

Selecting Files for Analysis

The Selecting Files for Analysis QC Wizard step specifies the results files to include in the inter-assay QC analysis.

The files could be added in the following ways:

Folder

Select this setting if the results you want to compare are stored in the same location and follow the same name convention.

- **Path** – The full path to the results folder location. Click the **Browse** button to select a folder in which your results files are stored.

- **Pattern** – Defines the pattern to extract results file with.

By default, the MyAssays Desktop organizes results files in accordance with the protocol name. For example, if a protocol is named "My Endpoint 12x8 Protocol," each run of the protocol will generate a results file that is named after "My Endpoint 12x8 Protocol" convention with a run number in brackets. For example, if the protocol was ran for three times, the newest results file is named "My Endpoint 12x8 Protocol (3)".

This organization of data simplifies the extraction of observation data from previous runs of a particular protocol. With this in place, the results are specified as:

Protocol Name*

> ℹ️ If the QC Wizard is launched in MAA, then the files to monitor are set up to match the configuration of the results naming setting.

For example, for the **My Endpoint 12x8 Protocol** results files, it would be **My Endpoint 12x8 Protocol***.

With this setting, all results for this protocol will be automatically added to QC analysis. In case you want to analyze only some of them, use the Specific Files setting.

Specific Files

This setting is useful if you want to track changes between specific results files or the results stored in different folders. For example, you might need to compare the results from first, fifth, and seventh run of an assay.

To add the files to the list, click the **Add** icon button and select the required results. For adding multiple files, hold the **Shift** or **Ctrl** key, if the files are or are not sequential.

To remove a file from the list, select it and click the **Remove** icon button.

Click **Next** to continue with the Wizard, and configure the observations to be tracked between the specified files.

> To use both file selection patterns at the same time or define several naming patterns, use the XML editor on the Configuring Observations step. See Advanced QC Wizard Settings to learn more.

Configuring Observations

This QC Wizard step allows you to add and configure the observations necessary to achieve your requirements of inter-assay quality control. Use the **Add Observation** or **Remove Observation** buttons to add observations as required.

Observations

Name

For each observation, a description can be specified under the **Name** column. Use this to provide a clear textual description for your QC monitoring. This will be used in the header for the **Observation Expression** column in the QC Results table to convey what has been monitored.

Data

For each Matrix-Transform Data Analysis Assays observation, specify which matrix the observation applies to. The numbering is sequential and starts from the index of the first matrix at 1 onward. The list of the available matrices (both raw and calculated) with their indexes is displayed in the Matrices tab. Any of the raw or calculated matrices that contain endpoint data can be referenced in an observation.

Matrix Name

If all selected assays have the same number of matrices and the same matrix names (e.g., Raw, Concentration, and Average), then a list box with the matrix names will be displayed.

Expression

An expression is used to define the observation data. The type of expression depends on the assay type:

- **Observation** (for Matrix-Transform Data Analysis Assays) – Enter an [expression](#) to query the data of the specified matrix. This could simply be the name of a sample group, e.g., **Control1** or a more sophisticated calculation expression. Non-matrix data can be queried by using [transform output variables](#).

- **XPath** (for other assays types) – An **XPath** expression that obtains single numerical value; that expression is then queried for each of the specified results.

> The type of expression to use will be reported in the column name.

Output

The inter-assay observation data can be plotted simply as a table of the values or as a CUSUM, Levey-Jennings, or Control Chart alongside. For all output types, a text summary is included under each Observation Table.

The Control Chart allows users to specify a target mean and standard deviation using the **XML** tab of the **Quality Control Wizard**. Add the attributes **Target** and **SpecifiedSD** to add the necessary parameters. An important distinction between the Levey-Jennings chart and the Control Chart is that with Control Charts, the parameters (Target Mean and Standard Deviation) are only updated when changes are made using the **Quality Control Wizard**, whereas with Levey-Jennings chart mean and standard deviation are updated in real-time.

```xml
<Observations>
  <Observation Name="Control" Expression="Control1" Matrix="3" SDLimits="3" Target="220" SpecifiedSD="22" Ou
    <NumericalFormatting Type="SignificantFigures" Precision="6" />
  </Observation>
</Observations>
```

The above configuration will set the target mean to 220, with one standard deviation equalling 22, with a +/-3 SD acceptability limit. [Video Walkthrough...](#)

SD±Limit

For each observation, control limits are expressed in terms of standard deviation range and are calculated automatically for the observation data.

You can define required range for the Table and CUSUM outputs and select the control rule for the Levey-Jennings and Control Chart.

The observation results for an assay run fall outside this range, they are highlighted in the resulting table.

Create QC Report Instantly

You can export a report to an Excel spreadsheet straight-away with the **Create Now** option. The report will be saved to your MyAssays **Reports** folder.

Configuring QC Observations in the XML Editor

After you have selected the files to monitor and configured at least one observation, you can select the XML tab to bring your quality-control setup to a new level. Using the built-in XML editor, you can configure your QC analysis to meet your needs. This includes:

- Monitoring multiple files, folders, or their combinations at the same time
- Modifying the display of resulting charts
- Formatting the results according to your lab's standards

Monitor Multiple Files, Folders, or Their Combination

The files you've included on the Selecting Files for Analysis step are stored in the **Files** element (the Folder option) or in its **File** child elements (the Specific Files option). You can define a combination of files to monitor by adding their associated elements.

Include Multiple Folders into a Single Observation

If your files are stored in several folders, or in the same folder with different naming patterns, add the following information for each folder:

<Files Folder="*Full Path*" Search="*Pattern*"/>

Replace **Full Path** with the actual full path to the folder and **Pattern** with the common filename component to search for applicable files, followed by an asterisk *****. For example,

<Files Folder="C:\Users\User1\Documents\MyAssays\Results\" Search="ELISA*"/>

<Files Folder="C:\Users\User1\Documents\MyAssays\Results\" Search="NEW*"/>

will include all .assay-results files that start with ELISA (e.g., "ELISA(1).assay-results", "ELISA (2).assay-results", etc.) and NEW (e.g., "NEW_ELISA(1).assay-results", "NEW 4PL.assay-results", etc.) into QC monitoring.

Compare Folder Against File

If you want to monitor the folder and a specific assay-results file in a single observation, for each file, add a File element as a child to Files and specify the full path to the file:

<File Path="*Full Path*"/>

For example:

```
<Files Folder="C:\Users\User1\Documents\MyAssays\Results\ELISA\"
Search="*">
        <File Path="C:\Users\User1\Documents\MyAssays\Results\ELISA
        (1).assay-results"/>
</Files>
```

This configuration will include ELISA(1).assay-results stored in the MyAssays\Results and all .assay-results files from its ELISA subfolder.

Modify the Appearance of the Chart

When selecting the output that includes CUSUM, Levey-Jennings or Control Chart, you can change the chart display as needed. The available settings include customizing the major and minor units of both axes and setting the number format for the axes values.

To customize the chart in your QC report, add the **ChartCustomization** element as a child of the associated **Observation** and set its attributes. See Change the Units and Number Format of the Charts to see all available attributes.

The editor adds the xmlns="http://www.myassays.com/ChartCustomizations" by default. This attribute is required for the customization.

For example:

```
<Observation Name="Control Values Check" Expression="Control1" Matrix="1"
SDLimits="2" Output="Levey-Jennings" />
        <ChartCustomization
        xmlns="http://www.myassays.com/ChartCustomizations"
        XAxisMajorUnits="10" XAxisMinorUnits="5" YAxisMajorUnits="0.2"
        YAxisMinorUnits="0.1" YAxisNumberFormat="[Red][&lt;1]0.00;
        [Green][&gt;=1]0.00"/>
</Observation>
```

Set Numerical Formatting of the Results

By default, the results in the QC report are displayed to 6 significant figures. To change the formatting, add the **NumericalFormatting** element as a child of the **Observation** and set its attributes. To learn about the numerical formatting settings, see Viewing Available Matrices and Configuring Their Settings.

> 📝 The **Type** settings are entered into XML without spaces.

For example:

```xml
<Observation Name="Observation1" Expression="Control1" Matrix="1" SDLimits="2" Output="Table" />
    <NumericalFormatting Type="DecimalPlaces" Precision="3"/>
</Observation>
```

Here the numerical formatting is set to 3 decimal places.

Set the Type of Observation Expression

Inside the **Observation** element, you can enter and set to true or false an optional Boolean **IsExpressionXPath** setting to treat the expression accordingly.

Observation Evaluations

Evaluations can be added to QC configurations to report important control parameters. Video Walkthrough...

Adding Observation Evaluations

In the QC Wizard, select the XML tab. For configured Observations, add the required Evaluations immediately following. For example:

```xml
<Observations>
    <Observation Name="Observation 1" Expression="Control1" Matrix="2" SDLimits="2" Output="Table">
        <Evaluations>
            <Evaluation Expression="head(obs,1)" />
            <Evaluation Expression="tail(obs,1)" />
            <Evaluation Expression="mean(head(obs,3))" Description="The mean of the first 3 collected 'Observation
            <Evaluation Expression="obscurrent" Description="The current observation" />
        </Evaluations>
    </Observation>
</Observations>
```

Using the above example, the output would be:

Observation	Observation 1	Date	File
3	0.201000	2021-04-23 / 15:53:11	ELISA (96 well) (1)
2	0.423000	2021-04-23 / 15:48:19	ELISA (96 well) (3)
1	0.346500	2021-04-14 / 18:33:13	ELISA (96 well) (2)

Result	Expression	Description
0.346500	head(obs,1)	head(obs,1)
0.201000	tail(obs,1)	tail(obs,1)
0.323500	mean(head(obs,3))	The mean of the first 3 collected 'Observation 1
0.201000	obscurrent	The current observation

Observation Evaluation Expressions

In addition to other supported Expressions, the below table displays additional functions that can be useful when configuring QC Observation Evaluations. Note **obs** refers to the Observation the Evaluation will apply to.

Function	Description	Syntax
head	Returns a subset of the provided observation list, beginning with the **first** observation.	**head(obs,{N})** Where N refers to the number of observations to include. Example: **head(obs,1)** Returns the first observation.
tail	Returns a subset of the provided observation list, beginning with the **last** observation.	**tail(obs,{N})** Where N refers to the number of observations to include. Example: **tail(obs,1)** Returns the last observation.
obscurrent	Returns the current observation.	**obscurrent**

Observation Rules

The Quality Control feature will automatically return pass or fail for configured observations depending upon whether the SD limits are satisfied. Additional rules can be configured to test for further conditions, also returning pass or fail. Video Walkthrough...

Configuring Observation Rules

In the QC Wizard, select the XML tab. For configured Observations, add the required Rules immediately following. For example:

```
<Observations>
  <Observation Name="Observation 1" Expression="Control1" Matrix="1" SDLimits="2" Output="Table">
    <NumericalFormatting Type="DecimalPlaces" Precision="3" />
    <Rules>
        <Rule Expression="x &lt; 20" Description="The latest result is less than 20"/>
        <Rule Expression="mean(obs) &lt; 20" Description="The mean of all observations are less than 20"/>
    </Rules>
  </Observation>
</Observations>
```

Using the above example, the output would be:

Quality Control:

Observation	Observation 1	Date	File
2 (Current)	5.61694	2021-04-26 / 14:45:11	ELISA (96 well) Linear Regression (2)
1	5.61694	2021-04-26 / 14:44:34	ELISA (96 well) Linear Regression (1)

Result	Expression	Description
✓ Pass	-	Within ±2SD range
✓ Pass	x < 20	The latest result is less than 20
✓ Pass	mean(obs) < 20	The mean of all observations are less than 20

Westgard Rules

Observation Rules functionality can be used to configure Westgard Rules. With the expressions available for Quality Control, rules can be configured to satisfy laboratory requirements for monitoring QC based on Westgard Rules.

QC Results

On this step, if the wizard is launched from MAA (with a protocol or results), generated results can be added to a report (and generated on the next calculation). Otherwise, the results can be saved to the QC Configuration file.

Press **Finish** to exit the wizard.

Observation Evaluation Issues

If one or more observations is not evaluated, they are listed in a separate table to indicate their exclusion from the inter-assay analysis. In this case, the error message describing the issue is displayed instead of result in Result column.

Message	Issue
QC not available for this file. Please open file and recalculate to enable QC	The latest version of results was generated before the QC feature was introduced and needs to be recalculated to enable QC.
Failed to evaluate expression: {expression}	The specified observation expression is not valid for the file.
Failed to parse value:{value}	The specified XPath expression returns non-numeric value and is thus not valid.
Failed to evaluate XPath expression	The specified XPath expression is not valid for the file.

QC Workflows

Here are described the typical workflows when working with the Quality Control. These can be combined to provide accurate and consistent results for all of your research needs.

Generate Report Instantly

In the simplest case, specify the results you want to compare, launch (in either MADE or MAA) and configure observations through the wizard, and click **Create Now**. The .XLSX report with your configured observation results is then generated and stored in your **Reports** folder.

Schedule QC Monitoring for all Future Runs of the Protocol

Typically, a protocol is created for an assay of a particular type (e.g., quantitative measurement of cortisol). This protocol is then run each time the assay is required. Running a protocol acquires the relevant measurement data and processes it in accordance with the calculations configured in the protocol; this generates a results file. If you set the QC to a protocol, it will be applied for all runs of this protocol in the future (so you don't need to repeat the configuration again next time).

Running this workflow is useful for designing systematic QC procedures. With this, the QC analysis is automatically performed as soon as a new results file is generated. For example, perhaps you are running a routine assay and want to monitor if the %CV of the measurements between runs does not go beyond a range of ±2*SD.

In this case, open the protocol and launch the QC Wizard. Select the **Add QC content to report** option if you want to include the QC Results in the report automatically when new results are calculated.

Compare Results and Add QC Results to Report

Perhaps, you want to determine if the response of control results in today's assay is significantly different from corresponding control's responses in the reference assays. The defined observations you want to include in the report for current assay run only.

In this case, launch today's results file, select the results for comparison, configure required observations in the wizard, and select the **Add QC content to report** option.

> When **Add QC content to report** option is selected, the results of the current assay are always included as the last observation and indicated with **(Current)** after the observation number.

QC Configuration File

For example, your lab has multiple analyses running under the same acceptable limits or works under general quality standards. In this case, you can run and configure typical validating observations and reuse them for every assay.

To create QC configuration file, select the **Save settings to file** check box when finishing working with QC Wizard. This file with all specified settings in place is stored under the QC subfolder in your MyAssays folder or any other specified location.

Note, this configuration may be tweaked depending on the analysis peculiarities (**Edit** or **Add Existing Configuration** commands) and optionally saved to another file, protocol, or results.

Reference

Transforms

Transforms can be described as sets of configurable operations that are performed to generate results. The results might be included in a report or used as inputs to other transforms. You can add multiple transforms in any order to perform a required data analysis with the leverage of transforms performed previously.

Most transforms use one input matrix and produce one output matrix (like Factor). However, this is not always the case. Here are the general rules:

- Each transform can have one or more input matrices.

- Each transform can produce one or more output matrices.

- A particular transform will always have the same number of input and output matrices.

- The input and output matrix types of a transform are fixed.

Matrices and Transforms

Input Matrices

A transform can accept one or more input matrices. Where an input matrix is used, the transform performs calculations using the data on those matrices. For example, the Factor transform multiplies all points on the input matrix by a specific value.

The input matrices available to a transform include the compatible raw data (i.e., of a particular data type) and compatible data that has been calculated prior to this transform.

For example, assuming all data is endpoint, the first transform can only access data on the **Raw** matrices, whereas a second transform can access data on the **Raw** matrices and/or the first **Calculated** matrix.

Output Matrices

Each transform will add one or more calculated matrices to the Matrices at each step. As each transform is evaluated, each container in the results will always contain the same number of matrices (raw and calculated) as all other containers in the results.

As you add transforms, you can configure output settings and display in the report for each of them.

Expressions and Transforms

In addition to the input matrices, any transform that uses MyAssays Analysis Expressions can access data directly from the current transform (including data that is not on the input

matrices). Similar to available input matrices, the data that can be accessed depends on the data that has been calculated up to this point of the evaluation (and data of the compatible type). Thus, the data accessible by an expression includes compatible raw and calculated matrices.

Transforms Tab

Transforms are added and configured via the **Transforms** tab.

How to Add a Transform

1. Launch an assay protocol or open a results file.

2. If you cannot see the **Assay Properties** panel, click **Properties** to open it.

3. Click **Add**.

4. Select a transform and click **Create**.

5. Review or edit the transform's input matrix and output matrix names as required.

6. Provide your required settings for the transform (see **Properties** section above).

7. Click **Calculate** to perform the calculations with the new settings and to see the results.

Each transform has a set of configurations to specify the parameters of the analysis. Some transforms can also add optional content to the report and be configured with specific calculation settings.

Transform Relevance

A transform may or may not be relevant to the current assay configuration. In this context, the configuration refers to:

- **Matrices (both raw and calculated)** – Certain transforms require a particular data type to be executed.

- **Layout** – Some transforms require specific layout rules to be followed.

General Transform Properties

With regard to flexibility of assay setup, each transform can be configured to fully match assay requirements with a number of settings.

Each transform has zero or more specific settings that allow customization of the transform operations. These are covered under each transform section specifically.

In addition to their specific settings, all transforms share the following common settings:

Advanced

Included Samples	The sample types to be computed by this transform.
Excluded Results	Sample types not selected in the **Included Samples** option will not be computed by this transform; for those cases, this setting specifies what the result will be for those excluded samples: • **Flagged With Value** – The result is flagged with the input value reported. This will appear in the report with the value with strikethrough, e.g., ~~1.23~~. • **Flagged No Value** – The result is flagged with no value reported. This will appear in the report as ~~Flagged~~. • **Equal Input** – The result is set to match the value of the input.

Units

Output Units	The measurement units to be included in the header of the Sample Table. If the output units of the transform are the same as the input, then use "ditto" units to automatically carry these units through (i.e., apply the same units to the transform's output). This shortcut means that it is not necessary to repeat settings across transforms. Ditto units are specified with two dots, i.e.: ..

In addition, the **XY** transforms and **XY Reduction** transforms can be configured with **Data** and **Range** settings.

Endpoint Transforms

Endpoint transforms operate on matrices of data that consist of a single numerical value at each position on the layout. An endpoint transform will compute a single numerical result for each position on the layout.

For example, with a typical ELISA microplate assay, a plate reader will measure and report a single numerical value for each successfully measured well on the plate. Each measurement value is the endpoint of the detection technology for the observed sample. The Standard Curve Fit transform is an endpoint transform that can compute the concentration endpoint from the measurement endpoint.

> For consistency, we refer to all matrices with a single numerical result as an **endpoint** matrix. Strictly speaking, of course an endpoint matrix might not actually be the final conclusion of the analysis. Using MyAssays Desktop, you can layer as many transforms as you need to perform the various analysis steps that are required (resulting in multiple "intermediary endpoint" matrices).

Flagged Endpoints

All transforms take into account the flagged status of each input value. Any data point that is flagged is not included in any calculation and ignored in any reference to the sample group that it belongs to.

For example, if a transform subtracts the average of a blank group from all samples, if the blank group is made up of 3 replicates but the 3rd replicate is flagged, then all the samples will be corrected by the average of the 2 non-flagged samples.

In addition, a transform computation for a position might result in a flagged endpoint result. This could be because of a calculation error or because the transform has performed some kind of automatic outlier detection (such as Auto Flag and Replicate Outlier Removal).

Sample Types to Process

For all endpoint transforms, by default the calculations are performed on all sample types.

For greater flexibility, you can use the **Advanced** settings of each transform to select to perform the transform's computations on only a subset of the sample types. In this case, it is possible to set what the excluded samples results should be (e.g., flagged or to equal the input endpoint).

For example, it might only make sense to perform a certain calculation on Unknown and Control samples but not with other sample types.

Endpoint Transforms

Transform	Operation
Auto Flag	Flags all data points that satisfy the specified Boolean expression.
Average	Calculates the average of replicates for each sample group.
Blank Correction	Subtracts the specified blank value from each input data point.
Dilution Factors	Multiplies sample groups of the selected type(s) by a specified factor (a unique value can be specified for each group).
Dose–Response Curves	Creates a dose–response chart, fit selected curve fitting method, and calculates the response for the specified dose from the curve for each group of the specified type.
Expression by Matrix (Dual)	Evaluates the expression in terms of x and y for each sample group. The x and y variables refer to the values on the first and on the second input matrix, respectively.
Expression by Matrix	Evaluates the expression in terms of x.
Expression by Position	Evaluates an expression in terms of x for each specified position.
Expression by Sample Type	Evaluates an expression in terms of x for each specified sample type.
Factor	Multiplies all input data points of the selected sample type(s) by a specified factor.
General Curve Fit	Fits selected fit method to the specified calibrators and then calculates either y or x values on the curve from input values for the selected sample types.
Matrix Difference	Calculates the difference between values on the first matrix and the second for each sample group.
Median	Calculates the median of the replicates for each sample group.
Percentage Coefficient of Variation	Calculates the %CV of the replicates for each sample group.
Percentage	Calculates a percentage value for each data point with respect to the specified 0% and 100%.
Replicate Outlier Removal	Flags the specified number of replicates for each sample group, in which %CV of its replicates is greater than specified threshold.
Standard Curve Fit	Constructs a standard curve by plotting the standard input concentration values versus data points.
Standard	Calculates concentrations of all included samples using a Library Curve.

Transform	Operation
Curve Fit (from Library)	
Standard Deviation	Calculates the standard deviation of the replicates for each sample group.
Standard Error of Mean	Calculates the standard error of the mean for replicates of each sample group.
Variance	Calculates the variance of the replicates for each sample group.

Auto Flag

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform flags positions where a Boolean condition is satisfied. This is useful for automatically rejecting and ignoring data points that are outside an expected range.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Auto Flag	The expression to evaluate, where a single *x* variable is set to value of each position of the input matrix.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to flag all positions with a value greater than 1.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

To flag values in this matrix where the measurement is greater than 1, specify an Auto Flag expression of *x>1*.

Calculated

The transform will generate an output matrix named **Calculated** with the value at each position matching the input data and positions that do not meet the specified condition

flagged. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	~~2.105~~	~~2.124~~	~~1.213~~	~~1.226~~	~~1.159~~	~~1.190~~	0.110	0.116	~~1.463~~	~~1.481~~
B	0.455	0.441	~~1.869~~	~~1.888~~	~~1.203~~	~~1.218~~	~~1.180~~	~~1.206~~	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	~~1.206~~	~~1.239~~	~~1.203~~	~~1.210~~	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	~~1.167~~	~~1.187~~	~~1.211~~	~~1.241~~	0.101	0.106	0.489	0.490
E	~~1.105~~	~~1.065~~	0.279	0.367	~~1.215~~	~~1.225~~	~~1.233~~	~~1.262~~	0.111	0.114	~~1.579~~	~~1.549~~
F	~~1.425~~	~~1.445~~	0.378	0.411	~~1.196~~	~~1.206~~	~~1.226~~	~~1.199~~	0.109	0.108	0.792	0.775
G	~~1.791~~	~~1.803~~	0.560	0.597	~~1.205~~	~~1.228~~	~~1.308~~	~~1.306~~	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	~~1.214~~	~~1.261~~	~~0.115~~	0.116	0.115	0.115	0.490	0.477

Average

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the average of the replicates in each sample group (flagged replicates are not included).

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to find the average position values in each sample group.

> This transform averages the replicates of the sample group and stores the resulting value to each sample group replicate of the output matrix. Therefore, the result will depend on the layout configuration.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in duplicate (e.g., **Unknown1** at **A1** and **A2**, **Unknown2** at **B1** and **B2**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	2	2	3	3	4	4	5	5	6	6
B	7	7	8	8	9	9	10	10	11	11	12	12
C	13	13	14	14	15	15	16	16	17	17	18	18
D	19	19	20	20	21	21	22	22	23	23	24	24
E	25	25	26	26	27	27	28	28	29	29	30	30
F	31	31	32	32	33	33	34	34	35	35	36	36
G	37	37	38	38	39	39	40	40	41	41	42	42
H	43	43	44	44	45	45	46	46	47	47	48	48

⬤ Unknown

Average

The transform will generate an output matrix named **Average** with the value at each position being the averaged input data for each sample group.

With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations. For each sample, the following details are reported:

Sample	Positions	My Raw Data	Average
⬤ Unknown1	A1	0.364	0.3435
	A2	0.323	
⬤ Unknown2	A3	2.105	2.1145
	A4	2.124	
⬤ Unknown3	A5	1.213	1.2195
	A6	1.226	
⬤ Unknown4	A7	1.159	1.1745
	A8	1.19	
⬤ Unknown5	A9	0.11	0.113
	A10	0.116	

- **Matrix Table**

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.344	0.344	2.115	2.115	1.220	1.220	1.175	1.175	0.113	0.113	1.472	1.472
B	0.448	0.448	1.879	1.879	1.211	1.211	1.193	1.193	0.131	0.131	0.777	0.777
C	0.581	0.581	0.494	0.494	1.223	1.223	1.207	1.207	0.115	0.115	0.620	0.620
D	0.790	0.790	0.371	0.371	1.177	1.177	1.226	1.226	0.104	0.104	0.490	0.490
E	1.085	1.085	0.323	0.323	1.220	1.220	1.248	1.248	0.113	0.113	1.564	1.564
F	1.435	1.435	0.395	0.395	1.201	1.201	1.213	1.213	0.109	0.109	0.784	0.784
G	1.797	1.797	0.579	0.579	1.217	1.217	1.307	1.307	0.127	0.127	0.656	0.656
H	0.262	0.262	0.467	0.467	1.238	1.238	0.116	0.116	0.115	0.115	0.484	0.484

Blank Correction

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform subtracts the average of a specified blank group (or groups) from each sample. This is useful for subtracting background noise from measurements.

The blank value is computed from the average of the ([non-flagged](#)) blank replicates.

In the simplest configuration, a single blank value is subtracted from all samples. More sophisticated correction methods are possible, including:

- 1-1 – Where each sample group is corrected by its associated blank group

- By-row – One blank group on each row

- By-column – One blank group on each column

> ℹ For more complicated blank correction calculations, an alternative approach is to use the [Expression by Position transform](#).

For viewing common transform settings, see [General Transform Properties](#).

To learn about adding this transform to your assay run, see [Transforms Tab](#).

Properties

Settings

Blank Group	The group number of the sample to use for correction. This can be defined as a number or as [an expression](#). The expression can refer to x, which is the group number of the sample to be corrected. For example, set this to x to perform a 1-to-1 correction where each group is corrected by the sample of the specified blank type with the same group number.
Blank Type	The sample type used as the blank.

Example: Single Blank

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to perform a blank correction using the average of one blank group. This blank group itself is measured in duplicate. The mean of these replicates will be subtracted from all other samples.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.192	0.199	0.347	0.346	0.325	0.321	0.803	0.797	1.589	1.593	0.241	0.246
B	0.293	0.300	0.586	0.584	0.800	0.793	0.402	0.401	0.839	0.837	0.562	0.564
C	0.537	0.534	0.549	0.547	0.878	0.875	0.471	0.471	0.759	0.756	1.039	1.043
D	0.858	0.855	0.320	0.325	0.531	0.530	1.552	1.551	0.429	0.427	0.424	0.424
E	1.523	1.527	0.486	0.490	1.289	1.283	1.430	1.438	1.494	1.501	1.427	1.429
F	1.622	1.621	0.621	0.626	0.667	0.663	1.350	1.347	0.631	0.634	1.695	1.694
G	0.001	0.001	0.356	0.352	0.418	0.412	1.172	1.174	1.572	1.570	0.595	0.590
H	0.297	0.297	0.796	0.801	1.517	1.515	0.960	0.965	0.534	0.527	0.585	0.584

This transform requires a layout with a minimum 1 **Blank** group.

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

● Standard ○ Blank ○ Control ○ Unknown

To subtract the mean of the blank positions from the measurements, specify **Blank Group** to **1** and **Blank Type** to **Blank**.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the blank value from the input data. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.191	0.198	0.346	0.345	0.324	0.320	0.802	0.796	1.588	1.592	0.240	0.245
B	0.292	0.299	0.585	0.583	0.799	0.792	0.401	0.400	0.838	0.836	0.561	0.563
C	0.536	0.533	0.548	0.546	0.877	0.874	0.470	0.470	0.758	0.755	1.038	1.042
D	0.857	0.854	0.319	0.324	0.530	0.529	1.551	1.550	0.428	0.426	0.423	0.423
E	1.522	1.526	0.485	0.489	1.288	1.282	1.429	1.437	1.493	1.500	1.426	1.428
F	1.621	1.620	0.620	0.625	0.666	0.662	1.349	1.346	0.630	0.633	1.694	1.693
G	0.000	0.000	0.355	0.351	0.417	0.411	1.171	1.173	1.571	1.569	0.594	0.589
H	0.296	0.296	0.795	0.800	1.516	1.514	0.959	0.964	0.533	0.526	0.584	0.583

Example: 1-1 Blank Correction

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to perform a 1-to-1 correction, where each sample group is corrected by the blank that it is associated with. The blank numbering used in the layout defines the associations.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.962	1.999	2.038	1.922	1.995	0.002	1.628	1.670	1.624	1.554	1.701	0.000
B	0.784	0.760	0.754	0.751	0.797	0.002	1.124	1.104	1.072	1.077	1.106	0.002
C	0.586	0.575	0.582	0.590	0.576	0.001	0.724	0.737	0.690	0.711	0.717	0.002
D	0.441	0.441	0.427	0.419	0.439	0.002	0.095	0.095	0.093	0.096	0.096	0.001
E	1.956	1.970	1.875	2.043	1.959	0.001	1.449	1.479	1.428	1.395	1.385	0.001
F	1.416	1.358	1.407	1.352	1.452	0.001	0.242	0.230	0.249	0.235	0.251	0.000
G	1.438	1.429	1.488	1.401	1.372	0.002	0.943	0.952	0.956	0.912	0.969	0.002
H	0.840	0.827	0.812	0.838	0.860	0.002	1.320	1.260	1.313	1.363	1.312	0.001

Layout

The example uses a layout with 16 **Unknowns** groups (with **Unknown1** in positions from **A1** to **A5**, **Unknown2** in positions from **B1** to **B5**, etc.) and 16 **Blank** singlets:

⚪ Blank ⚪ Unknown

To perform 1-1 correction, specify **Blank Group** to *x* and **Blank Type** to **Blank**.

With this specified, the value of each blank will be subtracted from every position of associated group. In other words, **Blank1** (stored in **A6**) value will be subtracted from **A1, A2, A3, A4, A5** (the members of **Unknown1**), and from **A6** itself. Therefore, the calculated matrix will contain blank corrected **Unknown** values and all **Blanks** will be 0.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the associated blank value from the input data. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.960	1.997	2.035	1.919	1.992	0.000	1.628	1.670	1.623	1.554	1.701	0.000
B	0.783	0.758	0.752	0.750	0.796	0.000	1.122	1.102	1.070	1.075	1.104	0.000
C	0.585	0.574	0.581	0.589	0.575	0.000	0.722	0.735	0.688	0.709	0.714	0.000
D	0.439	0.439	0.425	0.417	0.437	0.000	0.094	0.094	0.093	0.095	0.095	0.000
E	1.955	1.969	1.873	2.042	1.958	0.000	1.448	1.478	1.427	1.394	1.384	0.000
F	1.415	1.358	1.406	1.352	1.451	0.000	0.241	0.229	0.249	0.235	0.251	0.000
G	1.436	1.427	1.486	1.399	1.369	0.000	0.941	0.950	0.955	0.910	0.967	0.000
H	0.839	0.825	0.810	0.837	0.858	0.000	1.319	1.260	1.312	1.362	1.311	0.000

Advanced Example: By-Row Blank Correction

In this example, we would like to configure blank correction on a row-by-row basis to blank correct each sample by the average of the two blank samples of the same row.

For better clearness of the process, this example uses simplified endpoint data for a 12x8 microplate:

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	2	3	4	5	6	7	8	9	10	1
B	2	11	12	13	14	15	16	17	18	19	20	2
C	3	21	22	23	24	25	26	27	28	29	30	3
D	4	31	32	33	34	35	36	37	38	39	40	4
E	5	41	42	43	44	45	46	47	48	49	50	5
F	6	51	52	53	54	55	56	57	58	59	60	6
G	7	61	62	63	64	65	66	67	68	69	70	7
H	8	71	72	73	74	75	76	77	78	79	80	8

Layout

The example uses a layout with 80 singlet **Unknowns** and 8 **Blank** duplicates for each row (with **Blank1** in positions **A1** and **A12**, **Blank2** in positions **B1** and **B12**, etc.):

⬤ Blank ⬤ Unknown

With the **Blank Group** setting defined as the expression:

1+floor((x-1)/(LayoutWidth()-2),1)

This converts the group number of the sample to blank correct (x) to the blank number on its row. In other words, for $x=1$, this means **1+floor((1-1)/10),1)**, **floor=0** and the **Blank Group** is taken as 1. For the first row, x is in range from 1 to 10 and the expression outputs 1, thus for **Unknowns** from 1 to 10 the average of **Blank1** is subtracted.

For the second, x is from 11 to 20, **floor=1**, so the **Blank2** group is subtracted from **Unknown11-20**, etc.

Blank Corrected

	1	2	3	4	5	6	7	8	9	10	11	12
A	0	0	1	2	3	4	5	6	7	8	9	0
B	1	9	10	11	12	13	14	15	16	17	18	1
C	2	18	19	20	21	22	23	24	25	26	27	2
D	3	27	28	29	30	31	32	33	34	35	36	3
E	4	36	37	38	39	40	41	42	43	44	45	4
F	5	45	46	47	48	49	50	51	52	53	54	5
G	6	54	55	56	57	58	59	60	61	62	63	6
H	7	63	64	65	66	67	68	69	70	71	72	7

Dilution Factors

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform multiplies each selected sample group by a specified factor (a factor can be specified for each sample group).

> ℹ️ A sample prepared with a dilution of 1:2 would use a dilution factor of 2.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Factored Samples	The sample types to which the dilution factor should be applied
Factors	The dilution factor to use for each selected **Factored Samples**

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to multiply all odd **Unknown** sample groups by 2 and all even **Unknown** sample groups by 5.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	1	1	9	9	17	17	25	25	33	33
B	2	2	2	2	10	10	18	18	26	26	34	34
C	3	3	3	3	11	11	19	19	27	27	35	35
D	4	4	4	4	12	12	20	20	28	28	36	36
E	5	5	5	5	13	13	21	21	29	29	37	37
F	6	6	6	6	14	14	22	22	30	30	38	38
G	1	1	7	7	15	15	23	23	31	31	39	39
H	1	1	8	8	16	16	24	24	32	32	40	40

🔴 Standard 🟡 Blank 🔵 Control 🟢 Unknown

To multiply selected sample types in this matrix by specified factors, set **Factored Samples** to **Unknown** and specify **Factors** as **2** for every odd sample group and as **5** for every even sample group.

Concentration (x Dil. Factor)

The transform will generate an output matrix named **Concentration (x Dil. Factor)** with the value at each position of the selected Factored Samples multiplied by specified Factor and sample groups of other types matching the input data.

With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations for Unknown samples and the additional report content. For this transform, it is a Factor column displaying specified Factor for each sample group.

For each sample, the following details are reported:

Sample	Positions	Factor	My Raw Data	Concentration (x Dil. Factor)
🟢 Unknown1	A3	2	2.105	4.210
	A4		2.124	4.248
🟢 Unknown2	B3	5	1.869	9.345
	B4		1.888	9.440
🟢 Unknown3	C3	2	0.474	0.948
	C4		0.514	1.028
🟢 Unknown4	D3	5	0.364	1.820
	D4		0.378	1.890
🟢 Unknown5	E3	2	0.279	0.558
	E4		0.367	0.734

The location of Factor column in the Sample table can be customized in the XML tab.

How to: Set Factor Column Position in the Report

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Inside the **ReportContent** element, locate the **Factor** element.

3. Add the **SampleTableColumnPosition** element to the **Factor** element. Specify the column positioning with one of the following options:

   - **AfterOutputMatrix** – On the right of the output matrix
   - **LeftMost** – Before all matrix data
   - **RightMost** – After all matrix data

- **Matrix Table**

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	4.210	4.248	2.426	2.452	2.318	2.380	0.220	0.232	2.926	2.962
B	0.455	0.441	9.345	9.440	6.015	6.090	5.900	6.030	0.660	0.650	3.930	3.840
C	0.587	0.575	0.948	1.028	2.412	2.478	2.406	2.420	0.226	0.232	1.226	1.252
D	0.806	0.774	1.820	1.890	5.835	5.935	6.055	6.205	0.505	0.530	2.445	2.450
E	1.105	1.065	0.558	0.734	2.430	2.450	2.466	2.524	0.222	0.228	3.158	3.098
F	1.425	1.445	1.890	2.055	5.980	6.030	6.130	5.995	0.545	0.540	3.960	3.875
G	1.791	1.803	1.120	1.194	2.410	2.456	2.616	2.612	0.252	0.254	1.304	1.318
H	0.253	0.270	2.315	2.350	6.070	6.305	0.575	0.580	0.575	0.575	2.450	2.385

Dose–Response Curves

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform fits a dose–response curve for each sample group (with each sample group being dosed in the same way). The resulting dose–response curves are overlaid on a single chart for visual comparison.

The transform can also optionally compute and report values from each sample's curve, including:

- ED50/EC50/IC50, etc.

- ED(n)/EC(n)/IC(n), etc.

- Upper and lower bounds

- The dose at a specified response

- Any mathematical function (via an expression)

To learn about computing additional values from each curve, see Advanced Dose–Response Curves Evaluations.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Axes

X Axis Title	The name of the x-axis on the chart.
X Axis Type	The scale type to be used for the x-axis: - **Logarithmic** - **Linear**
Y Axis Title	The name of the y-axis on the chart.
Y Axis Type	The scale type to be used for the y-axis: - **Logarithmic** When y-axis is logged, negative (or zero) *y* values are not included in the plot. - **Linear**

Axes (Advanced)

Use these additional settings to adapt the chart's appearance to your needs.

X Axis Major Units	The numeric interval between numbers on the x-axis. Starting from the minimum value, a major unit is displayed at every increment.
X Axis Minor Units	The numeric interval between supplementary tickmarks on the x-axis. The minor units are not displayed unless this attribute is specified.
X Axis Numerical Formatting	The formatting for the **X Axis Major Units** values. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.
X Crosses Y At	Select where the x-axis will cross the y-axis from the drop-down: • **Automatic** – Determine the location that makes the most sense for your data automatically. • **Axis Value** – Cross y-axis at specified **X Crosses Y at Value**. • **Maximum Axis Value** – Cross y-axis at the maximum y value of the chart. • **Minimum Axis Value** – Cross y-axis at the minimum y value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
X Crosses Y at Value	The numerical value at which the x-axis will cross the y-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.
Y Axis Major Units	The numeric interval between the gridlines on the y-axis. Starting from the minimum value, a major unit is displayed at every increment.
Y Axis Minor Units	The numeric interval between supplementary tickmarks on the y-axis. The minor units are not displayed unless this attribute is specified.
Y Axis Numerical Formatting	The formatting for the **Y Axis Major Units** values. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.

	Select where the y-axis will cross the x-axis from the drop-down:
Y Crosses X At	• **Automatic** – Determine the location that makes the most sense for your data automatically. • **Axis Value** – Cross x-axis at specified **Y Crosses X at Value**. • **Maximum Axis Value** – Cross x-axis at the maximum *x* value of the chart. • **Minimum Axis Value** – Cross x-axis at the minimum *x* value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
Y Crosses X at Value	The numerical value at which the y-axis will cross the x-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.

These settings can be also applied to other charts as an advanced configuration. To learn more, see Change the Units and Number Format of the Charts and Customize X and Y Axes Positions for Curve Charts topics.

Chart

Overlay Multiple Plate Charts	Select to plot the data from multiple plates on a single chart rather than plotting separate charts for each plate.
Plot Response for Dose Calculation	Select to plot the **Response for Dose Calculation** (a black line showing the specified response) on the chart.

Dose–Response Curves

Doses	This specifies dose concentration values for each group of the specified **Type**. Click the drop-down to display the editor and specify doses settings. *Dose Replicates* Select the number of adjacent positions each dose value applies to. **Dose Replicates** are determined automatically and include all proper divisors (i.e., all divisors excluding itself) of the number of positions in each sample. For example, for a 12x8 layout with 8 **Unknown** sample groups, each group contains 12 positions. Thus, **Dose Replicates** options include 1, 2, 3, 4, 6. *Dose Concentrations* The left-hand **Doses** grid is used to select and indicate the dose value to edit. Select the dose to edit in a two-column grid. The **Sample** column is numbered from 1 upward. The number of rows is updated according to the selected **Dose Replicates** option. This is the number of replicates in a sample divided by the selected **Dose Replicates** option. In the **Dose** column, click the dose to edit its value. There are two modes for specifying dose values: • **Series** – Provide dose for the first sample of the specified **Type** and common series to apply to all samples. • **Non-Serial** – Provide a specific dose value for each sample separately. Click the **Series** button to switch between modes. > All sample groups are assumed to have the same number of positions defined on the layout (e.g., if **Unknown1** has 10 replicates, then all Unknowns on the layout must also have 10 replicates). *Paste Option* You can copy and paste the clipboard contents to the **Dose** column. The content is pasted starting from the first row on a line by line basis. This is useful if you have your dose values in another application (such as Excel or notepad). > When you click **Paste**, the mode automatically switches to **Non-**

	ℹ️ **Serial**.
Response for Dose Calculation	A numerical value or an [expression](#) representing the response value to calculate the dose for each sample.
Type	The sample type to use for dose calculation.

Fit

Fit Method	The curve-fitting method to construct a dose–response curve for your data based on the specified **Type**.
Weight Method	Specifies the weight function to use in the curve-fitting method.
X Transform	Determines how the *x* values are interpreted in the transform: • **None** – The *x* values remain as they are. • **Log10** – Each *x* point is taken as a common logarithm of *x*. • **Log2** – Each *x* point is taken as a binary logarithm of *x*. • **LogN** – Each *x* point is taken as a natural logarithm of *x*.
Y Transform	Determines how the *y* values are interpreted in the transform: • **None** – The *y* values remain as they are. • **Log10** – Each *y* point is taken as a common logarithm of *y*. • **Log2** – Each *y* point is taken as a binary logarithm of *y*. • **LogN** – Each *y* point is taken as a natural logarithm of *y*.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to fit a dose–response curve to each sample group of the **Unknown** type and calculate a dose that has a response of 1.5 from the curve.

Here is some example raw data displayed here to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.000	2.682	2.345	2.612	2.732	2.675	2.664	2.574	2.580	2.361	0.871	2.839
B	0.000	2.577	1.735	2.518	2.701	2.537	2.571	2.450	2.453	2.171	0.437	2.809
C	0.000	2.537	1.290	2.497	2.683	2.447	2.490	2.273	2.344	1.695	0.222	2.783
D	0.000	2.358	0.793	2.318	2.585	2.195	2.205	1.856	2.069	1.070	0.094	2.658
E	0.000	1.958	0.369	1.799	2.224	1.636	1.661	1.192	1.485	0.550	0.037	2.322
F	0.000	1.352	0.151	1.118	1.517	0.909	0.947	0.638	0.868	0.257	0.013	1.495
G	0.000	0.745	0.053	0.540	0.872	0.425	0.485	0.282	0.417	0.094	0.002	0.862
H	0.000	0.312	0.018	0.250	0.398	0.180	0.200	0.113	0.194	0.038	0.001	0.438

Layout

The example uses a layout with one **Unused** column (in positions from **A1** to **H1**) and **Unknowns** in columns (e.g., **Unknown1** at positions from **A2** downward to **H2**, **Unknown2** at **A3-H3**, etc.).:

○ Unused ● Unknown

To create a curve and calculate concentrations for this matrix, specify the following settings:

1. Set **X Axis Type** to **Logarithmic**.

2. Set **X Transform** to **None**.

3. Set **Y Axis Type** to **Linear**.

4. Set **Y Transform** to **None**.

5. Select the **Plot Response for Dose Calculation** check box.

6. In the Doses editor, set **Dose** for the **Sample 1** to 0.01 and **Series** to multiply by 3, and select **Dose Replicates** of 1.

7. Set a **Response for Dose Calculation** to 1.5.

8. Set **Type** to **Unknown**.

9. Set **Fit Method** of **4PL**.

10. Select a **Weight Method** of **None**.

11. Select an **X Transform** of **None**.

12. Select a **Y Transform** of **None**.

The transform generates a **Dose–Response Curves Table** and a **Dose–Response Curve Chart** by default. Other elements such as Matrix table and Notes can be added to report optionally.

Dose–Response Curves Table

This table lists coefficients calculated from the selected Fit Method and a resulting response value for each sample. With the example data provided above, the results are as follows:

Sample	a	b	c	d	R^2	Result
🟢Unknown1	2.67099	0.875198	2.65478	-0.0584816	0.999497	1.91503
🟢Unknown2	3.29931	0.606878	0.0441357	-0.0901615	0.997736	0.0541024
🟢Unknown3	2.59484	1.07281	1.69869	0.103291	0.999371	1.35375
🟢Unknown4	2.73875	1.10415	2.7794	0.176798	0.999281	2.61824
🟢Unknown5	2.64392	0.998377	1.25839	0.0355624	0.999147	0.982572
🟢Unknown6	2.66458	0.980399	1.28776	0.0581275	0.999619	1.03568
🟢Unknown7	2.60957	0.929062	0.682855	0.0190159	0.999764	0.500446
🟢Unknown8	2.57555	0.936045	1.10936	0.0468791	0.999425	0.804401
🟢Unknown9	2.53025	0.919968	0.194091	0.53025	0.999769	0.13033
🟢Unknown10	6.05263	0.681115	0.000740073	-0.00938084	0.999738	0.00374295
🟢Unknown11	2.83485	1.20751	2.35471	0.298789	0.999004	2.56967

Dose–Response Curve Chart

The chart contains a curve fit plotted with 4PL for dose and for each sample group.
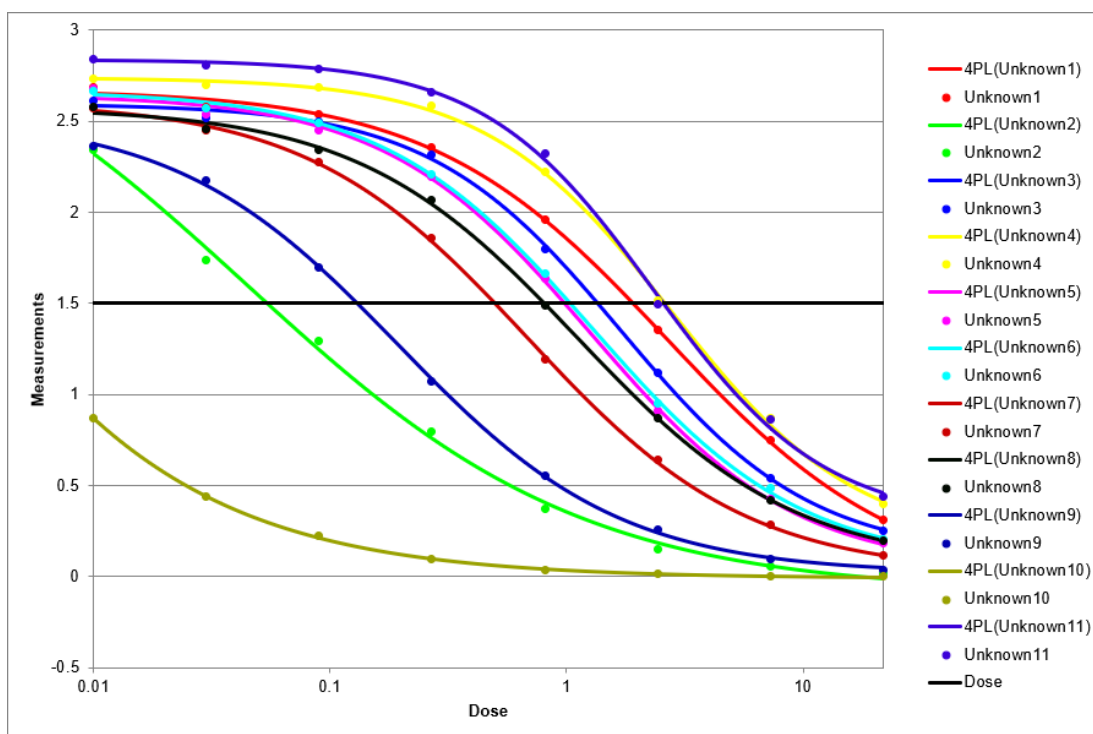
Dose–Response Curve Data Tables

For each fitting, these tables list the measurement and calculation details for the calibration doses used in the fit. Here is a snippet of the Dose–Response Curves Data Table for Dose 1 to 4 of **Unknown1** (using the data provided above):

Calibrator	Positions	Dose (Defined)	Raw	Dose (Calc.)	%CV (Dose Calc.)	% Accuracy
🟢Unknown1 (Dose 1)	A2	0.01	2.682	(NA)	0	(NA)
🟢Unknown1 (Dose 2)	B2	0.03	2.577	0.0588537	0	196.179
🟢Unknown1 (Dose 3)	C2	0.09	2.537	0.089809	0	99.7878
🟢Unknown1 (Dose 4)	D2	0.27	2.358	0.256915	0	95.1538

Dose

The output matrix named **Dose** can be optionally added to the report. It contains the calculated dose that has a response of 1.5 for each data point. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570
B	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570

	1	2	3	4	5	6	7	8	9	10	11	12
C	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570
D	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570
E	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570
F	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570
G	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570
H	~~Flagged~~	1.915	0.054	1.354	2.618	0.983	1.036	0.500	0.804	0.130	0.004	2.570

Example: Calculate EC(20), EC(50) and EC(80) from Each Dose–Response Curve

Using this transform, you can compute specific results from each dose–response curve and report them in a Dose–Response Fit Table.

Here is an example of how to compute EC(20), EC(50) and EC(80) from each dose-response curve taking the y-axis as the % with $c*(((a-d)/(EC(n)-d))-1)^{(1/b)}$ expression, where $EC(n)$ is the percentage value to calculate. This example uses the measurements data and layout from the Dose–Response Curves example to illustrate the results.

Assuming you have already added Dose–Response Curves transform, follow these steps to evaluate effective concentrations:

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Add the Dose–Response Fit Table.

3. Add evaluations as follows:

> Since the coefficient values in all curve fits from the example above are small, we add **abs** function to the formula to avoid negative results. So, the expression in this case is $c*\mathbf{abs}(((a-d)/(EC(n)-d))-1)^{(1/b)}$.

```
<FitTable>
    <Evaluation Description="EC(20)" Expression="c*abs(((a-d)/(20-d))-1)^
    (1/b)"/>
    <Evaluation Description="EC(50)" Expression="c*abs(((a-d)/(50-d))-1)^
    (1/b)"/>
```

```
<Evaluation Description="EC(80)" Expression="c*abs(((a-d)/(80-d))-1)^
(1/b)"/>
```

```
</FitTable>
```

> ℹ️ You can also optionally label the results in the table and change their numerical formatting. For details, see Advanced Dose–Response Curves Evaluations.

4. Add Dose–Response Fit Table to report.

5. Click **Apply** to accept changes and then click **Calculate**.

Here is a snippet that shows the calculated EC(n) results for **Unknown1** curve:

Sample	EC(20)	EC(50)	EC(80)
🟢 Unknown1	2.24619	2.49004	2.55162

Example: Use Area under Curve to Estimate the Difference between Dose–Response Curves

You also can assess and compare the areas under the fitted dose–response curves using **auc** function. This is handy for comparing curves with small number of doses, when determining EC50 (or IC50), slope, and maximum effect (or maximum inhibition) with reasonable precision is not always possible. With this, you can capture additional information about differential sensitivity (response).

To learn more about the **auc** function and its syntax, see Calculation Functions.

To evaluate area under curve (AUC) for each dose–response curve and assuming that you have already added Dose–Response Curves transform, follow these steps to calculate the areas under plotted curves:

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Add the Dose–Response Fit Table.

3. Add evaluation:

```
<FitTable>
```

```
<Evaluation Description="Area Under Curve" Expression="auc
('4PL',dosemin,dosemax,1000,a,b,c,d)"/>
```

```
</FitTable>
```

4. Add Dose–Response Fit Table to report.

5. Click **Apply** to accept changes and then click **Calculate** to generate new results.

Here is a snippet that shows the calculated area under **Unknown1** curve (using the example data from the Dose–Response Curves example above):

Sample	AUC
⬤ Unknown1	16.0385

Expression by Matrix (Dual)

Input: **Dual Endpoint** ➡ Output: **Endpoint**

This transform evaluates an expression defined in terms of *x* and *y* for all data points (excluding flagged samples). ***x*** refers to the data for the sample on the first input matrix, and ***y*** refers to the data for the same sample on the second input matrix.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Dual Matrix Expression	The expression to evaluate, where *x* and *y* variables are set to value of each position of the input matrices

> ℹ️ If the expression does not contain the *x* and *y* variables, the transform will output the same evaluation result for all positions. For example, if you enter **{2^3+4}**, the resulting matrix will contain 12 in each position.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw (1)** and **Raw (2)** matrices. In this example, we would like to summarize position values in these matrices.

Here is some example raw data displayed to 3 decimal places:

Raw (1)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Raw (2)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.204	0.201	0.213	0.209	0.206	0.208	0.216	0.217	0.216	0.213	0.205	0.218
B	0.216	0.200	0.214	0.214	0.204	0.201	0.215	0.216	0.203	0.219	0.207	0.204
C	0.206	0.210	0.208	0.203	0.201	0.218	0.212	0.217	0.216	0.213	0.208	0.204
D	0.215	0.215	0.214	0.203	0.214	0.213	0.219	0.219	0.213	0.201	0.202	0.219
E	0.215	0.220	0.219	0.212	0.210	0.211	0.214	0.214	0.201	0.202	0.202	0.207
F	0.214	0.212	0.202	0.200	0.201	0.217	0.213	0.209	0.218	0.207	0.216	0.216
G	0.211	0.211	0.218	0.209	0.214	0.213	0.201	0.211	0.205	0.210	0.201	0.212
H	0.216	0.209	0.215	0.206	0.218	0.206	0.209	0.219	0.215	0.219	0.216	0.217

To add values from **Raw(2)** to corresponding values of **Raw(1)**, specify an expression of **_x+y_**.

Calculated

The transform will generate an output matrix named **Calculated** with the value at each position being the point by point sum of the **Raw (1)** and **Raw (2)** matrices values. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.568	0.524	2.318	2.333	1.419	1.434	1.375	1.407	0.326	0.329	1.668	1.699
B	0.671	0.641	2.083	2.102	1.407	1.419	1.395	1.422	0.335	0.349	0.993	0.972
C	0.793	0.785	0.682	0.717	1.407	1.457	1.415	1.427	0.329	0.329	0.821	0.830
D	1.021	0.989	0.578	0.581	1.381	1.400	1.430	1.460	0.314	0.307	0.691	0.709
E	1.320	1.285	0.498	0.579	1.425	1.436	1.447	1.476	0.312	0.316	1.781	1.756
F	1.639	1.657	0.580	0.611	1.397	1.423	1.439	1.408	0.327	0.315	1.008	0.991
G	2.002	2.014	0.778	0.806	1.419	1.441	1.509	1.517	0.331	0.337	0.853	0.871
H	0.469	0.479	0.678	0.676	1.432	1.467	0.324	0.335	0.330	0.334	0.706	0.694

Expression by Matrix

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform evaluates an expression defined in terms of *x* for all data points (excluding flagged samples).

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Matrix Expression	The expression to evaluate, where a single *x* variable is set to value of each position of the input matrix

> ℹ If the expression does not contain the *x* variable, the transform will output the same evaluation result for all positions. For example, if you enter **{2^3+4}**, the resulting matrix will contain 12 in each position.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to square each measurement.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

The **Matrix Expression** setting is specified with expression of ***x*x***.

Calculated

The transform will generate an output matrix named **Calc** with the value at each position being the square of the input data. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.132	0.104	4.431	4.511	1.471	1.503	1.343	1.416	0.012	0.013	2.140	2.193
B	0.207	0.194	3.493	3.565	1.447	1.484	1.392	1.454	0.017	0.017	0.618	0.590
C	0.345	0.331	0.225	0.264	1.454	1.535	1.447	1.464	0.013	0.013	0.376	0.392
D	0.650	0.599	0.132	0.143	1.362	1.409	1.467	1.540	0.010	0.011	0.239	0.240
E	1.221	1.134	0.078	0.135	1.476	1.501	1.520	1.593	0.012	0.013	2.493	2.399
F	2.031	2.088	0.143	0.169	1.430	1.454	1.503	1.438	0.012	0.012	0.627	0.601
G	3.208	3.251	0.314	0.356	1.452	1.508	1.711	1.706	0.016	0.016	0.425	0.434
H	0.064	0.073	0.214	0.221	1.474	1.590	0.013	0.013	0.013	0.013	0.240	0.228

Expression by Position

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform enables an [expression](#) to be defined for each position in terms of *x* (where *x* refers to the value of position on the input matrix). This is useful for applying various tests to different samples simultaneously.

For viewing common transform settings, see [General Transform Properties](#).

To learn about adding this transform to your assay run, see [Transforms Tab](#).

Properties

Settings

This allows different [expressions](#) to be configured and calculated on the positions of the same index on different plates. Expressions are stored by container (1-based values are used for each container separately).

Click drop-down to open a **Position Expressions Editor** with grid-based view of input data. The configuration of the grid depends on the selected layout, thus each position's background is coloured to match its sample type.

Position Expressions	If the protocol contains >1 plate/analyte, select the one to specify expressions for from a drop-down list in the upper right corner of the Editor. To maximize its view, click the arrow button in the lower left corner of the Editor. Within each grid you can select and specify [an expression](#) in terms of *x* for: • A single position. • Multiple positions (within a single plate) to set to a same expression. Multiple positions can be selected by: • Dragging the mouse (for rectangular selection) • Using **Ctrl** to select random positions • Using **Shift** to select the end position (rectangular selection) ℹ **Paste**, **Copy**, and **Clear** commands are supported. For positions with default (simply *x*) or empty expression, the output position is equal to the input position.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to multiply positions from 1 to 5 by 10, positions 10 and 96 by 100, and position 50 by 2.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Provide expressions for positions in Position Expressions Editor:

- **A1**, **A2**, **A3**, **A4**, **A5** with the expression $x*10$
- **A10** and **H12** with the expression $x*100$
- **E2** with the expression $x*2$

Calculated

The transform will generate an output matrix named **Calculated** with the resulting values being the product of input data and specified expressions. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	3.640	3.230	21.050	21.240	12.130	1.226	1.159	1.190	0.110	11.600	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	2.130	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	47.700

Expression by Sample Group

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform enables an expression to be defined for each sample group of one of more sample types in terms of *x* (where *x* refers to the value of position on the input matrix). This is useful for applying different calculations to each sample group.

> The Expression by Sample Group transform is an Import Target. This means that it in addition to configuration through the Property Editor, it supports configuration through the Import Wizard, command line arguments or section data. For example, values or expressions to associate with each sample group can be automatically imported from a file. This is useful if your analysis depends on data values stored in a data file which vary from run-to-run; MyAssays Desktop can automatically import those values and use them as part of your data analysis.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Expression by Sample Group	Specify an expression to calculate for each sample group on the selected layout. Click the drop-down to display the editor, where you can enter an expression in terms of *x* for each sample group.
	ℹ **Paste**, **Copy**, and **Cut** commands are supported.
	For types with simply *x* (or empty expression), the output value is equal to the input value of the group.
Sample Types	Select which sample type or types an expression can be entered for. An expression can be provided for each group of the selected types.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to multiply Unknown1 by 2 and Unknown2 by 5.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

🔴 Standard 🟡 Blank 🔵 Control 🟢 Unknown

Select **Unknown** as the **Sample Types**

In **Expressions by Sample Group** Editor, provide:

- **Unknown1** type with the expression *x*2*
- **Unknown2** with the expression *x*5*

Calculated

The transform will generate an output matrix named **Calculated** with the resulting values of each specified type evaluated with provided expressions. With the example data provided above, the results are as follows (also displayed here to 3 decimal places). Here it can be seen that the values for Unknown1 (A3+A4) and Unknown2 (B3+B4) have been computed using the expressions provided.

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	4.210	4.248	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	9.345	9.440	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Advanced: Section Data

To add a section control for editing Expression by Sample Group expressions, add a section to the assay.xml as follows:

<section id="Parameters" type="analysis" customName="Values">

<ExpressionBySampleGroup TransNum="1" DataTitle="Custom Title" Description="Custom Description" />

</section>

Set **TransNum** to the 1-based transform number of the transform to associate the control with.

The optional **ExpressionBySampleGroup** attribute **ShowSampleTypesSelector** can be used to show or hide the Sample Types selector control.

Expression by Sample Replicates

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform enables an expression to be defined in terms of each replicate within each sample group (where *a* refers to the first replicate's value and *b* refers to the second, etc.). This is useful for applying calculations within each sample group.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Replicates Expression	Specify an expression to calculate for each sample in terms of the replicates of each sample.
	a = 1st replicate
	b = 2nd replicate
	c = 3rd replicate
	etc.
	Replicate ordering follows row-wise ordering. For example, if a sample group is replicated at positions A1, A2, B1 and B2, then the expression variables correspond as follows: *a*=A1, *b*=A2, *c*=B1, *d*=B2

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. All samples are arranged in duplicate. In this example, we would like to compute %D of each sample - that is the absolute difference between the replicates divided by the sum of the replicates.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

🔴 Standard 🟡 Blank 🔵 Control 🟢 Unknown

In **Replicates Expression** enter the %D expression which is: **100*abs(a-b)/(a+b)**

Calculated

The transform will generate an output matrix named **Calculated** with the resulting values of each specified type evaluated with provided expressions. With the example data provided above, the results are as follows displayed here to 2 decimal places). Here it can be seen that the values for all samples have been computed in accordance with the defined %D calculation:

	1	2	3	4	5	6	7	8	9	10	11	12
A	5.97	5.97	0.45	0.45	0.53	0.53	1.32	1.32	2.65	2.65	0.61	0.61
B	1.56	1.56	0.51	0.51	0.62	0.62	1.09	1.09	0.76	0.76	1.16	1.16
C	1.03	1.03	4.05	4.05	1.35	1.35	0.29	0.29	1.31	1.31	1.05	1.05
D	2.03	2.03	1.89	1.89	0.85	0.85	1.22	1.22	2.42	2.42	0.10	0.10
E	1.84	1.84	13.62	13.62	0.41	0.41	1.16	1.16	1.33	1.33	0.96	0.96
F	0.70	0.70	4.18	4.18	0.42	0.42	1.11	1.11	0.46	0.46	1.08	1.08
G	0.33	0.33	3.20	3.20	0.95	0.95	0.08	0.08	0.40	0.40	0.53	0.53
H	3.25	3.25	0.75	0.75	1.90	1.90	0.43	0.43	0.00	0.00	1.34	1.34

Expression by Sample Type

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform enables an expression to be defined for each sample type in terms of *x* (where *x* refers to the value of position on the input matrix). This is useful for applying different calculations to each sample type.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Expression by Sample Type	Specify an expression to calculate for each sample type on the selected layout. Click the drop-down to display the editor, where you can enter an expression in terms of *x* for the selected type.
	ℹ️ **Paste**, **Copy**, and **Cut** commands are supported.
	For types with simply *x* (or empty expression), the output value is equal to the input value at a position.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to multiply standards by 2 and unknowns by 5.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

In Expressions by Sample Type Editor, provide:

- **Standard** type with the expression *x*2*
- **Unknown** with the expression *x*5*

Calculated

The transform will generate an output matrix named **Calculated** with the resulting values of each specified type evaluated with provided expressions. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.728	0.646	10.525	10.620	6.065	6.130	5.795	5.950	0.550	0.580	7.315	7.405
B	0.910	0.882	9.345	9.440	6.015	6.090	5.900	6.030	0.660	0.650	3.930	3.840
C	1.174	1.150	2.370	2.570	6.030	6.195	6.015	6.050	0.565	0.580	3.065	3.130
D	1.612	1.548	1.820	1.890	5.385	5.935	6.055	6.205	0.505	0.530	2.445	2.450
E	2.210	2.130	1.395	1.385	6.075	6.125	6.165	6.310	0.555	0.570	7.895	7.745
F	2.850	2.890	1.890	2.055	5.980	6.030	6.130	5.995	0.545	0.540	3.960	3.875
G	1.791	1.803	2.800	2.985	6.025	6.140	6.540	6.530	0.630	0.635	3.260	3.295
H	0.253	0.270	2.315	2.350	6.070	6.305	0.575	0.580	0.575	0.575	2.450	2.385

Factor

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform multiplies data points by a common factor. The factor can be specified as a numeric value or as an expression to evaluate.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Factor	The value to multiply all data points by. This can be specified as a number or an expression to evaluate.

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to multiply each measurement by a common factor of 2.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

The **Factor** setting for this example is specified as 2.

Factored

The transform will generate an output matrix named **Factored** with the value at each position being the product of the input data and the factor. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.728	0.646	4.210	4.248	2.426	2.452	2.318	2.380	0.220	0.232	2.926	2.962
B	0.910	0.882	3.738	3.776	2.406	2.436	2.360	2.412	0.264	0.260	1.572	1.536
C	1.174	1.150	0.948	1.028	2.412	2.478	2.406	2.420	0.226	0.232	1.226	1.252
D	1.612	1.548	0.728	0.756	2.334	2.374	2.422	2.482	0.202	0.212	0.978	0.980
E	2.210	2.130	0.558	0.734	2.430	2.450	2.466	2.524	0.222	0.228	3.158	3.098
F	2.850	2.890	0.756	0.822	2.392	2.412	2.452	2.398	0.218	0.216	1.584	1.550
G	3.582	3.606	1.120	1.194	2.410	2.456	2.616	2.612	0.252	0.254	1.304	1.318
H	0.506	0.540	0.926	0.940	2.428	2.522	0.230	0.232	0.230	0.230	0.980	0.954

General Curve Fit

[Input: **Endpoint** ➡ Output: **Endpoint**]

> The **General Curve Fit** transform is suitable for performing a curve fit on any set of data with the calibrator points being defined as values, expressions or references to sample groups.
> For calculating concentrations from a standards curve, use the Standard Curve Fit transform.

This transform:

1. Plots specified calibration data (*x* and *y* values). These might be numeric values or expressions that can refer to samples on specific matrices or containers.

2. Fits a curve to the calibration data (optionally using weight methods).

3. Uses the resulting curve to predict either *x* or *y* value on the curve at each *y* or *x* input value for selected sample types.

> For multiple plate and multiplex assays, a single curve is plotted, used to compute values for all containers, and included in the report.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Axes

X Axis Title	The name of the x-axis on the chart.
X Axis Type	The scale type to be used for the x-axis: • **Logarithmic** • **Linear**
Y Axis Title	The name of the y-axis on the chart.

Y Axis Type	The scale type to be used for the y-axis: • **Logarithmic** When y-axis is logged, negative (or zero) *y* values are not included in the plot. • **Linear**

Axes (Advanced)

Use these additional settings to adapt the chart's appearance to your needs.

X Axis Major Units	The numeric interval between numbers on the x-axis. Starting from the minimum value, a major unit is displayed at every increment.
X Axis Minor Units	The numeric interval between supplementary tickmarks on the x-axis. The minor units are not displayed unless this attribute is specified.
X Axis Numerical Formatting	The formatting for the **X Axis Major Units** values. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.
X Crosses Y At	Select where the x-axis will cross the y-axis from the drop-down: • **Automatic** – Determine the location that makes the most sense for your data automatically. • **Axis Value** – Cross y-axis at specified **X Crosses Y at Value**. • **Maximum Axis Value** – Cross y-axis at the maximum *y* value of the chart. • **Minimum Axis Value** – Cross y-axis at the minimum *y* value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
X Crosses Y at Value	The numerical value at which the x-axis will cross the y-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.
Y Axis Major Units	The numeric interval between the gridlines on the y-axis. Starting from the minimum value, a major unit is displayed at every increment.
Y Axis Minor Units	The numeric interval between supplementary tickmarks on the y-axis. The minor units are not displayed unless this attribute is specified.

Y Axis Numerical Formatting	The formatting for the **Y Axis Major Units** values. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.
Y Crosses X At	Select where the y-axis will cross the x-axis from the drop-down: • **Automatic** – Determine the location that makes the most sense for your data automatically. • **Axis Value** – Cross x-axis at specified **Y Crosses X at Value**. • **Maximum Axis Value** – Cross x-axis at the maximum *x* value of the chart. • **Minimum Axis Value** – Cross x-axis at the minimum *x* value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
Y Crosses X at Value	The numerical value at which the y-axis will cross the x-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.

These settings can be also applied to other charts as an advanced configuration. To learn more, see Change the Units and Number Format of the Charts and Customize X and Y Axes Positions for Curve Charts topics.

Calibration Data

	Defines the *x* and *y* values of each calibration point.
	Click the **Calibrators** setting drop-down to display the editor. Each calibrator corresponds to a row where you specify *x* and *y* values under **X** and **Y** titled columns. These can be specified as numeric values or [expressions.](#)
	You can define *x* and *y* values of each calibrator as [sample references](#). When working with multiple plate assays, it is possible to [reference samples on a specific plate](#). For example, **Control1.1.1** refers to average of **Control1** sample replicates on the 1st matrix of the 1st container.
Calibrators	Click **Add** to add a calibrator. Select a cell and click **Remove** to remove the selected calibrator.

Pasting Calibration Data from Clipboard

With **Paste** option, you can insert the clipboard contents in the table. The content is pasted starting from the first cell (X) on the first row on a cell by cell basis. This is useful if you have your calibration data in another application (such as Excel or notepad).

The number of rows adjusts according to the inserted values. For example, if you insert 100 1 200 2 300 3 sequence, the values will be pasted as follows:

X	Y
100	1
200	2
300	3

Defining Output Units

In the **Units** field, you can define the measurement units to be included in the header of [Sample Table](#).

> If the output units of the transform are the same as its input, then use "ditto" units to automatically carry these units through (i.e., apply the same units to the transform's output). This shortcut means that it is not necessary to repeat settings across transforms. Ditto units are specified with two dots, i.e.:
>
> **..**

Chart

Points on Curve	In the drop-down editor, select any sample types to plot on the curve; this is useful to show where samples fall on the curve. The computed results of each selected sample will be plotted. In this case, all successfully computed non-flagged sample groups of the selected types will be displayed on the chart and in the report.
	Only non-calibrator sample types are applicable, e.g., **Unknown**, **Control**, **Blank**.

Fit

Calculate From	Defines how to calculate the output matrix results from the computed curve for each sample (i.e., is a result calculated from the curve for each replicate or for the average of the replicates?). Select either: • **Replicates** – Every position will contain the result calculated from value of every **Predict Input** replicate. • **Average** – Replicates from the same sample contain the result calculated from averaged value of **Predict Input** replicates. Any flagged positions on the input are also flagged in the output.
Fit Expression	When using the **Custom Fit**, you can enter or paste the equation to create your curve fit.
Fit Method	The curve-fitting method to construct a curve for your data. You can also use the **Best Fit** to plot the most appropriate fit for your data automatically or the **Custom Fit** to supply your own equation or model to fit the data.
Fit Methods	When using the **Best Fit**, this editor specifies the **Fit Methods** and **Weight Methods** to process your data with. You can select any combination of items in corresponding check box lists. At least 1 check box must be selected in each list.

Fit Score Method	When the **Best Fit** feature is selected, to construct the curve, you can additionally specify the [scoring method](#) to be used in evaluating the goodness of applied fit methods: • R^2 • R^2 with Low-End Accuracy • R^2 with High-End Accuracy • R^2 with Low-End and High-End Accuracy • 1/Standard-Error • 1/P-Value • -AIC • -AICc • -BIC
Weight Method	Specifies the weight function for the transform.
X Transform	Determines how the x values are interpreted in the transform: • **None** – The x values remain as they are. • **Log10** – Each x point is taken as a common logarithm of x. • **Log2** – Each x point is taken as a binary logarithm of x. • **LogN** – Each x point is taken as a natural logarithm of x.
Y Transform	Determines how the y values are interpreted in the transform: • **None** – The y values remain as they are. • **Log10** – Each y point is taken as a common logarithm of y. • **Log2** – Each y point is taken as a binary logarithm of y. • **LogN** – Each y point is taken as a natural logarithm of y.

General

	The resulting curve is used to make predictions of data by either calculating x or y values for the input matrix. The output matrix contains the results of these predictions. Select:
Predict Input	• **Y** – To compute x values from the resulting curve at each y value in the input matrix
	• **X** – To compute y values from the resulting curve at each x value in the input matrix

Example: Using General Curve Fit for a Standard Curve

Let's assume that we have endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to fit 4PL to the specified calibrators and calculate x values for the resulting matrix.

The Standard Curve Fit transform could be used to perform this analysis more conveniently, however, this example demonstrates performing the same analysis using the General Curve Fit to illustrate how to refer to samples defined on the layout along with values.

Raw

Here is some example raw data displayed to 3 decimal places:

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.192	0.199	0.347	0.346	0.325	0.321	0.803	0.797	1.589	1.593	0.241	0.246
B	0.293	0.300	0.586	0.584	0.800	0.793	0.402	0.401	0.839	0.837	0.562	0.564
C	0.537	0.534	0.549	0.547	0.878	0.875	0.471	0.471	0.759	0.756	1.039	1.043
D	0.858	0.855	0.320	0.325	0.531	0.530	1.552	1.551	0.429	0.427	0.424	0.424
E	1.523	1.527	0.486	0.490	1.289	1.283	1.430	1.438	1.494	1.501	1.427	1.429
F	1.622	1.621	0.621	0.626	0.667	0.663	1.350	1.347	0.631	0.634	1.695	1.694
G	0.001	0.001	0.356	0.352	0.418	0.412	1.172	1.174	1.572	1.570	0.595	0.590
H	0.297	0.297	0.796	0.801	1.517	1.515	0.960	0.965	0.534	0.527	0.585	0.584

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	1	1	9	9	17	17	25	25	33	33
B	2	2	2	2	10	10	18	18	26	26	34	34
C	3	3	3	3	11	11	19	19	27	27	35	35
D	4	4	4	4	12	12	20	20	28	28	36	36
E	5	5	5	5	13	13	21	21	29	29	37	37
F	6	6	6	6	14	14	22	22	30	30	38	38
G	1	1	7	7	15	15	23	23	31	31	39	39
H	1	1	8	8	16	16	24	24	32	32	40	40

● Standard ○ Blank ○ Control ● Unknown

To configure a **General Curve Fit** for this matrix, follow these steps:

1. Specify **Calibration Data**:

   - **X**=400 **Y**=Standard1
   - **X**=200 **Y**=Standard2
   - **X**=100 **Y**=Standard3
   - **X**=50 **Y**=Standard4
   - **X**=25 **Y**=Standard5
   - **X**=12.5 **Y**=Standard6

2. Set **Calculate From** to **Replicates**.
3. Select a **Fit Method** of **4PL**.
4. Select a **Weight Method** of **None**.
5. Set the **X Transform** to **None**.
6. Set the **Y Transform** to **None**.
7. Set **Predict Input** to **Y**.

Calculated

The transform will generate an output matrix named **Calculated** with *x* values from the calibration curve for each *y* value in the input matrix. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	~~Flagged~~	~~Flagged~~	141.821	142.385	155.949	158.981	58.993	59.443	17.416	17.180	345.017	309.761
B	186.523	178.336	80.170	80.434	59.217	59.747	118.015	113.354	56.393	56.533	83.466	83.180
C	87.237	87.715	85.380	85.683	53.755	53.952	99.439	99.439	62.426	62.672	44.297	44.084
D	55.086	55.290	159.767	155.949	88.200	88.363	19.495	19.549	109.743	110.304	111.160	111.160
E	21.026	20.819	96.313	95.520	32.112	32.388	25.589	25.210	22.494	22.145	25.731	25.636
F	15.385	15.450	75.832	75.251	70.807	71.217	29.307	29.445	74.680	74.341	9.612	9.715
G	~~Flagged~~	~~Flagged~~	137.012	139.091	112.924	114.764	37.594	37.498	18.392	18.505	79.005	79.648
H	181.711	181.711	59.519	59.142	21.334	21.436	48.695	48.405	87.715	88.856	80.302	80.434

Example: Variation Between Controls on 3 Plates of Data

In this example, we will show the variation of control values on different plates of data. To do so, we will fit the linear regression to the calibrators. For this example, we will use the control values on each plate (*y*) and plate numbers (*x*) the calibrators.

For conciseness, a small 3x4 layout with 3 plates of endpoint measurements is used.

Raw

Here is some example raw data displayed to 3 decimal places:

	Plate 1				Plate 2				Plate 3		
	1	2	3		1	2	3		1	2	3
A	1.503	1.490	1.499	**A**	1.521	1.521	1.523	**A**	1.501	1.500	1.497
B	1.801	1.849	1.838	**B**	0.927	0.893	0.959	**B**	1.094	1.076	1.074
C	1.824	1.871	1.781	**C**	1.866	1.917	1.958	**C**	1.028	1.031	1.072
D	0.509	0.519	0.494	**D**	1.731	1.677	1.693	**D**	2.046	2.105	2.070

Layout

All plates use the same layout with 1 **Control** and 3 **Unknown** sample groups in triplicates (i.e., **Control1** at **A1,A2**, **A3**; **Unknown1** at **B1**, **B2**, **B3**, etc.).

○ Control ● Unknown

To determine the variation between controls, follow these steps:

1. Specify **Calibration Data**:

   - **X**=1 **Y**=Control1..1
   - **X**=2 **Y**=Control1..2
   - **X**=3 **Y**=Control1..3

2. Set the **Calculate From** to **Replicates**.

3. Select a **Fit Method** of **Linear Regression**.

4. Select a **Weight Method** of **None**.

5. Set the **X Transform** to **None**.

6. Set the **Y Transform** to **None**.

7. Set the **Predict Input** to **Y**.

Chart

In this example, we are interested in seeing the variation of control values across plates rather than predicting values. With General Curve Fit, it is easy to plot such values on the chart and visually assess the stability of the samples. With the example data provided above, the chart is as follows:
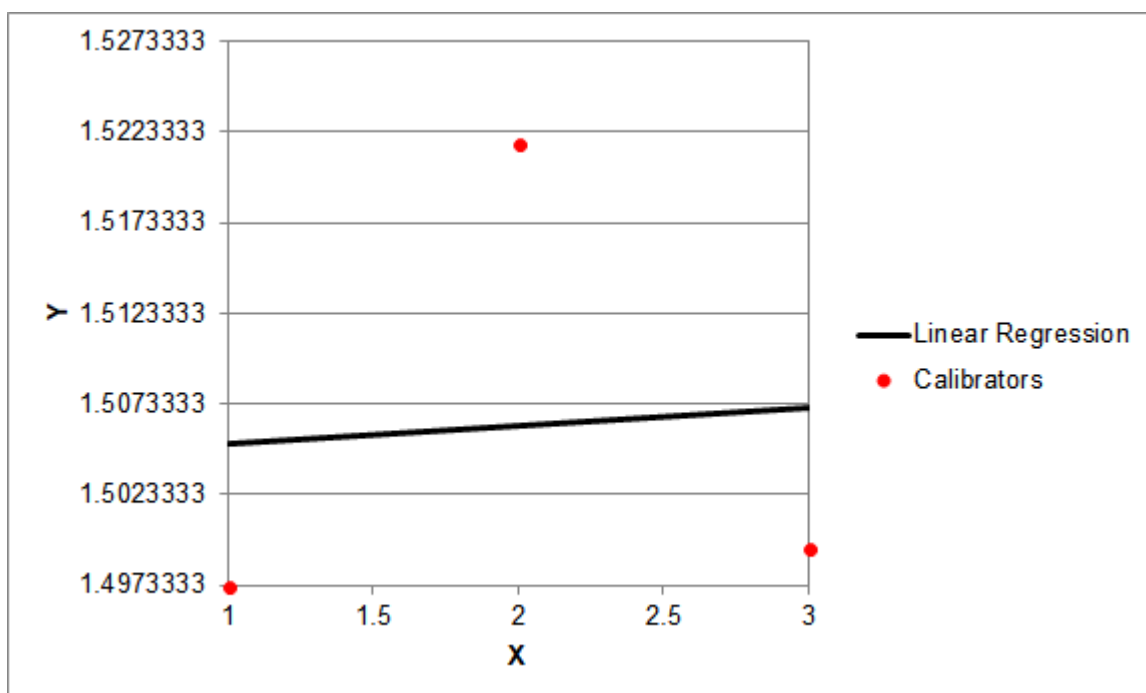
General Curve Fit TOVs:

This transform produces the following TOVs.

Here the **{n}** specifies the position of General Curve Fit in the sequence of transforms configured via **Transform** tab.

TOV	Refers to
Coefficients of the Fit Method	
The calculated values of the coefficients used in the selected fit method's equation.	
The actual coefficients available will depend on the fit method, please refer to Curve Fitting Methods for more details. For example, with Linear Regression, the coefficients **m** and **c** will be available.	
For example, the Four Parameter Logistic Regression:	
TOV{n}.a	The **a** coefficient value of 4PL
TOV{n}.b	The **b** coefficient value of 4PL
TOV{n}.c	The **c** coefficient value of 4PL
TOV{n}.d	The **d** coefficient value of 4PL
Goodness of Fit Measures	
The values of calculated goodness measures determined from the curve fit.	
TOV{n}.R2	The R^2 value

TOV	Refers to
TOV{n}.AR2	The adjusted R^2 value
TOV{n}.SE	The Standard Error value
TOV{n}.F	The F-Statistic value
TOV{n}.P	The P-value
TOV{n}.AIC	The Akaike's Information Criterion value
TOV{n}.AICc	The Akaike's Information Criterion corrected for small sizes value
TOV{n}.BIC	The Bayesian Information Criterion value
TOV{n}.DWS	The Durbin-Watson Statistic value
TOV{n}.DoF	The number of Degrees of Freedom If there are not enough **Degrees of Freedom**, then values for **P**, **F**, **SE** and **aR^2** cannot be computed.
TOV{n}.RMS	The Root Mean Square of the residuals value (reported for Auto Smoothed Spline only)
**Named Evaluations**
If there are any Named Evaluations defined for the General Curve Fit transform, they can also be referenced in the TOVs. For example:	
TOV{n}.LLD	The determined value of Lower Limit of Detection for the curve fit

Matrix Difference

Input: **Dual Endpoint** ⇒ Output: **Endpoint**

This transform calculates the difference between two input matrices sample-by-sample.

> 📝 If either of the matrix inputs are flagged, the result will be set to ~~Flagged~~.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw (1)** and **Raw (2)** matrices. In this example, we would like to find the difference between values in these matrices.

Here is some example raw data displayed to 3 decimal places:

Raw (1)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Raw (2)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.204	0.201	0.213	0.209	0.206	0.208	0.216	0.217	0.216	0.213	0.205	0.218
B	0.216	0.200	0.214	0.214	0.204	0.201	0.215	0.216	0.203	0.219	0.207	0.204
C	0.206	0.210	0.208	0.203	0.201	0.218	0.212	0.217	0.216	0.213	0.208	0.204
D	0.215	0.215	0.214	0.203	0.214	0.213	0.219	0.219	0.213	0.201	0.202	0.219
E	0.215	0.220	0.219	0.212	0.210	0.211	0.214	0.214	0.201	0.202	0.202	0.207
F	0.214	0.212	0.202	0.200	0.201	0.217	0.213	0.209	0.218	0.207	0.216	0.216
G	0.211	0.211	0.218	0.209	0.214	0.213	0.201	0.211	0.205	0.210	0.201	0.212
H	0.216	0.209	0.215	0.206	0.218	0.206	0.209	0.219	0.215	0.219	0.216	0.217

> ℹ️ If the data point values of the **Raw (2)** are greater than the values of **Raw (1)**, the resulting matrix will contain negative values.

Difference

The transform will generate an output matrix named **Difference** with the value at each position being the subtraction between values of the **Raw (1)** and **Raw (2)** matrices. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.160	0.122	1.892	1.915	1.007	1.018	0.944	0.973	-0.106	-0.097	1.258	1.263
B	0.239	0.241	1.656	1.674	0.999	1.017	0.965	0.990	-0.071	-0.089	0.579	0.564
C	0.381	0.365	0.266	0.311	1.005	1.021	0.991	0.993	-0.103	-0.097	0.405	0.422
D	0.591	0.559	0.150	0.175	0.953	0.974	0.992	1.023	-0.112	-0.095	0.287	0.271
E	0.890	0.845	0.060	0.155	1.005	1.014	1.019	1.048	-0.090	-0.088	1.377	1.342
F	1.211	1.234	0.176	0.211	0.995	0.989	1.013	0.990	-0.109	-0.099	0.576	0.559
G	1.580	1.592	0.342	0.389	0.991	1.016	1.107	1.095	-0.079	-0.083	0.451	0.447
H	0.037	0.061	0.248	0.264	0.996	1.055	-0.094	-0.103	-0.100	-0.104	0.274	0.260

Median

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the median of the replicates in each sample group (flagged replicates are not included).

> The median is the middle value of the values sorted into order. If there is an even number of values, the result is the average between the two middle values.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to find median value for each measurement sample group.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in triplets (e.g., **Unknown1** in positions from **A1** to **A3**, **Unknown2** in from **A4** to **A6**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	1	2	2	2	3	3	3	4	4	4
B	5	5	5	6	6	6	7	7	7	8	8	8
C	9	9	9	10	10	10	11	11	11	12	12	12
D	13	13	13	14	14	14	15	15	15	16	16	16
E	17	17	17	18	18	18	19	19	19	20	20	20
F	21	21	21	22	22	22	23	23	23	24	24	24
G	25	25	25	26	26	26	27	27	27	28	28	28
H	29	29	29	30	30	30	31	31	31	32	32	32

● Unknown

Median

The transform will generate an output matrix named **Median** with the value at each position being the median of replicates of each sample group. With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations. For each sample, the following details are reported:

Sample	Positions	My Raw Data	Median
● Unknown1	A1	0.364	0.364
	A2	0.323	
	A3	2.105	
● Unknown2	A4	2.124	1.226
	A5	1.213	
	A6	1.226	
● Unknown3	A7	1.159	1.159
	A8	1.190	
	A9	0.110	
● Unknown4	A10	0.116	1.463
	A11	1.463	
	A12	1.481	
● Unknown5	B1	0.455	0.455
	B2	0.441	
	B3	1.869	

- **Matrix Table**

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.364	0.364	1.226	1.226	1.226	1.159	1.159	1.159	1.463	1.463	1.463
B	0.455	0.455	0.455	1.218	1.218	1.218	1.180	1.180	1.180	0.768	0.768	0.768
C	0.575	0.575	0.575	1.206	1.206	1.206	1.203	1.203	1.203	0.613	0.613	0.613
D	0.774	0.774	0.774	1.167	1.167	1.167	1.211	1.211	1.211	0.489	0.489	0.489
E	1.065	1.065	1.065	1.215	1.215	1.215	1.233	1.233	1.233	1.549	1.549	1.549
F	1.425	1.425	1.425	1.196	1.196	1.196	1.199	1.199	1.199	0.775	0.775	0.775
G	1.791	1.791	1.791	1.205	1.205	1.205	1.306	1.306	1.306	0.652	0.652	0.652
H	0.270	0.270	0.270	1.214	1.214	1.214	0.115	0.115	0.115	0.477	0.477	0.477

Percentage Coefficient of Variation

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the %CV of the replicates in each sample group (flagged replicates are not included).

> ℹ The **%CV** is the Standard Deviation divided by the sample group mean and multiplied by 100. (If the mean or the Standard Deviation is 0, then the result is forced to 0.)

> 📝 For groups with less than 2 non-flagged replicates, the result for the group will be set to ~~Flagged~~.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to find the percentage coefficient of variation for each sample group of the input matrix.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

● Standard ○ Blank ○ Control ● Unknown

%CV

The transform will generate an output matrix named **%CV** with the value at each position being the percentage coefficient of variation in each sample group. The %CV is useful for measuring the deviation between the replicates. The %CV is calculated for each sample group as the % of the standard deviation of the replicate measurements divided by their mean. Typically, for replicates one might expect a %CV value to be < 15. A value greater than this might indicate a preparation or layout error. Acceptable limits depend on the application.

With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations. For each sample, the following details are reported:

Sample	Positions	My Raw Data	%CV
● Standard1	A1	0.364	8.440
	A2	0.323	
● Standard2	B1	0.455	2.210
	B2	0.441	
● Standard3	C1	0.587	1.460
	C2	0.575	
● Standard4	D1	0.806	2.864
	D2	0.774	
● Standard5	E1	1.105	2.607
	E2	1.065	

- **Matrix Table**

Here all calculated %CV data is displayed in a [Matrix Table](#).

	1	2	3	4	5	6	7	8	9	10	11	12
A	8.440	8.440	0.635	0.635	0.754	0.754	1.866	1.866	3.755	3.755	0.865	0.865
B	2.210	2.210	0.715	0.715	0.876	0.876	1.541	1.541	1.080	1.080	1.638	1.638
C	1.460	1.460	5.726	5.726	1.909	1.909	0.410	0.410	1.853	1.853	1.484	1.484
D	2.864	2.864	2.668	2.668	1.202	1.202	1.730	1.730	3.416	3.416	0.144	0.144
E	2.607	2.607	19.265	19.265	0.580	0.580	1.644	1.644	1.886	1.886	1.356	1.356
F	0.986	0.986	5.915	5.915	0.589	0.589	1.575	1.575	0.652	0.652	1.534	1.534
G	0.472	0.472	4.523	4.523	1.337	1.337	0.108	0.108	0.559	0.559	0.755	0.755
H	4.597	4.597	1.061	1.061	2.686	2.686	0.612	0.612	0.000	0.000	1.901	1.901

Percentage

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates a percentage value for each sample with respect to the specified 0% and 100% values.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

P0 and **P100** can be defined as sample groups, evaluated in the context of the container. For example, if a multiple container layout contains 2 containers of data, both container 1 and container 2 include 2 **Control** groups (but in different places on each container). If **P0** is defined as **Control1** and **P100** is **Control2**, then when the analysis is performed, the %s for container 1 will be calculated using **Control1** and **Control2** on container 1, whereas the %s for container 2 will calculate %s using the **Control1** and **Control2** from container 2.

P0	The value treated as "0%." This can be defined as a number or as an expression. All values less than **P0** will have negative value in resulting matrix.
P100	The value treated as "100%." This can be defined as a number or as an expression. All values greater than **P100** will have values greater than 100 in resulting matrix.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to calculate each measurement percentage value with respect to 0-3 range.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

To calculate all percentage values in this matrix, specify a **P0** of 0 and **P100** of 3.

%

The transform will generate an output matrix named **%**. The value at each position will equal its percent rank with respect to the specified 0% and 100%. With the example data provided above, the results are as follows (displayed here to 2 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	12.13	10.77	70.17	70.80	40.43	40.87	38.63	39.67	3.67	3.87	48.77	49.37
B	15.17	14.70	62.30	62.93	40.10	40.60	39.33	40.20	4.40	4.33	26.20	25.60
C	19.57	19.17	15.80	17.13	40.20	41.30	40.10	40.33	3.77	3.87	20.43	20.87
D	26.87	25.80	12.13	12.60	38.90	39.57	40.37	41.37	3.37	3.53	16.30	16.33
E	36.83	35.50	9.30	12.23	40.50	40.83	41.10	42.07	3.70	3.80	52.63	51.63
F	47.50	48.17	12.60	13.70	39.87	40.20	40.87	39.97	3.63	3.60	26.40	25.83
G	59.70	60.10	18.67	19.90	40.17	40.93	43.60	43.53	4.20	4.23	21.73	21.97
H	8.43	9.00	15.43	15.67	40.47	42.03	3.83	3.87	3.83	3.83	16.33	15.90

Replicate Outlier Removal

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform flags up to a specified number of outlier data points in each sample group. The output matrix values match the input matrix values with any outlier(s) flagged. Outliers are determined and removed as follows:

For each sample group, the transform:

1. Calculates the **%CV** of its replicates (including only the replicates not already flagged).

2. If the **%CV** is greater than the specified **%CV Threshold**, then the replicate furthest from the mean is removed.

These steps are repeated until either the new **%CV** of the replicates that are not flagged is below the threshold, or until the specified number of outliers to remove has been removed.

> ℹ This transform can be used to perform automatic outlier rejection (useful when samples are measured in replicate groups of 3 or more).

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Outliers To Remove	Specifies the maximum number of outliers to remove. The minimum and default value for this setting is 1.
%CV Threshold	Defines threshold percentage coefficient of variance. Data point with superior or inferior values will be flagged. The default value is 15%.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to remove 1 outlier from each sample group.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in columns (e.g., **Unknown1** vertically at positions from **A1** to **H1**, **Unknown2** from **B2** to **H2**, etc.). I.e.:

⬤ Unknown

To flag 1 outlier data point for each sample group, specify an **Outliers To Remove** as 1 and **%CV Threshold** as 15%.

Calculated

The transform will generate an output matrix named **Calculated** with the value at each position matching the input data and outlier data points flagged. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	~~2.105~~	~~2.124~~	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	~~1.579~~	~~1.549~~
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	~~1.791~~	~~1.803~~	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	~~0.115~~	~~0.116~~	0.115	0.115	0.490	0.477

> ℹ️ If there are only 2 remaining replicates (before the flag), both of them will be flagged and a message will be added to the calculation log.

Standard Curve Fit

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform:

1. Plots the specified concentration values (*x*) against the measurement data (*y*) for each standard

2. Fits a curve to the standard data points (optionally using weight methods)

3. Calculates concentration values from the curve

4. Determines LLOQ and ULOQ using the specified quantification limits

5. Optionally computes any additional values from the curve (such as LLD)

> ℹ️ To use **Standard Curve Fit** transform, select or create a layout with a minimum of 2 **Standard** sample groups.

> 📝 You can use **Library Curve** to save the curve created by this transform for use in other assays (perhaps in assays where standards are not measured).

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Axes

X Axis Title	The name of the x-axis on the chart.
X Axis Type	The scale type to be used for the x-axis: • **Logarithmic** • **Linear**
Y Axis Title	The name of the y-axis on the chart.

	The scale type to be used for the y-axis:
Y Axis Type	• **Logarithmic** 📝 When y-axis is logged, negative (or zero) *y* values are not included in the plot. • **Linear**

Axes (Advanced)

Use these additional settings to adapt the chart's appearance to your needs.

X Axis Major Units	The numeric interval between numbers on the x-axis. Starting from the minimum value, a major unit is displayed at every increment.
X Axis Minor Units	The numeric interval between supplementary tickmarks on the x-axis. The minor units are not displayed unless this attribute is specified.
X Axis Numerical Formatting	The formatting for the **X Axis Major Units** values. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.
X Crosses Y At	Select where the x-axis will cross the y-axis from the drop-down: • **Automatic** – Determine the location that makes the most sense for your data automatically. • **Axis Value** – Cross y-axis at specified **X Crosses Y at Value**. • **Maximum Axis Value** – Cross y-axis at the maximum *y* value of the chart. • **Minimum Axis Value** – Cross y-axis at the minimum *y* value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
X Crosses Y at Value	The numerical value at which the x-axis will cross the y-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.
Y Axis Major Units	The numeric interval between the gridlines on the y-axis. Starting from the minimum value, a major unit is displayed at every increment.
Y Axis Minor Units	The numeric interval between supplementary tickmarks on the y-axis. The minor units are not displayed unless this attribute is specified.

Y Axis Numerical Formatting	The formatting for the **Y Axis Major Units** values.
	To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.
Y Crosses X At	Select where the y-axis will cross the x-axis from the drop-down:
	• **Automatic** – Determine the location that makes the most sense for your data automatically.
	• **Axis Value** – Cross x-axis at specified **Y Crosses X at Value**.
	• **Maximum Axis Value** – Cross x-axis at the maximum *x* value of the chart.
	• **Minimum Axis Value** – Cross x-axis at the minimum *x* value. If axis type is set to **Logarithmic**, then it is the lowest positive value.
Y Crosses X at Value	The numerical value at which the y-axis will cross the x-axis. This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.

These settings can be also applied to other charts as an advanced configuration. To learn more, see Change the Units and Number Format of the Charts and Customize X and Y Axes Positions for Curve Charts topics.

Calibrators

	Defines the *x* value (the concentration) of each calibration point.
	Click the **Concentrations** setting drop-down to display the editor. Concentration values can be specified using two different modes:
Concentrations	• **Series** – Provide the concentration value of the first calibrator and define a series to compute the remaining calibrators. This is useful if your samples are in a serial dilution.
	• **Non-Serial** – Provide concentrations values for every calibrator.
	Click **Series** to switch the concentration specification mode.
	When working with multiple plate assays, it is possible to set different standard concentrations for each plate.
	With a multiplex assay, concentration values can be specified for each analyte using the Multiplex Concentration Editor.
Standard Type	Defines a sample type to treat as a standard.

Chart

	In the drop-down editor, select any sample types to plot on the curve; this is useful to show where samples fall on the curve. The computed results of each selected sample will be plotted. In this case, all successfully computed non-flagged sample groups of the selected types will be displayed on the Fit Chart and in the report. (Only non-calibrator sample types are applicable e.g., **Unknown**, **Control**, **Blank**.)
Points on Curve	

Fit

Calculate From	Defines how the output matrix results are calculated from the computed curve for each sample (i.e., is a result calculated from the curve for each replicate or for the average of the replicates?). Select either: • **Replicates** – Every position will contain the result of x, calculated from value of every replicate (y). • **Average** – Replicates from the same sample contain the result of x, calculated from averaged value of replicates (y). ⓘ Any flagged positions on the input are also flagged in the output.
Fit Expression	When using the **Custom Fit**, you can enter or paste the equation for your curve fit.
Fit Method	The curve-fitting method to construct a curve for your data based on the specified **Standard Type**. If your license is Pro, you can also use the **Best Fit** feature to plot the most appropriate fit for your data automatically or the **Custom Fit** feature to supply your own equation/model to fit the data with.
Fit Methods	When using the **Best Fit** feature, this editor specifies the **Fit Methods** and **Weight Methods** to process your data with. You can select any combination of items in corresponding check box lists. 📝 At least 1 check box must be selected in each list.

Fit Score Method	When the **Best Fit** feature is selected, to construct the curve, you can additionally specify the <u>scoring method</u> to be used in evaluating the goodness of applied fit methods: • R^2 • R^2 with Low-End Accuracy • R^2 with High-End Accuracy • R^2 with Low-End and High-End Accuracy • 1/Standard-Error • 1/P-Value • -AIC • -AICc • -BIC
Fit To Standard	Defines which points are used as the calibrators to fit the curve to: • **Replicates** – All replicate points from each **Standard** sample group are used as calibrators. • **Average** – Average of the replicates from each **Standard** sample group are used as the calibration points for the curve.
Weight Method	Specifies the weight function for the transform.
X Transform	Determines how the *x* values are interpreted in the transform: • **None** – The *x* values remain as they are. • **Log10** – Each *x* point is taken as a common logarithm of *x*. • **Log2** – Each *x* point is taken as a binary logarithm of *x*. • **LogN** – Each *x* point is taken as a natural logarithm of *x*.
Y Transform	Determines how the *y* values are interpreted in the transform: • **None** – The *y* values remain as they are. • **Log10** – Each *y* point is taken as a common logarithm of *y*. • **Log2** – Each *y* point is taken as a binary logarithm of *y*. • **LogN** – Each *y* point is taken as a natural logarithm of *y*.

Quantification Limits

Accuracy (±%)	Defines a [percentage limit of accuracy](#) for **Standard Type** sample groups. This is used to verify whether the accuracy of the calibrators' fits in required limits. The default value is 20%.
Precision (%CV)	Defines a [%CV precision limit](#). This is used to verify whether %CV for each **Standard Type** sample group is lower than required limit. The default value is 20%.

The Quantification limits properties are used to determine the Lower Limit of Quantification (LLOQ) and Upper Limit of Quantification (ULOQ) from the fit. The LLOQ and ULOQ are computed and added to the report automatically.

The method used to calculate LLOQ and ULOQ can be overridden by setting [named evaluations](#) with corresponding **Name** settings. In this case, the custom calculated values will replace the default values.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to construct a curve fit and calculate concentrations for input matrix.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.192	0.199	0.347	0.346	0.325	0.321	0.803	0.797	1.589	1.593	0.241	0.246
B	0.293	0.300	0.586	0.584	0.800	0.793	0.402	0.401	0.839	0.837	0.562	0.564
C	0.537	0.534	0.549	0.547	0.878	0.875	0.471	0.471	0.759	0.756	1.039	1.043
D	0.858	0.855	0.320	0.325	0.531	0.530	1.552	1.551	0.429	0.427	0.424	0.424
E	1.523	1.527	0.486	0.490	1.289	1.283	1.430	1.438	1.494	1.501	1.427	1.429
F	1.622	1.621	0.621	0.626	0.667	0.663	1.350	1.347	0.631	0.634	1.695	1.694
G	0.001	0.001	0.356	0.352	0.418	0.412	1.172	1.174	1.572	1.570	0.595	0.590
H	0.297	0.297	0.796	0.801	1.517	1.515	0.960	0.965	0.534	0.527	0.585	0.584

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

● Standard ○ Blank ○ Control ● Unknown

To configure a **Standard Curve Fit** for this matrix, provide following settings:

1. Set **X Axis Title** to Concentration.

2. Set **X Axis Type** to Logarithmic.

3. Set **Y Axis Title** to Raw.

4. Set **Y Axis Type** to Linear.

5. Set **Concentrations** in **Standard1** to 0.125 and a **Series** to multiply by 2.

6. Set **Standard Type** to **Standard**.

7. Select **Show Points on Curve** to **None**.

8. Set the **Calculate From** to **Average**.

9. Select a **Fit Method** of **4PL**.

10. Set **Fit To Standard** to **Average**.

11. Select a **Weight Method** of **None**.

12. Set the **X Transform** to **None**.

13. Set the **Y Transform** to **None**.

14. Set **Accuracy (±%)** to 20%.

15. Set **Precision (%CV)** to 20%.

Concentration

The transform will generate an output matrix named **Concentration** with concentrations (*x*) calculation results for all samples using the curve fit. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	~~Flagged~~	~~Flagged~~	0.352	0.352	0.318	0.318	0.844	0.844	2.890	2.890	0.153	0.153
B	0.274	0.274	0.623	0.623	0.841	0.841	0.423	0.423	0.886	0.886	0.600	0.600
C	0.572	0.572	0.585	0.585	0.928	0.928	0.503	0.503	0.799	0.799	1.131	1.131
D	0.906	0.906	0.317	0.317	0.566	0.566	2.561	2.561	0.454	0.454	0.450	0.450
E	2.390	2.390	0.521	0.521	1.550	1.550	1.969	1.969	2.240	2.240	1.947	1.947
F	3.243	3.243	0.662	0.662	0.704	0.704	1.702	1.702	0.671	0.671	5.174	5.174
G	~~Flagged~~	~~Flagged~~	0.362	0.362	0.439	0.439	1.332	1.332	2.710	2.710	0.630	0.630
H	0.275	0.275	0.843	0.843	2.338	2.338	1.030	1.030	0.566	0.566	0.622	0.622

To learn how to configure this transform for an assay measured on more than one plate, see Multiple Plate Standard Curve Fit Analysis.

Example Additional XML Evaluation and Flagging Configuration

In addition to plotting a curve fit and calculating concentrations, additional values can be obtained with Advanced Curve Fit Evaluations. Moreover, with Custom Flag Labels by Fit Transform Calculations, you can exclude from analysis and mark with a custom label samples that are, for example, outside the range of the standard calibrator.

In this example (using the data provided above):

- Lower Limit of Detection (LLD) is computed from the curve by calculating the concentration at the average of the blank measurements + 3 * standard deviation of the blank positions.

- The **Name** attribute for LLD is specified and is used as a variable to flag condition $x < LLD$.

XML Configuration

The set attributes are highlighted in yellow.

<Settings>

```xml
        <StandardCurveFit StandardType="2" FitMethod="4PL" Concentrations="0.25,0.5,1,2,4,8"
XAxisTitle="Concentration" YAxisTitle="OD" FitToStandard="Average"
CalculateFrom="Average">
                <Evaluations>
                    <Evaluation Type="CalcY" Expression="Blank+(3*sd(Blank))"
        Description="My LLD"Name="LLD" />
                </Evaluations>
                <Flags>
                    <Flag Type="Input"Condition="x &lt; LLD"Label="Below LLD"
            />
                </Flags>
        </StandardCurveFit>
    </Settings>
```

Upon calculating data with the aforementioned XML configuration defined, the LLD evaluation is computed and added to the report below an interactive chart. It is displayed in the table below LLOQ and ULOQ, which are calculated from the curve automatically.

LLOQ	0.25
ULOQ	2
My LLD	0.222063

With the example data provided above, the results are computed as follows:

	1	2	3	4	5	6	7	8	9	10	11	12
A	Below LLD	Below LLD	0.352	0.352	0.318	0.318	0.844	0.844	2.890	2.890	0.153	0.153
B	0.274	0.274	0.623	0.623	0.841	0.841	0.423	0.423	0.886	0.886	0.600	0.600
C	0.572	0.572	0.585	0.585	0.928	0.928	0.503	0.503	0.799	0.799	1.131	1.131
D	0.906	0.906	0.317	0.317	0.566	0.566	2.561	2.561	0.454	0.454	0.450	0.450
E	2.390	2.390	0.521	0.521	1.550	1.550	1.969	1.969	2.240	2.240	1.947	1.947
F	3.243	3.243	0.662	0.662	0.704	0.704	1.702	1.702	0.671	0.671	5.174	5.174
G	Below LLD	Below LLD	0.362	0.362	0.439	0.439	1.332	1.332	2.710	2.710	0.630	0.630
H	0.275	0.275	0.843	0.843	2.338	2.338	1.030	1.030	0.566	0.566	0.622	0.622

Standard Curve Fit TOVs:

This transform produces the following TOVs.

Here the **{n}** specifies the position of Standard Curve Fit in the sequence of transforms configured via **Transform** tab.

TOV	Refers to
Coefficients of the Fit Method	
The calculated values of the coefficients used in the selected fit method's equation.	
📝 The actual coefficients available will depend on the fit method, please refer to Curve Fitting Methods for more details. For example, with Linear Regression, the coefficients **m** and **c** will be available.	
For example, the Four Parameter Logistic Regression:	
TOV{n}.a	The **a** coefficient value of 4PL
TOV{n}.b	The **b** coefficient value of 4PL
TOV{n}.c	The **c** coefficient value of 4PL
TOV{n}.d	The **d** coefficient value of 4PL
Goodness of Fit Measures	
The values of calculated goodness measures determined from the curve fit.	
TOV{n}.R2	The R^2 value
TOV{n}.AR2	The adjusted R^2 value
TOV{n}.SE	The Standard Error value
TOV{n}.F	The F-Statistic value
TOV{n}.P	The P-value
TOV{n}.AIC	The Akaike's Information Criterion value
TOV{n}.AICc	The Akaike's Information Criterion corrected for small sizes value
TOV{n}.BIC	The Bayesian Information Criterion value
TOV{n}.DWS	The Durbin-Watson Statistic value
TOV{n}.DoF	The number of Degrees of Freedom 📝 If there are not enough **Degrees of Freedom**, then values for **P**, **F**, **SE** and **aR^2** cannot be computed.
TOV{n}.RMS	The Root Mean Square of the residuals value (reported for Auto Smoothed Spline only)

TOV	Refers to
Quantification Limits	
The lower and upper <u>concentration values</u> determined from the curve.	
TOV{n}.ULOQ	The determined ULOQ value of the curve fit
TOV{n}.LLOQ	The determined LLOQ value of the curve fit
Sum of Squares	
The sum of squared distances from the fit to the data.	
TOV{n}.SSR	The sum of squares computed from input y replicates and y average (flagged points not included)
TOV{n}.SSC	The sum of squares computed from input y average and y' average (flagged points not included) ⓘ The y' is computed from curve at x
Named Evaluations	
If there are any <u>Named Evaluations</u> defined for the Standard Curve Fit transform, they can also be referenced in the TOVs. For example:	
TOV{n}.LLD	The determined value of Lower Limit of Detection for the curve fit

Standard Curve Fit (from Library)

> Play Video

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform uses a Library Curve to calculate concentration values.

> 📝 This transform will compute concentrations values using a standards curve that was measured and constructed in a previous assay run. In this way, concentrations can be computed from a library curve without needing to measure new standards as part of this protocol.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Library Curve File	Specifies the full file path to the Library Curve file.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to use a curve created from a previous assay run that used the Standard Curve Fit transform. This library curve has been saved with the name "My Library Curve".

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.529	1.540	1.379	1.261	0.940	1.040	0.846	0.845	1.739	1.755	0.552	0.557
B	1.130	1.136	0.719	0.728	1.123	1.074	1.641	1.648	1.274	1.232	2.429	2.322
C	1.771	1.730	2.169	2.151	0.954	0.926	0.472	0.463	1.368	1.319	1.055	1.049
D	1.140	1.151	2.351	2.304	0.287	0.279	0.228	0.235	0.435	0.425	1.999	2.006
E	1.550	1.553	0.333	0.320	1.275	1.325	0.127	0.126	1.489	1.547	0.740	0.758
F	1.600	1.617	1.976	1.973	1.006	1.050	1.013	1.073	1.404	1.388	1.136	1.109
G	0.830	0.817	1.070	1.046	0.198	0.192	1.218	1.200	1.174	1.154	1.188	1.060
H	0.192	0.184	1.952	2.030	0.510	0.502	0.975	0.982	0.734	0.711	1.656	1.658

Layout

The example uses a layout with **Unknowns** in duplicate (e.g., **Unknown1** in **A1** and **A2**, **Unknown2** at **B1** and **B2**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	9	9	17	17	25	25	33	33	41	41
B	2	2	10	10	18	18	26	26	34	34	42	42
C	3	3	11	11	19	19	27	27	35	35	43	43
D	4	4	12	12	20	20	28	28	36	36	44	44
E	5	5	13	13	21	21	29	29	37	37	45	45
F	6	6	14	14	22	22	30	30	38	38	46	46
G	7	7	15	15	23	23	31	31	39	39	47	47
H	8	8	16	16	24	24	32	32	40	40	48	48

⬤ Unknown

To reuse an existing curve, select "My Library Curve" file from Curve Library and apply it to calculate results for an assay.

Concentration

The transform will generate an output matrix named **Concentration** with concentrations (**X**) calculation results for all samples using the curve from the specified library curve file. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	2.448	2.448	1.629	1.629	1.064	1.064	0.894	0.894	~~Flagged~~	~~Flagged~~	0.591	0.591
B	1.266	1.266	0.764	0.764	1.213	1.213	3.608	3.608	1.480	1.480	~~Flagged~~	~~Flagged~~
C	~~Flagged~~	~~Flagged~~	~~Flagged~~	~~Flagged~~	1.002	1.002	0.499	0.499	1.689	1.689	1.147	1.147
D	1.286	1.286	~~Flagged~~	~~Flagged~~	0.249	0.249	0.105	0.105	0.457	0.457	~~Flagged~~	~~Flagged~~
E	2.561	2.561	0.323	0.323	1.582	1.582	~~Flagged~~	~~Flagged~~	2.349	2.349	0.790	0.790
F	3.079	3.079	~~Flagged~~	~~Flagged~~	1.114	1.114	1.134	1.134	1.839	1.839	1.250	1.250
G	0.870	0.870	1.155	1.155	~~Flagged~~	~~Flagged~~	1.395	1.395	1.317	1.317	1.252	1.252
H	~~Flagged~~	~~Flagged~~	~~Flagged~~	~~Flagged~~	0.541	0.541	1.050	1.050	0.763	0.763	3.865	3.865

> All TOVs, produced by the original Standard Curve Fit transform can be referenced from where the Standard Curve Fit (from Library) transforms is used.

Standard Deviation

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the standard deviation of the replicates in each sample group (flagged replicates are not included). The sample of population method is used.

> ℹ The standard deviation is a measure of how widely the replicate values are dispersed from the average of the group.

> 📝 For groups with less than 2 non-flagged replicates, the result for the group will be set to ~~Flagged~~.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to find the deviation between replicates in each sample group.

Here is some example raw data displayed here to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

Standard ● Blank ○ Control ○ Unknown ●

SD

The transform will generate an output matrix named **SD** with the value at each position being the product of the input data and deviation between positions of each sample group. With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations. For each sample, the following details are reported:

Sample	Positions	My Raw Data	SD
● Standard1	A1	0.364	0.029
	A2	0.323	
● Standard2	B1	0.455	0.010
	B2	0.441	
● Standard3	C1	0.587	0.008
	C2	0.575	
● Standard4	D1	0.806	0.023
	D2	0.774	
● Standard5	E1	1.105	0.028
	E2	1.065	

- **Matrix Table**

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.029	0.029	0.013	0.013	0.009	0.009	0.022	0.022	0.004	0.004	0.013	0.013
B	0.010	0.010	0.013	0.013	0.011	0.011	0.018	0.018	0.001	0.001	0.013	0.013
C	0.008	0.008	0.028	0.028	0.023	0.023	0.005	0.005	0.002	0.002	0.009	0.009
D	0.023	0.023	0.010	0.010	0.014	0.014	0.021	0.021	0.004	0.004	0.001	0.001
E	0.028	0.028	0.062	0.062	0.007	0.007	0.021	0.021	0.002	0.002	0.021	0.021
F	0.014	0.014	0.023	0.023	0.007	0.007	0.019	0.019	0.001	0.001	0.012	0.012
G	0.008	0.008	0.026	0.026	0.016	0.016	0.001	0.001	0.001	0.001	0.005	0.005
H	0.012	0.012	0.005	0.005	0.033	0.033	0.001	0.001	0.000	0.000	0.009	0.009

Standard Error of Mean

[Input: **Endpoint** ⇒ Output: **Endpoint**]

This transform calculates the standard error of the mean (SEM) of the replicates in each sample group ([flagged](#) replicates are not included). The sample of population method is used.

> ℹ️ The standard error of the mean quantifies how precisely the average of the replicates estimates the true mean of the population. Lower values of SEM indicate more precise estimates of the population mean. Typically, increasing the number of replicates will result in a smaller SEM value and a more precise estimate.

> 📝 For groups with less than 2 non-flagged replicates, the result for the group will be set to ~~Flagged~~.

For viewing common transform settings, see [General Transform Properties](#).

To learn about adding this transform to your assay run, see [Transforms Tab](#).

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to find the SEM of each sample group.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in triplets (e.g., **Unknown1** in positions from **A1** to **A3**, **Unknown2** in from **A4** to **A6**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	1	2	2	2	3	3	3	4	4	4
B	5	5	5	6	6	6	7	7	7	8	8	8
C	9	9	9	10	10	10	11	11	11	12	12	12
D	13	13	13	14	14	14	15	15	15	16	16	16
E	17	17	17	18	18	18	19	19	19	20	20	20
F	21	21	21	22	22	22	23	23	23	24	24	24
G	25	25	25	26	26	26	27	27	27	28	28	28
H	29	29	29	30	30	30	31	31	31	32	32	32

⬤ Unknown

SEM

The transform will generate an output matrix named **SEM** with the value at each position being the product of the input data and the standard deviation divided by the square root of the number of non-flagged replicates in each group. With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations. For each sample, the following details are reported:

Sample	Positions	My Raw Data	SEM
● Unknown1	A1	0.364	0.587
	A2	0.323	
	A3	2.105	
● Unknown2	A4	2.124	0.302
	A5	1.213	
	A6	1.226	
● Unknown3	A7	1.159	0.355
	A8	1.190	
	A9	0.110	
● Unknown4	A10	0.116	0.452
	A11	1.463	
	A12	1.481	
● Unknown5	B1	0.455	0.474
	B2	0.441	
	B3	1.869	

- **Matrix Table**

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.587	0.587	0.587	0.302	0.302	0.302	0.355	0.355	0.355	0.452	0.452	0.452
B	0.474	0.474	0.474	0.226	0.226	0.226	0.354	0.354	0.354	0.216	0.216	0.216
C	0.036	0.036	0.036	0.236	0.236	0.236	0.365	0.365	0.365	0.168	0.168	0.168
D	0.142	0.142	0.142	0.266	0.266	0.266	0.375	0.375	0.375	0.128	0.128	0.128
E	0.269	0.269	0.269	0.284	0.284	0.284	0.379	0.379	0.379	0.483	0.483	0.483
F	0.352	0.352	0.352	0.263	0.263	0.263	0.368	0.368	0.368	0.225	0.225	0.225
G	0.412	0.412	0.412	0.207	0.207	0.207	0.394	0.394	0.394	0.176	0.176	0.176
H	0.067	0.067	0.067	0.256	0.256	0.256	0.000	0.000	0.000	0.123	0.123	0.123

Variance

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the variance of the replicates in each sample group (flagged replicates are not included). The sample of population method is used.

> ℹ The variance is the sum of the squares of the difference of each replicate and the mean divided by **n-1** (where **n** is the number of the replicates).

> 📝 For groups with less than 2 non-flagged replicates, the result for the group will be set to ~~Flagged~~.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to find the variance between measurements in each sample group.

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	1	1	9	9	17	17	25	25	33	33
B	2	2	2	2	10	10	18	18	26	26	34	34
C	3	3	3	3	11	11	19	19	27	27	35	35
D	4	4	4	4	12	12	20	20	28	28	36	36
E	5	5	5	5	13	13	21	21	29	29	37	37
F	6	6	6	6	14	14	22	22	30	30	38	38
G	1	1	7	7	15	15	23	23	31	31	39	39
H	1	1	8	8	16	16	24	24	32	32	40	40

● Standard ○ Blank ○ Control ○ Unknown

Variance

The transform will generate an output matrix named **Variance** with the values at each sample group being the product of the input data variance. With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations. For each sample, the following details are reported:

Sample	Positions	My Raw Data	Variance
● Standard1	A1	0.364	0.001
	A2	0.323	
● Standard2	B1	0.455	0.000
	B2	0.441	
● Standard3	C1	0.587	0.000
	C2	0.575	
● Standard4	D1	0.806	0.001
	D2	0.774	
● Standard5	E1	1.105	0.001
	E2	1.065	

- **Matrix Table**

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
B	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	0.000	0.000	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000
D	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
E	0.001	0.001	0.004	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
F	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
G	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000

General Transform Properties for XY Data

The transforms that operate on the XY Data are configured with:

- General settings for all transforms
- General settings for XY and XY Reduction transforms (described below)
- Specific settings (if available)

General Settings for XY and XY Reduction Transforms

Data

X Axis	This setting determines which values to use in the x-axis on the chart and for evaluations:
	
	• **Index** – The 1-based position number of the data point in the collection.
	
	• **X** – Depending on the measurements data type, this option is displayed as:
	
	    • **X (Cycle)** – For kinetic data with no time values, **X** equals the **Index**.
	
	    • **X (Time)** – For kinetic data, if time values are stored, then this is the time stamp associated with the data point.
	
	    • **X (Wavelength)** – For spectral data, if wavelength values are stored, then this is the wavelength of the data point.
	
	• **Y** – Each value is set to a *y* value of the corresponding input matrix's data point.

Y Axis	This setting determines which values to consider in the y-axis on the chart and for evaluations:
	
	• **Index** – The 1-based position number of the data point in the collection.
	
	• **X**– Depending on the measurements data type, this option is displayed as:
	
	    • **X (Cycle)** – For kinetic data with no time values, **X** equals the **Index**.
	
	    • **X (Time)** – For kinetic data, if time values are stored, then this is the time stamp associated with the data point.
	
	    • **X (Wavelength)** – For spectral data, if wavelength values are stored, then this is the wavelength of the data point.
	
	• **Y** – Each value is set to a *y* value of the corresponding input matrix's data point.

Range

The range settings enable the specification of a subset of the data points to consider; only data points within the specified range will be processed. When a range is set, data points outside the specified range are excluded from the calculation. Thus, only the data points inside the specified minimum and maximum range (non-flagged) are processed by the transform.

The range can be defined by setting the **X Minimum** and **X Maximum** properties to a value or expression:

X Minimum	A numerical value or expression that defines the minimum *x* data point to include within the subset. If this is not specified, then all data points less than **X Maximum** are included.
X Maximum	A numerical value or expression that defines the maximum *x* data point to include within the subset. If this is not specified, then all data points greater than **X Minimum** are included.

To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix. This is useful to set the range of calculations for each sample to be based on the results of previous calculation steps.

In addition, the range can be adjusted interactively by positioning range bars. The range bars are displayed as vertical dashed lines on the chart that you can either:

- Drag with mouse to correct range values

- Double-click to reset minimum or maximum value

XY Transforms

XY transforms operate on matrices of data that consist of XY data and result in a new XY data matrix.

For example, the XY Baseline Correction transform can be used to remove the inherent baseline from each sample to result in a new XY plot with the measurements shifted down the y-axis.

XY Data

Throughout MyAssays Desktop, we refer to measurements that yield a 2-dimensional data sets for each sample in general terms as "XY Data". This encompasses:

- Kinetic data with measurements made over time (with or without time values).

- Spectral data measured at different wavelengths.

- Scan data measured as a single line (with a distance from an origin).

XY Axes

With certain measurement types, there might be different data available to plot on the x- and y-axis. For example, with kinetic data measured over time, you might want to use the time values as the x-axis or the cycle number instead. The axes settings specify what data should be processed by the transform. For additional details, see General Transform Properties for XY Data subsection.

Flagged XY Data Points

Any data point that is part of an XY data set can be flagged. Flagged data points are excluded from the calculation.

For example, with the XY Baseline Correction transform, if the baseline is computed using the average of the 4 lowest measurements but the lowest measurement is flagged, then the baseline will be computed using the next 4 lowest data points.

In addition to each data point, each position can also be flagged to completely exclude the sample from any further analysis. This follows the same convention as Flagged Endpoint.

XY Range

By default, XY data transform calculations are performed on all XY data points that are not flagged. However, it is also possible to define a range of points to process. This is useful if the area of interest is only a subset of the measurements. The range minimum and maximum values can be set as an absolute value or as an expression (that can in turn refer to other computed results).

For example, the XY Expression transform could be configured to work with input XY data that has 100 data points and to use only points >=20 and <= 80. In this case, the resulting output XY matrix would contain only this subset.

Refer to the General Transform Properties for XY Data subsection for more details.

XY Transforms

Transform	Operation
Baseline Correction	This transform removes the inherent variable background, or baseline, from each input position.
Blank Correction	Subtracts the average of specified Blank group(s) from each input position.
Expression (Dual)	Evaluates an expression in terms of x and y, where variables are set to the value of each position of the first (x) and second (y) input matrices.
Expression	Evaluates the specified expression for each input position.
Fit	Fits a curve to each used XY plot.
Join	Creates new combined XY plot from two input XY matrices for each position by appending data points from the second matrix to those of the first.
Outlier Removal	Flags data points that are considered to be outliers. The values of the output matrix match the input matrix (the only difference being that outlier(s) might be flagged).
Outlier Removal (for Horizontal)	Flags the specified number of data points for each plot, in which %CV of its points is greater than specified threshold.
Replicates Average	Calculates the XY average plot for each sample group.
Replicates Function	Calculates the new plot for each sample group by using specified function on its replicates.

XY Baseline Correction

[Input: **XY** ➡ Output: **XY**]

This transform removes the inherent variable background (or baseline) from each XY position.

Flagged positions or points are not included in the calculations. The operation is only performed on data within specified range.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Method	The method for a baseline correction: • **Average Between X1 And X2** – Correct points by the average *y* of the non-flagged points between and including points **X Index 1** and **X Index 2**. • **Average Of N Lowest** – Correct points by the average *y* of the lowest non-flagged **N**. • **Proportional N1 Lowest and N2 Highest** – Proportional percentage between average of the **N1** lowest and **N2** highest non-flagged points.
	The visibility of the following settings depend on the selected **Method**. For example, if you choose the **Average Of N Lowest**, then only the **N** setting will be displayed.
X Index 1 **X Index 2**	These settings are used in the **Average Between X1 And X2** method. These are 1-based index numbers and apply to the data sets with or without time values. Only non-flagged points that are **<= X Index 1** and **>= X Index 2** are used. **X Index 1** and **X Index 2** must be **>=1** and **X Index 2** must be **>= X Index 1**. If there are no included points between **X Index 1** and **X Index 2**, then no correction will be made and the output position will be flagged.

N	This setting is used in the **Average Of N Lowest** method. It is the number of lowest non-flagged data points within a subset. If the number of included points **< N**, then the output position will be flagged. If the number of included points **= N**, then the result is that all points are corrected by the average of all points.
N1 **N2**	These settings are used in the **Proportional N1 Lowest and N2 Highest** method. **N1** is the number of the lowest points, **N2** is the number of the highest points used for correction. **N1** and **N2** must be **>= 1**. The average of each of these is computed. Then each y value is scaled between these points (e.g., if a point equals the average of the lowest, then it is set to 0; or if a point equals the average of the highest, it is set to 100). Also, note results here are clipped. In other words, all results will fall within the range 0 and 100, so values which are calculated to < 0 or > 100 will be set to 0 and 100, respectively. If the average of the lowest values is equal to the average of the highest values, then this cannot be calculated and the output position will be flagged. If there are less than **N1** or **N2** valid readings, then the output position will be flagged.

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to remove the inherent variable background from each point. Here this background is measured as the average of five lowest points for each XY plot and is then subtracted from each point of this plot. The calculations for the **A1** position are shown for illustration of the transform.

Raw

Here is an **XY** matrix with each position containing 80 XY data points. Position data plots of the matrix are displayed in Plate Scale.

The raw data is displayed here to 3 decimal places:

A1 317.780;0.235 377.710;0.230 437.630;0.231 497.530;0.232 557.440;0.229 617.360;0.232 677.280;0.234 737.180;0.242 797.080;0.360 856.980;0.567 916.900;0.705 976.840;0.766 1036.760;0.791 1096.680;0.798 1156.580;0.800 1216.480;0.797 1276.410;0.786 1336.330;0.769 1396.230;0.746 1456.150;0.721 1516.050;0.696 1575.980;0.666 1635.900;0.634 1695.850;0.599 1755.750;0.560 1815.670;0.518 1875.590;0.470 1935.510;0.416 1995.410;0.364 2055.320;0.319 2115.220;0.277 2175.120;0.261 2235.020;0.255 2294.970;0.251 2354.890;0.233 2414.790;0.231 2474.690;0.228 2534.620;0.227 2594.520;0.229 2654.420;0.226 2714.340;0.226 2774.280;0.225 2834.180;0.226 2894.100;0.225 2954.030;0.226 3013.970;0.225 3073.900;0.224 3133.800;0.227 3193.700;0.225 3253.600;0.224 3313.500;0.225 3373.420;0.225 3433.340;0.224 3493.270;0.224 3553.210;0.223 3613.130;0.223 3673.030;0.224 3732.950;0.223 3792.860;0.224 3852.760;0.223 3912.660;0.223 3972.580;0.223 4032.510;0.223 4092.460;0.222 4152.390;0.222 4212.330;0.225 4272.230;0.223 4332.130;0.223 4392.030;0.223 4451.930;0.223 4511.830;0.223 4571.730;0.222 4631.650;0.221 4691.560;0.220 4751.500;0.224 4811.420;0.222 4871.350;0.222 4931.280;0.222 4991.180;0.222 5051.080;0.222

To correct each point with the specified baseline:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Specify **Settings**: **Method** as **Average Of N Lowest**, **N** as **5**.

4. Click **Calculate**.

Corrected

The transform will generate an output XY matrix named **Corrected** where each position will contain the plot with the specified baseline subtracted from each input point.

With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows:
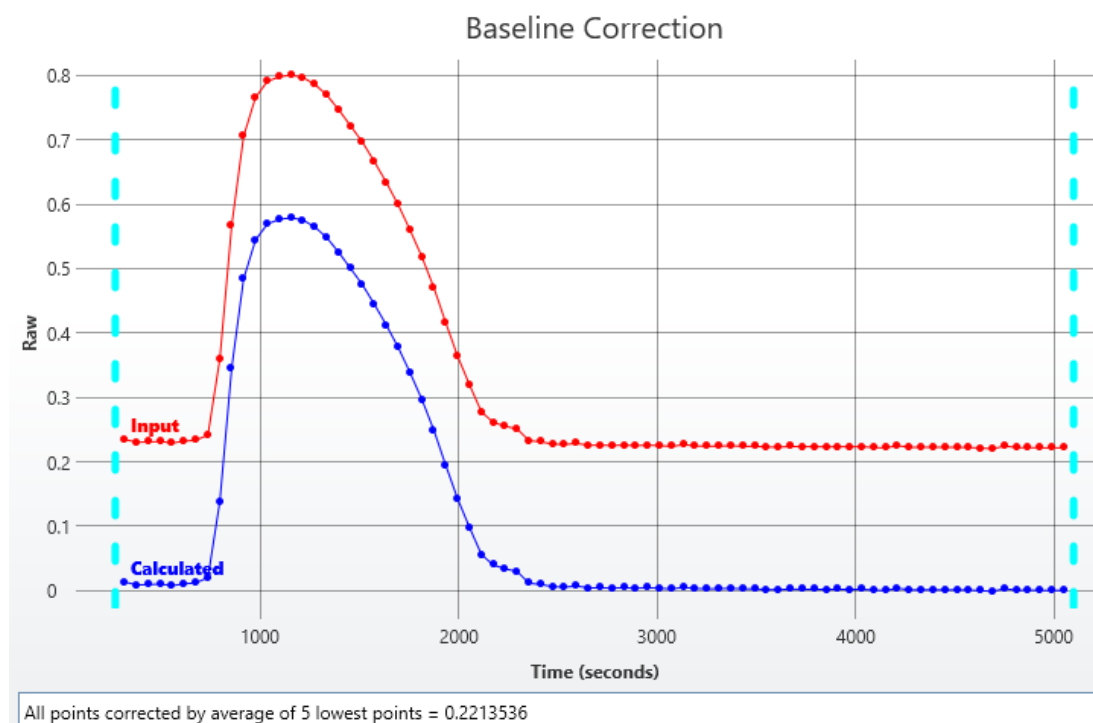
- **Sample Table**

Here is a Sample Table snippet, which shows the difference between input and output plot at the **A1** position. For each sample, the following details are reported:

Sample	Positions	Raw	Corrected
⬤ Unknown1	A1	∿	∿

XY Blank Correction

[Input: **XY** ➡ Output: **XY**]

This transform subtracts the average of a specified blank group (or groups) from each sample on a point-by-point basis. This is useful for subtracting background noise from measurements.

The background plot is first determined by creating an average XY plot of all replicates of the blank group. This background plot is then subtracted from each associated sample on a point-by-point basis.

Flagged positions or points are not included in the calculations. The operation is only performed on data within specified range.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

> 📝 This transform requires a layout with at least 1 **Blank** group.

Blank Group	The group number of the sample to use for correction. This can be defined as a number or as an expression. The expression can refer to *x* which is the group number of the sample to be corrected.
	For example, set this to *x* to perform a 1-to-1 correction where each group is corrected by the sample of the specified blank type with the same group number.
Blank Type	The sample type used as the blank.

Example: Single Blank

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to perform a blank correction using the average of one blank group. This blank group itself is measured in duplicate. The mean of these replicates will be subtracted from all other samples.

Layout

The example uses a layout with **Standards**, **Control**, **Blank**, and **Unknowns** in duplicate (e.g., **Standard1** in **A1** and **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4**, etc.):

To subtract the mean of the blank positions from the measurements, specify **Blank Group** to **1** and **Blank Type** to **Blank**.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the average of **Blank1** sample group from the input data.

Example: 1-1 Blank Correction

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to perform a 1-to-1 correction, where each sample group is corrected by the blank that it is associated with. The blank numbering used in the layout defines the associations.

Layout

The example uses a layout with 16 **Unknowns** groups (with **Unknown1** in positions from **A1** to **A5**, **Unknown2** in positions from **B1** to **B5**, etc.) and 16 **Blank** singlets:

⬤ Blank ⬤ Unknown

Specify **Blank Group** to *x* and **Blank Type** to **Blank** to perform 1-1 correction.

With this specified, the value of each blank will be subtracted from every replicate of associated sample group. In other words, **Blank1** (stored in **A6**) value will be subtracted from **A1, A2, A3, A4, A5** (the members of **Unknown1**), and from **A6** itself.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the associated blank value from the input data. Therefore, calculated matrix will contain blank corrected **Unknown** values and all **Blanks** will be 0.

Advanced Example: By-Row Blank Correction

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to configure blank correction on a row-by-row basis to blank correct each sample by the average of the two blank samples of the same row.

Layout

The example uses a layout with 80 singlet **Unknowns** and 8 **Blank** duplicates for each row (with **Blank1** in positions **A1** and **A12**, **Blank2** in positions **B1** and **B12**, etc.):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	9	17	25	33	41	49	57	65	73	1
B	2	2	10	18	26	34	42	50	58	66	74	2
C	3	3	11	19	27	35	43	51	59	67	75	3
D	4	4	12	20	28	36	44	52	60	68	76	4
E	5	5	13	21	29	37	45	53	61	69	77	5
F	6	6	14	22	30	38	46	54	62	70	78	6
G	7	7	15	23	31	39	47	55	63	71	79	7
H	8	8	16	24	32	40	48	56	64	72	80	8

◯ Blank ◯ Unknown

The **Blank Group** setting uses the expression:

1+floor((x-1)/(LayoutWidth()-2),1)

This converts the group number of the sample to blank correct **(x)** to the blank number on its row. In other words, for **x=1** this means **1+floor((1-1)/10),1)**, **floor=0** and the **Blank Group** is taken as 1. For the first row, x is in range from 1 to 10 and the expression outputs 1, thus for **Unknowns** from 1 to 10 the average of **Blank1** is subtracted.

For the second, x is from 11 to 20, **floor=1**, so the **Blank2** group is subtracted from **Unknowns11-20**, etc.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the average of the associated **Blank** group from the input data.

XY Expression (Dual)

[Input: **Dual XY** ➡ Output: **XY**]

This transform evaluates an expression defined in terms of *x* and *y* for each non-flagged input XY data point within the specified range. In this case *x* refers to the data for the sample on the first input matrix and *y* refers to the data for the same sample on the second input matrix.

> ℹ️ This transform is useful when it is necessary to perform a common operation on two sets of XY data. For example, this transform could be used to create a plot for each sample, that is the difference or ratio of two sets of XY measurements.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Expression	The expression to evaluate, where variables are set to the value of each position of the first (*x*) and second (*y*) input matrices. Default expression value is ***x-y***. 📝 To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix.
Plot Input on Chart	When the check box is selected, the chart includes both the input and the calculated plot. If it is cleared, the chart shows the calculated plot only.

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** and **Corrected** matrices. In this example, we would like to calculate a new plot by summarizing input plot values in these matrices point-by-point. The calculations for the **A1** position are shown for illustration of the transform.

Here are **XY** matrices with each position containing 80 XY data points. Position data plots of the matrices are displayed in Plate Scale.
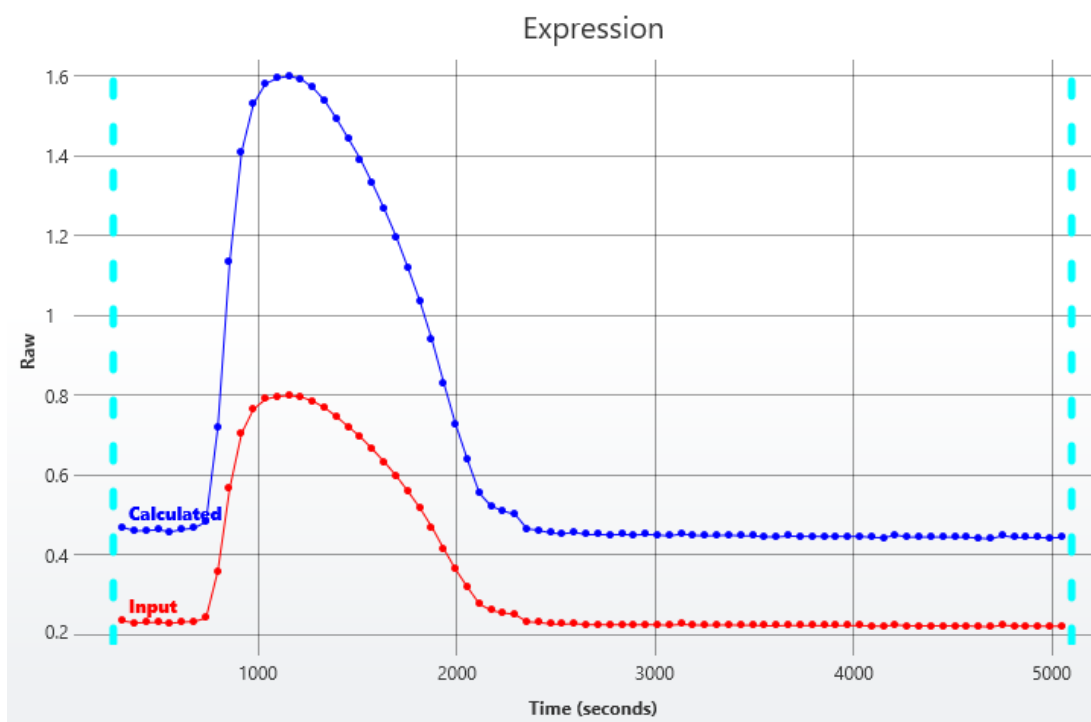
Raw
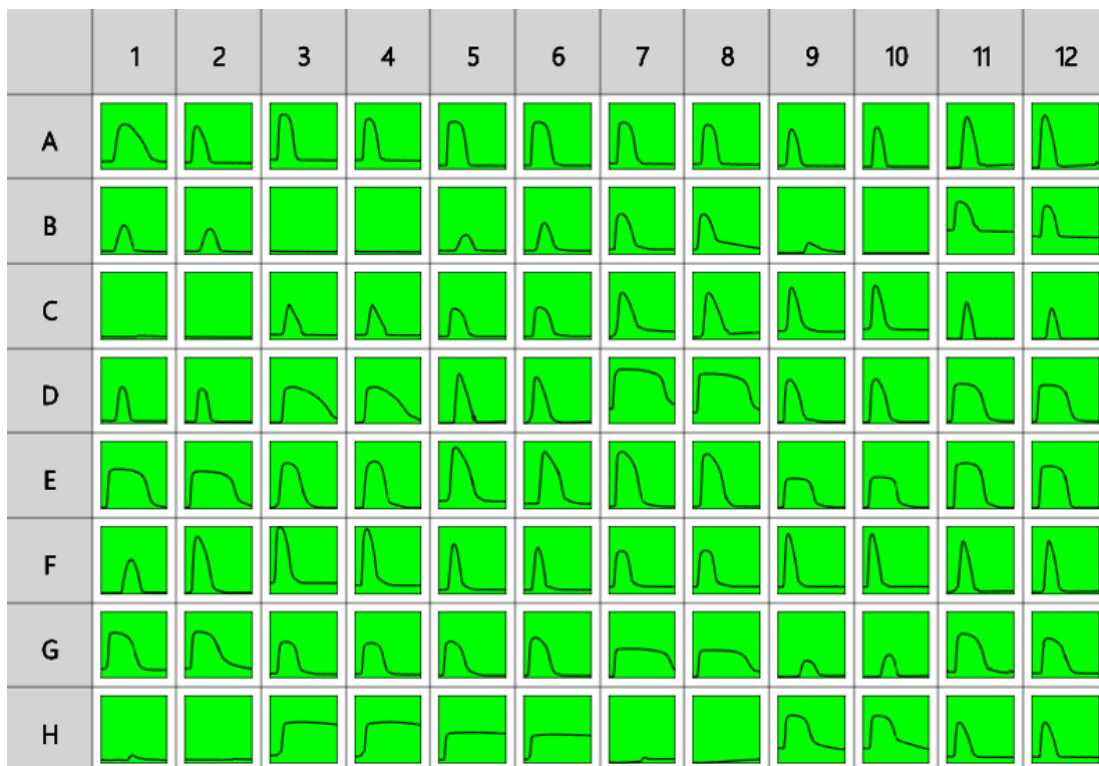
Corrected
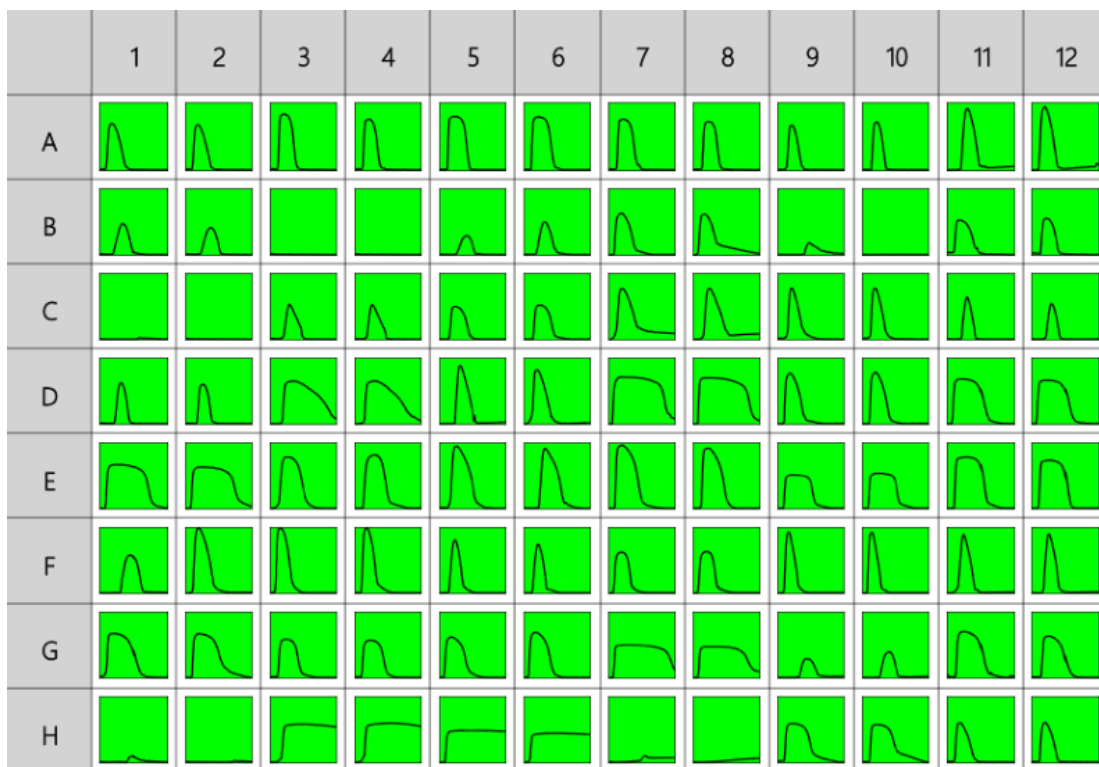
To add plot values of the input matrices and calculate a new plot for each position:

1. Specify output matrix name as **Raw+Corrected**.

2. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

3. Leave **X Minimum** and **X Maximum** blank.

4. Specify **Settings**: **Expression** as *x+y*, select the **Plot Inputs on Chart** check box.

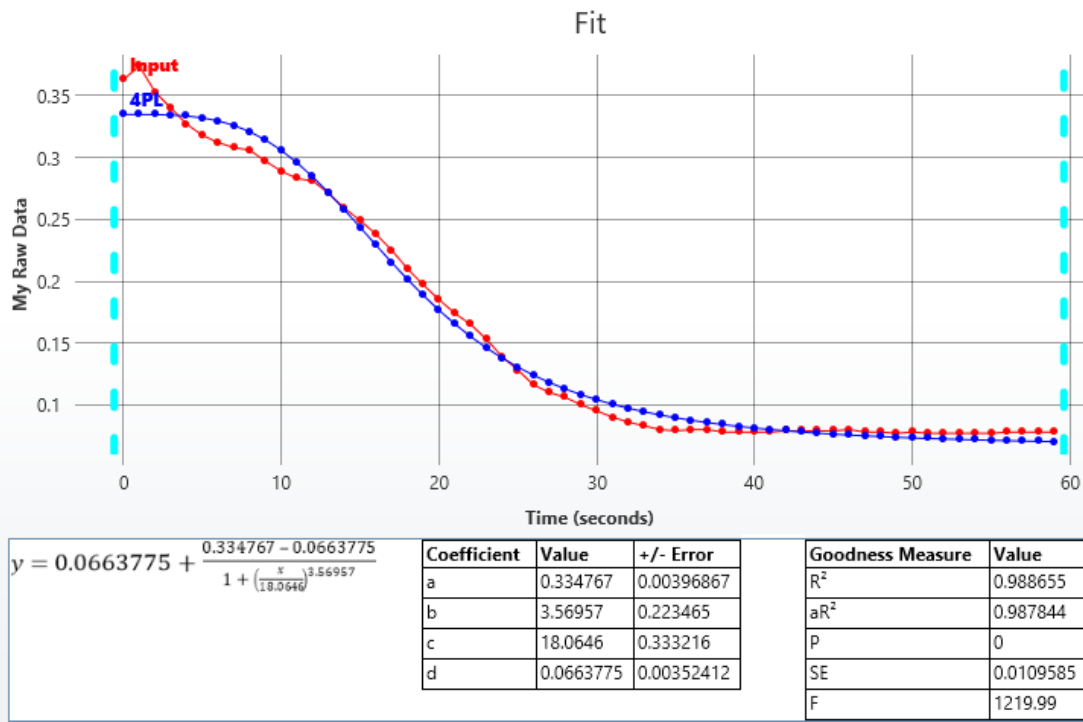5. Click **Calculate**.

Raw+Corrected

The transform will generate an output XY matrix named **Raw+Corrected** where each position will contain the plot with each data point being point by point sum of the **Raw** and **Corrected** matrices plots.

With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows:
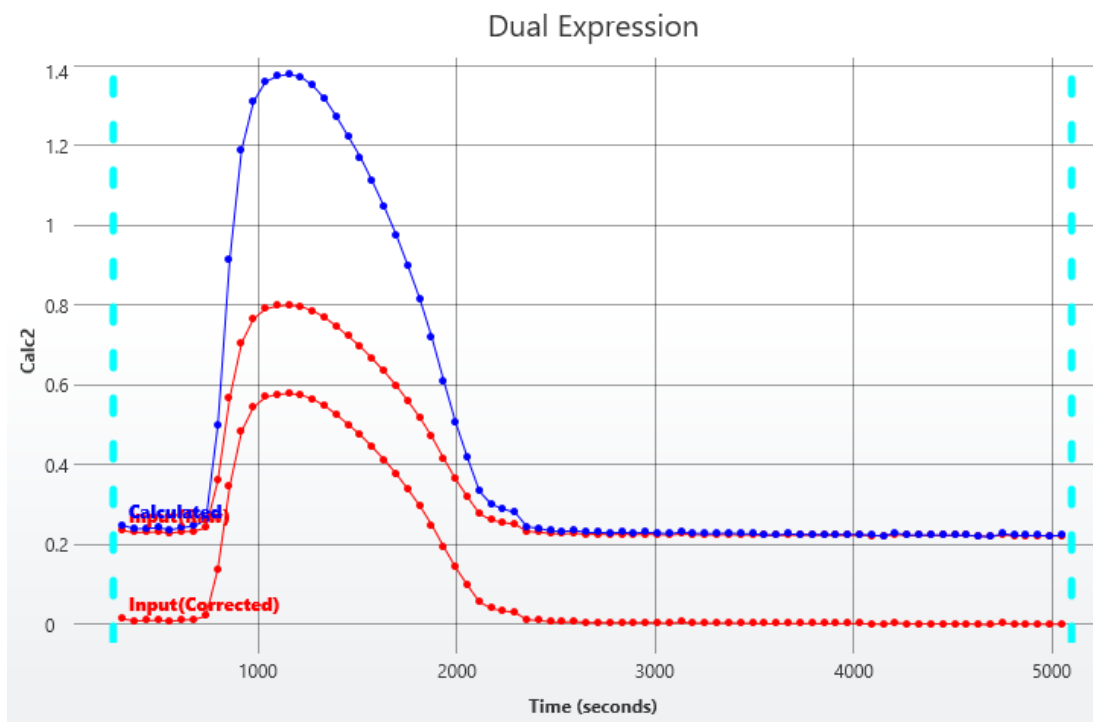
- **Sample Table**

Here is a Sample Table snippet, which shows the input plots and calculated resulting plot at the **A1** position. For each sample, the following details are reported:

Sample	Positions	Raw	Corrected	Raw+Corrected
⬤ Unknown1	A1	⌐⌐	⌐⌐	⌐⌐

XY Expression

[Input: **XY** ➡ Output: **XY**]

This transform evaluates a specified expression for each input XY data point (only points within the specified range that are not flagged are processed). The resulting XY plot is generated from this expression.

> ℹ️ This transform is useful when it is necessary to perform an operation on all input points to calculate a new plot for each sample. For example, this transform could be used to subtract, correct, or multiply all plots by a specified value.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Expression	The expression to evaluate, where the *y* variable is set to the value of each position of the input matrix. 📝 To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix.
Plot Input on Chart	When the check box is selected, the chart includes both the input and the calculated plot. If it is cleared, the chart shows the calculated plot only.

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to double data points in each input plot. The calculations for the **A1** position are shown for illustration of the transform.

Raw

Here is an **XY** matrix with each position containing 80 XY data points. Position data plots of the matrix are displayed in Plate Scale.
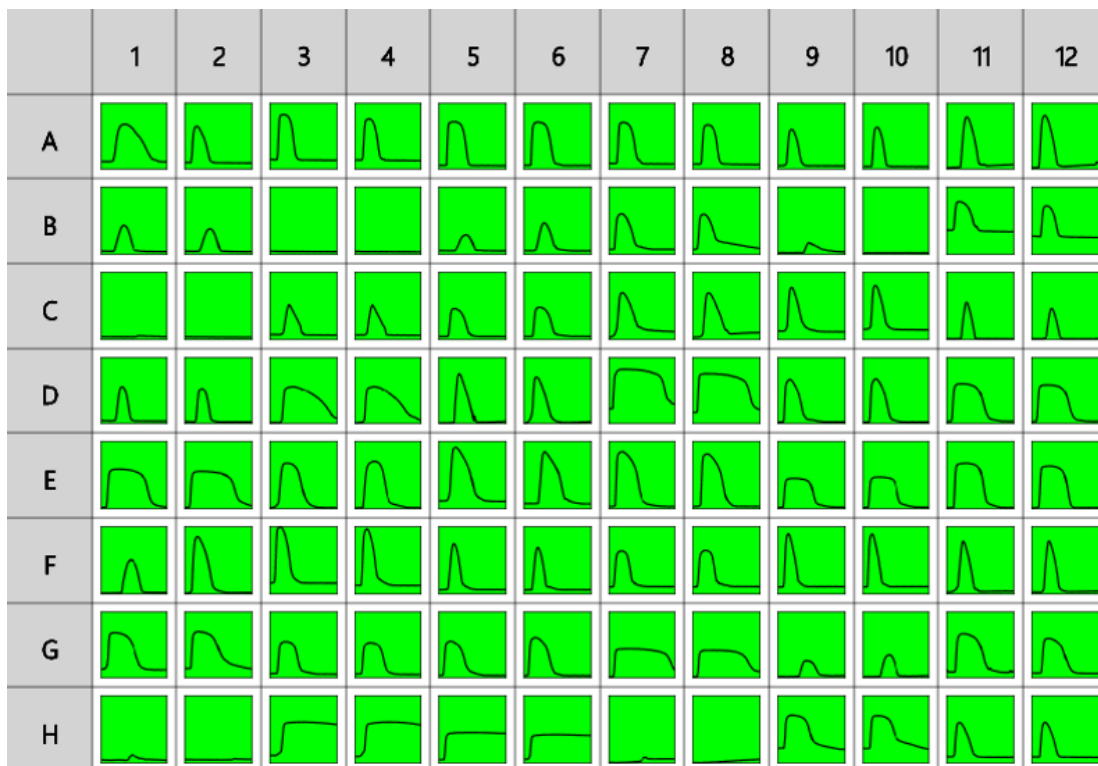
To double each data point in each plot:

1. Specify output matrix name as **Raw *2**.

2. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

3. Leave **X Minimum** and **X Maximum** blank.

4. Specify **Settings**: **Expression** as *y*2*, select the **Plot Input on Chart** check box.

5. Click **Calculate**.

Raw *2

The transform will generate an output XY matrix named **Raw*2** where each position will contain the plot with each input point multiplied by 2.

With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows:

Expression

- **Sample Table**

Here is a Sample Table snippet, which shows the input plot and calculated resulting plot at the **A1** position. For each sample, the following details are reported:

Sample	Positions	Raw	Raw *2
⬤Unknown1	A1		

XY Fit

[Input: **XY** ➡ Output: **XY**]

This transform fits a curve to each XY plot and generates a new XY plot from the calculated curve.

The resulting plot is computed by calculating the *y* value of each *x* point using the fitted curve. (Only points within the specified range that are not flagged are processed.)

> ⓘ This transform can be used to smooth each XY plot using a particular curve fitting model. If you are interested in a fitting parameter of the curve fit (such as the slope of linear regression or midpoint of 4PL), then use the XY Reduction Fit Parameter transform.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Fit Method	The curve-fitting method to construct the curve (from each XY plot).

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to fit a 4PL curve for each input plot. The calculations for the **A1** position are shown for illustration of the transform.

Raw

Here is an **XY** matrix with each position containing 80 XY data points. Position data plots of the matrix are displayed in Plate Scale.
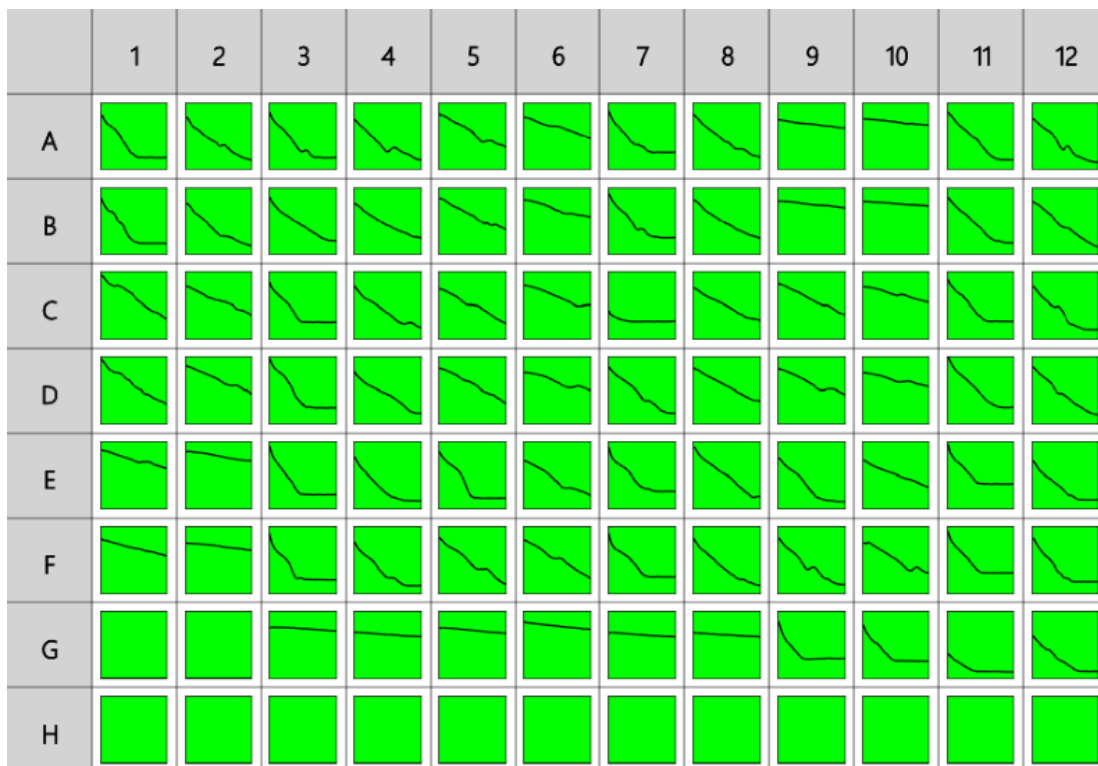
To fit a 4PL curve to each input data plot:

1. Specify output matrix name as **Smoothed**.

2. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

3. Leave **X Minimum** and **X Maximum** blank.

4. Specify **Settings**: **Fit Method** as 4PL.

5. Click **Calculate**.

Smoothed

The transform will generate an output XY matrix named **Smoothed** where each position will contain the 4PL curve fitted to each input plot.

With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows:

Fit

	Coefficient	Value	+/- Error		Goodness Measure	Value
$y = 0.0663775 + \dfrac{0.334767 - 0.0663775}{1 + \left(\frac{x}{18.0646}\right)^{3.56957}}$	a	0.334767	0.00396867		R²	0.988655
	b	3.56957	0.223465		aR²	0.987844
	c	18.0646	0.333216		P	0
	d	0.0663775	0.00352412		SE	0.0109585
					F	1219.99

- **Sample Table**

Here is a Sample Table snippet, which shows the input plot and calculated resulting plot at the **A1** position. For each sample, the following details are reported:

Sample	Positions	My Raw Data	Smoothed
⬤ Unknown1	A1		

XY Join

[Input: **Dual XY** ➡ Output: **XY**]

This transform accepts two XY input matrices and creates new combined XY plot for each position by appending data points from the second matrix to those of the first (Any flagged data points are not included in the output matrix).

> ℹ This transform can be used to combine two separate sets of XY measurements to a single plot (for each sample) for further analysis or reporting.

> 📝 When using this transform, consider the **X Axis** setting of the **Data** group. The joined data will use the data from both input matrices. To make sure that the resulting joined contents has sequential *x* values, set the **X Axis** setting to **Index**.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

> 📝 **Advanced** and **Range** settings do not apply to this transform.

Data

> ℹ If **X** is set as **Index**, then the first index of the joined matrix is 1 plus the last used index.
> If **X** is set as **X**, then the *x* values specified in each input matrix are used (unchanged) in the output matrix.

Units

Output Units	The measurement units to be included in the header of the Sample Table. If the output units of the transform are the same as the input, then use "ditto" units to automatically carry these units through (i.e., apply the same units to the transform's output). This shortcut means that it is not necessary to repeat settings across transforms. Ditto units are specified with two dots, i.e.: ..

Second Matrix X Range Correction

|	
CorrectSecondMatrixX	This setting defines how the *x* values used in the second matrix are corrected if **X Axis** is not **Index**. This can be used to ensure that the *x* values of the joined data are contiguous with a regular interval. • **None** – The results are merged on a point-by-point basis (i.e., first data point from the second matrix is appended to the first point of the first matrix, etc.) • **GapIsAverageInterval** – For each plot, the average interval of the data points in the first input matrix is computed. The first *x* value of the second input matrix is set to equal the *x* value of the last data point plus the computed average interval. The subsequent data points are first normalized by subtracting the original value of the first data point. Then, the computed *x* of the first data point is added to ensure a contiguous range of *x* values ℹ️ In this case, flagged data points are considered and used in these *x* correction calculations (however, any flagged data points in the input matrices will also be flagged in the output).

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to create a new combined plot for each position. The calculations for the **A1** position are shown for illustration of the transform.

Here are **XY** matrices with each position containing 60 XY data points. Position data plots of the matrices are displayed in Plate Scale.
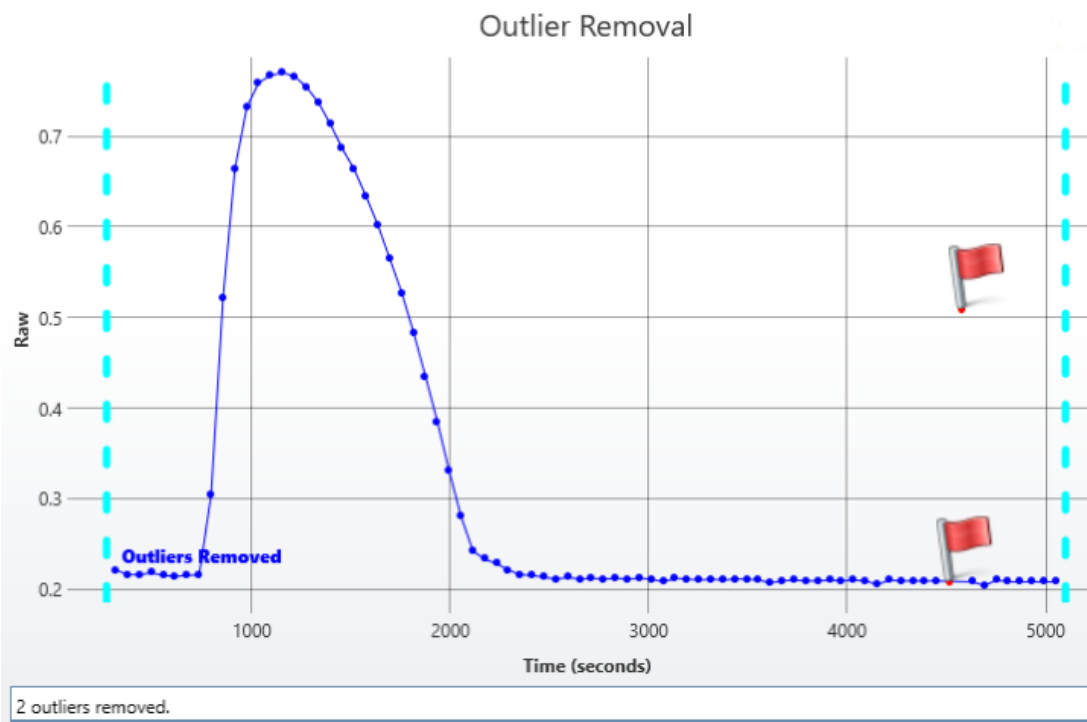
Read 1
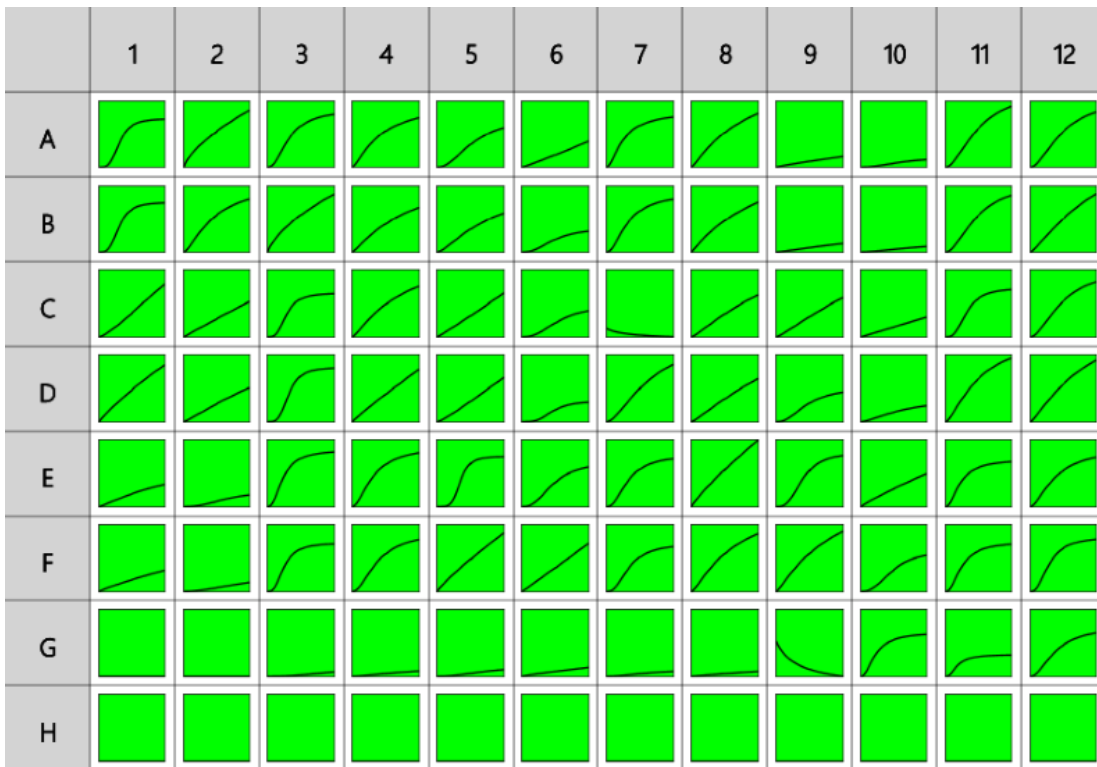
Read 2
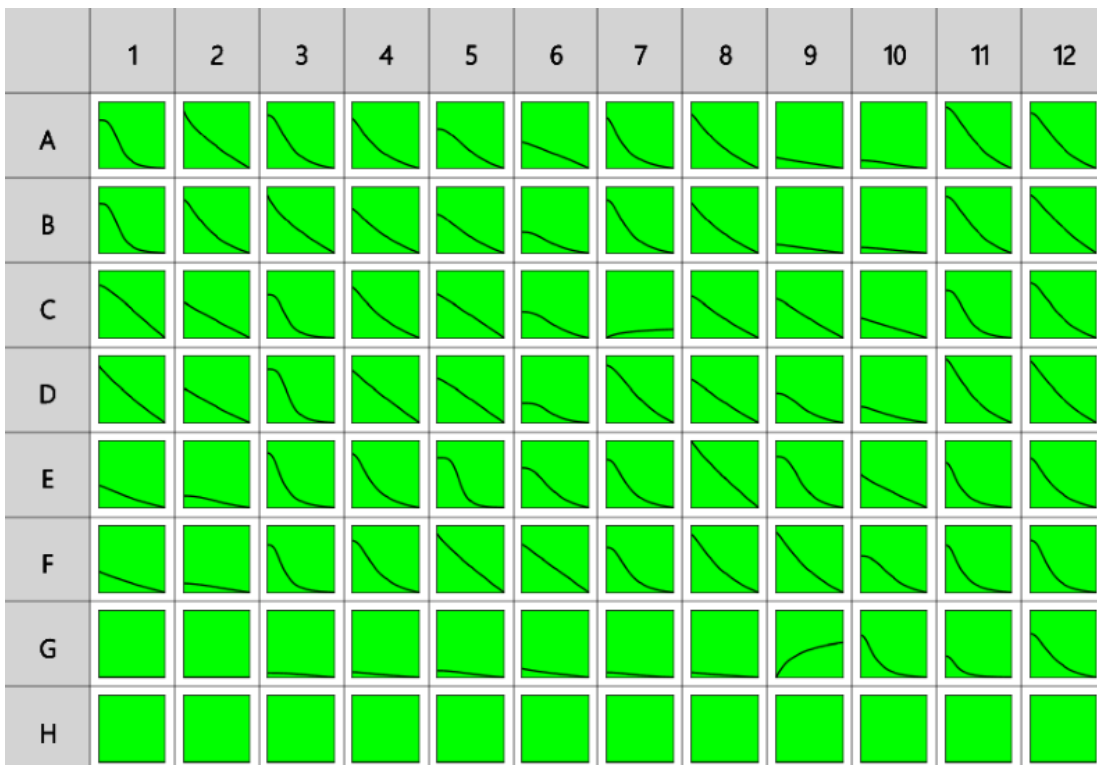
To append the data points from the second matrix to those of the first for each plot:

1. Specify output matrix name as **Joined**.

2. Specify **Data**: **X Axis** as **Index**, **Y Axis** as **Y**.

3. Click **Calculate**.

Joined

The transform will generate an output XY matrix named **Joined** where each position will contain a new XY plot which is simply the plot from the first matrix with the plot from the second matrix appended to it.

With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows:
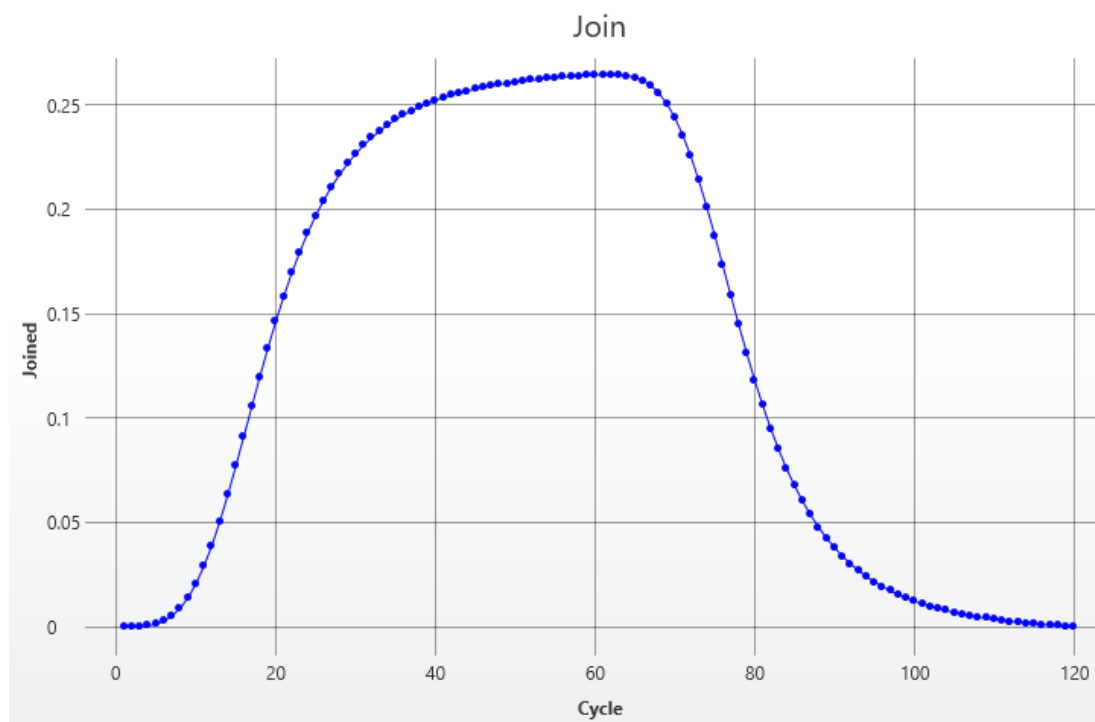
- **Sample Table**

Here is a Sample Table snippet, which shows the input plots and output appended plot at the **A1** position. For each sample, the following details are reported:

XY Outlier Removal

[Input: **XY** ➡ Output: **XY**]

This transform flags data points that are considered to be outliers. The values of the output matrix match those of the input matrix (the only difference being that any specified outlier(s) are flagged).

For each XY plot, the transform:

1. Calculates the linear regression of the specified number of adjacent points (segment)

2. Uses the calculated line to calculate y from each x in the segment

3. Compares each calculated y with the original y and flags the points where the % difference is > than the specified threshold

This process is repeated across each sequential segment in the plot for adjacent point sets.

> ℹ This transform can be used to automatically remove outlier points in XY data.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Num Regression Points	The number of regression points used for each linear regression segment when determining the maximum slope. The default and minimum value is 2.
Threshold	Defines the threshold % accuracy to flag outliers. It calculates absolute % difference between back fit value and the original y value. The back fit is computed from slope and intercept for each x value in the regression set. If this % difference is **>** the specified **Threshold**, then the data point is flagged on the output matrix. 📝 Points that are flagged in one regression set are not included in calculations of following regression sets.

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the

Raw matrix. In this example, we would like to remove up to 3 outliers from each input plot. The calculations for the **A1** position are shown for illustration of the transform.

Raw

Here is an **XY** matrix with each position containing 80 XY data points. Position data plots of the matrix are displayed in Plate Scale.
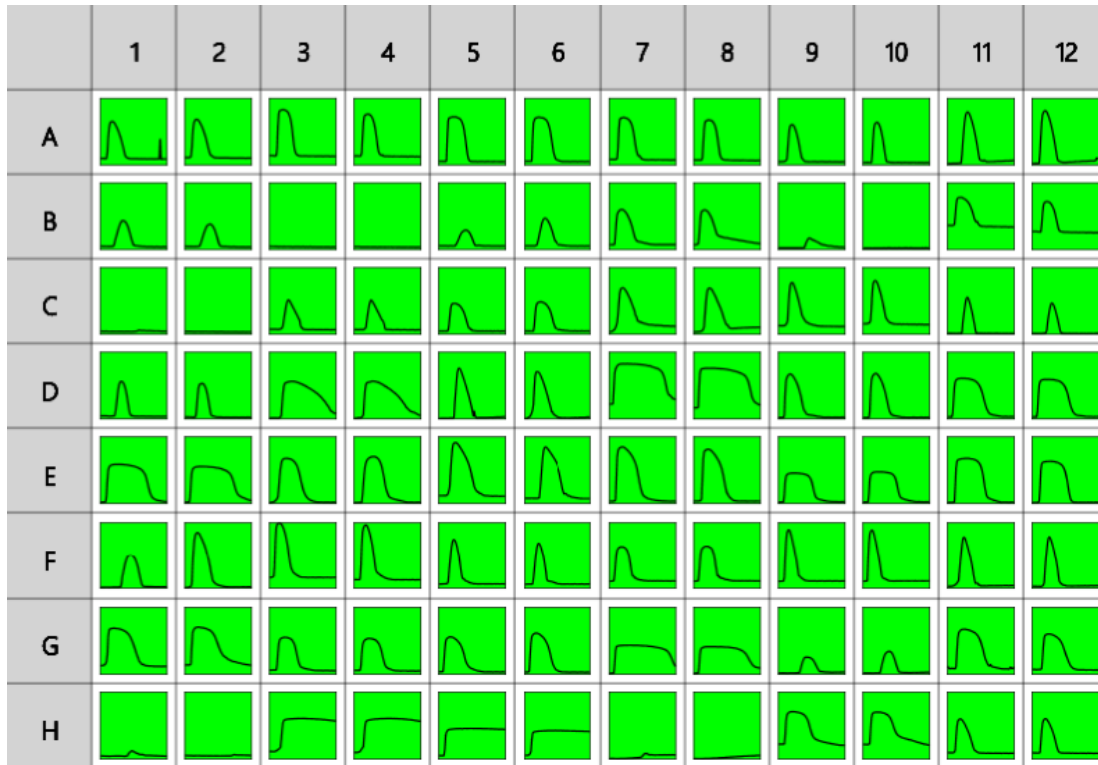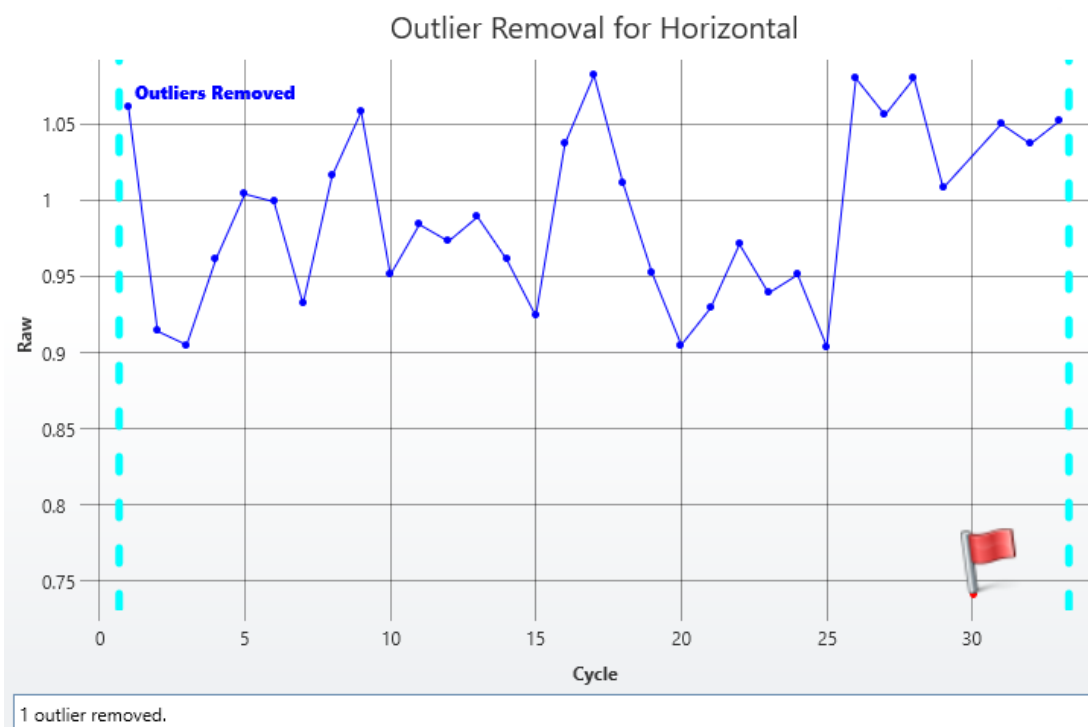

To flag outliers for each plot:

1. Specify output matrix name as **Outliers Removal**.

2. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

3. Leave **X Minimum** and **X Maximum** blank.

4. Specify **Settings**: **Number of Regression Points** as **6** and the **Threshold** as **45**.

5. Click **Calculate**.

Outliers Removal

The transform will generate an output XY matrix named **Outliers Removal** where each position will contain the plot matching the input plot and outlier data points flagged.

With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows:

Outlier Removal

2 outliers removed.

- **Sample Table**

Here is a Sample Table snippet, which shows the input plot and calculated resulting plot at the **A1** position. For each sample, the following details are reported:

Sample	Positions	Raw	Outliers Removal
⬤ Unknown1	A1		

XY Outlier Removal (for Horizontal)

[Input: **XY** ➡ Output: **XY**]

This transform flags data points that are considered to be outliers. The values of the output matrix match those of the input matrix (the only difference being that any specified outlier(s) are flagged).

For each XY plot, the transform:

1. Calculates the **%CV** of each set of its XY points (including only the points not already flagged).

2. If the **%CV** is greater than the specified **%CV Threshold**, then the point furthest from the mean is removed.

These steps are repeated until either the new **%CV** of the data points that are not flagged is below the threshold, or until the specified number of outliers to remove has been removed. Calculations are performed on the non-flagged replicates within the specified range of each XY plot.

> ℹ This transform can be used to automatically remove outlier points in XY data.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

% CV Threshold	Defines threshold percentage coefficient of variance. Data points with values resulting in a %CV greater than the specified threshold will be flagged. The default value is 15%.
Outliers To Remove	Specifies the maximum number of outliers to remove. The minimum and default value for this setting is 1.

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to remove 1 outlier from each input plot. The calculations for the **A1** position are shown for illustration of the transform.

Raw

Here is an **XY** matrix with each position containing 33 XY data points. Position data plots of the matrix are displayed in Plate Scale.
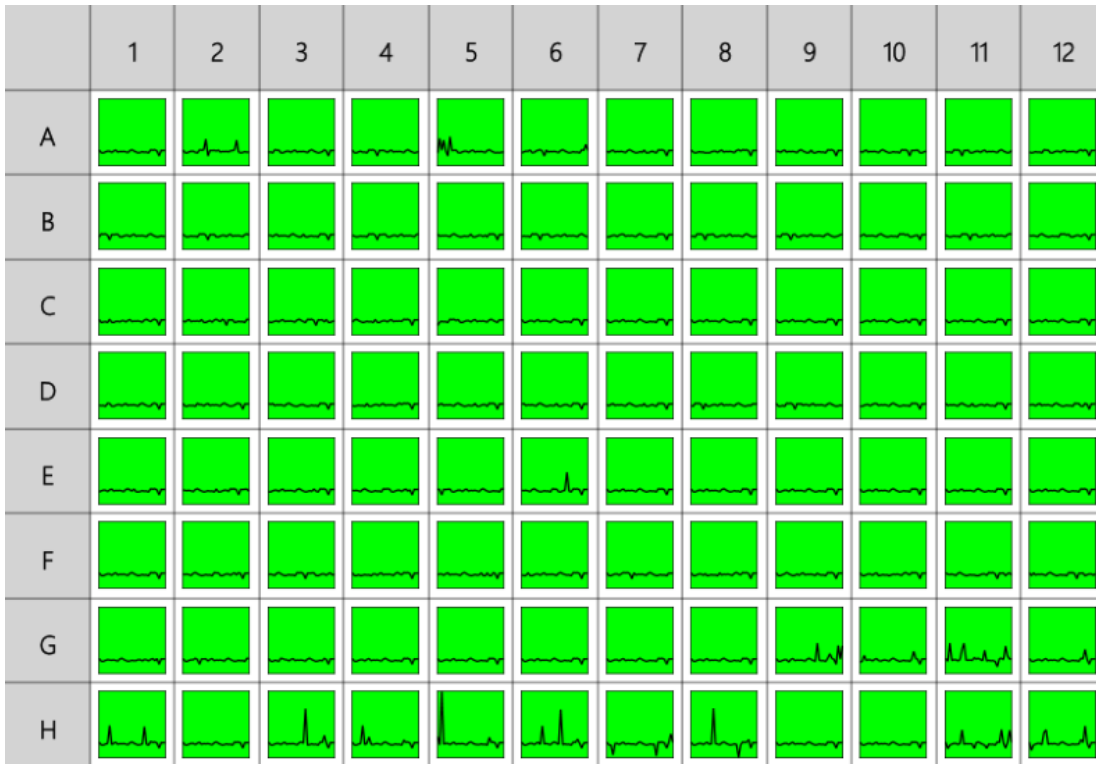
To flag 1 outlier for each plot:

1. Specify output matrix name as **Outlier Removal (Horizontal)**.

2. Specify **Data**: **X Axis** as **X (Cycle)**, **Y Axis** as **Y**.

3. Leave **X Minimum** and **X Maximum** blank.

4. Specify **Settings**: **%CV Threshold** as **5** and the **Outliers To Remove** as **1**.

5. Click **Calculate**.

Outlier Removal (Horizontal)

The transform will generate an output XY matrix named **Outliers Removal** where each position will contain the plot matching the input plot and outlier data points flagged.

With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows:

Outlier Removal for Horizontal

1 outlier removed.

- **Sample Table**

Here is a [Sample Table](#) snippet, which shows the input plot and calculated resulting plot at the **A1** position. For each sample, the following details are reported:

Sample	Positions	Raw	Outliers Removal
◯ Unknown1	A1		

XY Replicates Average

[Input: **XY** ➡ Output: **XY**]

This transform calculates the average XY (kinetic/spectral) plot for each sample group. Both the *x* and *y* values of the replicates in each group are averaged.

> If your XY data features unique *x* values for each point (such as ascending time values that are unique for each sample), you may prefer to set the x-axis type to **Index** so that the resulting plot is sequential with an increment of 1. Alternatively, if another x-axis setting is used, please note that the resulting XY plot will contain the average of the input *x* values.

Any flagged data points are not included in the analysis.

As with other XY transforms, the calculations are performed on data within the specified ranges only.

> To use this transform, select a layout with at least one sample group that contains more than one replicate.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like calculate the average plot of the replicate plots for each sample group. The calculations for the **Unknown1** group are shown for illustration of the transform.

Raw

Here is an **XY** matrix with each position containing 80 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Layout

The example uses a layout with 32 **Unknowns** groups in triplicates (with **Unknown1** in positions from **A1** to **A3**, **Unknown2** in positions from **A4** to **A6**, etc.). I.e.:


To calculate averaged data plot for each sample group:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Click **Calculate**.

Average

The transform will generate an output XY matrix named **Average** where each position will contain the averaged data plot for each sample group.

With the example data provided above, the result for the **Unknown1** averaged plot is displayed on the Kinetic/Spectral Analysis Chart as follows:
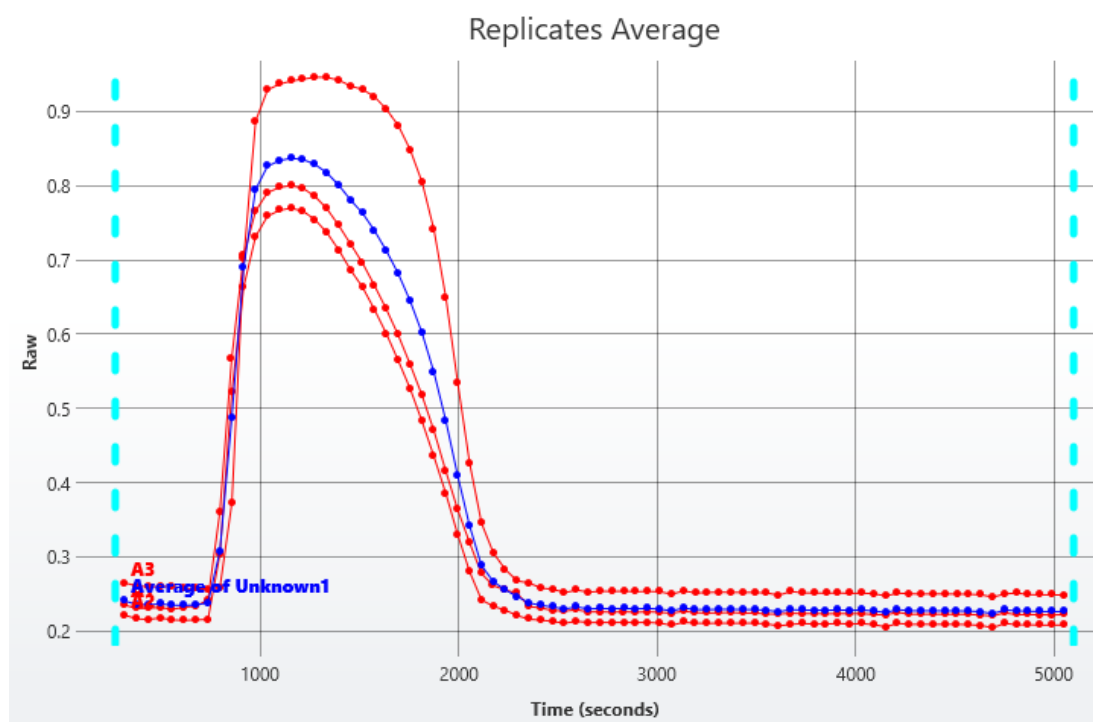
- **Sample Table**

Here is a Sample Table snippet, which shows the input plots and averaged output plot at the **Unknown1** group. For each sample, the following details are reported:

XY Replicates Function

[Input: **XY** ➡ Output: **XY**]

This transform computes a new plot for each XY (kinetic/spectral) replicate group where the *y* values of the resulting plot are computed from the selected function applied to the corresponding replicate values of the group.

> ℹ️ Selecting the **Average** function will yield the same results at the XY Replicates Average transform, i.e., an average XY plot of the replicates.

The *y* value of each point in the plot is the result of the selected function applied to each *y* value of the point for the replicate. The *x* value of each point is the average of the *x* values of the replicates.

> 📝 If your XY data features unique *x* values for each point (such as ascending time values that are unique for each sample), you may prefer to set the x-axis type to **Index** so that the resulting plot is sequential with an increment of 1. Alternatively, if another x-axis setting is used, please note that the resulting XY plot will contain the average of the input *x* values.

Any flagged data points are not included in the analysis.

As with other XY transforms, the calculations are performed on data within the specified ranges only.

> ℹ️ To use this transform, select a layout with at least one sample group that contains more than one replicate.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

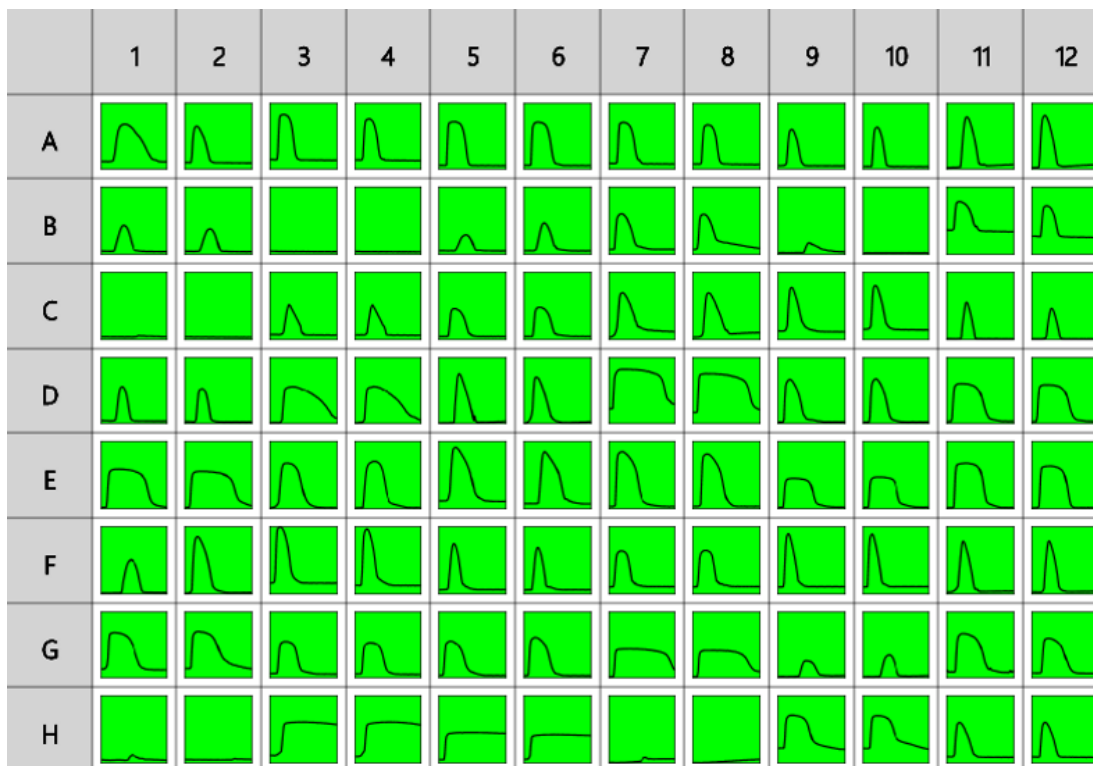|	For each sample group, the *y* values are plotted as:
Function	- **Average** – The point-to-point average of the replicates *y* values - **Median** – The point-to-point median of the replicates *y* values - **Standard Deviation** – The point-to-point standard deviation between the replicates *y* values - **%CV** – The point-to-point percentage coefficient of variation between the replicates *y* values - **Sum** – The point-to-point sum of the replicate plots - **Minimum** – For each sample, the point-to-point minimum *y* value of each point is used to create the resulting plot - **Maximum** – For each sample, the maximum *y* value of each point is used to create the resulting plot

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like calculate the standard deviation of the replicate plots for each sample group. The calculations for the **Unknown1** group are shown for illustration of the transform.

Raw

Here is an **XY** matrix with each position containing 80 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Layout

The example uses a layout with 32 **Unknowns** groups in triplicates (with **Unknown1** in positions from **A1** to **A3**, **Unknown2** in positions from **A4** to **A6**, etc.). I.e.:


To find the standard deviation between input replicate plots for each sample group:

1. Specify output matrix name as **Replicates SD**.

2. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

3. Leave **X Minimum** and **X Maximum** blank.

4. Specify **Settings**: **Function** as **Standard Deviation**.

5. Click **Calculate**.

Replicates SD

The transform will generate an output XY matrix named **Replicates SD** where each position will contain the calculated plot with deviation between input plots of each sample group.

With the example data provided above, the results for the **Unknown1** averaged plot are displayed on the Kinetic/Spectral Analysis Chart as follows:
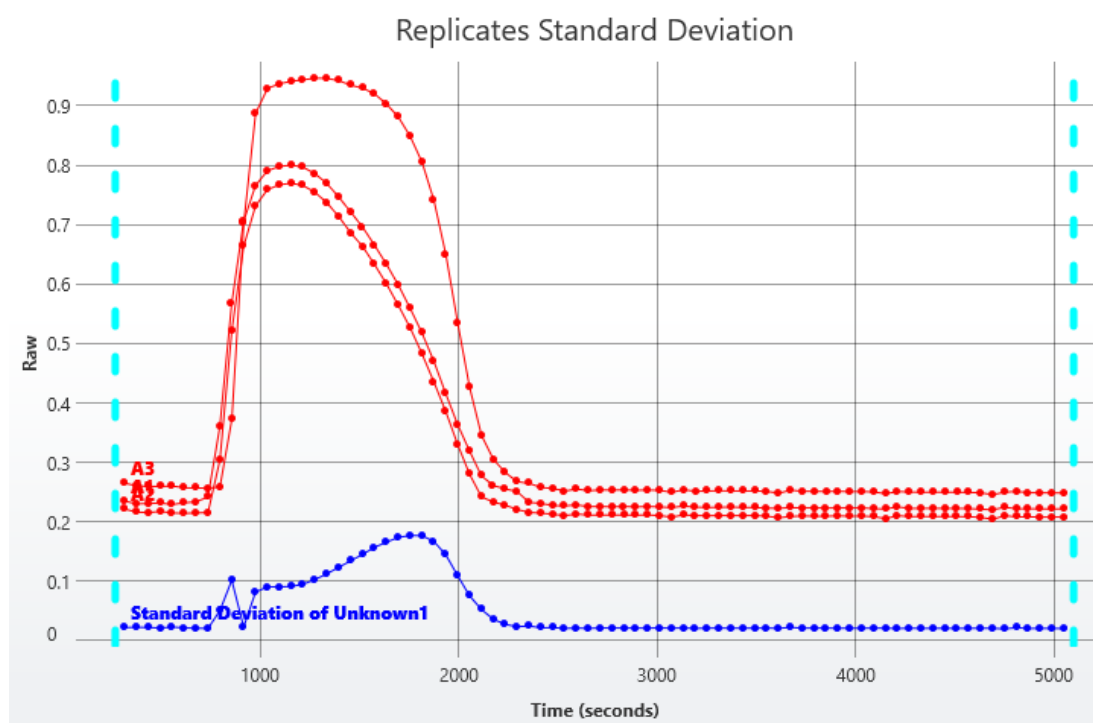
- **Sample Table**

Here is a Sample Table snippet, which shows the input plots and output plot at the **Unknown1** group. For each sample, the following details are reported:

Sample	Positions	Raw	Replicates SD
🟢 Unknown1	A1		
	A2		
	A3		

XY Reduction Transforms

XY transforms operate on matrices of data that consist of XY data and result in a new endpoint data matrix.

For example, the XY Reduction Peak Point transform will compute the peak value of each XY plot.

XY Data

Throughout MyAssays Desktop, we refer to measurements that yield a 2-dimensional data sets for each sample in general terms as "XY Data". This encompasses:

- Kinetic data with measurements made over time (with or without time values).

- Spectral data measured at different wavelengths.

- Scan data measured as a single line (with a distance from an origin).

XY Axes

With certain measurement types, there might be different data available to plot on the x- and y-axis. For example, with kinetic data measured over time, you might want to use the time values as the x-axis or the cycle number instead. The axes settings specify what data should be processed by the transform. For further details, see General Transform Properties for XY Data subsection.

Flagged XY Data Points

Any data point that is part of an XY data set can be flagged. Flagged data points are excluded from the calculation.

For example, with the XY Reduction Peak Point transform, if the peak is set to minimum and is computed using the lowest measurement but the lowest measurement is flagged, then the peak will be computed using the next lowest data point.

In addition to each data point, each position can also be flagged to completely exclude the sample from any further analysis. This follows the same convention as for Flagged Endpoint.

XY Range

By default, XY data transform calculations are performed on all XY data points that are not flagged. However, it is also possible to define a range of points to process. This is useful if the area of interest is only a subset of the measurements. The range minimum and maximum values can be set as an absolute value or as an expression (that can in turn refer to other computed results).

For example, the XY Reduction Average transform could be configured to work with input XY data that has 100 data points and to use only points >=20 and <= 80. In this case, the resulting output endpoint matrix would contain only mean value from this subset at each position.

Refer to the General Transform Properties for XY Data subsection for more details.

XY Reduction

Transform	Reduces Data To
Area Under Curve	The area under the curve computed using either the trapezia or summation method.
Average	The average of non-flagged data points within a subset at each position.
Fit Parameter	The specified parameter for non-flagged data points within specified range at each position.
Maximum Slope	Determined maximum slope between two adjacent points within specified range at each position.
Peak from Fit	Determined peak (minimum or maximum) value interpolated from the curve fitted to the of non-flagged points within specified range at each position.
Peak Point	Determined peak (minimum or maximum) data point within the specified range of the non-flagged points at each position.
Total	The sum of non-flagged data points within specified range at each position.
X at Y	The x value at which the specified y value crosses the evaluated plot of non-flagged points within the specified range at each position.
X between Y	The difference between the first two x points that equal or cross specified y value at each position.
Y at X	Determined y value for a specified x value within the specified range of the non-flagged points at each position.

XY Reduction Area Under Curve

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform computes the area under the curve of each XY plot using either the trapezia or summation method (within the specified range of points to consider). Flagged positions or points are not included in the calculations.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data in each position to the area under data points and store resulting value to corresponding position of an endpoint matrix.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

To reduce **XY** data to an average endpoint value:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Click **Calculate**.

Area Under Curve

The transform will generate an endpoint matrix named **Area** with the value at each position being the area under the curve. With the example data provided above, the resulting computed area using the sum of trapezia method for the **A1** plot is (displayed here to 3 decimal places): **2.555**

XY Reduction Average

[Input: **XY data** ⮕ Output: **Endpoint**]

This reduction transform computes the average *y* value of each XY plot (within the specified range of points to consider). Flagged positions or points are not included in the calculations.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data in each position to average of its data points and store resulting value to corresponding position of an endpoint matrix.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491
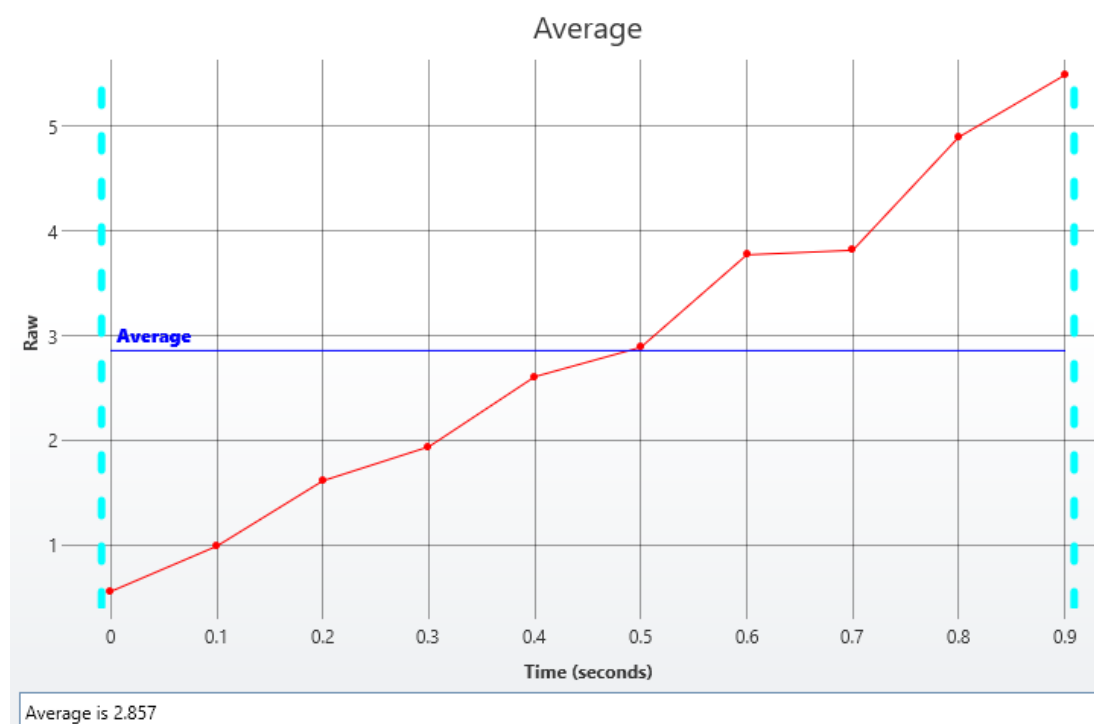
To reduce **XY** data to an average endpoint value:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Click **Calculate**.

Average

The transform will generate an endpoint matrix named **Average** with the value at each position being the averaged value of the *Y* input data points. With the example data provided above, the resulting averaged value for the **A1** plot is displayed on the [Kinetic/Spectral Analysis Chart](#) as follows (also displayed here to 3 decimal places):

2.857

Average is 2.857

XY Reduction Function

[Input: **XY data** ⇒ Output: **Endpoint**]

This reduction transform performs the selected mathematical function on all of the (not-flagged) *y* values of each XY plot (within the specified range of points to consider). Flagged positions or points are not included in the calculations.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data in each position to the average of its data points and store resulting value to corresponding position of an endpoint matrix.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

To reduce **XY** data to an average endpoint value:

1. Select **Average** as the **Function**.

2. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

3. Leave **X Minimum** and **X Maximum** blank.

4. Click **Calculate**.

Function

The transform will generate an endpoint matrix named with the value at each position being the averaged value of the *Y* input data points. With the example data provided above, the resulting averaged value for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows (also displayed here to 3 decimal places):

2.857
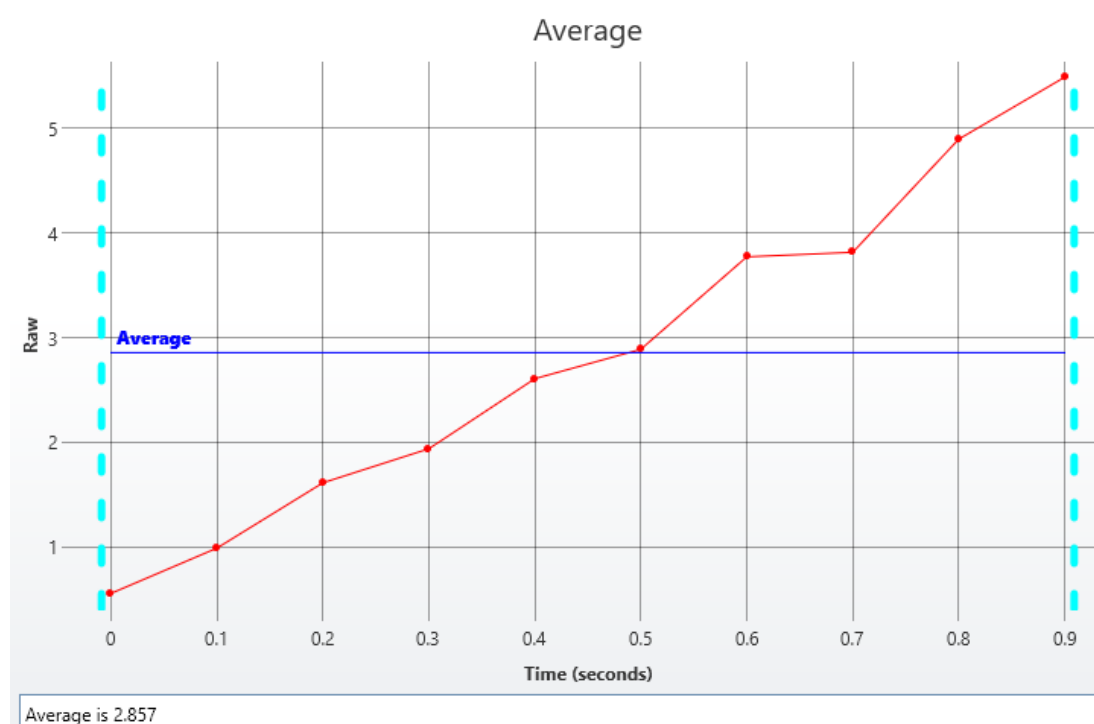
XY Reduction Fit Parameter

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform performs the selected curve fit on each XY plot and sets the result to the value of a specified fit parameter. Points outside the specified range and flagged positions/points are excluded from calculations.

> ℹ This transform can be used to obtain the specific fitting parameter of a curve fit to each plot (such as the slope of linear regression or midpoint of 4PL).

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Fit Method	The curve-fitting method to construct a curve for your data.
Parameter	Represents the Fit Transform Context Parameter to fit data points by.

Example

Let's assume that we have some kinetic measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to fit the Linear Regression and calculate the R^2 parameter for each position plot.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

To reduce the plot at each position to its R^2 parameter:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Select Linear Regression **Fit Method** and specify **Parameter** as R2 (with the syntax, provided in Fit Transform Context Parameters).

4. Click **Calculate**.

Calculated

The transform will generate an output endpoint matrix named **Calculated** with the value at each position R^2 measure for each input plot. With the example data provided above, the resulting averaged value for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows (also displayed here to 3 decimal places):

0.987

Fit Parameter
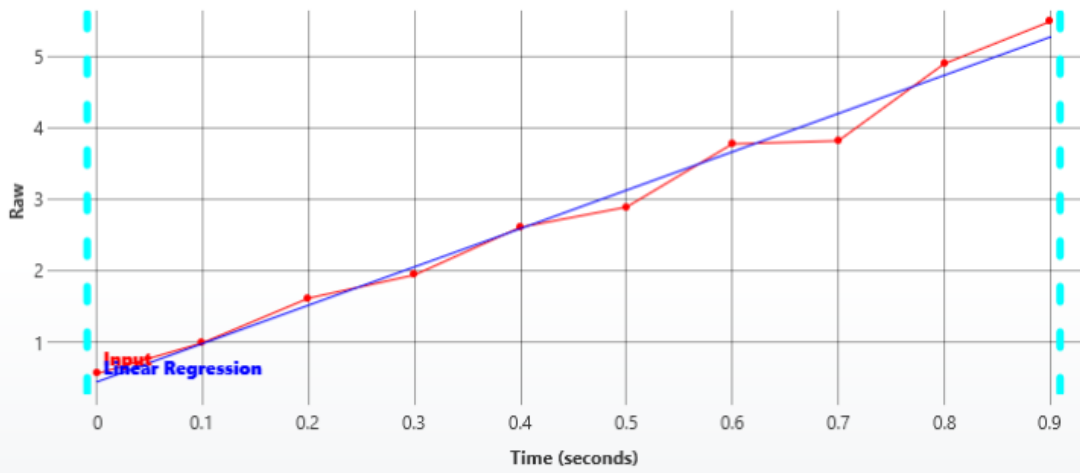
$$y = 5.36915x + 0.440824$$

Coefficient	Value	+/- Error
m	5.36915	0.221636
c	0.440824	0.118321

Goodness Measure	Value
R^2	0.986551
aR^2	0.98487
P	0.00000000899332
SE	0.201311
F	586.856

XY Reduction Maximum Slope

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform finds the maximum slope of each XY plot. The result can be set to the slope, or to the *x* or *y* value at the maximum slope (absolute or relative to the start *x*).

> ℹ️ This transform can be used in kinetic applications to calculate the time to reach a maximum rate or to find the maximum rate in a reaction.

The maximum slope is determined by computing the linear regressions of adjacent points (using the specified number of linear regressions points) and determining the slope with the maximum (upward or downward) value.

Where the result is set to be the *x* or *y* value of the maximum slope:

- The *x* value is calculated as the centre of the points with the maximum slope.

  > 📝 This may not exactly equal an *x* data point.

- The *y* value is computed from the linear regression of the calculated center *x*.

Flagged positions or points or those outside specified ranges are not included in the calculations.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Max is	Determines the type of slope to be found by this transform. The settings are: • **Auto** – The maximum slope is determined from the general direction of each plot by using the linear regression. If the slope of the plot is positive, the **Fastest Increase** is used; if negative, the **Fastest Decrease** is used. • **Fastest Increase** – The maximum slope is the slope with the highest positive value. • **Fastest decrease** – The maximum slope is the slope with the greatest negative value.
Num Regression Points	The number of regression points used for each linear regression segment when determining the maximum slope. The default and minimum value is 2.

Result is	Specifies the result of the analysis. The settings are: • **Slope** – The result is the slope of the determined maximum slope. • **X At Centre Absolute** – The result is the x at the center of the determined maximum slope. (The center is the midpoint of the data points with the maximum linear regression slope). • **Y At Centre Absolute** – The result is the y at the center of the determined maximum slope. (The center is the y value computed from the x midpoint of the data points with the maximum linear regression slope). • **X At Centre Relative** – The result is the x at the center of the determined maximum slope relative to the first non-flagged data point that is greater than **X Minimum**. (The center is the midpoint of the data points with the maximum linear regression slope). • **Y At Centre Relative** – The result is the y at the center of the determined maximum slope relative to the first non-flagged data point that is greater than **X Minimum**. (The center is the y value computed from the x midpoint of the data points with the maximum linear regression slope). • **Extrapolated Y** – A value of y is calculated from the determined maximum slope using the x value specified with **X For Extrapolation**.
X for Extrapolation	When **Extrapolated Y** option in the **Result Is** setting is chosen, then this can be used to <u>specify an expression</u> used to determine the x value to calculate y for.

Example

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data for each replicate to maximum slope between its data points and store resulting value to corresponding position of an endpoint matrix.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

To reduce **XY** plot at a position to a maximum slope to an endpoint value:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Define **Max is** as **Auto**, **Num Regression Points** as 2, and **Result is** as **Slope**.

4. Click **Calculate**.

Maximum Slope

The transform generates an endpoint matrix named **Maximum Slope** with the value at each position being the maximum slope between points at each kinetic/spectral plot. With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows (also displayed here to 3 decimal places):

10.815

Maximum Slope

Maximum slope (10.8147705928176)

Maximum slope is 10.815
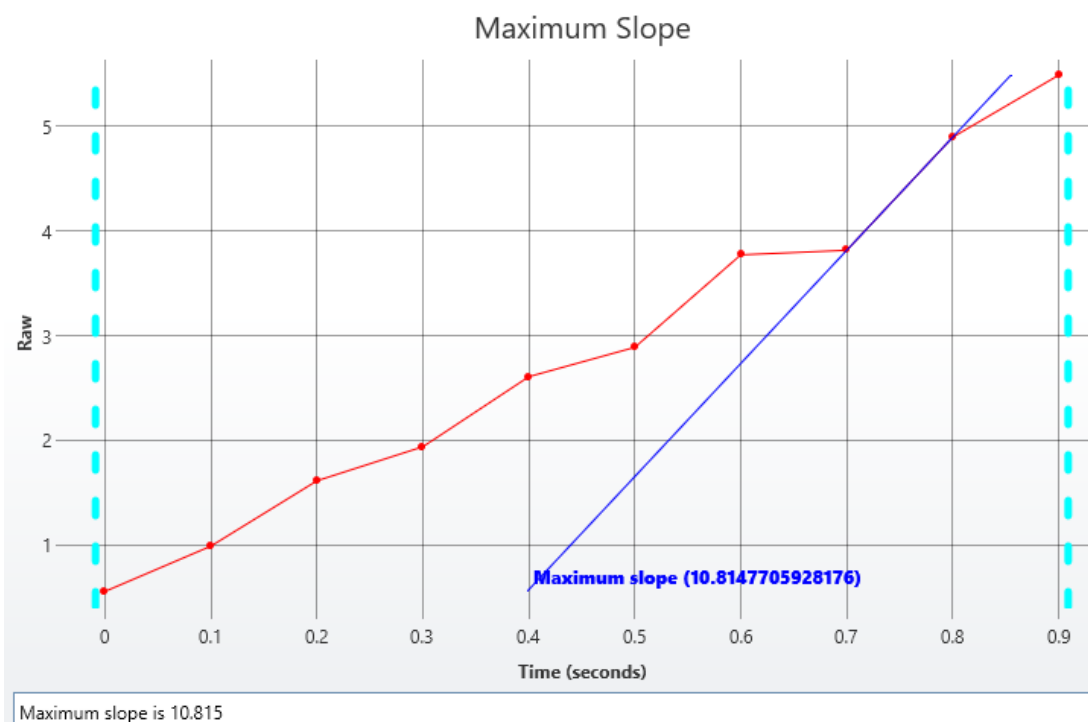
XY Reduction Peak from Fit

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform:

1. Fits a specified curve to each XY plot.
   Flagged positions or points and points outside the specified range are not included in the calculations.

2. Interpolates y for each x value at every specified increment between the lowest and highest x values of included points.

3. Determines the peak — maximum or minimum — from interpolated y values

4. Reports specified value (x or y) of the determined peak.

> ℹ This transform is useful for finding a peak that might fall between points by using interpolation. To reduce each position to the value of its highest or lowest data point, use XY Reduction Peak Point.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

<u>Settings</u>

Fit Method	Select a curve-fitting method to construct a curve for your data: • Cubic Regression • Cubic Spline Akima • Cubic Spline Natural • Cubic Spline Smoothed • Cubic Spline Smoothing • Polynomial Order 4 Regression • Polynomial Order 4 Regression • Quadratic Regression • Quintic Regression
Interpolation Increment	Specify the increment between x values to use for computing y values from the fitted curve.
Peak	Select which data point to consider as the peak: • **Max** – The point with the maximum y value • **Min** – The point with the minimum y value
Plot Fit At Increments	Select this check box to plot the interpolated value at every increment. If not selected, the interpolated value will be plotted for each input data point.
Result	Select which axis's coordinate is stored in the resulting matrix: • **X** – Projection of **Peak** value on x-axis • **Y** – Projection of **Peak** value on y-axis

Example

Let's assume that we have some spectral measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we will reduce each input plot to the x of the peak (maximum) value. We will determine the peak by fitting Polynomial Order 4 Regression, interpolating the curve at 0.1 increments in the 430-450 wavelength range.

Raw

Here is an **XY** matrix with each position containing 61 XY data points. Position data plots of the matrix are displayed in Plate Scale.
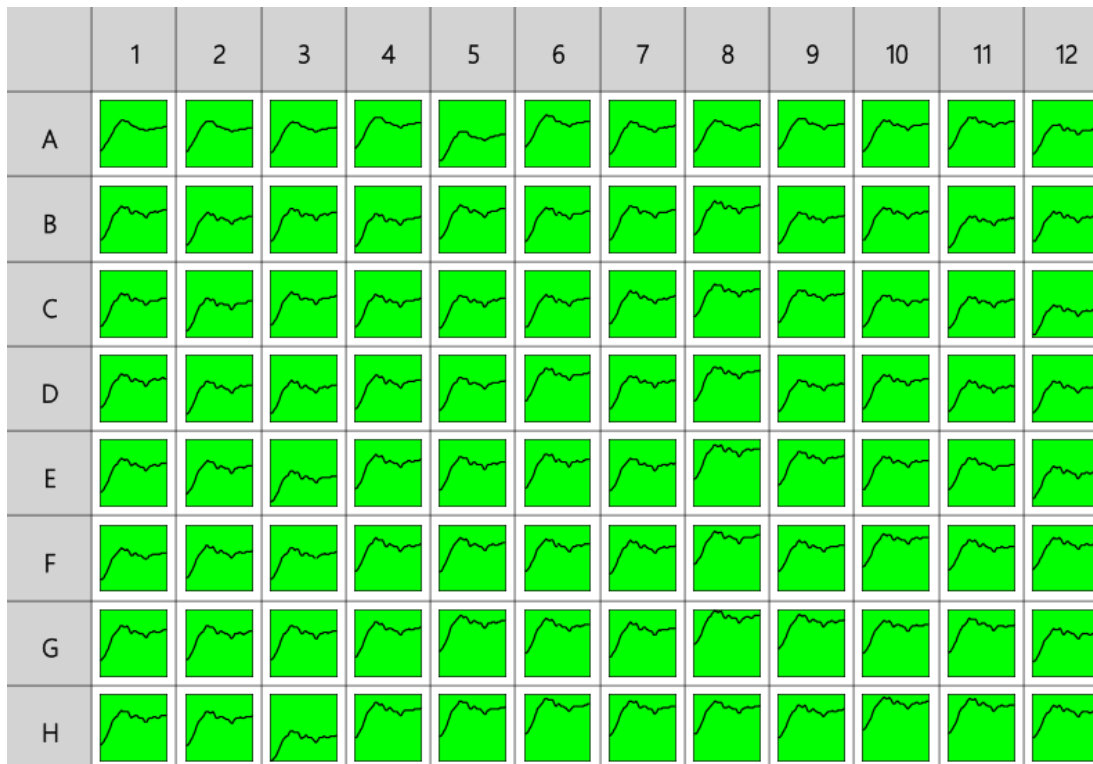
Here the reduction of data in the **A1** position is shown for illustration of the transform:

A1 420;0.142 421;0.143 422;0.144 423;0.145 424;0.147 425;0.148 426;0.149 427;0.15 428;0.152 429;0.153 430;0.155 431;0.156 432;0.158 433;0.16 434;0.161 435;0.162 436;0.163 437;0.164 438;0.165 439;0.166 440;0.166 441;0.166 442;0.165 443;0.165 444;0.165 445;0.165 446;0.164 447;0.163 448;0.162 449;0.162 450;0.161 451;0.161 452;0.161 453;0.16 454;0.16 455;0.159 456;0.159 457;0.159 458;0.159 459;0.159 460;0.158 461;0.158 462;0.158 463;0.158 464;0.159 465;0.159 466;0.159 467;0.159 468;0.159 469;0.159 470;0.16 471;0.16 472;0.16 473;0.16 474;0.16 475;0.16 476;0.16 477;0.161 478;0.161 479;0.161 480;0.161

To reduce spectral plot in each position to its fitted maximum endpoint value:

1. Specify **Data**: **X Axis** as **X (Wavelength)**, **Y Axis** as **Y**.

2. Provide **X Minimum** of 430 and **X Maximum** of 450.
   Only data points within this range will be considered when evaluating the transform.

3. Select **Fit Method** of **Polynomial Order 4 Regression**.

4. Enter **Interpolation Increment** of 0.1.

5. Define **Peak** as **Max** and **Result** as **X**.

6. Click **Calculate**.

Peak Fit

The transform will generate an output endpoint matrix named **Peak Fit** with the value at each position being the *x* projection of the interpolated maximum *y* value of each input replicate plot. With the example data provided above, the result for the **A1** plot is displayed on the [Kinetic/Spectral Analysis Chart](#) as follows:

441

Maximum point is (441, 0.16582), result is 441
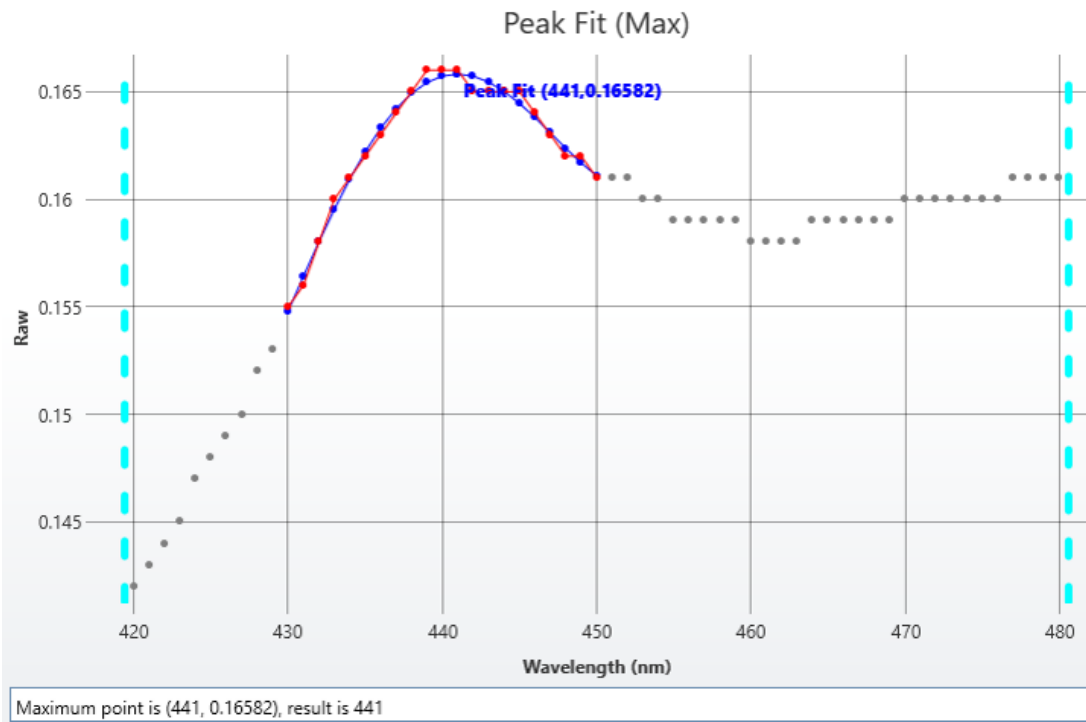
XY Reduction Peak Point

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform computes the peak of all values for each XY plot (within the specified range of points to consider). Flagged positions or points are not included in the calculations.

The result can be set to the *x* or *y* value at the peak, with the peak being defined as either the minimum or maximum value.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Peak	This setting determines which data point is considered as the peak: • **Max** – The point with the maximum *y* value • **Min** – The point with the minimum *y* value
Result	This setting determines which axis's coordinate is stored in resulting matrix: • **X** – Projection of **Peak** value on x-axis • **Y** – Projection of **Peak** value on y-axis

Example

Let's assume that we have some kinetic measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce each input plot to the value at its peak point (maximum).

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 300.000;0.002 350.000;0.021 400.000;0.106 450.000;0.279 500.000;0.384 550.000;0.279 600.000;0.106 650.000;0.021 700.000;0.002

To reduce kinetic plot in each position to its maximum endpoint value:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Define **Peak** as **Max** and **Result** as **X**.

4. Click **Calculate**.

Peak

The transform will generate an output endpoint matrix named **Peak** with the value at each position being the maximum *y* point of each input replicate plot. With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows (also displayed here to 3 decimal places):

500.000

Peak (Max)

Maximum point is (500, 0.384), result is 500.000
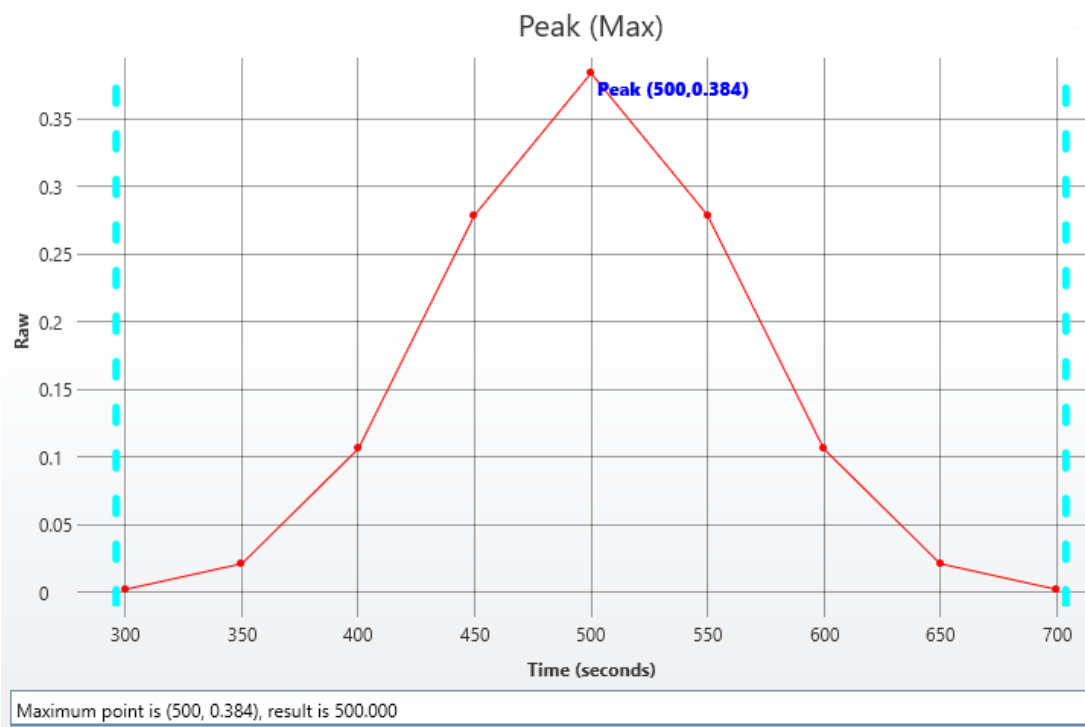
XY Reduction Total

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform computes the sum of all *y* values for each XY plot (within the specified range of points to consider). Flagged positions or points are not included in the calculations.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some kinetic measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data in each position to sum of its data points and store the resulting value to the corresponding position of an endpoint matrix.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.
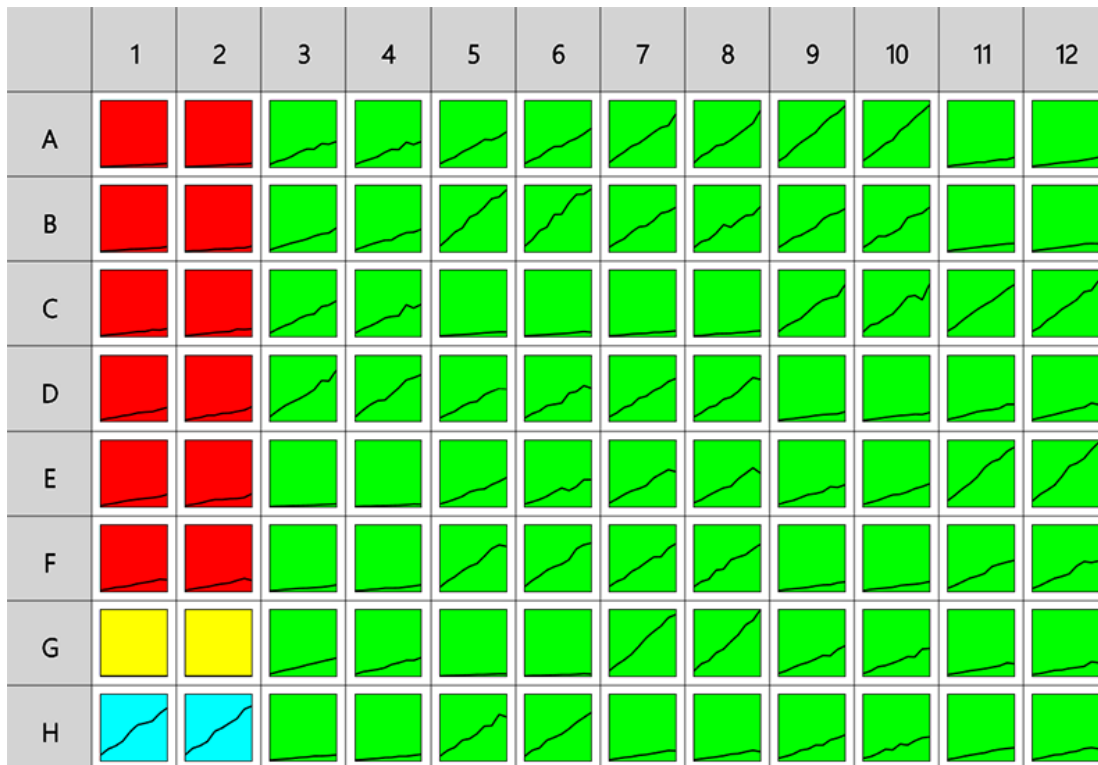
Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

To reduce **XY** data to a sum of its data points:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Click **Calculate**.

Total

The transform will generate an endpoint matrix named **Total** with the value at each position being the sum of *y* input data point values. With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows (also displayed here to 3 decimal places):

28.569

Total is 28.569
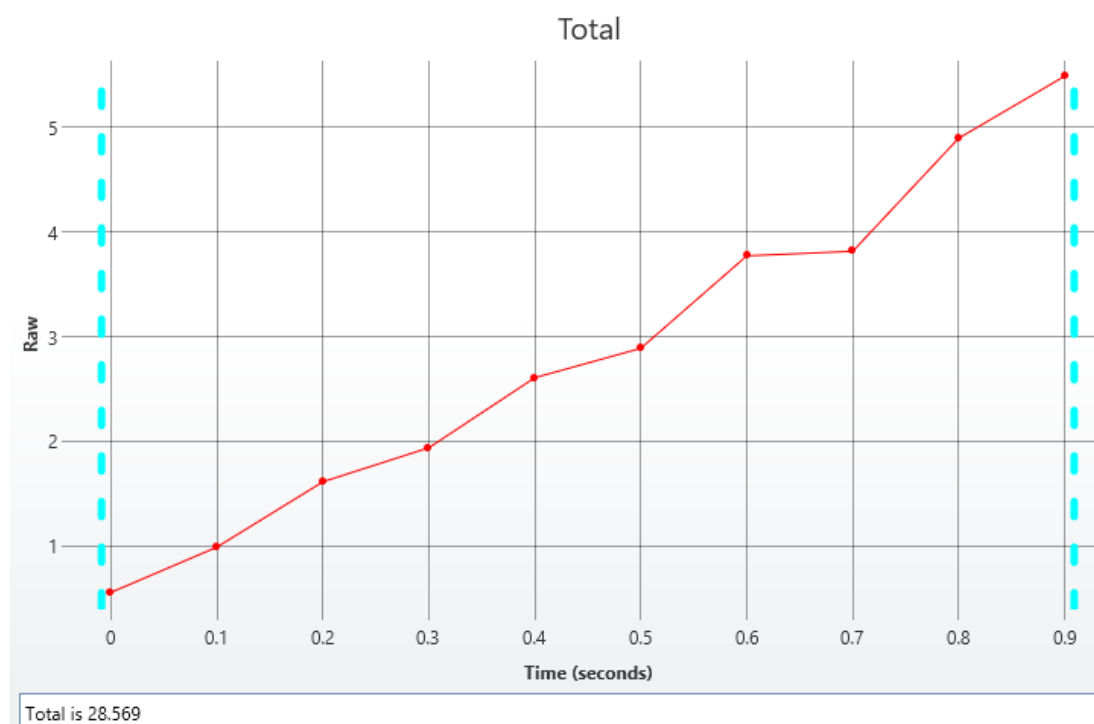
XY Reduction X at Y

[Input: **XY data** ⮕ Output: **Endpoint**]

This reduction transform finds the *x* value at which the specified *y* value (**Cursor**) crosses the plot (within the specified range). If the *y* position is between two adjacent data points, then an interpolated value is calculated from the bounding points.

X and *y* values can be specified as a relative to the first point or as an absolute value. Flagged positions and points are not included in calculations.

> ℹ️ This transform can be used to determine the *x* value at the point where the horizontal (defined by *y*) value crosses each plot.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Cursor	The expression evaluated for each position that represents the target in *Y* value. The default value is 1. 📝 To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix.
Cursor Type	This defines how the **Cursor** is treated for each position. The settings are: • **Absolute** – The value specified by **Cursor** is the value to use in the calculation of *x*. • **Relative From First Measured** – The value of **Cursor** is added to the *y* value of the first point for the position (even if the first point is ~~Flagged~~ or outside the range). • **Relative From First In Range** – The value of **Cursor** is added to the *y* value of the first non-flagged data point within the range.

	Specifies the result of the analysis. The settings are:
Result is	• **Absolute** – The computed *x* value. • **Relative From First Measured** – The computed *x* value minus the *x* value of the first point for the position (even if the first point is ~~Flagged~~ or out of range). • **Relative From First In Range** – The computed *x* value minus the *x* value of the first non-flagged data point within the range.

Example

Let's assume that we have some kinetic measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data in each position to the value of *x* at which the specified *y* value crosses the plot.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

To reduce the plot at each position to the value of *x* when crossing/equaling specified **Cursor**:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Specify **Settings**: **Cursor** as 1, **Cursor Type** and **Result is** as **Absolute**.

4. Click **Calculate**.

X

The transform will generate an endpoint matrix named **X** with the value at each position being kinetic/spectral plot reduced to resulting numeric value (as defined in specified settings). With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows (also displayed here to 3 decimal places):

0.102
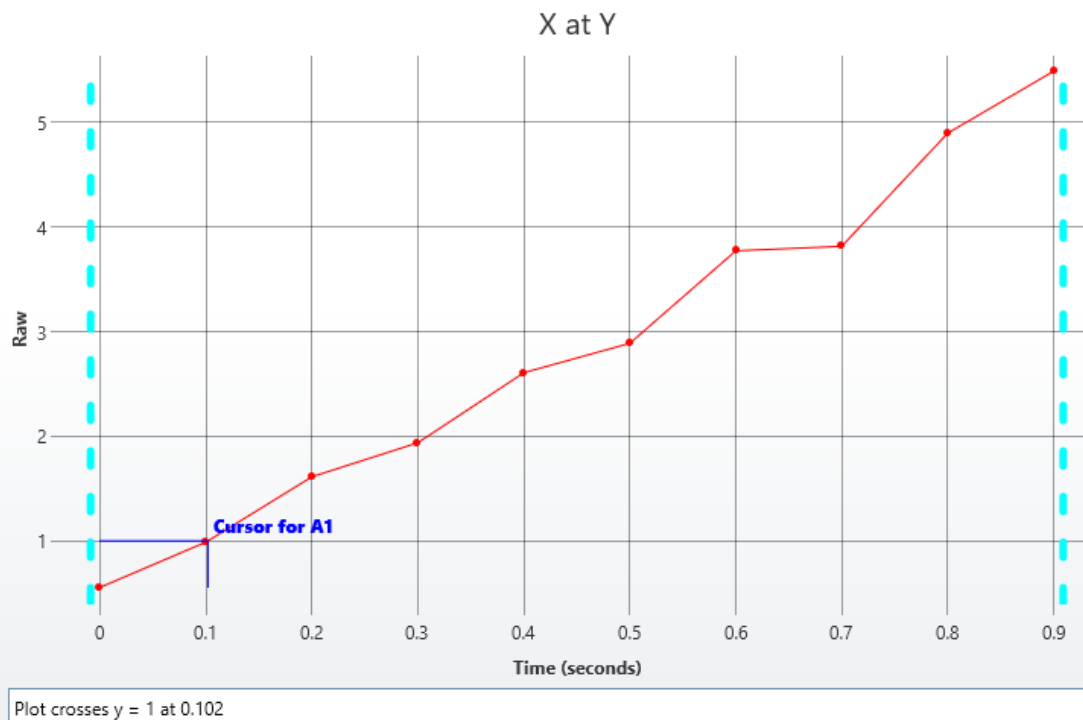
XY Reduction X between Y

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform computes the difference between the first two *x* points at which the specified *y* value (**Cursor**) crosses or equals the plot.

Y value can be specified as relative to the first point or as an absolute value. Flagged positions and points outside the specified range are not included in calculations.

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Cursor	The expression evaluated for each position that represents the target in *y* value. The default value is 1. 📝 To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix.
Cursor Type	This defines how the **Cursor** is treated for each position. The settings are: • **Absolute** – The value specified by **Cursor** is the value to use in the calculation of *x*. • **Relative From First Measured** – The value of **Cursor** is added to the *y* value of the first point for the position (even if the first point is ~~Flagged~~ or outside the range). • **Relative From First In Range** – The value of **Cursor** is added to the *y* value of the first non-flagged data point within the range.

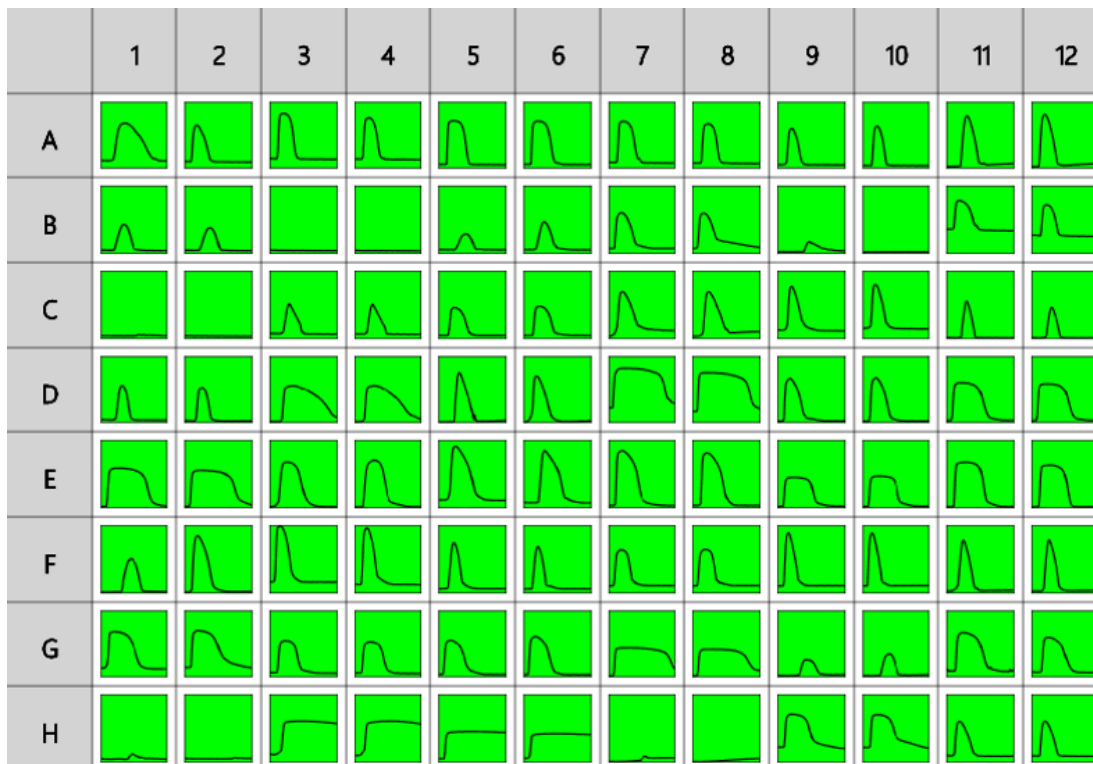📝 If the plot is not crossed or only crossed once, the result will be flagged.

Example

Let's assume that we have some XY measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to calculate the difference between the first two *x* points that equal or cross the specified **Cursor** (*y*) and then reduce data to the difference

between these *x* points in each position.

Raw

Here is an **XY** matrix with each position containing 40 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Raw data kindly provided by Andreas Engel Krag, Aarhus Universitetshospital.

The reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 317.780;0.235 377.710;0.230 437.630;0.231 497.530;0.232 557.440;0.229 617.360;0.232 677.280;0.234 737.180;0.242 797.080;0.360 856.980;0.567 916.900;0.705 976.840;0.766 1036.760;0.791 1096.680;0.798 1156.580;0.800 1216.480;0.797 1276.410;0.786 1336.330;0.769 1396.230;0.746 1456.150;0.721 1516.050;0.696 1575.980;0.666 1635.900;0.634 1695.850;0.599 1755.750;0.560 1815.670;0.518 1875.590;0.470 1935.510;0.416 1995.410;0.364 2055.320;0.319 2115.220;0.277 2175.120;0.261 2235.020;0.255 2294.970;0.251 2354.890;0.233 2414.790;0.231 2474.690;0.228 2534.620;0.227 2594.520;0.229 2654.420;0.226

To reduce the plot at each position to the difference between the first and the second *x* value when crossing/equaling specified **Cursor**:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Specify **Settings**: **Cursor** as 0.7, **Cursor Type** as **Absolute**.

4. Click **Calculate**.

Difference

The transform will generate an endpoint matrix named **Difference** with the value at each position being the XY plot reduced to resulting numeric value (as defined in specified settings). With the example data provided above, the result for the **A1** plot is as displayed on the Kinetic/Spectral Analysis Chart follows (also displayed here to 3 decimal places):

591.737

Plot crosses y = 0.7 at X1 = 914.729 and X2 = 1506.466, difference = 591.737
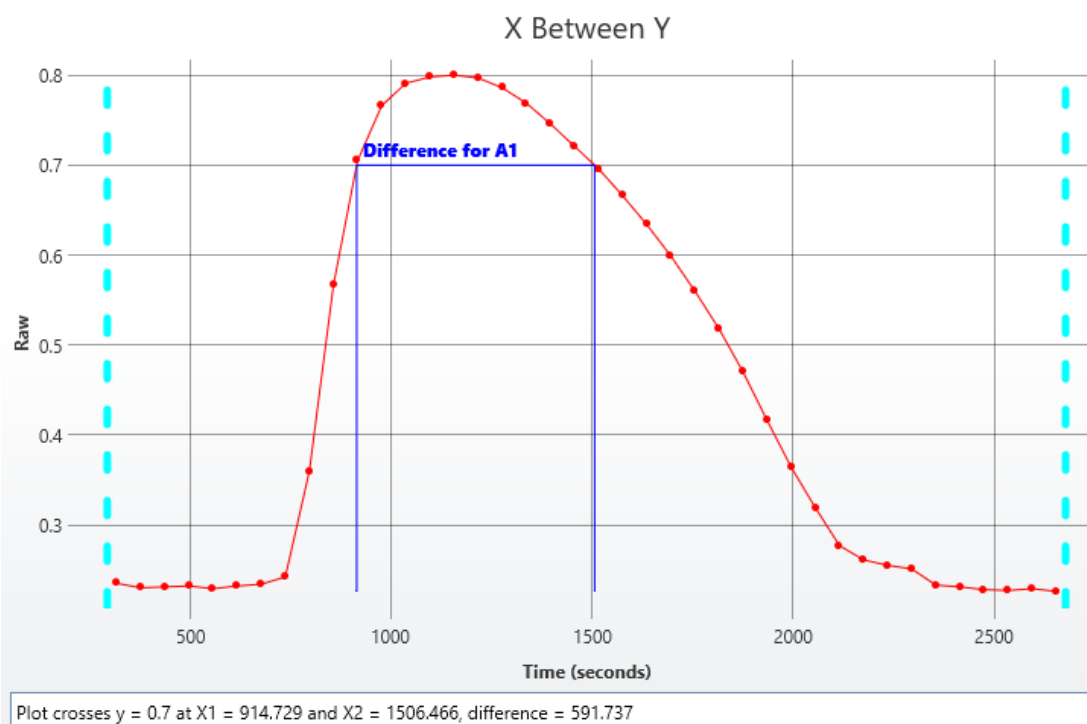
XY Reduction Y at X

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform finds the *y* value at which the specified *x* value (**Cursor**) crosses the plot (within the specified range). If the *x* position is in between two adjacent data points, then an interpolated value is calculated from the bounding points.

The *x* value can be specified as a relative to the first point or as an absolute value. Flagged positions and points are not included in calculations.

> ℹ This transform can be used to determine the *y* value at the point where the vertical (defined by *x*) value crosses each plot (or more simply the *y* at a given *x*).

For viewing XY data common settings, see General Transform Properties for XY Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Settings

Cursor	The expression evaluated for *x* value of each position. 📝 To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix.
Cursor Type	This defines how the **Cursor** is treated for each position. These settings are used to handle scenarios where *x* values for each position may be out of sync by adding an offset to the cursor. The settings are: • **Absolute** – The value specified by the **Cursor** is the value to use in the calculation of *y*. • **Relative From First Measured** – The **Cursor** value is added to the *x* value of the first point for the position (even if the first point is **Flagged** or out of range). • **Relative From First In Range** – The **Cursor** value is added to the *x* value of the first non-flagged data point within the range

Example

Let's assume that we have some kinetic measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data in each position to the *y* value at which the specified **Cursor** (*x*) crosses the plot. The resulting value is then stored to corresponding position of an endpoint matrix.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in the **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

To reduce **XY** data to the defined by the **Cursor** data points in each position:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.

2. Leave **X Minimum** and **X Maximum** blank.

3. Specify **Settings**: **Cursor** as 0.2, **Result is** as **Absolute**.

4. Click **Calculate**.

Y

The transform will generate an endpoint matrix named **Y** with the value at each position being the *x* value defined by the specified **Cursor**. With the example data provided above, the result for the **A1** plot is displayed on the Kinetic/Spectral Analysis Chart as follows (also displayed here to 3 decimal places):

1.613

At x = 0.2 y = 1.613
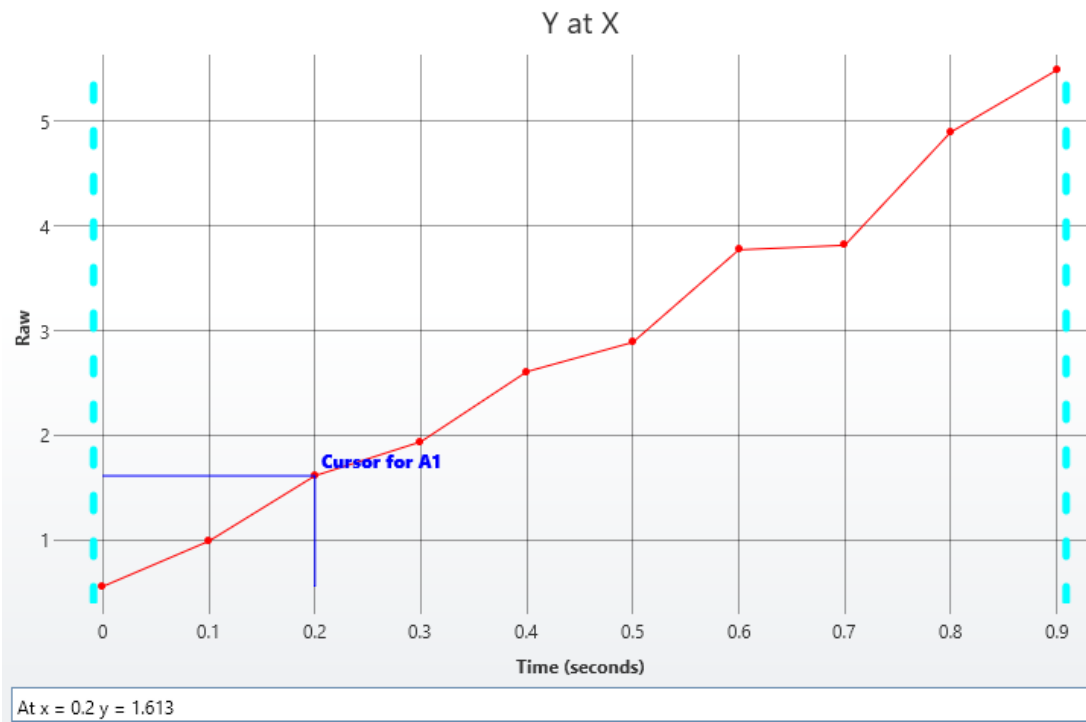
Scan Data General Transform Properties

The transforms that operate on the Scan Data are configured with:

- General settings for all transforms
- General settings for Scan and Scan Reduction transforms (described below)
- Specific settings (if available)

General Settings for Scan and Scan Reduction Transforms

Data

X Axis	This setting determines which values to use in the x-axis on the chart and for evaluations: • **Index** – The 1-based position number of the data point in the collection. • **X** – Each value is set to an *x* value of the corresponding input matrix's data point • **Y** – Each value is set to a *y* value of the corresponding input matrix's data point. • **Z** - Each value is set to a *z* value of the corresponding input matrix's data point (the z-value normally corresponds to the sample position).
Y Axis	This setting determines which values to consider in the y-axis on the chart and for evaluations: • **Index** – The 1-based position number of the data point in the collection. • **X** – Each value is set to an *x* value of the corresponding input matrix's data point • **Y** – Each value is set to a *y* value of the corresponding input matrix's data point. • **Z** - Each value is set to a *z* value of the corresponding input matrix's data point (the z-value normally corresponds to the sample position).
Z Axis	This setting determines which values to consider in the z-axis on the chart and for evaluations: • **Index** – The 1-based position number of the data point in the collection. • **X** – Each value is set to an *x* value of the corresponding input matrix's data point • **Y** – Each value is set to a *y* value of the corresponding input matrix's data point. • **Z** - Each value is set to a *z* value of the corresponding input matrix's data point (the z-value normally corresponds to the sample position).

Range

The range settings enable the specification of a subset of the data points to consider; only data points within the specified range will be processed. When a range is set, data points

outside the specified range are excluded from the calculation. Thus, only the data points inside the specified minimum and maximum range (non-flagged) are processed by the transform.

The range can be defined by setting the **X Minimum**, **X Maximum**, **Y Minimum**, and **Y Maximum** properties to a value or expression:

X Minimum	A numerical value or expression that defines the minimum *x* data point to include within the subset. If this is not specified, then all data points less than **X Maximum** are included.
X Maximum	A numerical value or expression that defines the maximum *x* data point to include within the subset. If this is not specified, then all data points greater than **X Minimum** are included.
Y Minimum	A numerical value or expression that defines the minimum *y* data point to include within the subset. If this is not specified, then all data points less than **Y Maximum** are included.
Y Maximum	A numerical value or expression that defines the maximum *y* data point to include within the subset. If this is not specified, then all data points greater than **Y Minimum** are included.

> To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix. This is useful to set the range of calculations for each sample to be based on the results of previous calculation steps.

Scan Reduction Transforms

Scan Reduction Transforms

Scan transforms operate on matrices of data that consist of Scan data and result in a new endpoint data matrix.

For example, the Scan Reduction Average transform will compute the average of each scan plot.

Throughout MyAssays Desktop, we refer to measurements where each position contains multiple measurements in a 2D grid in general terms as "Scan Data". This includes well-Scan data and other similarly arranged data set.

Scan Axes

With certain measurement types, there might be different data available to plot on the x-, y-, and z-axes. The axes settings specify which data should be processed by the transform. For additional details, see General Transform Properties for Scan Data.

Flagged Scan Data Points

Any data point that is part of a scan data set can be flagged. Flagged data points are excluded from the calculation.

In addition to each data point, each position can also be flagged to completely exclude the sample from any further analysis. This follows the same convention as for Flagged Endpoint.

Scan Range

By default, scan data transform calculations are performed on all scan data points that are not flagged. However, it is also possible to define a range of points to process. This is useful if the area of interest is only a subset of the measurements. The range minimum and maximum values can be set as an absolute value or as an expression (that can in turn refer to other computed results).

Refer to the General Transform Properties for Scan Data subsection for more details.

Scan Reduction

Transform	Reduces Data To
Scan Reduction Average	The average of non-flagged data points at each position.
Scan Reduction Count	The number of non-flagged data points at each position.
Scan Reduction Median	The median value of non-flagged data points at each position.
Scan Reduction Peak	Determined peak (minimum or maximum) data point within the specified range of non-flagged data points at each position.
Scan Reduction Percentage CV	The percentage coefficient of variation of non-flagged data points at each position.
Scan Reduction Standard Deviation	The standard deviation of non-flagged data points at each position.

Scan Reduction Average

[Input: **Scan Data** ➡ Output: **Endpoint**]

This reduction transform calculates the average value for each position. Flagged positions or points are not included in the calculations.

For viewing Scan data common settings, see General Transform Properties for Scan Data.

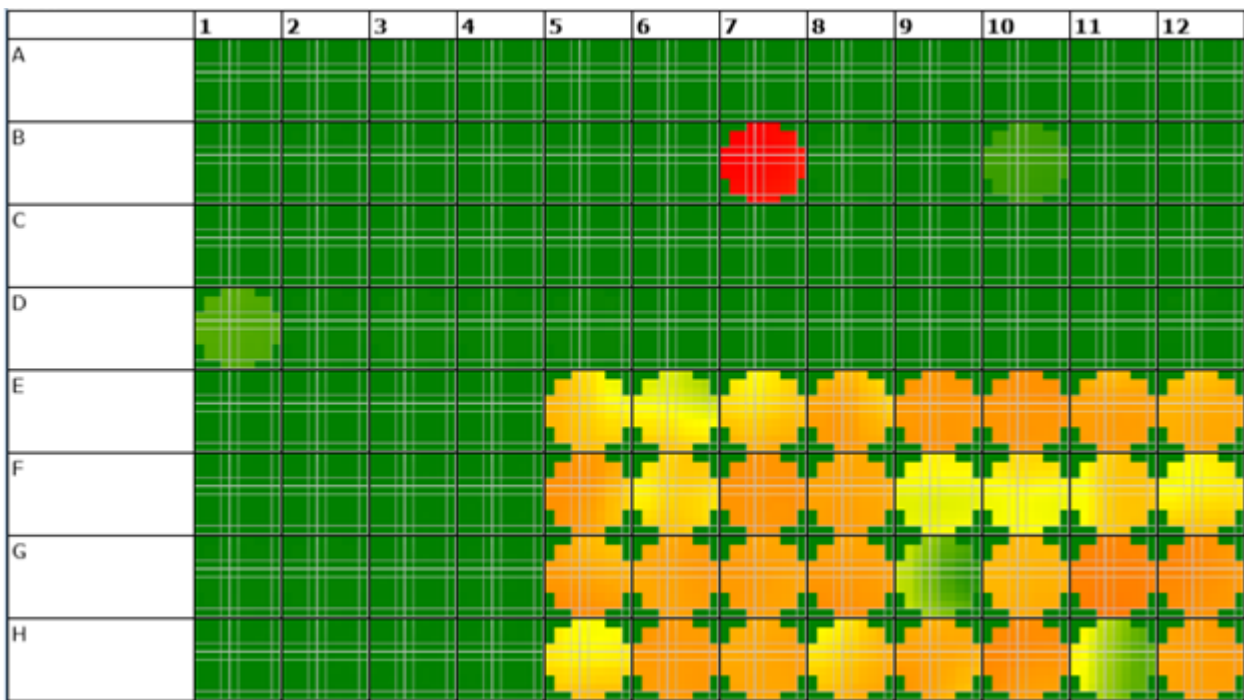For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some **scan** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce data in each position to average of its data points and store resulting value to corresponding position of an endpoint matrix.

Raw

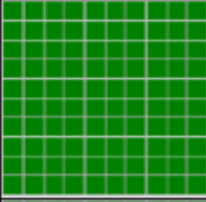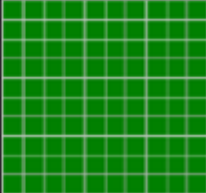## Here is some example scan data displayed in heatmap thumbplots:

Average

The transform will generate an output matrix named Average with the average value for each position. With the example data provided, the results are as follows (displayed to 3 decimal places):

• Sample Table

Here is a Sample Table snippet, which lists the details of the calculations. For each samples, the following details are reported:

Sample	Positions	Raw (OD)	Average
🟢 Unknown1	B1		139.990
🟢 Unknown2	B2		175.480
🟢 Unknown3	B3		132.510
🟢 Unknown4	B4		131.430

Matrix Table

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	124.060	119.670	122.870	110.660	118.800	118.490	105.030	116.540	117.630	121.300	115.330	134.800
B	139.990	175.480	132.510	131.430	146.320	127.940	183845	661.110	130.170	6593.86	138.700	165.720
C	135.610	134.060	139.660	152.820	137.850	142.920	146.890	139.540	133.810	142.350	153.760	151.610
D	9862.43	503.420	651.310	527.230	717.750	150.250	181.840	166.790	176.020	157.120	147.300	271.210
E	144.640	167.880	167.330	166.210	61816.8	45512.9	63126.4	77318.7	87187.3	88363.2	81861.0	76273.6
F	156.240	158.230	179.420	179.350	82458.8	60500.6	88656.8	81135.2	43352.1	48362.1	61186.6	54900.7
G	438.860	426.480	174.690	201.870	81311.0	82046.2	83018.9	85331.2	15769.4	74224.5	98039.8	90767.4
H	165.810	189.940	188.700	210.130	54996.2	85725.9	80111.3	66346.0	79319.7	90032.8	24436.4	83309.6

Scan Reduction Count

[Input: **Scan Data** ➡ Output: **Endpoint**]

This reduction transform reports the count of data points for each position. Flagged positions or points are not included in the calculations.

For viewing Scan data common settings, see General Transform Properties for Scan Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some **scan** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce the data in each position to the count of non-flagged data points and store the results value to the corresponding position of an endpoint matrix.

Raw

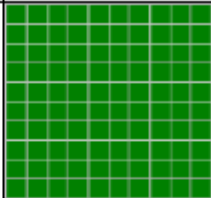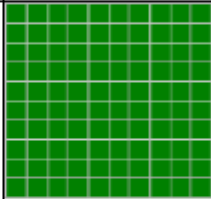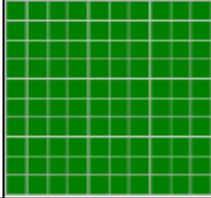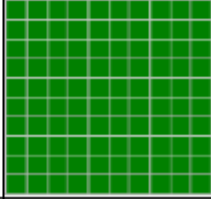## Here is some example scan data displayed in heatmap thumbplots:
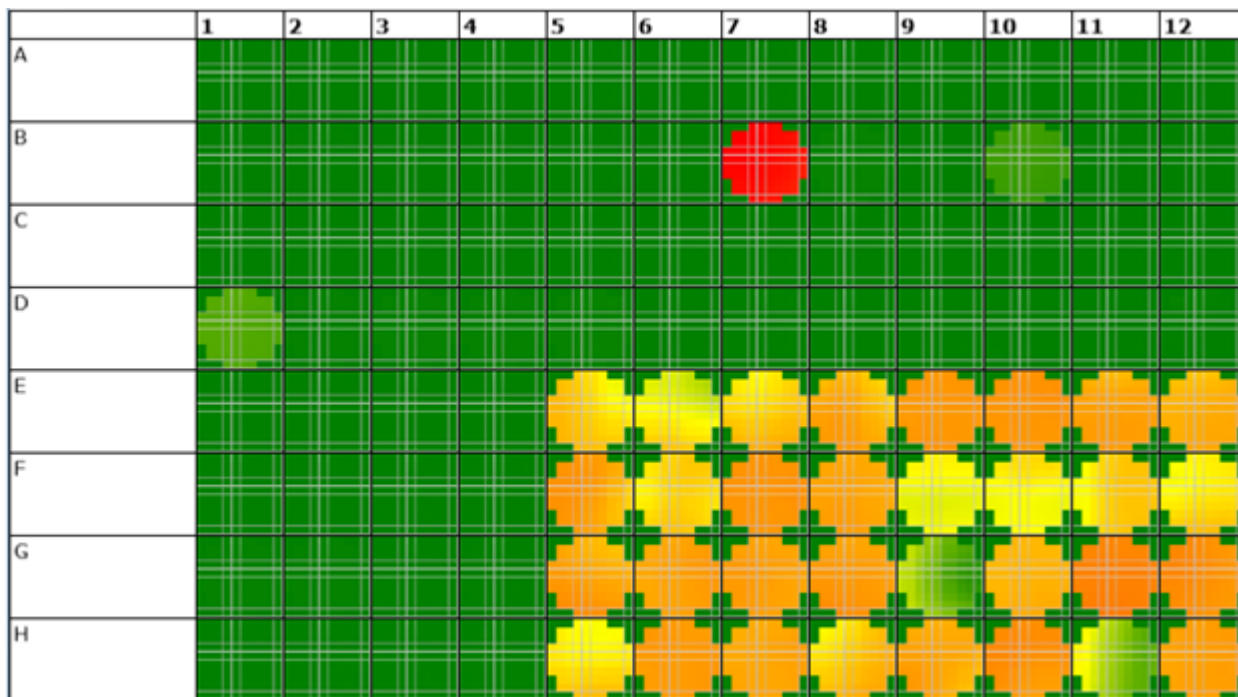
Count

The transform will generate an endpoint matrix named **Count** with the value at each position being the count of input data point values. With the example data provided above, the results are as follows (displayed to 3 decimal places):

• Sample Table

Here is a Sample Table snippet, which lists the details of the calculations. For each samples, the following details are reported:

Sample	Positions	Raw (OD)	Count
🟢 Unknown1	B1		100.000
🟢 Unknown2	B2		100.000
🟢 Unknown3	B3		100.000
🟢 Unknown4	B4		100.000

Matrix Table

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
B	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
C	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
D	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
E	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
F	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
G	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
H	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000

Scan Reduction Median

[Input: **Scan Data** ➡ Output: **Endpoint**]

This reduction transform reports the median of data points for each position. Flagged positions or points are not included in the calculations.

For viewing Scan data common settings, see General Transform Properties for Scan Data.

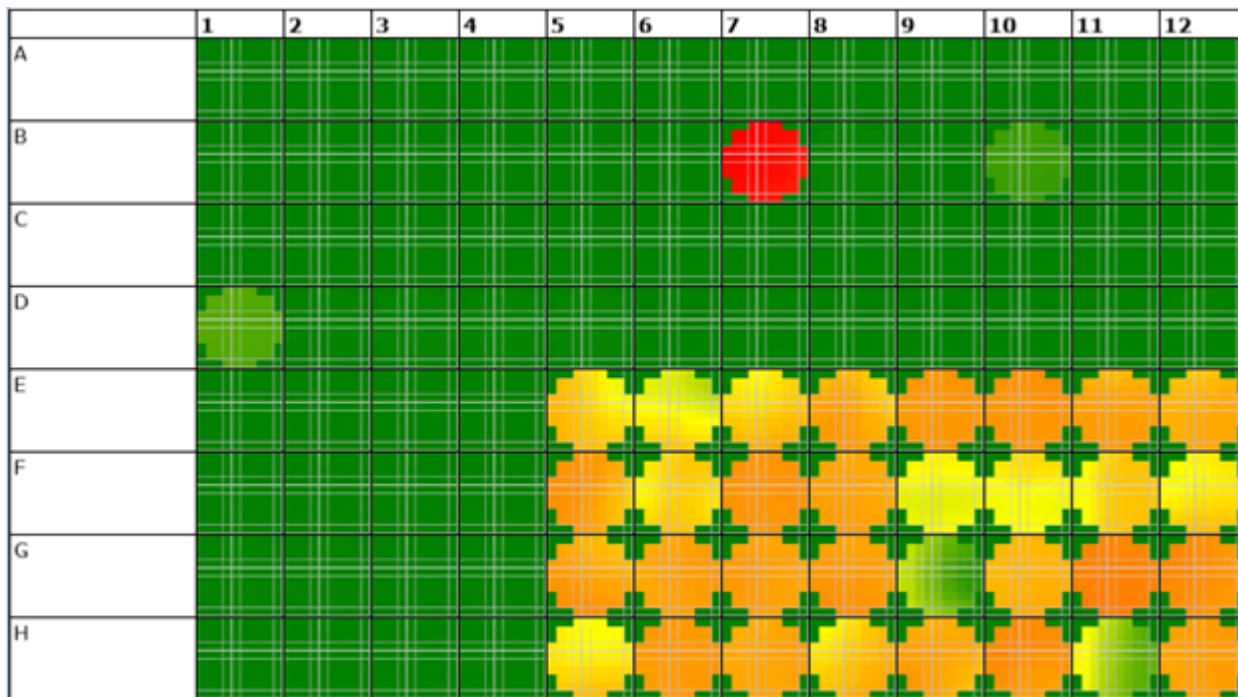For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some **scan** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce the data in each position to the median of non-flagged data points and store the results value to the corresponding position of an endpoint matrix.

Raw

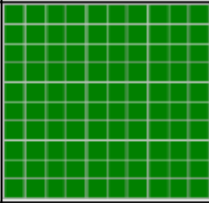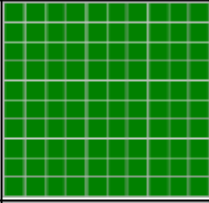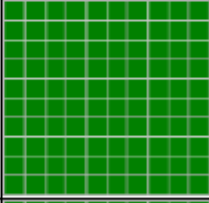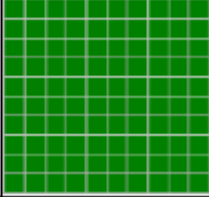**Here is some example scan data displayed in heatmap thumbplots:**

Median

The transform will generate an endpoint matrix named **Median** with the value at each position being the median of input data point values. With the example data provided above, the results are as follows (displayed to 3 decimal places):

• Sample Table

Here is a Sample Table snippet, which lists the details of the calculations. For each samples, the following details are reported:

Sample	Positions	Raw (OD)	Median
● Unknown1	B1		170.500
● Unknown2	B2		187.500
● Unknown3	B3		160.500
● Unknown4	B4		160.000

Matrix Table

Here all calculated data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	150.500	144.500	151.000	133.500	144.500	145.500	126.000	142.000	144.000	146.000	140.000	164.000
B	170.500	187.500	160.500	160.000	179.500	156.000	227684	815.500	158.000	8155.00	168.000	200.500
C	166.000	165.000	168.500	187.000	169.500	174.000	179.000	171.500	163.500	170.500	188.000	184.500
D	12151.5	617.500	802.500	650.000	851.500	182.000	214.000	204.000	215.500	188.000	176.000	211.000
E	176.500	203.000	202.000	201.000	74817.5	50875.0	75459.5	94388.0	108828	109959	102751	95015.5
F	188.500	192.500	219.500	218.500	103167	74971.0	110587	100615	51391.5	56704.0	77120.5	65020.5
G	538.000	526.500	216.000	242.500	98950.5	101146	102587	104764	14261.5	91395.5	121680	112016
H	201.500	228.000	232.500	259.500	63987.5	106731	99591.0	80198.0	98110.0	112406	21737.5	103803

Scan Reduction Peak

[Input: **Scan Data** ➡ Output: **Endpoint**]

This reduction transform reports the maximum value for each position. Flagged positions or points are not included in the calculations.

For viewing Scan data common settings, see General Transform Properties for Scan Data.

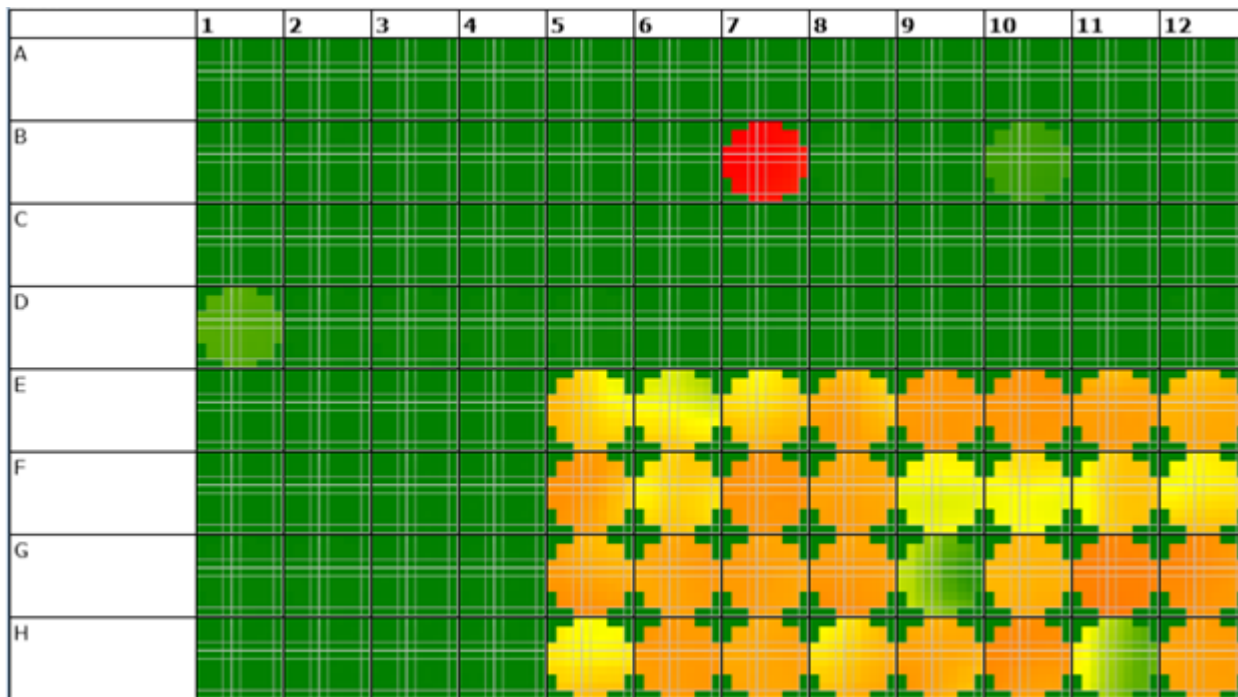For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Example

Let's assume that we have some **scan** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce the data in each position to the maximum value of non-flagged data points and store the results value to the corresponding position of an endpoint matrix.

Raw

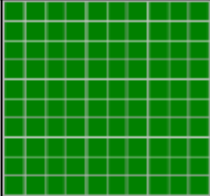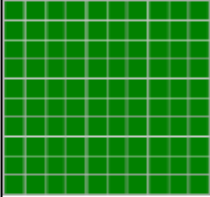### Here is some example scan data displayed in heatmap thumbplots:
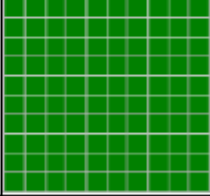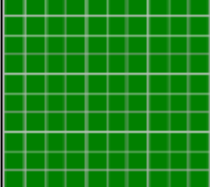

Peak

The transform will generate an endpoint matrix named **Peak** with the value at each position being the maximum of input data point values. With the example data provided above, the results are as follows (displayed to 3 decimal places):

• Sample Table

Here is a Sample Table snippet, which lists the details of the calculations. For each samples, the following details are reported:

Sample	Positions	Raw (OD)	Peak
● Unknown1	B1		209.000
● Unknown2	B2		396.000
● Unknown3	B3		199.000
● Unknown4	B4		192.000

Matrix Table

Here all calculated data is displayed in a [Matrix Table](#).

	1	2	3	4	5	6	7	8	9	10	11	12
A	194.000	182.000	181.000	172.000	185.000	172.000	158.000	169.000	183.000	192.000	170.000	205.000
B	209.000	396.000	199.000	192.000	229.000	193.000	243945	919.000	204.000	9014.00	204.000	246.000
C	198.000	194.000	213.000	230.000	205.000	214.000	216.000	206.000	205.000	215.000	226.000	224.000
D	13200.0	737.000	893.000	719.000	1108.00	245.000	302.000	245.000	258.000	269.000	226.000	887.000
E	209.000	245.000	254.000	252.000	92276.0	83772.0	98221.0	108347	110827	113695	106580	100404
F	239.000	227.000	271.000	264.000	113058	84368.0	112755	106761	63995.0	75452.0	85900.0	87905.0
G	633.000	589.000	256.000	340.000	115392	108590	107702	114708	38268.0	97927.0	126119	119652
H	255.000	286.000	292.000	305.000	87740.0	109543	104767	99776.0	108602	118303	63013.0	107666

Scan Reduction Percentage Coefficient of Variation

[Input: **Scan Data** ➡ Output: **Endpoint**]

This reduction transform calculates the percentage CV for each position. [Flagged positions or points](#) are not included in the calculations.

For viewing Scan data common settings, see [General Transform Properties for Scan Data](#).

For viewing common transform settings, see [General Transform Properties](#).

To learn about adding this transform to your assay run, see [Transforms Tab](#).

Example

Let's assume that we have some **scan** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce the data in each position to the %CV of non-flagged data points and store the results value to the corresponding position of an endpoint matrix.

Raw

Here is some example scan data displayed in heatmap thumbplots:
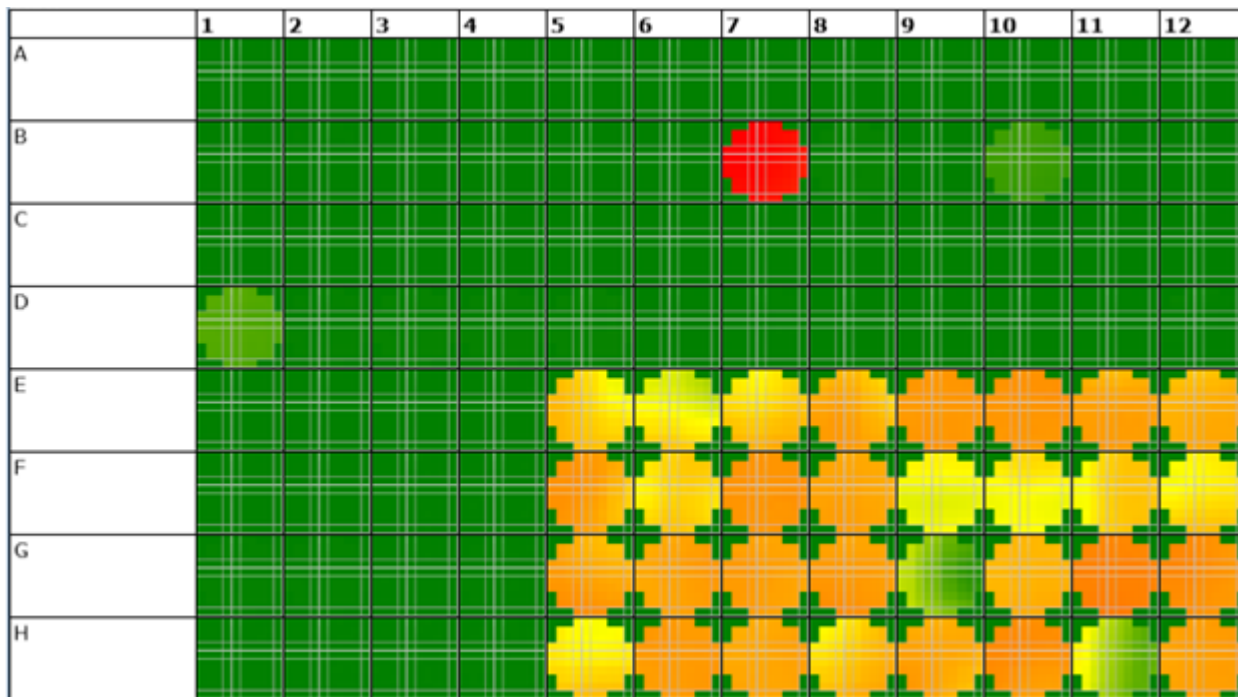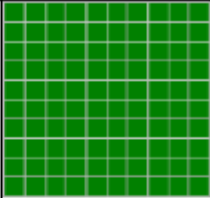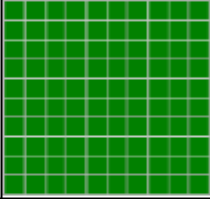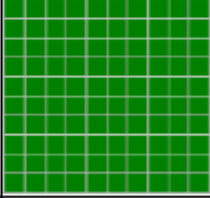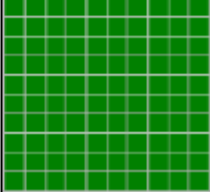

Peak

The transform will generate an endpoint matrix named **%CV** with the value at each position being the maximum of input data point values. With the example data provided above, the results are as follows (displayed to 3 decimal places):

• Sample Table

Here is a Sample Table snippet, which lists the details of the calculations. For each samples, the following details are reported:

Sample	Positions	Raw (OD)	%CV
🟢 Unknown1	B1		51.0560
🟢 Unknown2	B2		57.6856
🟢 Unknown3	B3		50.9935
🟢 Unknown4	B4		50.9976

Matrix Table

Here all calculated data is displayed in a [Matrix Table](#).

	1	2	3	4	5	6	7	8	9	10	11	12
A	51.0463	51.1235	50.9883	51.2311	51.1648	50.9141	51.3557	50.9840	51.2160	51.2394	51.0535	50.9427
B	51.0560	57.6856	50.9935	50.9976	50.8967	51.1522	50.4802	50.4652	51.1120	50.6114	50.8508	50.9394
C	51.0028	50.9238	51.1687	51.1074	50.9526	50.9395	51.1477	50.9374	50.9264	51.1446	50.8831	50.8804
D	50.4336	50.6418	50.4340	50.4941	51.4646	51.1150	52.2972	50.6974	50.8478	51.8436	51.4883	79.0033
E	50.8940	50.9707	50.9729	51.0158	52.6367	56.0930	52.0700	51.2242	50.2609	50.2729	50.4805	50.4734
F	51.0715	50.8059	50.9597	51.0097	51.2966	50.9408	50.2594	50.3181	51.2383	51.5960	52.2338	52.0472
G	50.6284	50.4672	50.7539	52.2126	50.9606	50.3523	50.3012	50.4062	74.9086	50.3173	50.2792	50.3877
H	51.1794	51.3760	50.9637	50.6966	52.2378	50.2640	50.3038	52.1195	50.5092	50.4327	75.3082	50.2846

Scan Reduction Standard Deviation

[Input: **Scan Data** ➡ Output: **Endpoint**]

This reduction transform calculates the standard deviation for the data contained at each position [Flagged positions or points](#) are not included in the calculations.

For viewing Scan data common settings, see [General Transform Properties for Scan Data](#).

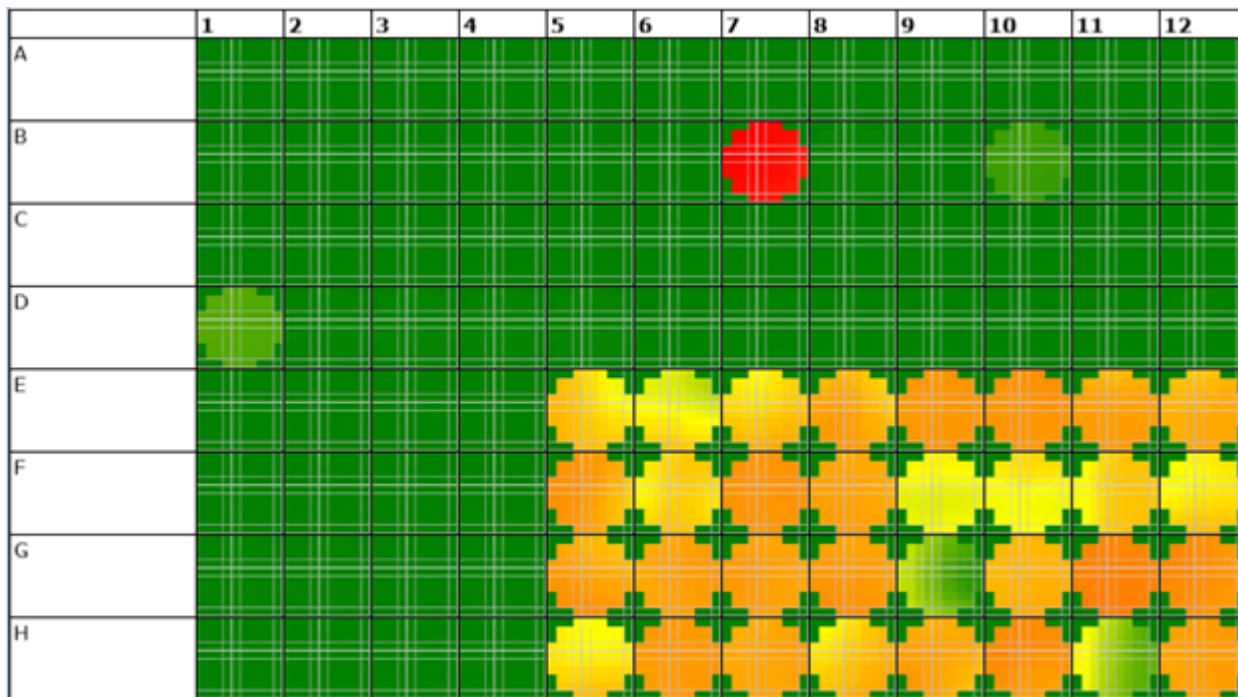For viewing common transform settings, see [General Transform Properties](#).

To learn about adding this transform to your assay run, see [Transforms Tab](#).

Example

Let's assume that we have some **scan** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example, we would like to reduce the data in each position to the standard deviation of non-flagged data points and store the results value to the corresponding position of an endpoint matrix.

Raw

Here is some example scan data displayed in heatmap thumbplots:

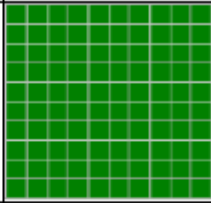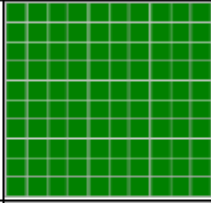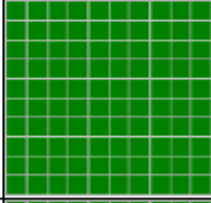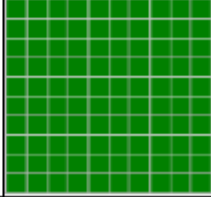Standard Deviation

The transform will generate an endpoint matrix named **SD** with the value at each position being the maximum of input data point values. With the example data provided above, the results are as follows (displayed to 3 decimal places):

• Sample Table

Here is a Sample Table snippet, which lists the details of the calculations. For each samples, the following details are reported:

Sample	Positions	Raw (OD)	SD
● Unknown1	B1		71.4733
● Unknown2	B2		101.227
● Unknown3	B3		67.5715
● Unknown4	B4		67.0262

Matrix Table

Here all calculated data is displayed in a [Matrix Table](#).

	1	2	3	4	5	6	7	8	9	10	11	12
A	63.3280	61.1795	62.6494	56.6924	60.7838	60.3281	53.9389	59.4168	60.2454	62.1534	58.8800	68.6708
B	71.4733	101.227	67.5715	67.0262	74.4720	65.4441	92805.1	333.631	66.5324	3337.24	70.5301	84.4168
C	69.1648	68.2685	71.4622	78.1023	70.2382	72.8027	75.1308	71.0781	68.1446	72.8043	78.2378	77.1398
D	4973.98	254.941	328.481	266.220	369.387	76.8003	95.0973	84.5582	89.5022	81.4566	75.8423	214.265
E	73.6130	85.5697	85.2930	84.7934	32538.3	25529.5	32869.9	39605.9	43821.1	44422.7	41323.8	38497.9
F	79.7941	80.3902	91.4320	91.4859	42298.5	30819.5	44558.3	40825.7	22212.9	24952.9	31960.1	28574.3
G	222.188	215.232	88.6621	105.402	41436.6	41312.1	41759.5	43012.2	11812.6	37347.8	49293.7	45735.6
H	84.8606	97.5836	96.1685	106.529	28728.8	43089.2	40299.1	34579.2	40063.8	45406.0	18402.6	41891.9

Scan Transforms

Scan Transforms

Scan transforms operate on matrices of data that consist of scan data and result in either an endpoint matrix (for [Scan Reduction Transforms](#)), or a new scan data matrix.

Scan Data

Throughout MyAssays Desktop, we refer to measurements where each position contains multiple measurements in a 2D grid in general terms as "Scan Data". This includes well-scan data and other similarly arranged data set.

Scan Axes

With certain measurement types, there might be different data available to plot on the x-, y-, and z-axes. The axes settings specify which data should be processed by the transform. For additional details, see General Transform Properties for Scan Data subsection.

Flagged Scan Data Points

Any data point that is part of a scan data set can be flagged. Flagged data points are excluded from the calculation.

In addition to each data point, each position can also be flagged to completely exclude the sample from any further analysis. This follows the same convention as Flagged Endpoint.

Scan Range

By default, scan data transform calculations are performed on all scan data points that are not flagged. However, it is also possible to define a range of points to process. This is useful if the area of interest is only a subset of the measurements. The range minimum and maximum values can be set as an absolute value or as an expression (that can in turn refer to other computed results).

Refer to the General Transform Properties for Scan Data subsection for more details.

Scan Transforms

Transform	Operation
Scan Blank Correction	Calculates the average scan measurement of non-flagged samples in the specified blank, and subtracts that value from each scan value for all included positions.
Scan Flag	Flags positions where a Boolean condition is satisfied. This is useful for automatically rejecting and ignoring data points that are outside an expected range.

Scan Blank Correction

[Input: **Scan** ➡ Output: **Scan**]

This transform calculates the average scan measurement of non-flagged samples in the specified blank, and subtracts that value from each scan value for all included positions. This is useful for subtracting background noise from measurements.

Flagged positions or points are not included in the calculations. The operation is only performed on data within specified range.

For viewing Scan data common settings, see General Transform Properties for Scan Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Range

The range settings enable the specification of a subset of the data points to consider; only data points within the specified range will be processed. When a range is set, data points outside the specified range are excluded from the calculation. Thus, only the data points inside the specified minimum and maximum range (non-flagged) are processed by the transform.

The range can be defined by setting the **X Minimum**, **X Maximum**, **Y Minimum**, and **Y Maximum** properties to a value or expression:

X Minimum	A numerical value or expression that defines the minimum *x* data point to include within the subset. If this is not specified, then all data points less than **X Maximum** are included.
X Maximum	A numerical value or expression that defines the maximum *x* data point to include within the subset. If this is not specified, then all data points greater than **X Minimum** are included.
Y Minimum	A numerical value or expression that defines the minimum *y* data point to include within the subset. If this is not specified, then all data points less than **Y Maximum** are included.
Y Maximum	A numerical value or expression that defines the maximum *y* data point to include within the subset. If this is not specified, then all data points greater than **Y Minimum** are included.

To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix. This is useful to set the range of calculations for each sample to be based on the results of previous calculation steps.

Settings

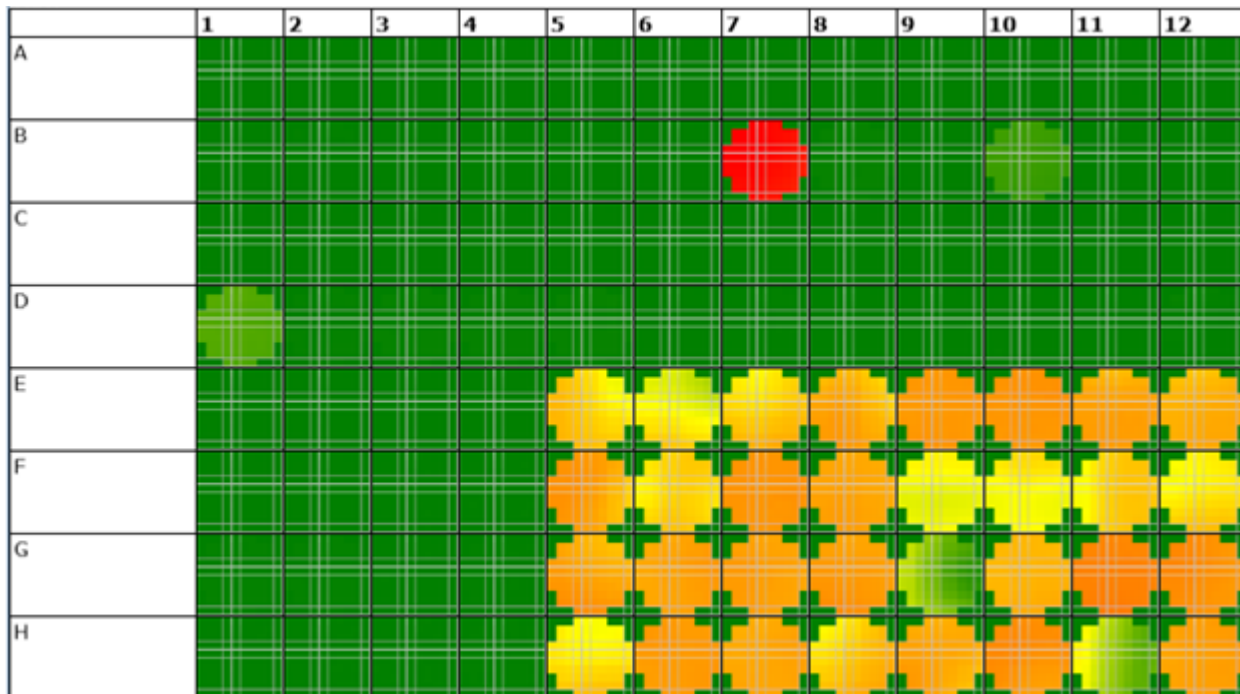|	
Flag Expression	The Expression to evaluate, where a single x variable is set to the value of each position of the input matrix.

Example

Let's assume we have Scan measurement data for a 12x8 (10x10) microplate stored in the

Raw matrix. In this example, we would like to subtract the average of the specified **Blank** samples from each scan value for all included positions.

Raw

## Here is some example data displayed in heatmap thumbplots:

The average of each position is reported in the below table:

	1	2	3	4	5	6	7	8	9	10	11	12
A	124.0	119.6	122.8	110.6	118.8	118.4	105.0	116.5	117.6	121.3	115.3	134.8
B	139.9	175.4	132.5	131.4	146.3	127.9	18384	661.1	130.1	6593.	138.7	165.7
C	135.6	134.0	139.6	152.8	137.8	142.9	146.8	139.5	133.8	142.3	153.7	151.6
D	9862.	503.4	651.3	527.2	717.7	150.2	181.8	166.7	176.0	157.1	147.3	271.2
E	144.6	167.8	167.3	166.2	61816	45512	63126	77318	87187	88363	81861	76273
F	156.2	158.2	179.4	179.3	82458	60500	88656	81135	43352	48362	61186	54900
G	438.8	426.4	174.6	201.8	81311	82046	83018	85331	15769	74224	98039	90767
H	165.8	189.9	188.7	210.1	54996	85725	80111	66346	79319	90032	24436	83309

Calculated

The transform will generate an output matrix named **Blank Corrected** with the thumbplot at each position reporting the blank corrected values. With the example provided above, the results are as follows:
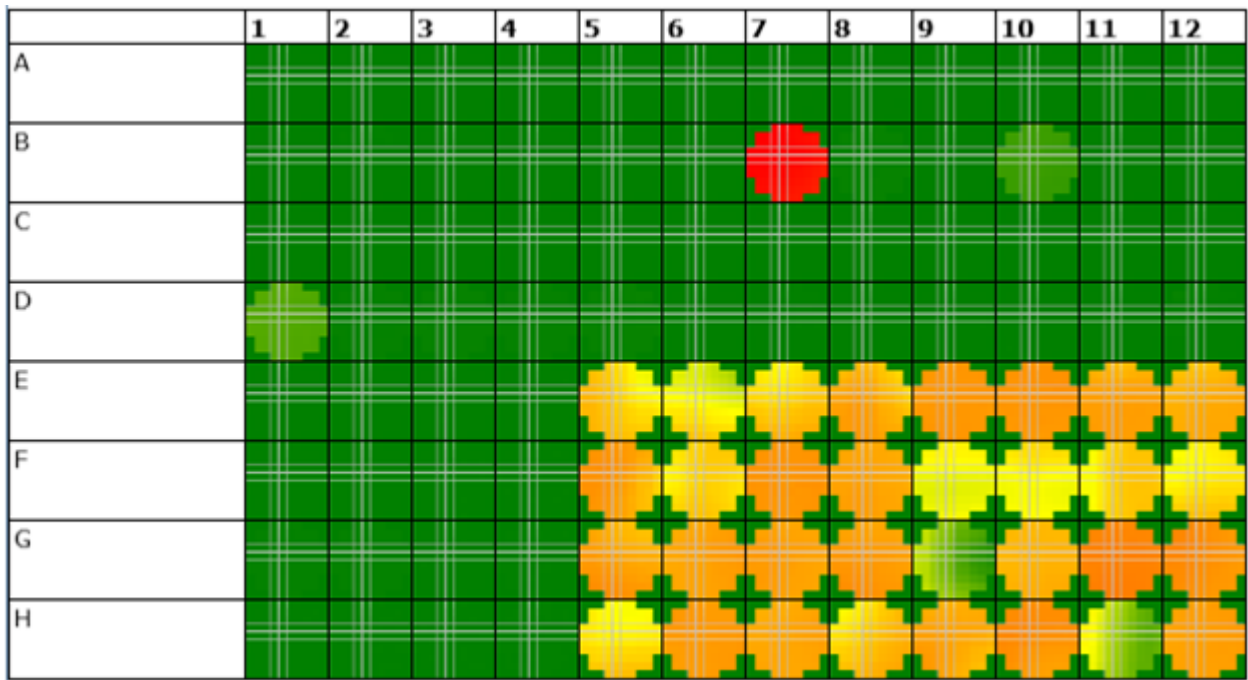
The average blank corrected value is listed in the table below:

	1	2	3	4	5	6	7	8	9	10	11	12
A	5.30	0.91	4.11	-8.10	0.04	-0.27	-13.7	-2.22	-1.13	2.54	-3.43	16.04
B	21.23	56.71	13.75	12.67	27.56	9.17	18372	542.3	11.41	6475.	19.94	46.95
C	16.85	15.30	20.90	34.06	19.09	24.16	28.13	20.78	15.05	23.59	35.00	32.85
D	9743.	384.6	532.5	408.4	598.9	31.49	63.07	48.02	57.25	38.36	28.54	152.4
E	25.88	49.11	48.56	47.44	61698	45394	63007	77199	87068	88244	81742	76154
F	37.48	39.47	60.65	60.58	82340	60381	88538	81016	43233	48243	61067	54781
G	320.1	307.7	55.92	83.11	81192	81927	82900	85212	15650	74105	97921	90648
H	47.04	71.17	69.93	91.37	54877	85607	79992	66227	79200	89914	24317	83190

Scan Flag

[Input: **Scan** ➡ Output: **Scan**]

This transform flags positions where a Boolean condition is satisfied. This is useful for automatically rejecting and ignoring data points that are outside an expected range.

Flagged positions or points are not included in the calculations. The operation is only performed on data within specified range.

For viewing Scan data common settings, see General Transform Properties for Scan Data.

For viewing common transform settings, see General Transform Properties.

To learn about adding this transform to your assay run, see Transforms Tab.

Properties

Range

The range settings enable the specification of a subset of the data points to consider; only data points within the specified range will be processed. When a range is set, data points outside the specified range are excluded from the calculation. Thus, only the data points inside the specified minimum and maximum range (non-flagged) are processed by the transform.

The range can be defined by setting the **X Minimum**, **X Maximum**, **Y Minimum**, and **Y Maximum** properties to a value or expression:

X Minimum	A numerical value or expression that defines the minimum *x* data point to include within the subset. If this is not specified, then all data points less than **X Maximum** are included.
X Maximum	A numerical value or expression that defines the maximum *x* data point to include within the subset. If this is not specified, then all data points greater than **X Minimum** are included.
Y Minimum	A numerical value or expression that defines the minimum *y* data point to include within the subset. If this is not specified, then all data points less than **Y Maximum** are included.
Y Maximum	A numerical value or expression that defines the maximum *y* data point to include within the subset. If this is not specified, then all data points greater than **Y Minimum** are included.

> To refer to the position's corresponding data on an endpoint matrix, use a Matrix Position Reference (e.g., **#2**) to refer to the data on the second matrix. This is useful to set the range of calculations for each sample to be based on the results of previous calculation steps.
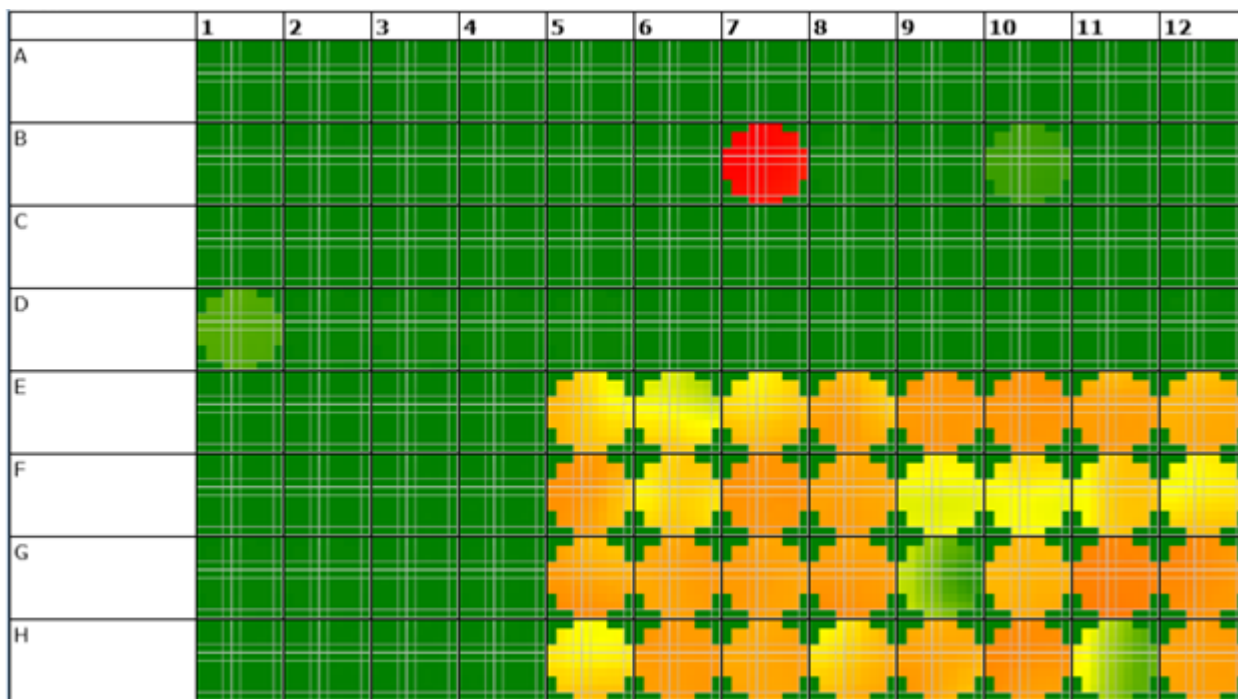
Settings

Flag Expression	The Expression to evaluate, where a single x variable is set to the value of each position of the input matrix.

Example

Let's assume we have Scan measurement data for a 12x8 (10x10) microplate stored in the **Raw** matrix. In this example, we would like to subtract the average of the specified **Blank** samples from each scan value for all included positions.

Raw

Here is some example data displayed in heatmap thumbplots:

In this example, we have calculated the average of the blank samples using a Scan Reduction Average transform. This transform resulted in an average value contained in an endpoint matrix - Matrix #2. To flag values in this matrix where the measurement is less than the average of the Blank samples, specify a Flag Expression of **x<Blank1.2**

Calculated

The transform will generate an output matrix named **Calculated** with the thumbplot at each position matching the input data and positions that meet the specified condition flagged. With the example provided above, the results are as follows:
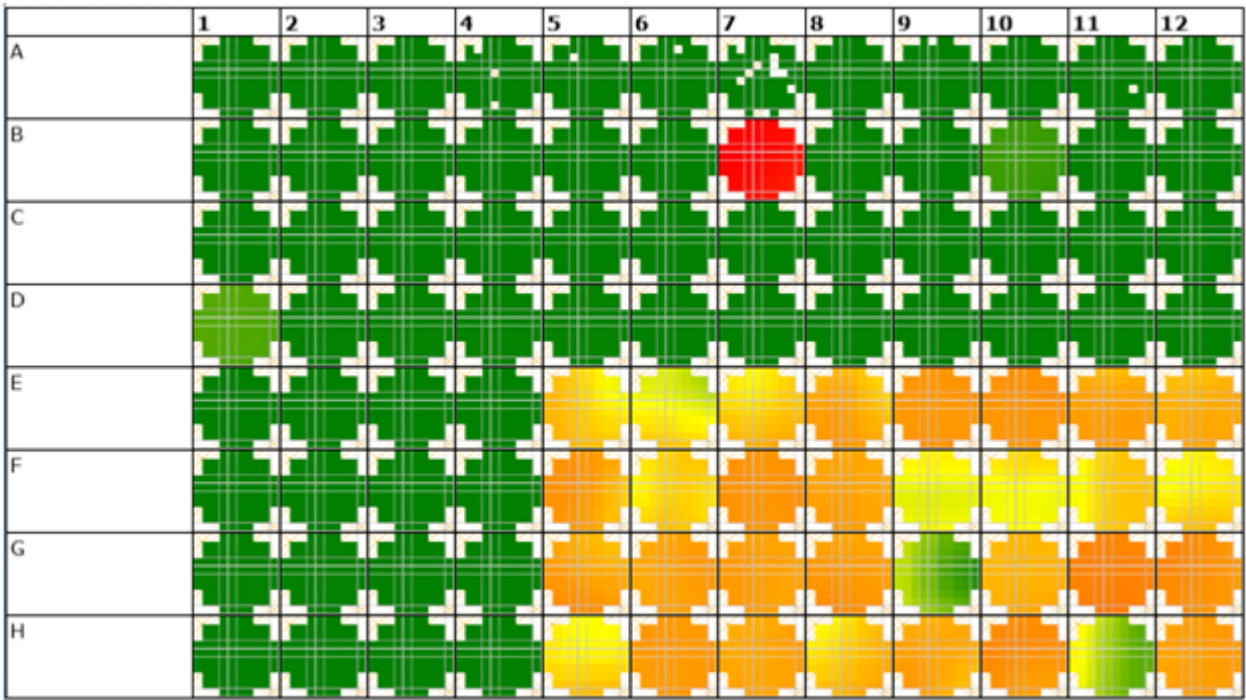
General Assay Advice

Common ELISA Problems and Solutions

Enzyme-linked immunosorbent assays (ELISA) are widely used tests to detect and quantify biological molecules. They are relatively simple and inexpensive to perform. However, one needs to fully understand the principles of an ELISA to properly interpret the results. As with any biological assay, things occasionally don't go as planned. In this article, we will describe useful controls to include with each assay run and how to interpret results, and suggest solutions to try when the controls indicate a problem with the assay.

ELISAs come in many forms. For the purpose of this article, we will refer to a relatively straightforward and common ELISA format: the antigen capture.

Prototype Antigen Capture Assay
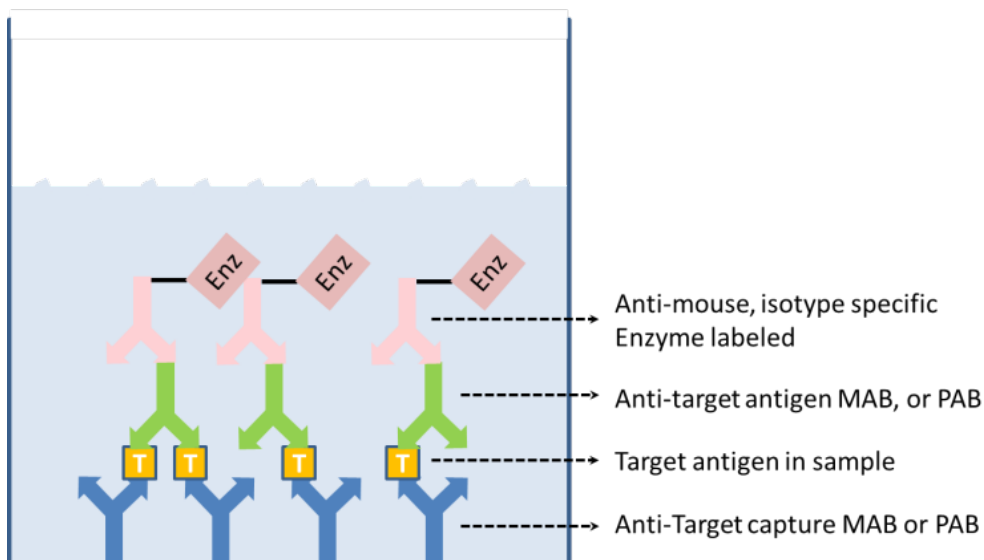
Each reagent is made in optimized buffers. One starts by adsorption of the anti-target capture monoclonal (MAB) to the microtiter plate. Excess MAB is washed out of the wells, and a blocking buffer is added to prevent further binding of any reagents to the plate itself. Typically there is a wash step between all reagent addition steps of the ELISA. A sample containing the target antigen is added and bound by the capture antibody. A second anti-target MAB, known as the detector, is added. This also binds to the target antigen. The detector MAB may be labeled in some way, or a third anti-mouse isotype-specific MAB which binds to the detector MAB is added to the wells. This third antibody will be labeled. Typically the label is an enzyme, but it may be any easily detectable entity. If an enzyme is used, then a substrate for that enzyme is added to the wells. The substrate is designed such that the action of the enzyme will produce a colorimetric change in the well, which may easily be measured at the proper wavelength of light by spectrographic instrumentation. This colorimetric change is usually

reported as an optical density (OD, the log of the absorbance at the chosen wavelength). The optical density is then proportional to the amount of captured antigen in the sample.

Of course, controls should be performed along with the sample to ensure proper interpretation of the results for a given assay run. It is these controls that allow one to ensure that the assay is performed according to expectations. There is a short list of common controls typically included with each ELISA. Below we will define those controls and discuss what they can tell us about the performance of a given ELISA run.

The Blank (B)

The B control consists of a microtiter well or wells that are coated with the capture antibody and blocked with blocking buffer. These wells do not receive any sample or detector antibodies. The blank wells control for any variation, or contribution, of the plate itself to the measured OD. Expected values for the blank are quite low, approaching zero. Each assay typically has a few wells designated for the blank control. These wells may be placed adjacent to each other, or randomly across the plate to make the statisticians happy. If all goes well, then one can assume that the plates were manufactured properly and the blocking agent is performing as expected. However, if the blank well OD is higher than normally seen, the assay may have a problem. High ODs in the blank well may indicate a plate-washer problem. Further investigation of the plate-washing procedure, buffers, and instrumentation are warranted. The problem may be as simple as a clogged tube on the washer, especially if the problem is isolated to a single well. If the problem occurs in more than one well, a more thorough investigation of the wash process is needed. Once the washer checks out, then consideration of the substrate preparation should be investigated. Too much substrate can push the blank well ODs up as well.

Zero Concentration (ZC)

This ZC control is similar to the blank but contains all buffers and reagents from each step of the assay. The sample should contain only sample buffer with no target antigen. This is sometimes difficult to achieve, especially if one is measuring a common antigen that is found at measurable concentrations in the likely sample matrix. Sometimes one has to be creative to obtain or create a true zero concentration control. Once created or obtained, a ZC control allows one to determine the contribution of all reagents and buffers to our assay signal, absent any target antigen. Thus we have determined the true "background" of the assay.

If all goes well with the assay, one should expect to see OD values in the ZC wells that are only slightly higher than our blank wells. The actual values seen will likely vary among different assays for different target antigens. For each given assay, the control values should be consistent across runs. This control is also necessary if one wants to calculate a true limit of detection for an assay. Once the zero concentration is established, it serves as a benchmark for the sum of all reagents and buffers in the assay. Changes to the signal, either up or down,

indicate a change to the assay that requires investigation. As with most ELISA performance issues, double-check the plate washer as described before. It cannot be stressed enough that proper care and maintenance of your plate washer will prevent many assay problems. However, once you have ruled out a plate-washer problem, it will be necessary to double-check reagent preparation, storage, and delivery. One needs to understand the stability profiles of all ELISA reagents. Adhering to the commercial kit guidelines usually prevents problems, but not always, so be aware.

Non-Specific Binding (NSB)

This is a variation on the blank and zero concentration wells. The goal is to further isolate the performance of assay reagents to ensure their proper function in the assay. For the NSB control, the wells are blocked as usual, but then blocking or wash buffer is added in place of the reagents at each step of the assay. The final addition of the labeled detector antibody is performed in the usual manner. Subsequent substrate development then occurs. This control allows one to assess the contribution of the labeled detector antibody to the overall OD signal of the assay. Desired OD results for NSB wells are slightly over the B control wells, but not over the ZC wells. Any differences in signal, up or down, can be attributed to the performance of the labeled detector antibody and may need to be investigated. Look carefully at reagent preparation and delivery. Improperly prepared detector antibody or substrate will easily affect this control and of course the rest of the assay.

Maximum Binding (B0)

We have been focusing on controls that look at the low end, or background, of the assay signal. Of equal importance is a good estimate of the maximum signal possible in the assay. This can be achieved by adding saturating amounts of sample to the capture assay, followed by saturating amounts of the labeled detector. After addition of substrate, a maximum colorimetric response will be determined.

A maximum binding control is necessary if one wants to subsequently calculate a % bound of sample. This calculation is performed when utilizing a competitive format antigen capture assay. In this case, the labeled target antigen would compete with unlabeled from the sample. However, even without using the competitive format, it is a good idea to perform a maximum binding control. By using this control, one will know the upper limit of the signal generated by the assay. Depending on how the assay has been developed, values for such a control may actually exceed the ability of the instrument to measure OD. If this is the case, it may be necessary to cut back on the target antigen concentration until the OD is reduced to measurable levels. If the maximum binding OD values then drop, or even rise, one knows that there has been a change in the assay performance. As always, give the washer and the wash procedure a good review. After determining that the washer is working well, examine assay procedures and reagent preparation and delivery. Typically this control will pick up sample,

substrate, or detector antibody issues. If a problem occurs, it is likely the B0 control will come in lower than expected, which may indicate a preparation or delivery problem in one or more of the three key reagents.

Summary

The use of the controls described above will help in determining the probable cause and hopefully lead to solutions to any problems encountered in the performance of an ELISA. In summary, there are really only a few things that can go wrong with an ELISA. As stressed above, the plate-wash instrumentation, buffers, and procedure are always likely causes of problems. Plate-wash problems frequently mimic reagent issues, so it is always wise to ensure that the washer is not the source of problems before pursuing other ends. Assuming the washer is not the problem, one typically can categorize the problems as follows: low or no signal, high background, inconsistent results between replicate samples or controls, or samples out of range (high or low).

If the entire plate is blank or has minimal signal, one can conclude that a procedural error has occurred or a key reagent was bad. Since the low signal is seen across the plate, it is likely that the labeled detector antibody was not added to the assay system. It is also possible that the enzyme is non-functional, but this is rare. A quick test for enzyme functionality is to add some correctly prepared enzyme labeled MAB directly to the substrate. The expected colorimetric change should occur rapidly. Another possibility is that the substrate is bad or was improperly prepared. Double-check procedures to make sure that the appropriate substrate buffer was used, as this may severely inhibit the expected colour change. If you have an old lot of substrate, you can compare this to the new lot to ensure activity is relatively similar.

A high background is likely a reagent preparation problem. Too much labeled detector may cause this type of response in an assay. One has to double-check that the blocking step was also performed correctly. Was the right amount of block used in the right buffer?

Inconsistent results across replicate samples or controls are one of the most difficult issues to deal with. Assuming we have ruled out the plate washer, then one might have to consider a bad lot of plates or manufacturing issues. To rule out manufacturer problems, it may be necessary to test different kit lots. Be sure to track the lot numbers of the individual components of each test kit. Frequently, kit lots share the lot numbers of one or more components. In addition to bad plates, one has to look at the ability of the operator to pipette accurately. Small variations in pipetting across multiple reagents can produce results that will not pass quality control limits of variability.

Sometimes the controls all pass quality control criteria, but the samples themselves appear to be problematic. On occasion one may notice that the samples are exhibiting higher or lower than normal OD signals. Depending on the expected variability of samples, this can be difficult to notice. It is likely due to procedural issues such preparing the wrong sample dilution, using

the wrong buffer, or pipetting the incorrect amount. One should also be aware of sample handling. While it is relatively easy to document sample handling in one's own laboratory, it can be quite difficult to determine if problems have occurred somewhere else in the sample's chain of custody. Be aware that sample handling is of the utmost importance for reliable results, both within one's own laboratory and outside the laboratory.

Should your assay not behave as expected, the solutions discussed above will provide good starting points to quickly resolve your problems.

Written by James E. Drummond Ph.D

How to Choose and Optimize ELISA Reagents and Procedures

ELISAs have been used for detection of biological molecules since the 1970s. Over time, scientists have developed and utilized many variations of this assay format. The various types of ELISAs (Antibody detection, Antigen capture, Sandwich, Competitive, etc.) are really variations on a theme. The overarching themes of ELISAs are to specifically and sensitively detect a biological molecule (antibody, cell receptor, cytokine, etc.) in a biological matrix. Virtually any type of molecule (protein, lipid, carbohydrate, nucleic acid, etc.) can be detected by an appropriately developed ELISA.

Briefly, the ELISA works by attaching a capture moiety to a microtiter plate, allowing a sample to bind, and detecting the sample via another binding moiety coupled to a signal generating molecule. The capture and detector components are usually added at saturating concentrations and allowed to come to binding equilibrium. Excess unbound material is washed out of the wells in between each assay step. The sample concentration will, of course, be variable. This article will describe general concepts to keep in mind as you choose and optimize ELISA reagents and procedures.

In this day and age it is usually possible to find many commercially available ELISA reagents. These include a wide variety of antibodies to many different biologically important molecules, multiple buffers, and a wide assortment of detection and signal generation molecules. However, sometimes appropriate reagents are not available and will need to be developed. The rest of this article will assume the development of an antigen capture ELISA for detection of a serum cytokine. In general, try to maximize desired binding events while minimizing the unintended binding events. Optimization of reagents is accomplished by maximizing "signal to noise" ratios between positive and negative samples. Using the example assay, key areas that need attention in the development of every ELISA assay will be addressed.

The Target

First and foremost one must understand the target of the ELISA. By this I mean more than just what the target is, although that is definitely an important first step. One must understand the biological and chemical characteristics of the target molecule. Both aspects of a target cytokine can affect the ELISA. Understanding the chemical nature of the target molecule is essential to choosing appropriate sample buffers to obtain, store, and test the target molecule. Obtaining some purified target material will assist with preliminary stability testing in likely buffers and matrices. On the biological front, some easy questions, which might not have easy answers, need to be asked. First, how much target cytokine is likely to be present in the desired sample? If there is very little target present, such as picograms or less, then one will need to spend time and effort to find or develop sensitive capture and detector reagents. If

the target is present at milligram quantities or greater, then it will probably be easier to find or develop the capture and detection reagents.

Secondly, how does the target cytokine exist in its normal matrix? Does the target have any interactions with other biological molecules and to what extent? Does it exist as whole molecules or as various metabolic fragments? Cytokines frequently exist in serum bound to other molecules. These other binding partner molecules may confound the binding of capture and/or detection reagents to the cytokine. Capture and detector reagents that work in the presence of these target binding partners need to be carefully chosen or developed to accurately detect the target cytokine. If the target can exist in the sample matrix as a whole molecule along with some number of metabolic fragments, then internal competition of fragments with whole molecules may occur within the ELISA. One fragment may bind nicely to the capture reagents, but not present a suitable epitope for the detector reagents. Many variations of this problem will impact the accuracy of the ELISA. In essence, one needs to develop and optimize the capture and detector reagents as a pair, not as stand-alone molecules.

The Capture

Assuming one has the target identified and well characterized; it is time for a first go at the cytokine detection assay. It is necessary to line up the anticipated capture antibody, samples, detector antibody, signal generator, and all the appropriate buffers to go along with them. Choose an assay format that can fit with the available laboratory tools and instrumentation (i.e., pipetters, plate washers, plate readers, etc.). The 96 well polystyrene microtiter plate is generally a great place to start. There are many variations of microtiter plate with different binding characteristics. For initial attempts, a generic ELISA plate is recommended. Once the assay is established, one can decide if the more expensive high binding plates will improve the assay or not.

The cytokine antigen assay will utilize an anti-cytokine polyclonal antibody (PAB) to capture the target cytokine. The choice of capture reagent will change depending on the needs of each assay. It is important to optimally attach the capture PAB to the plate. This can usually be accomplished via passive adsorption. A fairly minimalist buffer such as phosphate buffered saline (PBS pH 7.4), or carbonate/bicarbonate buffer (pH 9.5), is typically used to dissolve the capture PAB. Adjusting the pH is an easy way to alter the charge on the capture PAB or other protein that one may be adsorbing to a plate. Try a few different concentrations of capture PAB because the buffer/antibody/plate combination may vary in binding capacity. A good PAB concentration to bracket around is 1 µg/ml. This may vary for other proteins. It is recommended that you test the binding of the PAB to the plate by completing the assay. Since the rest of the assay has yet to be optimized you need to use reasonable reagent concentrations and chemistries for choosing the remaining reagents. These will subsequently be optimized. Initial capture PAB binding to the microtiter plate should incubate for at least 1

hour. Incubation times may need further optimization to ensure complete binding has occurred to the microtiter plate.

The Wash

After the capture PAB incubation one needs to utilize a wash buffer. The purpose of the wash buffer is to remove assay components that are not bound to the plate in an intended fashion. Wash buffers are usually formulated at physiologic pH and salt concentrations (e.g., PBS). The goal is to be gentle and prevent denaturation of any assay components while at the same time removing excess material not specifically and tightly bound to the well. To accomplish this, it may be necessary to add some mild detergents to the wash buffer. A good place to start is with Tween-20, or something similar, at 0.5% or thereabouts.

The type of detergent and its concentration must be compatible with all assay reagents. Too much detergent, or the wrong one, may wash capture PAB off the plate or inhibit binding of assay components. Sometimes additional proteins may be added to help stabilize assay components. It will be necessary to do some empirical testing to make sure of complete assay compatibility. For ease of use a single wash buffer is generally used for a given ELISA. Rarely certain assay reagents may require different wash buffers. Understanding the chemistry and biology is a must. The proper wash will greatly stabilize the assay leading to sensitive and accurate results.

The number of washes is arrived at empirically. In essence, washing is just diluting the soluble components of the well. Think about how much of a dilution is needed at each step in the ELISA. One needs to balance washing out the undesired components with reducing the amount of the desired components in the assay. Stability of the wash fluid is often overlooked, especially in laboratories with low throughput. Wash fluids can begin to grow unwanted "things" if left sitting. Adding a preservative or ensuring the wash is made fresh for each assay will likely prevent any stability problems. Don't forget plate washer maintenance to prevent clogging of tubes. Nothing creates false positives faster than a faulty plate washer.

The Block

After the first wash to remove excess capture molecules, it is necessary to block the well. The purpose of the blocking step is to prevent any non-specific (i.e., unintended) binding of other assay components to the well. The blocking agent usually consists of some assay neutral protein that is unlikely to interfere with any of the other binding events in the assay. Try readily available solutions first, such as 1-5% albumin or casein, before investigating more exotic blocking mixes. There are many commercial blocking mixes that work very well and can sometimes serve as a starting point for further modification to achieve optimal blocking. A good blocking buffer may also contain detergents. The detergents may be similar to the wash buffer or may vary. Understanding the interactions of a detergent with the chosen microtiter plate and other assay reagents is necessary to help in the selection. Be careful with detergents

as they sometimes have a tendency to remove desired components from the well, thereby decreasing sensitivity. All components of a blocking solution should be tested to ensure they are not inhibiting any of the subsequent binding events in the assay. The last step of the block is to wash out the excess blocking solution in preparation for sample addition.

The Sample

The sample is, of course, the key component to any ELISA. Take care in acquiring, transporting, and storing samples. These are critical components of any assay. It is essential that everything under your control happens as you planned. Things out of your control need to be documented and the impact on the sample well understood. For instance, one should be able to tell that the samples sat under the equatorial sun for three days and therefore may not be suitable for the assay. But, let's get back to the things happening in the lab that are under your control.

When the sample arrives in the lab, it should be stored in a manner that will stabilize the target molecules and minimize any other degradation that could interfere with the assay. Many samples are not assay ready as collected. They will need to be further processed to alter the concentration and sample matrix/buffer. This buffer should be well thought out to prevent any degradation to the target molecule in the sample. In addition, the sample buffer must be compatible with all other components in the assay. A good first choice of sample buffer is, in fact, the blocking buffer. Depending on the sample, the buffer may be adjusted (i.e., pH, salts, detergent, stabilizers) based on the biologic and chemical constraints of the target molecule. The sample incubation must achieve binding equilibrium with the capture molecules. The timing of this will vary depending on sample concentration and affinity for the capture reagents. As always the microtiter plates are washed prior to the next step.

The Detector

There are many different detection systems employed by ELISAs. The goal of each is sensitive and specific detection of the target molecule. The cytokine detection assay will employ a standard monoclonal antitarget Monoclonal antibody (MAB). There are many fine commercially available antibodies to many biologic molecules. Of course, you will have to test a given MAB in the assay to ensure that it meets your needs. The detector MAB is usually unlabeled. This ensures that the MAB has not been altered in any way and will provide the desired sensitivity and specificity. The detection antibody is usually diluted in the blocking buffer, or perhaps in a manufacturers recommended buffer. Either buffer is a great place to start, but always keep in mind that modifications may be necessary based on the chemical needs of the target and other assay components. The proper dilution is usually arrived at empirically by titering the antibody and comparing relative sample to background signal strength between known positive and negative samples. The goal of the assay to measure very low concentration or perhaps high concentration samples may drive the final choice for

detector MAB concentration and buffer. After suitable sample incubation which allows for binding equilibrium, excess non-bound detector is washed from the wells.

The Signal

At this point the signal generation components are added. For the cytokine assay an anti-species antibody directed against our detector MAB is utilized. The anti-species antibody is conjugated to an enzyme. Some popular enzymes are alkaline phosphatase and horseradish peroxidase. There are many commercially available antibody-enzyme signal generation combinations for a multitude of species. However, they are not all created equal, and it is usually prudent to test several. In the end, price and convenience may also drive the choice of signal system. Test the signal system by bracketing test dilutions around the manufacturer's recommendation. Frequently you can choose lower concentrations and save some money, but sometimes you may need to have a higher concentration to get the desired assay signal strength. If the manufacturer has a recommended buffer compatible with your assay, then start with that. If you need to use your own buffer, a good place to start is with the blocking buffer. As with all buffer decisions, ensure compatibility with all other assay components.

After signal reagent incubation and wash, an appropriate substrate is added. There are many commercially available stable substrates. It is recommended to go with the commercially available substrates because most of the stability issues have already been solved by the manufacturer. The substrate incubation time will need to be arrived at empirically depending on the amount of target molecule in the samples and the absolute sensitivity of the assay. The substrates will undergo a distinct colorimetric change in the presence of the enzyme. The substrate should show little to no conversion in blank or negative wells. Some substrate systems require a stop solution to be added to the wells after the incubation period. This has the advantage of stopping the reaction across multiple plates at approximately the same time, thereby preventing the last plates read from incubating longer than the first plates read. The plate is now read using any one of many suitable microtiter plate spectrophotometers to measure the optical density of the wells. The optical density is proportional to the amount of target captured in the wells.

There are many different molecules besides enzymes that can generate signals in ELISAs. Some of these include fluorescent molecules, chemiluminescent molecules, and even colloidal gold. Discussion of the relative merits of the different signal generation molecules is best left to another article.

The Incubations

The term incubation has been mentioned several times above. Clearly each step of the ELISA has an incubation component. For an ELISA to work, the various components of the capture, sample, detector, and signal generation must be allowed to come together. Incubation time and temperature are two additional components that greatly affect the outcome of the ELISA.

Sufficient time for binding equilibrium to occur must be achieved at each step. The higher the affinity between components the faster this equilibrium can be achieved. Typical ELISA steps require a minimum 30 minutes of incubation and may easily require more. Sufficient time to achieve equilibrium between surface bound and soluble components at each step of the ELISA must be achieved.

It is much better to use some sort of controlled temperature incubator rather than to trust the building maintenance man to keep the room air at a constant temperature. Even 2-3â° C differences will affect ELISA results, especially if one is trying to quantitate or measure samples near the lower cutoff of the assay. Time and temperature optimization and consistency will greatly add to assay stability over time or between labs.

In addition, gentle mixing of the microtiter plate is sometimes recommended. If mixing is needed, it can best be addressed with an optimized assay. Remember that the conditions the assay has been optimized under need to be replicated whenever and wherever the assay is performed. Will the likely users of the assay have all the necessary equipment and reagents to successfully execute the ELISA? Keep this in mind if your assay users will be in clinically regulated laboratories or out in the bush.

The Analysis

During the reagent optimization the assay signal from known positive samples is continuously compared with the signal from known negative samples. Assay reagent concentrations, buffers, and incubations are adjusted to maximize this "signal to noise" ratio. Now one has an optimized assay format along with all key reagents and buffers. The assay is ready to be put to the test. Can the ELISA distinguish between true positive and negative samples? What are the upper and lower limits of the assay? How reproducible is the assay? If necessary, work with your organization's internal review board to ensure that appropriate consent has been obtained if you are planning to use human samples.

It is essential to obtain or create a panel of samples consisting of positives, negatives, and blanks. The panels should be 10 or more samples from populations likely to serve as actual sample sources. If the ELISA will be used on many different populations, then these populations should be represented in the panels. The positives need to cover the expected range of target molecules one is likely to acquire under real use conditions. In the case of the cytokine we are seeking, it may not be possible to obtain strong enough positives unless we acquire samples from ill individuals or "create" them by spiking known amounts of purified cytokine into negative samples. On the other hand, it may not be possible to obtain negative samples if the cytokine is normally at detectable levels in all people. In that case some thought may be needed on how to create a negative that is as similar to the real sample matrix as possible. Depleting samples of the target may be a viable option to create negative samples. This needs to be done in a manner that is not harmful to the sample matrix. Substituting with

other species samples can be done but should be approached with caution due to specificity concerns.

However one obtains or creates the appropriate positive and negative samples, it is now time to test the system. Consulting with a statistician trained in the art of assay development would be wise at this juncture. The statistician can help with plans to show the limits of the assay and how to set a cutoff. Repeat assay runs can easily document the true reproducibility of the assay. That being said, a good place to start with a cutoff is 2-3 standard deviations above the average response of your negative samples. Multiple runs will be necessary to accurately determine the reproducibility of the ELISA. The goal is to set a cutoff that minimizes false negatives and positives.

With all that has been discussed, one should be well equipped to develop and optimize a reasonable ELISA. Remember that every target/Ab combination is unique. If one is ready for surprises, they can usually be addressed.

Written by James E. Drummond Ph.D

Curve Fitting

Is My Fit a Good Fit?

The term "good fit" can cover a number of factors. To evaluate how good your curve fit is, you can assess your curve and verify if it fits with the following suggested evaluations.

First, it is always important to view each curve critically to check for sample preparation errors or an erratic fit and to verify that the curve's general direction matches the expectations for the assay type.

One common goodness measure is R^2. If this metric is > 0.9, then generally speaking, the model is considered to be a good fit to the data (the closer to 1 the better). Each laboratory will likely define an acceptable threshold for the goodness measure used to validate the assay. Other goodness measures are also available.

In addition, it is important to consider how good the fit is across the standards by considering the precision and accuracy of the fit at each point. This is why the software computes LLOQ and ULOQ and includes the calibrator table to clearly indicate where the precision (%CV) and accuracy (% Accuracy) are within range.

It is quite common to see poorer accuracy at the upper or lower ranges of the standards. In this case, you may want to consider reassaying those samples that fall outside of this range (by diluting or concentrating and applying a suitable dilution factor).

Where precision is poor an outlier might be the cause. In this case, the software can be used to flag and ignore the outlier, and the results can be recalculated excluding the outliers.

To automate the determination of a good fit, controls can be included. These will typically have a known concentration (or an acceptable concentration range) with validations used to automatically check that the computed concentrations match these expected quantities.

Goodness of Fit Measures

The goodness of fit measures are calculated when each fit method is used. These measures indicate how well the curve model fits the data.

The following table describes these measures and how they can be used to assess the fit.

Name	Description
R^2	R^2 is 1 minus the ratio of the sum of the squares of the residuals divided by the sum of the squares of the differences between y fit and the mean y value). This will equal 1 for a perfect fit and tend toward 0 for a bad fit. In other words, R^2 is the ratio of variation that is explained by the curve-fitting model to the total variation in the model. In most situations, irreducible errors in measurement will prevent the model from explaining all the variation. Models using a larger set of factors may produce an R^2 value that is closer to 1. However, it may be that the additional factors are essentially modeling noise.
aR^2	aR^2 is the adjusted R^2 value. aR^2 is R^2 adjusted downward to compensate for overfitting. The larger the number of independent variables is (compared to the number of observations), the lower the adjusted R^2 value will be. When using curve fitting models with a larger number of independent variables, the additional variables may be simply modeling noise.
P	P is the P-value. P is the significance of the model as a probability. It is the P-value of F for the curve-fitting model. This compares the variance attributed to the model with the variance of the residual.
SE	SE is the standard error. The standard error is the root mean square of the residuals.
F	F is the F-statistic. F is the ratio of the variance explained by the curve fitting model to the residual variance.
AIC	AIC is Akaike's Information Criterion; this provides an estimate of the quality of the curve-fitting model for comparison against other models. AIC can be used to compare curve-fitting models and determine which is the best. The model with the lowest AIC value is most likely to be correct (AIC values can be negative). AIC will favour simpler curve-fitting models over those with more parameters (it achieves this by applying a penalty proportional to the number of parameters).
AICc	AICc is Akaike's Information Criterion corrected for small sample sizes. Use this method instead of AIC when comparing curve-fitting models for smaller

Name	Description
	sample sizes (number of calibrators).
	📝 This method is only applicable when the number of calibrators is at least two greater than the number of parameters.
BIC	BIC is Bayesian Information Criterion; this is very similar to AIC. The key difference is that BIC imposes a higher penalty for the number of parameters in the model.
DWS	DWS is the Durbin-Watson Statistic; this is used to detect the presence of autocorrelation (at lag 1) in the residuals of the regression. DWS values range between 0 and 4. A value close to zero indicates a positive autocorrelation between the residuals. A value close to 4 indicates a negative autocorrelation between the residuals. A value around 2 indicates there is no significant autocorrelation.
DoF	DoF is Degrees of Freedom; this is computed as the number of calibrators minus the number of parameters in the fit. The number of calibrators depends on the selected **Fit To Standard** option; for **Replicates** (if there are replicates) will be more degrees of freedom than for **Average**.
	📝 If there are not enough **Degrees of Freedom**, then values for **P**, **F**, **SE** and **aR^2** cannot be computed.
RMS	RMS is the Root Mean Square of the residuals (reported for Auto Smoothed Spline only). RMS is the square root of the residual mean squared.
SSE	SSE is the Sum of Squared Errors, the sum of squares of the residuals of the model.

Accuracy and Precision

This section describes how the accuracy and precision of the Standard Curve Fit are defined, used, and computed in a quantitative analysis.

Definition

Accuracy is a measure of how close a measurement matches its known value (standard).

Precision is a measure of how close replicated measurements are to each other.

Limits

You will typically want to define acceptable limits of accuracy and precision for your assays. The acceptable limits depend on the application of the assay. MyAssays Desktop default limits are as follows:

- Accuracy ±20%
- Precision ≤20%

> These values can be adjusted through the Accuracy and Precision Quantification Limits of the Standard Curve Fit.

With a Standard Curve Fit, the accuracy and precision are likely to vary across the standards. Because of this, it is useful to determine the upper and lower limits of quantification (ULOQ and LLOQ) and only use the curve to compute values within that range.

These quantification limits are determined by computing the accuracy and precision of each standard measurement and computed concentration from the curve.

Computation

Accuracy

To measure the accuracy of the curve at a particular standard, the *x* value of the known concentration (expected) is compared against the *x* value at this point computed from the curve (actual).

So % Recovery or % Accuracy is simply:

= 100 * Actual / Expected

= 100 * (calculated concentration) / (defined concentration)

Precision

To measure the precision of the curve for a particular calibrator (**Standard Type** sample), the %CV is calculated as the % of the standard deviation (SD) of the standard's replicate measurements divided by their mean.

This way % CV Precision is calculated as:

100 * SD / Average

= 100* (standard deviation of calibrator)/(average value of calibrator's replicates)

Evaluation and Results

Accuracy and precision are calculated from the curve with the LLOQ and ULOQ determined from these values; the results for each standard are included in right-most columns of Curve Data Table.

To clearly indicate whether each standard is within the acceptable range or not, each row is highlighted based on whether it satisfies the specified precision and accuracy rules (rows in light-red fail the test).

Fit Methods

Which Fit Method Should I Use?

A single fit method that works perfectly for all assays sadly does not exist. Any curve fitting model is a compromise and simplification of reality in some way or another.

As a first step of evaluating any applied fit, it is important to critically view the curve to check for sample preparation errors or an erratic fit.

In general, the 4PL or 5PL are the best models for dose–response curves; these model the sigmoidal nature of saturation curves very well. These methods are widely used, cited, and recommended. However, where samples fall outside these saturation limits (the upper and lower asymptotes) no result can be computed and this can be frustrating. Where this occurs, the common advice is to dilute/concentrate the sample and reassay. Alternatively, with weighting applied to these models, the fit can be biased to go through specific points (such as those nearer the *x* or *y* axis). This is useful, if it is important to have good curve accuracy at one end of the curve and to ensure the fit has an expected range of usage.

For certain assays (and especially when working with validated kits), a statistician or manufacturer may recommend a specific 4PL or 5PL model with a particular weighting. In those cases, it is important to use the same method for each run of the assay (and, of course, MyAssays Desktop supports that).

However, without this guidance, it can become tedious to try out different methods and models for each assay run. It is for this reason that MyAssays Desktop Pro includes the Best Fit feature. With this option, MyAssays Desktop will perform multiple fits with different weighting options and automatically pick and apply the "best". What is deemed to be the best is open to interpretation and it is for this reason that the software allows you to select different scoring methods. The fit with the highest score is considered to be the best.

After selecting the **Best Fit** fit method, select which fits and weighting methods to consider. For example, with:
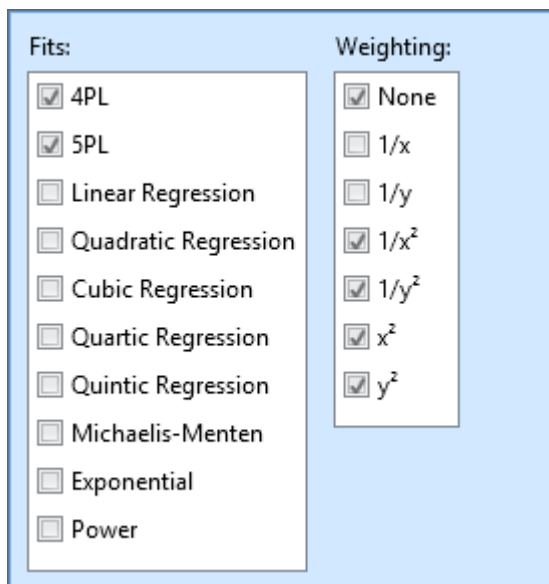
10 methods will be compared.

Next, specify a fit score method from:

- R^2
- R^2 with Low-End Accuracy
- R^2 with High-End Accuracy
- R^2 with Low-End and High-End Accuracy
- 1/Standard-Error
- 1/P-Value
- -AIC
- -AICc
- -BIC

R^2 is a common method for evaluating a fit, however, care should be taken when using this to compare different fit models (it does not take into account the differences between models). 1/Standard-Error is a good choice for finding the fit with the lowest standard error. The AIC, AICc, and BIC methods are useful for evaluating different models and these penalize more complicated models (i.e., those with more terms).

For even further flexibility, it is also possible to define your own fit score methods. To learn more about this feature, see Custom Fit.

Alternatively, MyAssays Desktop includes legacy fits like the Auto Smoothed Spline method in an attempt to provide a "set-it and forget-it" solution. This may be preferable in some situations (like RIAs) where a good fit is acceptable, as opposed to identifying a more accurate

fit that requires operator intervention. Auto Smoothed Spline is based on the cubic spline fit, so the accuracy can be poor and can lead to unnatural looking curves and erratic behaviour. The pure Cubic Spline method will exactly trace through every data point so the Auto Smoothed method attempts to smooth the fit automatically. The Cubic Spline Smoothed applies a fixed smoothing parameter.

Linear Regression

It is a basic and easy regression model that fits data linearly.

Linear regression sets the linear relationship between the dependent variable (*y*) and a single independent variable (*x*). This model provides starting approximation and, although is seldom used for biological systems, is often used to visualize data relationship at a glance.

The equation for the model is:

$$y = mx + c$$

Variables

In this model we have the following:

y = the dependent variable (i.e., what you measure as the signal)

x = the independent variable (i.e., what you control, such as dose, concentration, etc.)

Coefficients of the Fit

m = the slope of the fitted line

c = the intercept of the dependent axis

The rearranged equation to solve *x* is:

$$x = \frac{y - c}{m}$$

The goal is to determine values of **m** and **c** that minimize the sum of squares (SS) of the residuals between the observed values (i.e., your data) and the predicted values (i.e., the fitted curve). As some observed values will likely be above the fitted curve and some below, you will get positive and negative residuals. SS is used to square each of the residuals, which render all the values positive, then sum them. The smaller the SS, the closer the observed values are to the predicted, the better the model predicts your data.

The fitted plot may show the data to be nonlinear. In this case, it is advised to consider using different methods.

Four Parameter Logistic Regression (4PL)

This nonlinear symmetrical sigmoidal model is known as 4-parameter logistic regression (4PL).

It is quite useful for dose–response and/or receptor–ligand binding assays, or other similar types of assays. As the name implies, it has 4 parameters that need to be determined in order to "fit the curve." The model fits data that makes a sort of S-shaped curve that is symmetrical around its inflection point.

The equation for the model is:

$$y = d + \frac{a-d}{1+\left(\frac{x}{c}\right)^b}$$

Variables

In this model we have the following:

y = the dependent variable (i.e., what you measure as the signal)

x = the independent variable (i.e., what you control, such as dose, concentration, etc.)

Coefficients of the Fit

The 4 parameters consist of the following:

- **a** = the minimum value that can be obtained (i.e., what happens at 0 dose).
- **d** = the maximum value that can be obtained (i.e., what happens at infinite dose).
- **c** = the point of inflection (i.e., the value of x at the point on the S-shaped curve halfway between a and d).
- **b** = Hill's slope of the curve (i.e., this is related to the steepness of the curve at point **c**). It could either be positive or negative.

The rearranged equation to solve x is:

$$x = c\left(\frac{a-d}{y-d} - 1\right)^{\frac{1}{b}}$$

> The **a** and **d** values might be flipped; however, **a** and **d** will always define the upper and lower asymptotes (horizontals) of the curve. **a** and **d** are the same units at y. The curve can only be used to calculate concentrations for signals within **a** and **d**. Samples outside the range of the determined **a** and **d** cannot be calculated.

4PL and IC50

A common requirement is to calculate IC50 from the fit. The IC50 is the concentration of an inhibitor where the response (or binding) is reduced by half. There are actually two ways to do this depending on what you consider IC50 to be:

- Firstly, the midpoint of the sigmoid of the 4PL is equal to the **c** coefficient of the 4PL. In this case you can simply look at the calculated **c** coefficient. Use this method if you consider the midpoint of the sigmoid to be equal to IC50. Mathematically, this is the case as it is the x point at exactly half way between the two horizontal asymptotes.

- Alternatively, if the response is measured between 0 and 100% and you consider IC50 to be where $y = 50$, then you can calculate where $y = 50$ using the equation to solve x (above), substituting in the calculated coefficients.

Best Fit

The Best Fit feature will automatically find the most appropriate fit for your data. The feature processes your data using multiple curve fits and weighting methods and automatically chooses and applies the best performing fit.

> When working with multiplex data and best fit, a best fit search is performed on each analyte. Thus, the results for each analyte in an assay may use different fit methods — the best for each analyte.

Which Fits?

The default configuration will compare the 4PL and 5PL fit methods each with unweighted and various weighting models. These fit methods are the most widely used fit methods for most assays.

Beyond this default configuration, you can select which fit methods and which weighting models to compare. It is also possible to define your own curve fit equation.

What Is Best?

The method used to evaluate which fit is best can be customized. For example, you might consider the fit with the highest R^2 to be the best. You also might want to consider the accuracy of the curve at certain regions of the fit (e.g., at the low or high end of your standards data).

To achieve this flexibility, the system uses a fit score method to quantify how good each fit is. The fit with the highest score is considered to be the best fit.

Fit Score Methods

On completion of each fit, the fit is scored using a fit score method equation. The scores of each fit are compared, and the fit with the highest score is considered to be the best. Thus, the score method equation should quantify how good the fit is.

For convenience, the following preset fit score methods are available for selection:

- R^2
- R^2 with Low-End Accuracy
- R^2 with High-End Accuracy
- R^2 with Low-End and High-End Accuracy
- 1/Standard-Error
- 1/P-Value

- -AIC

- -AICc

- -BIC

Beyond these presets, you can define your own fit score methods to evaluate and compare each attempted fit.

Fit Score Method Expressions

This section describes how to define your own fit score method expressions to evaluate a fit. The fit score method equation can reference the goodness measures determined from the fit:

Goodness Measures

To learn more about available measures and how they can be used to assess the fit, see Goodness of Fit Measures.

Name	Description
R^2	R^2 is 1 minus the ratio of the sum of the squares of the residuals divided by the sum of the squares of the differences between *y* fit and the mean *y* value). This will equal 1 for a perfect fit and tend toward 0 for a bad fit. In other words, R^2 is the ratio of variation that is explained by the curve-fitting model to the total variation in the model. In most situations, irreducible errors in measurement will prevent the model from explaining all the variation. Models using a larger set of factors may produce an R^2 value that is closer to 1. However, it may be that the additional factors are essentially modeling noise.
aR^2	aR^2 is the adjusted R^2 value. aR^2 is R^2 adjusted downward to compensate for overfitting. The larger the number of independent variables is (compared to the number of observations), the lower the adjusted R^2 value will be. When using curve fitting models with a larger number of independent variables, the additional variables may be simply modeling noise.
P	P is the P-value. P is the significance of the model as a probability. It is the P-value of F for the curve-fitting model. This compares the variance attributed to the model with the variance of the residual.
SE	SE is the standard error. The standard error is the root mean square of the residuals.
F	F is the F-statistic. F is the ratio of the variance explained by the curve fitting model to the residual variance.

Name	Description
AIC	AIC is Akaike's Information Criterion; this provides an estimate of the quality of the curve-fitting model for comparison against other models. AIC can be used to compare curve-fitting models and determine which is the best. The model with the lowest AIC value is most likely to be correct (AIC values can be negative). AIC will favour simpler curve-fitting models over those with more parameters (it achieves this by applying a penalty proportional to the number of parameters).
AICc	AICc is Akaike's Information Criterion corrected for small sample sizes. Use this method instead of AIC when comparing curve-fitting models for smaller sample sizes (number of calibrators). This method is only applicable when the number of calibrators is at least two greater than the number of parameters.
BIC	BIC is Bayesian Information Criterion; this is very similar to AIC. The key difference is that BIC imposes a higher penalty for the number of parameters in the model.
DWS	DWS is the Durbin-Watson Statistic; this is used to detect the presence of autocorrelation (at lag 1) in the residuals of the regression. DWS values range between 0 and 4. A value close to zero indicates a positive autocorrelation between the residuals. A value close to 4 indicates a negative autocorrelation between the residuals. A value around 2 indicates there is no significant autocorrelation.
DoF	DoF is Degrees of Freedom; this is computed as the number of calibrators minus the number of parameters in the fit. The number of calibrators depends on the selected **Fit To Standard** option; for **Replicates** (if there are replicates) will be more degrees of freedom than for **Average**. If there are not enough **Degrees of Freedom**, then values for **P**, **F**, **SE** and aR^2 cannot be computed.
RMS	RMS is the Root Mean Square of the residuals (reported for Auto Smoothed Spline only). RMS is the square root of the residual mean squared.
SSE	SSE is the Sum of Squared Errors, the sum of squares of the residuals of the model.

Accuracy Functions

In addition to the Goodness Measures, various accuracy functions are available to assess the accuracy of the fit at various points. These accuracy functions enable a comparison to be

made between the expected value (the known *x* of the calibrator) and its actual value calculated from the curve.

The calibration data set is the known concentration values of the standards (*x*) plotted against their measurements (*y*). Each curve is fitted to the calibration data set.

To simplify combining accuracy functions together and with other measures (such as R^2), the accuracy functions return a value between 0 and 1 (where 1 is perfectly accurate).

Function	Description
AccuracyRatio	Calculates the accuracy ratio of the expected value and its actual value. This is similar to % recovery; however, here a value between 0 and 1 where 1 is perfect accuracy (i.e., 100% recovery). A % Recovery of 120% or 80% both equal an Accuracy Ratio of 0.8. With AccuracyRatio, if the actual value differs from the expected by a factor of 2 or more, the accuracy ratio is 0.
AccuracyFactor	Calculates an accuracy factor of the expected value and its actual value. This is computed using % Recovery and a Gaussian function such that: <table><tr><th>% Recovery</th><th>Accuracy Factor</th></tr><tr><td>100</td><td>1</td></tr><tr><td>0</td><td>0.5</td></tr><tr><td>200</td><td>0.5</td></tr><tr><td><0%</td><td>Value between 0.5 and 0</td></tr><tr><td>>200%</td><td>Value between 0.5 and 0</td></tr></table> This function avoids reporting a value of 0 for scenarios where the % Recovery is <0% and >200%.
Diff	The absolute difference between the expected value, and is the actual value.

Accuracy Function Forms

Each accuracy function comes in three forms:

- At Specified X Point

- From Low end (ends with Low)

- From High end (ends with High)

The following table provides example expressions calling accuracy functions and their result:

Expression	Result
AccuracyRatio (0.125)	The accuracy ratio for calibrator where x=0.125
AccuracyRatioLow (1)	The accuracy ratio for the calibrator with the lowest x value
AccuracyRatioLow (2)	The accuracy ratio for the calibrator with the second-lowest x value
AccuracyRatioHigh (1)	The accuracy ratio for the calibrator with the highest x value
AccuracyRatioHigh (2)	The accuracy ratio for the calibrator with the second-highest x value

Combining Measures

A fit score method can reference various goodness measures and accuracy calculations. Remember that the fit with the highest score is considered to be the best. Therefore, if you plan to consider multiple measures, it is recommended that each measure is a value between 0 and 1 and that the various measures are multiplied together.

Score Method Preset Expressions

To illustrate example scoring methods, the following table lists the expressions used for each of the preset scoring methods:

Preset	Expression
R^2	R^2
R^2 with Low-End Accuracy	R^2*AccuracyFactorLow(1)
R^2 with High-End Accuracy	R^2*AccuracyFactorHigh(1)
R^2 with Low-End and High-End Accuracy	R^2*AccuracyFactorLow(1)*AccuracyFactorHigh(1)
1/Standard-Error	1/SE
1/P-Value	1/P
Akaike's Information Criterion	-AIC
Akaike's Information Criterion corrected	-AICc
Bayesian Information Criterion	-BIC

> For the goodness measures **P-Value** and **Standard-Error** the model with the value closest to zero is likely to have the best fit. In this case, the associated score is computed as the reciprocal of the goodness measure; the value closest to zero will have the highest score and be selected as the best-fit.
> Similarly, for the goodness measures **AIC**, **AICc** and **BIC** the model with the lowest

value is likely to have the best fit. In this case the associated scoring methods are computed as the negative of these computed values; the result is that the fit with the lowest value (highest score) is considered to be the best fit.

Custom Fit Method

With this feature, you can define your own curve equation to use when fitting a curve to your calibration data. The software will automatically determine the best set of values for each unknown coefficient in your equation. In this way you can model your data using your own method.

Writing a Custom Fit Expression

Your curve equation must be defined as an expression as follows:

- Write the equation in terms of *x* (i.e., there must be at least one *x* reference)
- Use mathematical operators
- Use any single letter (excluding *x* and *y*) for each coefficient to compute. For longer coefficient names, enclose the name in square brackets (e.g., **[intercept]**)

> 📋 At least 1 unknown coefficient must be determined by the fit.

Also, you can optionally:

- Refer to TOVs of previous transforms (e.g., calculated coefficients, goodness measures)
- Include Group References, Position References, and Type References in your custom fit.
- Insert constants (numerical values)
- Specify a custom name, weighting, inverse equation and define heuristic rules to improve the curve-fitting accuracy (see Advanced topic)

Examples of Custom Fit Expressions

For example, here are the alternatives for custom fit equation of **4PL with r (from expression)**:

- **d+((a-d)/(1+(r*x/c)^b))** – The expression with single-letter coefficients
- **tov1.d+((tov2.a-tov1.d)/(1+(r*x/tov2.c)^tov1.b))** – The expression uses TOVs from previous transforms as coefficients
- **1.23+((a-1.23)/(1+(r*x/c)^b))** – Here the **d** coefficient is a constant (1.23)
- **d+((a-d)/(1+(r*x/[Slope])^b))** – Here the **c** coefficient is named **Slope**
- **(m*x)+Standard1** - Here the **c** coefficient uses the value of **Standard1** Video Walkthrough...

In addition to defining the expression, you can configure Custom Fit Method further by using advanced custom fit method settings.

Library Curve

The Library Curve feature can be used to save a curve that was measured and computed in one assay for reuse in other assays (perhaps where no standards are measured).

Storing a Curve to the Library

Any curve created with the Standard Curve Fit or General Curve Fit transform can be extracted and saved to a Curve Library file.

The Curve Library file contains all of the data necessary to reproduce the curve and the chart in future analyses. This includes:

- **Curve Configuration** – All the transform settings (e.g., Fit Method, Calculate From, etc.) specified for the original curve
- **Curve Plot Data** – Calibration data (and average points) used in the curve fit
- **Transform Output Content** – Transform-specific report content (as specified in the assay-results file from which it was created)
- **Origin** – The full path to the assay-results file from which it was created

Save a Curve to the Library

1. Add the Standard Curve Fit or General Curve Fit transform.

2. In the **Results** tab, select the **Standard Curve Fit** or **General Curve Fit** subtab. If your assay comprises multiple plates, select the one that contains the analysis view for your data.

3. Click the **Save to Library** button. If there are changes to the Standard Curve Fit or General Curve Fit settings that have not yet been calculated, then a message box will appear with the prompt to choose which results version the curve should be saved.

4. Review and edit a name and (optionally) description for your curve library file as required.

5. Click the **Finish** button.
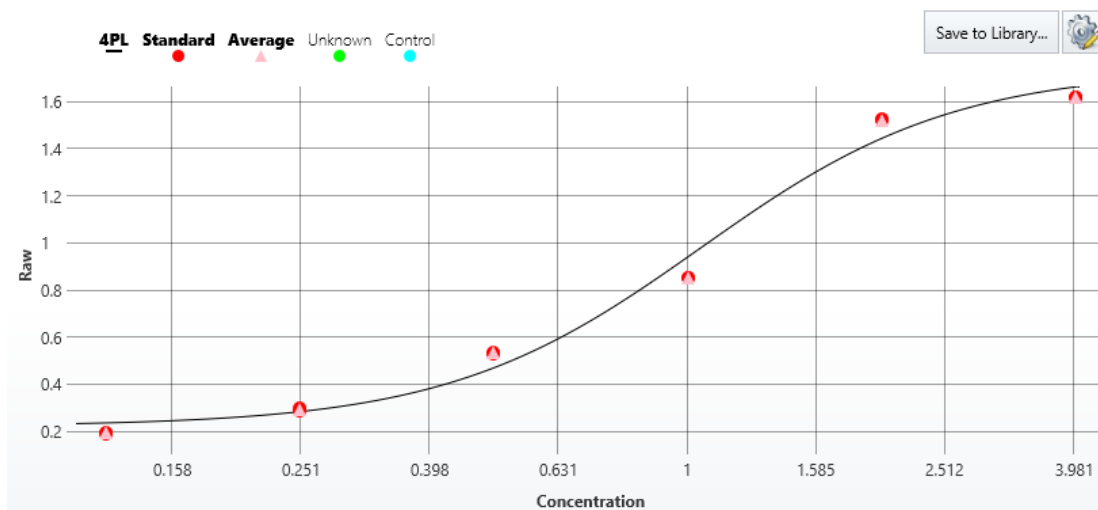
Curve Library files are stored in the **Curves** folder of your MyAssays root folder.

Calculating Results with a Curve from the Library

After the curve is saved, you can apply it by adding a Standard Curve Fit (from Library) transform. The selected curve file is used to recreate the curve for computing the concentrations of all samples measured in the referring assay.

> When using the Standard Curve Fit (from Library) transform on an assay that also includes **Standards** defined on the layout, concentrations for these standards will be computed from the original curve. These standards will not be used to recompute the curve. It can be useful to include controls or a subset of the original standards in subsequent assay runs and use the Validation feature to define expected results to detect sample preparation issues.

Library Curve Details

When reviewing the curve used by the Standard Curve Fit (from Library) transform, click the **Library Curve Details** button on the Standards Chart to review the name, description, and assay results file, from which the Curve Library file is created. Click the results hyperlink to open the containing folder and open then original results file from where the curve was created.
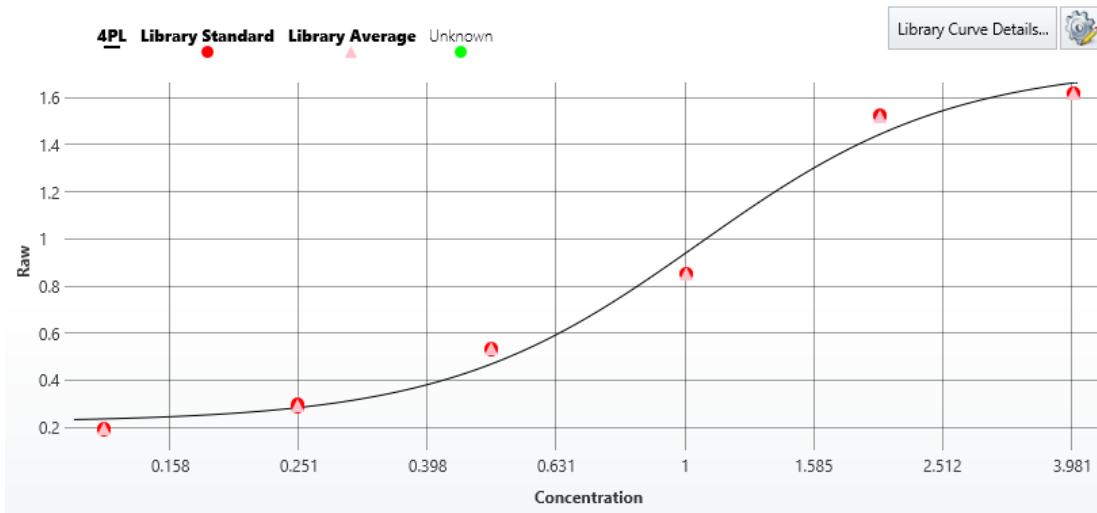
Curve-Fitting Transforms Settings and Configuration

Standard Curve Fit Settings

Multiplex Concentration Editor for Standard Curve Fit

This editor is used to specify concentration values and units of each analyte for the Standard Curve Fit transform when working with a multiplex assay.

The editor is displayed by clicking on the **Concentrations** setting drop-down.

Multiplex concentrations data can be specified in a number of different ways including:

- A start concentration for each analyte with a common dilution/concentration series
- Unique concentration values for each calibrator (standard) of each analyte
- Common concentration units for all multiplexed analytes
- Unique concentration units for each analyte

The display and behaviour of the editor depends on the way in which the data will be specified.

For example, here the editor is displaying a start concentration and dilution series for each analyte with the same concentration units applying to all analytes:

Analyte	Start Conc.		Series		Calibrator	Kim1 Conc. (nm/ml)
Kim1	700		× ÷		● Standard1	700
Clusterin	1000				● Standard2	1400
OPN	10		2		● Standard3	2800
IL8	50				● Standard4	5600
CystatinC	10		≡ Units		● Standard5	11200
NGAL	20		nm/ml		● Standard6	22400
50	10				● Standard7	44800

Selecting the Analyte to Edit

The **Analyte** column of the left-hand **Analyte** grid is used to select and indicate the analyte to edit. Click an analyte name to select to edit its concentration settings.

Concentration Modes

There are two modes for specifying concentrations:

- **Series** – Provide a **Start Conc.** and common series to apply to all analytes. Use this if all of the analytes share a common concentration/dilution series.

- **Non-Serial** – Provide a specific concentrations value for each calibrator of each analyte. Use this if your analytes do not share a common concentration/dilution series or if your concentration values are not in a simple mathematical series.

Click **Series** to switch between the modes.

Series Mode

This mode allows you to define a series to calculate the concentrations of each analyte (from a specified starting concentration). The series calculations are specified using the selection of the multiplication or division operator along with a specified factor or divisor.

With the **Series** turned on, enter or paste the starting calibrator concentration values for each **Analyte** in the **Start Conc.** column of the left-hand **Analyte** grid. The right-hand grid shows the computed concentrations of the selected analyte.

For example, for the selected Kim1 analyte with a **Start Conc.** specified as 700 and **Series** mode on, with multiplication selected and a factor of 2 specified, the concentrations of the analyte are computed and displayed in the right-hand grid as shown here:

Non-Serial Mode

Non-Serial mode allows the specification of the concentration of each calibrator separately.

With the **Series** turned off, select an analyte in the left-hand **Analyte** grid and enter or paste concentration values on the right-hand **Calibrators** grid.

For example, here Kim1 analyte concentration values are specified in non-serial mode.

Analyte	Series	Calibrator	Kim1 Conc. (nm/ml)
Kim1		● Standard1	700
Clusterin	≡ Units	● Standard2	1400
OPN	nm/ml	● Standard3	2800
IL8		● Standard4	5600
CystatinC		● Standard5	11200
NGAL		● Standard6	22400
50		● Standard7	44800

Units Mode

There are two modes for specifying the concentration units of the analytes:

- The same concentration units applies to all analytes

- Concentration units specified for each analyte

Click ≡ **Units** to switch the concentration mode state.

Identical Units for All Analytes

When ≡ **Units** is turned on, the single specified units of concentrations applies to all analytes. In this case, enter the units below the ≡ **Units** button.

Different Units per Analyte

When ≡ **Units** is turned off, you can enter or paste different output units for each analyte in the **Units** column of the left-hand Analytes grid.

Analyte	Start Conc.	Units	Series	Calibrator	Clusterin Conc. (nm/ml)
Kim1	700	pmol/uL	× ÷	● Standard1	1000
Clusterin	1000	nm/ml		● Standard2	2000
OPN	10	ng/ml	2	● Standard3	4000
IL8	50	nm/µl	≡ Units	● Standard4	8000
CystatinC	10	nm/ml		● Standard5	16000
NGAL	20	ng/ml		● Standard6	32000
50	10	nm/µl		● Standard7	64000

Paste Option

For all columns with a paste icon at the bottom, you can copy and paste the clipboard contents to the corresponding column. The content is pasted starting from the first row on a

line by line basis. This is useful if you have your concentration data in another application (such as Excel or notepad).

Standard Curve Fit Analysis for Multiple Plates

For quantitative assays, you may arrange standards on every plate in the batch or you may decide to measure standards only on some plates in the batch. Also, you can specify how the standard curve is generated and which curve to use to calculate concentrations from for each plate.

Common Scenarios

- Measure standards on every plate in the batch. You may select to calculate concentrations using the standard curve on the same plate as the samples. **Example**: 3 plates are read, each uses the same layout, a curve is created for each plate, and concentrations are calculated using the standard curve on the same plate as the samples being calculated.

- Measure standards on some or all plates and generate a single standard curve using standard replicates from across plates. In this case sample concentrations are calculated using a common curve. **Example**: 3 plates are read, each uses the same layout, and a single curve is created using the standard measurements from each plate. The common standard curve is then used to calculate concentrations for all samples on all plates.

- Using a different layout on each plate read. **Example**: 3 plates are read, each uses a different layout, and a single curve is created using the standard measurements from each plate.

- Combine these options and configure a layout that uses a specific curve or common curve for each plate.

Standard Curve Fit Evaluation with Multiple Plate

The additional complexity with evaluating the Standard Curve Fit transform across multiple plates is that for each plate the concentrations must be calculated using the correct curve as specified in the Layout Editor (and taking into account if there are more plates of data than defined in the layout).

For the details of the general procedure, see Multiple Plate Support.

For performance reasons, curves should not be unnecessarily recalculated, thus for evaluating the Standard Curve Fit analysis with a multiple plate assay:

1. Identify the curve to use for each plate.

2. Prepare the calibration data for each required curve.

3. Fit each curve once.

Then, after the curve data has been prepared, go through each plate and use the associated fitted curve to calculate the concentration values.

> ℹ️ There may be more than one curve generated.

Preparing Calibration Data

1. Where the **Curve selection** for a plate refers to the curve on a specific plate (and not the average), the calibration data is prepared using the calibrator data from the specified plate number.

2. If the curve selection is an **Average Across Plate** selection, then the calibration data for the curve is obtained from all layouts with this setting; to be clear, all plates with this selection will use the same common curve that is computed from points across separate plates.

> 📝 As with all other analyses, flagged points are not included in the fit.

If the Standard Curve Fit transform's **FitToStandard** is **Replicates**, then this is the data that will be used for the fit. If **FitToStandard** is **Average**, then the replicates are averaged (i.e., for each x value, there is only 1 y value and that y value is the average of the non-flagged replicates).

Different Concentrations per Container/Plate

When the data for the curve is obtained from the same plate that is being evaluated, you can provide different concentration values per plate/container. With this configuration, the standard concentrations used for the fit are as defined in the Plates section in the XML Editor.

How to: Specify Different Concentrations per Container/Plate

```
<StandardCurveFit StandardType="2" FitMethod="4PL"
Concentrations="0.125,0.25,0.5,1,2,4" XAxisTitle="Concentration" YAxisTitle="Raw"
FitToStandard="Average" CalculateFrom="Replicates">

<Plates>

<Container Concentrations="1,2,4"/>

<Container Concentrations="10,20,40"/>

<Container Concentrations="100,200,400"/>

</Plates>

</StandardCurveFit>
```

If there are more data containers than Container elements defined, then those additional containers will use the primary Concentrations attribute of the Standard Curve Fit properties.

If there are less containers in the data containers than Container elements defined, then those additional Container elements are simply ignored.

Zero Concentration Calibrator

Using a theoretical zero concentration as a standard curve calibrator can be the source of many mathematical problems when fitting standard curves. Firstly, a zero standard can skew the fitting process with certain fit methods leading to an unexpected curve. Also, with any fit method, a zero value cannot be plotted on a logarithmic x-axis (as is typically used to plot a standard curve). Another issue is that a zero concentration will break fit methods with weighting models such as $1/x^2$. A common workaround is to use a suitably small specified concentration value instead (such as 0.001).

If using a suitably small value is not ideal there are some other options.

Measure Zero Without Using It as a Calibrator

In this scenario the zero standard is measured but not included as a calibrator for the fit; the zero standard is used as a control (and not as a calibrator). To achieve this, add the **Zero** sample type to your layout configuration to denote the location of the zero concentration sample(s).

Including a Zero Standard Calibrator

In this case standards are added to the layout as normal, however, the first standard (**Standard1**) is given a known concentration of 0. In some cases, this might not map directly to your actual standard numberings and you might prefer for **Standard1** to map to the first non-zero standard. In this case, please try the following scenario.

Including a Zero Calibrator

With this scenario, you can specify a **Zero** sample group to be used as a calibrator along with the **Standard** groups. If included, the curve fit will include this sample (i.e., all of its replicates) as a part of the calibrators (with a zero concentration value). The values will be added in the same way as for the standards (i.e., **Average** or **Replicates** using **Calculate From** setting). The *x* value of these points will be zero.

To achieve this, first add the **Zero** sample type to your layout along with your standards. Next, to include the Zero group in the calibrators of the curve, an additional configuration step is required:

Add Zero Concentration to a Standard Curve Fit

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.
2. Locate the **StandardCurveFit** element.

3. Add a **ZeroType** and optionally **ZeroGroup** attributes (inside the **StandardCurveFit**).

4. Click **Apply** to save changes to the protocol.

Attributes and Syntax

The Zero concentration is calibrated via XML with the following attributes:

ZeroType	The sample type index for a zero sample.
ZeroGroup	The sample group number for a zero sample. If **ZeroType** is specified but this value is omitted, then a default value of 1 is applied.

For example:

<Settings>

    <StandardCurveFit StandardType="2" FitMethod="4PL" Concentrations="0.25,0.5,1,2,4,8" XAxisTitle="Concentration" YAxisTitle="OD" FitToStandard="Average" CalculateFrom="Average" ZeroType="27" ZeroGroup="1">

This will set the zero type to **Zero** sample type and zero group to 1.

> The zero data points are included in Fit Chart in the same way as standards (i.e., with pink average triangle when relevant) but only if the **X Axis Type** is **Linear**. If it is **Logarithmic**, then these values do not appear on the chart as a calibrator.

Weighting Infinity Resolution

Applying weighting on calibration data points can lower the overall error of the method and therefore improve the quality of the results. However, weighting could result in the weight for a zero point to be infinite and thus skew the curve. An infinite weight can occur if the weight method is one of the forms: 1/y or 1/x (or $1/y^2$, etc.) and the calibration point has a 0 value in the axis of the denominator (e.g., (0,0)).

The notification will advise you if this issue has occurred. In this case, to avoid the infinite weights, you can use the following XML attributes:

	Specifies how to resolve infinite weights for the curve:
WeightInfinityResolution	• **None** – Any infinite weights are used. • **MaxFiniteMultipliedByFactor** – Any infinite weight will be replaced by a finite weight which is computed as the maximum finite weight in the calibrators multiplied by the specified factor (**WeightInfinityReplacementFiniteMax Factor**).
WeightInfinityReplacementFiniteMax Factor	When **WeightInfinityResolutionWeighting** is **MaxFiniteMultipliedByFactor**, this is the factor to multiply the maximum finite weight by, the result is used in place of any infinite weights.

For example:

<Settings>

   <StandardCurveFit StandardType="2" FitMethod="4PL" Concentrations="0.25,0.5,1,2,4,8" XAxisTitle="Concentration" YAxisTitle="OD" FitToStandard="Average" CalculateFrom="Average" WeightInfinityResolution="MaxFiniteMultipliedByFactor" WeightInfinityReplacementFiniteMaxFactor="1">

With this configuration, the infinite weight will be replaced with the maximum finite weight multiplied by 1.

Advanced Fit Charts Configuration

Customize X and Y Axes Positions for Curve Charts

You can define at which point the vertical axis (y-axis) crosses the horizontal axis (x-axis) and vice versa. You can specify axes crossing settings for:

- Charts generated by endpoint curve-fitting transforms (Standard Curve Fit, General Curve Fit, and Dose–Response Curves)
- Curve Overlay, Histogram, and XY Plot report element charts
- QC Output Levey-Jennings, CUSUM and Control charts

> To learn about customizing chart appearance for QC results, see Configuring QC Observations in the XML Editor.

> You can also use **Axes (Advanced)** settings in the transform properties and Histogram settings.

About Axes Crossing

By default, the axes cross each other at the minimum data point values. Using axis crossing XML attributes, you can set custom crossing points such as a specific value, maximum point on either axis, or allow the software to determine the best position automatically. For example, the default chart for the ELISA protocol is displayed:
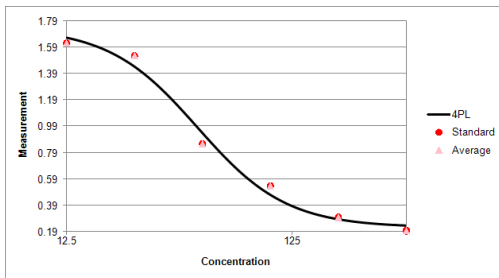
With the **VerticalAxisCrosses="MaximumAxisValue"** attribute added to the StandardCurveFit element in the XML editor, the chart will be displayed:
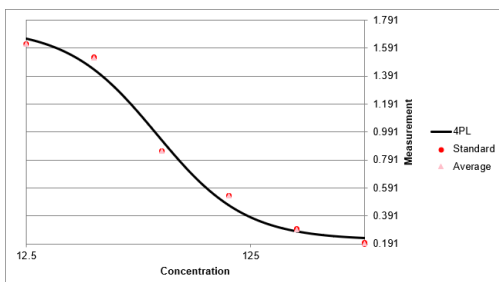
Specify How the Axes Cross in the XML

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Depending on which chart you would like to customize, locate:

   - For Standard Curve Fit, the **StandardCurveFit** element.

   - For General Curve Fit, the **GeneralCurveFit** element.

   - For Dose–Response Curves, the **DoseResponseCurves** element.

   - For Curve Overlay, under the **Report** element, the **Curve** child element.

   - For Histogram, under the **Report** element, the **Histogram** child element.

   - For XY Plot, under the **Report** element, the **XYPlot** child element.

3. Add the child element **ChartCustomization** to the appropriate element.

4. Inside the **ChartCustomization** element, add axis crossing attributes and specify their syntax.
   The editor adds the xmlns="http://www.myassays.com/ChartCustomizations" by default. This attribute is required for the customization.

5. Click **Apply** to save changes and then **Calculate** to generate new results.

Axis Crossing Attributes and Syntax

With these attributes, you can choose where you want the x-axis to cross the y-axis and vice versa. By default, the axes cross each other at the minimum axes values. For axes of logarithmic type, that is the lowest positive value.

VerticalAxisCrosses	Specify where the vertical axis (y-axis) should cross the horizontal axis (x-axis): • **Automatic** - Automatically determines the location that makes the most sense for your data. • **AxisValue** - Cross horizontal axis at specified **VerticalAxisCrossesValue**. • **MaximumAxisValue** - Cross horizontal axis at the maximum horizontal value of the chart. • **MinimumAxisValue** - Cross horizontal axis at the minimum horizontal value. If axis type is set to logarithmic, then it is the lowest positive value.
VerticalAxisCrossesValue	The numerical value at which the vertical axis (y-axis) will cross the horizontal axis (x-axis). This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.
HorizontalAxisCrosses	Specify where the horizontal axis (x-axis) should cross the vertical axis (y-axis): • **Automatic** - Automatically determines the location that makes the most sense for your data. • **AxisValue** - Cross vertical axis at specified **VerticalAxisCrossesValue**. • **MaximumAxisValue** - Cross vertical axis at the maximum vertical value of the chart. • **MinimumAxisValue** - Cross vertical axis at the minimum vertical value. If axis type is set to logarithmic, then it is the lowest positive value.
HorizontalAxisCrossesValue	The numerical value at which the vertical axis (y-axis) will cross the horizontal axis (x-axis). This value must be in the range of calculated results. If axis type is set to logarithmic, the provided value must be greater than 0.

Example in the XML:

For example, with Dose–Response Curves the configuration will look like:

<DoseResponseCurves Type="*Type*" Doses="*List of Doses*" FitMethod="*Method*"

```
PlotResponseForDoseCalculation="true"
ResponseForDoseCalculation="Response" >

    <ChartCustomization
    xmlns="http://www.myassays.com/ChartCustomizations"
    VerticalAxisCrosses="AxisValue"  VerticalAxisCrossesValue="5"
    HorizontalAxisCrosses="MinimumAxisValue"/>

</DoseResponseCurves>
```

Change the Units and Number Format of the Charts

To make the chart data easier to interpret, you can adjust the major and minor units displayed on the chart's axes. You can also define custom formatting for values shown on the axes.

You can apply custom settings to:

- Fit charts generated by endpoint curve-fitting transforms (Standard Curve Fit, General Curve Fit, and Dose–Response Curves)
- Curve Overlay, Histogram, and XY Plot report element charts
- QC Output Levey-Jennings, CUSUM, and Control charts

> To learn about customizing chart appearance for QC results, see Configuring QC Observations in the XML Editor.

> You can also use **Axes (Advanced)** settings in the transform properties and Histogram settings.

About Units and Number Format

By default, MyAssays Desktop determines the chart's major units automatically based on your data. Changing these units will affect the intervals and values displayed on the axes as well as the gridlines of the y-axis. Minor units are not displayed unless specified, but they can help you estimate the data point values at a glance.

Also, for Excel outputs, you can specify the convention for formatting the numbers displayed on either axis. The options include setting the required number of decimal places or significant figures, changing font colour, rounding options, and much more.

For example, this is how the chart for the ELISA protocol can appear:
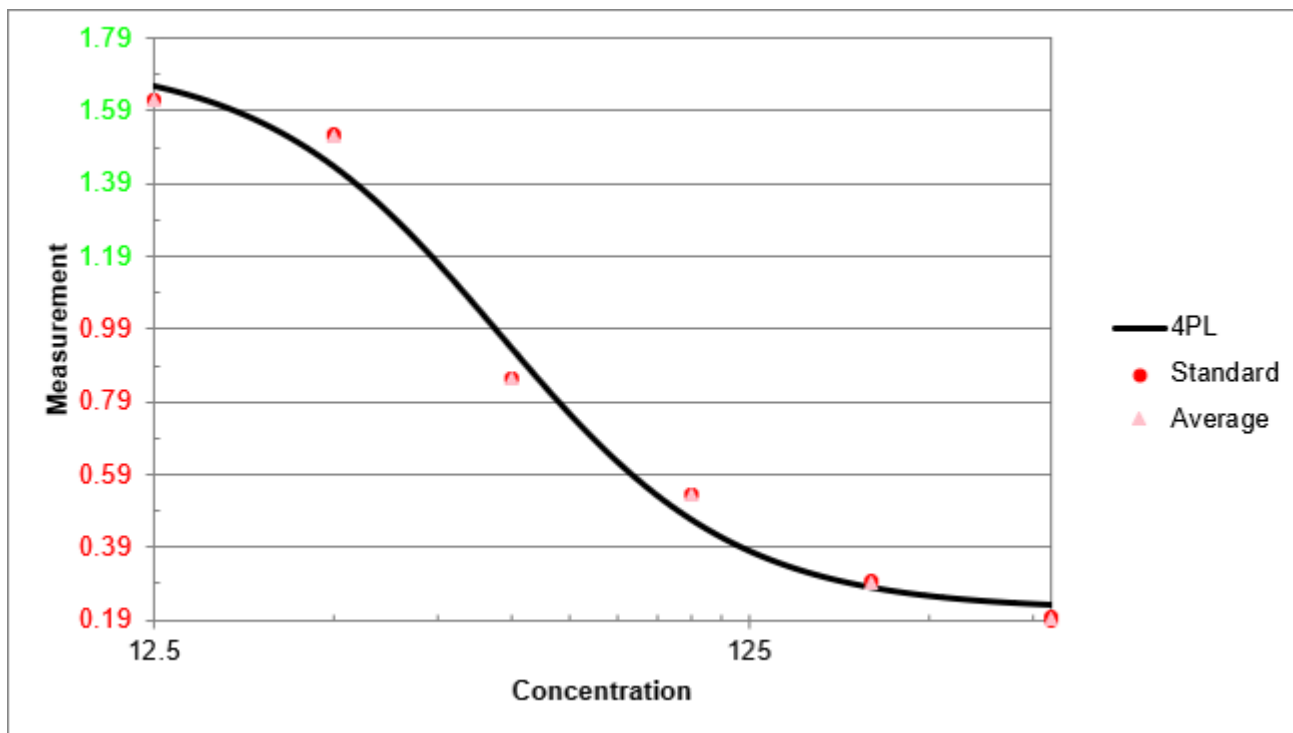
Specify the Axes Display Settings in the XML Tab

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Depending on which chart you would like to customize, locate:

   - For Standard Curve Fit, the **StandardCurveFit** element.

   - For General Curve Fit, the **GeneralCurveFit** element.

   - For Dose–Response Curves, the **DoseResponseCurves** element.

   - For Curve Overlay, under the **Report** element, the **Curve** child element.

   - For Histogram, under the **Report** element, the **Histogram** child element.

   - For XY Plot, under the **Report** element, the **XYPlot** child element.

3. Add the child element **ChartCustomization** to the appropriate element.

4. Inside the **ChartCustomization** element, aadd display units, number format attributes, or both and specify their syntax.
   The editor adds the xmlns="http://www.myassays.com/ChartCustomizations" by default. This attribute is required for the customization.

5. Click **Apply** to save changes and then **Calculate** to generate new results.

Attributes and Syntax

With these attributes, you can set the chart's appearance according to your needs.

XAxisMajorUnits	The major unit to use as the numeric interval between numbers on the x-axis. Starting from the minimum value, a major unit is displayed at every increment.
XAxisMinorUnits	The minor unit that defines the numeric interval between supplementary tickmarks on the x-axis. The minor units are not displayed unless this attribute is specified.
XAxisNumberFormat	Specify the number formatting for the values displayed on the x-axis. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.
YAxisMajorUnits	The major unit to use as the numeric interval between the gridlines on the y-axis. Starting from the minimum value, a major unit is displayed at every increment.
YAxisMinorUnits	The minor unit that defines the numeric interval between supplementary tickmarks on the y-axis. The minor units are not displayed unless this attribute is specified.
YAxisNumberFormat	Specify the number formatting for the major unit values of the y-axis. To learn about available formatting options, see Custom Format Codes for Numbers of the Chart.

Example in XML:

Here is the XML snippet that shows the configuration of the Fit Chart from the example image above:

```
<StandardCurveFit StandardType="2" FitMethod="4PL"
Concentrations="400,200,100,50,25,12.5" XAxisTitle="Concentration"
YAxisTitle="Measurement" FitToStandard="Average"
CalculateFrom="Replicates">
    <ChartCustomization
    xmlns="http://www.myassays.com/ChartCustomizations"
    XAxisMajorUnits="10" XAxisMinorUnits="5" YAxisMajorUnits="0.2"
    YAxisMinorUnits="0.1" YAxisNumberFormat="[Red][&lt;1]0.00;
    [Green][&gt;=1]0.00"/>
</StandardCurveFit>
```

Advanced Settings for Curve-Fitting Transforms

Advanced Curve Fit Evaluations

When using the Standard Curve Fit and General Curve Fit transform, you can evaluate expressions that compute values from the determined curve. This topic describes how to configure, report, and optionally use evaluations as variables in other calculations.

> 📝 This is an advanced feature that can only be configured through the XML editor.

About Curve Fit Evaluations

In addition to performing curve fit and computing values from the curve, you can evaluate expressions that:

- Calculate x or y values on the curve (using interpolation or extrapolation)
- Reference the coefficients and goodness measures of the curve
- Can be referred to as a variables in other evaluations or Curve Fit Custom Flag Labels
- Can be referenced as the Transform Output Variables

This capability is useful for a range of scenarios, including calculating and reporting limits of detection and quantification.

Add Evaluations to the Transform Configuration

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.
2. Depending on the transform you are using, locate:

   - For Standard Curve Fit, the **StandardCurveFit** element.
   - For General Curve Fit, the **GeneralCurveFit** element.

3. Add an **Evaluations** child element.
4. Add an **Evaluation** child element for each required evaluation. Set the evaluation attributes in accordance with the table below.
5. Click **Apply** to save changes and then **Calculate** to generate new results.

Evaluation Attributes and Syntax

Expression	The expression to evaluate. It can refer to: • The Fit Transform Context Parameters and TOVs • Sample values of the input matrix • Any existing Curve Fit Evaluation result using its **Name** attribute (the referenced evaluation must be defined prior to where it is referenced) 📝 A curve fit evaluation expression should not refer to *x* or *y* variables.
Type	This setting describes how the expression is treated in report: • **CalcX** – Calculates the *x* value from the fit line using **Expression** as *y* value. The resulting values are reported using numerical formatting of input matrix. • **CalcY** – Calculates the *y* value from the fit line using **Expression** as *x* value. The resulting values are reported using standard numerical formatting. • **Parameter** – Outputs the computed **Expression** value.
Plot	Optional setting with Boolean type values: • **true** – Plots the **Expression** result for **CalcX** or **CalcY Type** on the curve. The calculated point (*x,y*) is connected to x-axis and y-axis with solid blue lines. • **false** – An **Expression** result is not plotted on the curve.
Description	Optional setting to define a textual description of the expression. If this is not specified, the **Expression** itself is used in the report.
Name	Optional setting to define a name for evaluation. If it is specified, the **Name** can be used as a variable for other XML configurations (as described below).

Named Curve Fit Evaluations

If the **Name** attribute is set, then the evaluation can be referred to by this **Name** as a variable in:

• Context variables in evaluations that are defined in the XML editor below it

• Curve Flag Label conditions

• Transform Output Variables

> ℹ️ The **LLOQ** and **ULOQ** are computed automatically and can be used as an evaluation and flag variables too.

Example XML Configuration

In this example, we will configure evaluation of the Lower Limit of Detection (LLD). The LLD is often computed as the concentration (*x*) at the average of the blank replicates + 3 * standard deviation of the blank replicates. This can be computed by calculating the *x* value on the curve where **y=Blank+3*sd(Blank)**:

```
<Evaluations>
    <EvaluationType="CalcX" Expression="Blank1+ (3* sd(Blank1))" Description="LLD"Name="LLD" />
</Evaluations>
```

In this XML snippet, the expression defines the *y* value to compute, the expression's type **CalcX** indicates that the *x* value on the curve which equals the Expression should be computed.

Customizing LLOQ and ULOQ in Standard Curve Fit

For Standard Curve Fit, the LLOQ and ULOQ calculations are included by default and equal a defined concentration value. If you create a named evaluation using LLOQ or ULOQ, it will replace the default LLOQ and ULOQ calculation:

```
<Evaluations>
    <Evaluation Type="CalcY" Expression="Control1 + (10 * sd(Control1))" Description="My LLOQ"Name="LLOQ" />
</Evaluations>
```

Results and Report

The evaluation results are displayed below the interactive Fit Chart and in the report as a simple two-column Fit Evaluations table. The first column contains **Description** if specified or **Expression** if it was not. The second column contains the numerical value of the evaluated result or any syntax/computation error in red (in same way as the Evaluation feature).

For Standard Curve Fit, the LLOQ and ULOQ are the first entries; any further evaluations follow them.

Advanced Dose–Response Curves Evaluations

Using the Dose–Response Curves transform, you can assess and report many more analytical values from each sample's curve. The additional evaluations are arranged and reported in a Dose–Response Fit Table. The below topics cover how to add, configure, and report the fit table, including an example configuration of common estimation factors.

About Dose–Response Fit Table

Expression-based calculations from curves, computed by the Dose–Response Curves transform, result in a single numerical value for each curve. They are arranged and reported in a Dose–Response Fit Table. If there is an error in evaluating the expression, then the error message is reported (in red) as the result.

You can also specify the numerical formatting and label for each evaluation in the report.

> When configuring expressions directly in the XML editor, it is necessary to follow XML conventions. To learn about XML syntax and settings, see XML Editor.

Add Dose–Response Fit Table and Configure Evaluations

Assuming you have already added Dose–Response Curves transform, configure custom evaluations as follows:

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Locate the **DoseResponseCurves** element and add a **FitTable** child element.

3. For each required evaluation, add a child element **Evaluation** and set the attributes:

Expression	An expression to evaluate for each sample. The expression can refer to any matrix and/or non-matrix data (i.e., contains no *x* references) and results in a single numerical value.
Description	A header for column with the results of the **Expression** in the report.

Also, for each defined evaluation, you can optionally specify numerical formatting settings under the **NumericalFormatting** child element.

> The **Type** settings are entered into XML without spaces.

Example in the XML:

<FitTable>

```
        <Evaluation Description="Description" Expression="Expression"/>
        <Evaluation Description="Description" Expression="Expression">
            <NumericalFormatting Type="DecimalPlaces" Precision="3"/>
        </Evaluation>
</FitTable>
```

Add Dose–Response Fit Table to Report

Because this is an advanced configuration, add the following XML elements to include the Dose–Response Fit Table in the report:

1. Locate the **ReportContent** element and add a child element **Item** with the following attributes:

Id	A unique identifier that is used to identify the report element in the Report Elements pane and when configuring custom report templates. For example, DoseResponseCurvesFitTable1.
Name	Enter or paste **DoseResponseCurvesFitTable**.
Type	Select **Table** from a drop-down list.

Example in the XML:

```
<Item Id="DoseResponseCurvesFitTable1" Name="DoseResponseCurvesFitTable"
Type="Table" />
```

2. Locate the **TransformContent Id="TransformContentDoseResponseCurves1"** (inside the **Report** element) and, for each defined Fit Table, add a child element **Content** with the following attributes:

ItemId	Enter or paste the **Id** from **Item** element.
Include	Select **1** or **true** to include the table in the report.
SheetName	Optionally include the table on a separate sheet. For more details, see Sheet Name.

Example in the XML:

```
<Content ItemId="DoseResponseCurvesFitTable1" Include="true" SheetName="Fit
Table" />
```

Click **Apply** to save changes to the protocol and **Calculate** to inspect the results with the new settings.

Label Dose–Response Fit Table Evaluation Result in the Report

You can also highlight the Fit Table results with sample labels.

Assuming you have already added Dose–Response Curves Fit Table and specified needed evaluations, configure the conditions in the XML as follows:

1. Locate the **Evaluation** element for which you want to set the label.

2. Add a child element **SampleReportLabel**.

3. For each required evaluation, add a child element **Rule** and set the attributes:

Condition	Boolean condition to evaluate (typically a conditional expression) in terms of *x*. The *x* value specified in the expression refers to the sample.
Label	The label to be displayed in the Fit Table if the **Condition** is satisfied. Use **{x}** to refer to the data value that was used in the condition (i.e., the original data point).
Symbol	A graphical icon to display to the left of the **Label** if the **Condition** is satisfied: • **None** – Display no icon • **Pass** – Display a ✔ icon • **Fail** – Display a ✖ icon • **Question** – Display a ❔ icon
BackColour	This sets the background colour for the cell when **Condition** is satisfied. Where there are multiple **Conditions** satisfied, the colour of the first satisfied **Condition** is applied.
ForeColour	This sets the text colour for the cell when **Condition** is satisfied. Where there are multiple **Conditions** satisfied, the colour of the first satisfied **Condition** is applied.

Example XML Configuration

With this XML snippet, all calculated R^2 values that are greater than 0.999 are displayed as *x* **HIGH** in red and with a yellow background.

```
<FitTable>
    <Evaluation Description="R²" Expression="R2">
```

```
                    <SampleReportLabel>

                            <Rule Condition="x &gt; 0.999" Label="{x} HIGH"
        Symbol="None" BackColour="#FFFFFF00"
        ForeColour="#FFFF0000" />

                    </SampleReportLabel>

            </Evaluation>

    </FitTable>
```

With the measurements data and layout from the [Dose–Response Curves example](#), the results for **Unknown1** are as follows:

Sample	R^2
🟢Unknown1	0.999497 HIGH

Dose–Response Curves Context Parameters

When configuring evaluations in Dose–Response Fit Table, you can use Fit Transform Context Parameters.

Parameter	Description	Example in XML
groupnum	Refers to the group number of the dose-response curve.	**GroupValue("Unknown", (groupnum*2)-1)** Returns the value of each **Unknown1** on a dynamic rack layout.
dosemin	Refers to the minimum numerical value from the **Doses** drop-down.	**auc ('4PL',dosemin,dosemax,1000,a,b,c,d)** Calculates the area under each [4PL](#) curve.
dosemax	Refers to the maximum numerical value from the **Doses** drop-down.	

For information about functions you can use when configuring expressions, see [Functions](#).

To learn how to apply **auc** to your assay run, see [Use Area under Curve to Estimate the Difference between Dose–Response Curves](#).

Configure Contents of Curve Data Tables

Curve Data Tables list the measurement and calculation details for the calibrators or doses used in the Standard Curve Fit or the Dose–Response Curves transforms. You can customize the content included in Curve Data Tables by including additional or excluding existing columns. For example, you may prefer to collect more statistical data about the fitting, or limit the table to the input or calculated data only.

> 📝 This is an advanced feature that can only be configured through the XML editor.

Configure Curve Data Table in XML

To configure how the Curve Data Table appears in the report, follow these steps:

1. In the **Assay Properties** panel, select the **XML** tab.

   This opens the built-in XML editor. If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Inside the **Report** element, locate the **TransformContent** element with the **Id** of the transform you are using:

   - For Standard Curve Fit, the **TransformContentStandardCurveFit**, and then locate **Content** child element with **CurveDataTable ItemId**.

   - For Dose–Response Curves, the **TransformContentDoseResponseCurves**, and then locate **Content** child element with **DoseResponseCurveDataTables ItemId**.

3. Add child element **Setting** for each column you'd like to modify and specify their attributes:

Property	Enter or paste the **Column** name from the Available Curve Data Table Contents table below.
Value	Boolean setting that determines how to treat the columns. Enter: • **true** to include the column in the report. • **false** to exclude the column from the report.

   Example in the XML:

   ```
   <Setting Property="Column" Value="Boolean"/>
   ```

4. Click **Apply** to save changes, and then **Calculate** to generate report with new settings.

Available Curve Data Table Contents

Here the columns that you can include in or exclude from the Curve Data Tables are listed in the order they will appear. The columns that are included by default are marked with asterisk (*****).

Column	Content
IncludeRaw	The raw measurements — the first raw matrix.
IncludeRawAverage	The average of the raw measurements.
IncludeRawPCV	The %CV of the replicates of each group of the raw measurements.
IncludeRawSD	The standard deviation calculation of the raw measurements.
IncludeTransformInput*	The transform input data.
IncludeCalculated*	The concentrations or calibration doses calculated from the curve. Depending on the selected **Calculate From** setting of the Standard Curve Fit, a value will be displayed for each non-flagged replicate (**Replicates**) or per sample group (**Average**).
IncludeCalculatedPCV*	The percentage coefficient of variation of the calculated concentrations or doses. This column is included only if the calibrators are replicated (one or more of the standard groups of the specified standard type contains more than one replicates). If the **CalculateFrom** setting of the Standard Curve Fit is set to **Average**, this column will be excluded.
IncludeRawStandardError	The Standard Error (SEM) of the raw data. This column is included only if the calibrators are replicated (one or more of the standard groups of the specified standard type contains more than one replicates).
IncludeCalculatedStandardError	The Standard Error (SEM) of the concentrations or doses calculated from the curve.

Column	Content
	This column is included only if the calibrators are replicated (one or more of the standard groups of the specified standard type contains more than one replicates). If the **CalculateFrom** setting of the Standard Curve Fit is set to **Average**, this column will be excluded.
IncludePercentAccuracy*	The % Accuracy column ratio of the average of the calculated value against the original specified concentration or dose.
IncludeSampleNumbers	Includes the Sample Numbers in a column directly to the right of the Calibrators column.
SampleNumbersText	Specify the column title for **IncludeSampleNumbers**
IncludeSamplePositions	Includes the Sample Positions.

Additional Settings

The below table contains additional settings that be specified in the XML.

Column	Content
IncludeRowHighlighting	Include or exclude row highlighting
StandardErrorNumericalFormattingType	Specify the numerical formatting type (decimal places or significant figures) for the Standard Error column
StandardErrorNumericalFormattingPrecision	Specify the precision (number of decimal places or significant figures) for the Standard Error column
StandardDeviationNumericalFormattingType	Specify the numerical formatting type (decimal places or significant figures) for the Standard Deviation column
StandardDeviationNumericalFormattingPrecision	Specify the precision (number of decimal places or significant figures) for the Standard Deviation column
PCVNumericalFormattingType	Specify the numerical formatting type (decimal places or significant figures) for the Percent CV column

Column	Content
PCVNumericalFormattingPrecision	Specify the precision (number of decimal places or significant figures) for the Percent CV column
PercentAccuracyNumericalFormattingType	Specify the numerical formatting type (decimal places or significant figures) for the Percent Accuracy column
PercentAccuracyNumericalFormattingPrecision	Specify the precision (number of decimal places or significant figures) for the Percent Accuracy column

The numerical formatting for concentration columns is as defined in the associated concentration matrix (available through the Matrices settings). The below XML excerpt shows how to set the numerical formatting of %CV columns in thee CurveDataTable to use 3 decimal places:

<Content ItemId="CurveDataTable1" Include="true">

    <Setting Property="PCVNumericalFormattingPrecision" Value="3"/>

    <Setting Property="PCVNumericalFormattingType" Value="DecimalPlaces"/>

<Content/>

Example XML Configuration

With this XML snippet, the Curve Data Table of Standard Curve Fit will feature two additional columns in the report. These columns will present the standard deviation between replicates of calibrator samples and the standard error for calculated concentrations.

<Content ItemId="CurveDataTable1" Include="true">

    <Setting Property="IncludeRawSD" Value="true"/>

    <Setting Property="IncludeCalculatedStandardError" Value="true"/>

<Content/>

Constrain Coefficients of the Fit

For certain types of curve-fitting applications, it is useful to be able to constrain one or more coefficients of the fit to specific values or ranges. With coefficient constraints imposed, the resulting curve fit equation will follow these constraints.

For example, when using the 4PL or 5PL model, it might be useful to constrain the upper and/or lower asymptotes of the curve to equal known saturation points (such as **NSB** or **B0**). These constraints could be based on measurements from specific samples in the assay and used to set limits on the computed curve.

Also, where the resulting fit is expected to fall within certain ranges, you can define constraints to guide the curve fitting process as required. For example, you may be using a curve-fitting equation that uses a coefficient that must be within a certain range (such as positive), a range constraint defined with a bound can be applied to direct the curve fit accordingly.

Where and How to Apply Coefficient Constraints

You may constrain one or more of the coefficients of the selected fit method when working with the following endpoint transforms:

- Dose–Response Curves
- General Curve Fit
- Standard Curve Fit

Each coefficient can be constrained using either:

- A fixed value (specified using an expression that can refer to samples or mathematical operations)
- Bound (upper, lower or both)

The values of these constraints can be specified using an expression and may refer to a TOV.

Coefficient Constraints and Parallel Line Analysis

Coefficient Constraints are useful when performing Parallel Line Analysis. In this case, an unconstrained fit can be performed followed by constrained fits that use limits defined from the unconstrained fit. The resulting constrained fits can then be compared and considered for parallelism.

> When working with Standard Curve Fit or General Curve Fit transforms, you can define a Custom Fit expression with a constant value instead of using a fixed coefficient constraint.

How to: Add Coefficient Constraints to a Curve-Fitting Transform Configuration

1. In the **Assay Properties** panel, select the **Transforms** tab.
   If the **Transforms** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Depending on the transform you're using, locate the:

   - For Standard Curve Fit, the **StandardCurveFit** Transform.

   - For General Curve Fit, the **GeneralCurveFit** Transform.

   - For Dose–Response Curves, the **DoseResponseCurves** Transform.

3. Under the **Fit** settings, open the **Constraints** dropdown box.

4. Select **Add** and specify the **Fit Parameter**, whether the parameter is **Fixed** or a **Boundary**, and the **Value**

5. Press **Calculate** to generate new results.

Syntax

The value of these constraints can be specified using an expression (that results in a single numerical value) and may refer to a TOV. The interpretation of the constraint depends on the type of restriction setting:

- **Fixed** – Sets a coefficient to a fixed value

- **LowerBound** – Limits the search range for the coefficient to be greater than specified constraint

- **UpperBound** – Limits the search range for the coefficient to be less than specified constraint

> The **UpperBound** and **LowerBound** can be used separately or in a conjunction. However, **Fixed** type overrides any **UpperBound** or **LowerBound** setting.

Example Configuration

Here is a screengrab that shows a configuration of the **StandardCurveFit** element with **Constraints** for the 4PL fit coefficients.
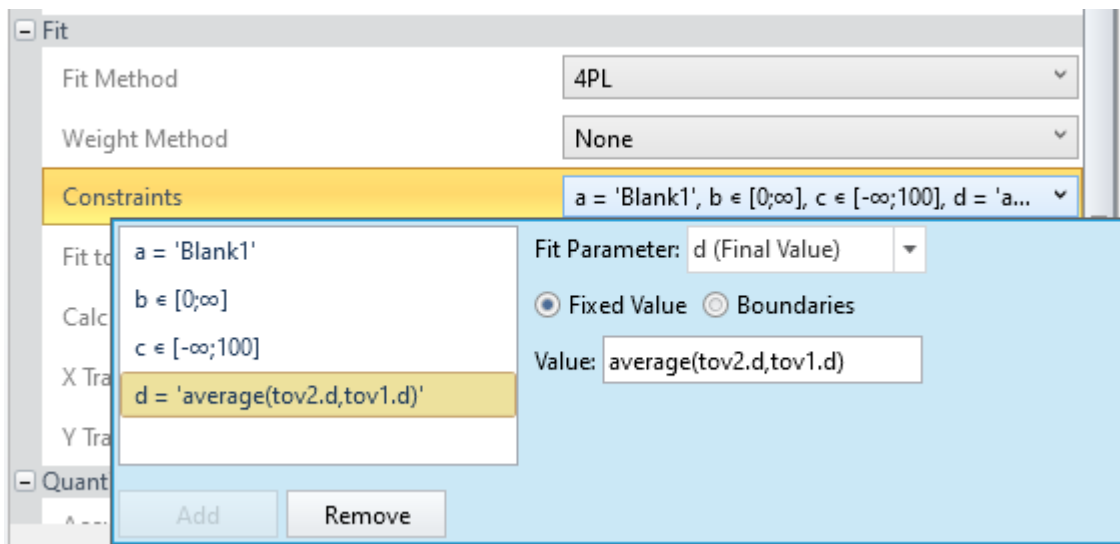
With this configuration the coefficients will be constrained as follows:

- **a** will equal the average of **Blank1** sample replicates

- **b** will be greater than 0

- **c** will be less than 100

- **d** will equal the average of the d coefficients as computed from two previous Standard Curve Fit transforms (referenced using TOVs)

Custom Fit Advanced Settings

When using the Standard Curve Fit's or General Curve Fit's **Custom** curve fit option, it is possible to define further fit settings via the XML editor including:

- **Name** – A name for your custom fit to be displayed on chart and in the report

- **Weighting** – A weighting model to apply

- **Inverse Equation** – How to compute *x* values from *y* (i.e., provide an equation in terms of *y*)

- **Coefficient Estimate Heuristics** – Rules for estimating each coefficient's starting value

- **Coefficient Constraints/Ranges** – Constraints or acceptable ranges for each coefficient

> This is an advanced feature that can only be configured through the XML editor.

To learn about Custom Fit feature, see Custom Fit.

How to: Add Attributes to a Custom Fit Configuration

1. In the **Assay Properties** panel, select the **XML** tab.
   If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Depending on the transform you would like to create a custom fit, locate:

   - For Standard Curve Fit, the **StandardCurveFit** element.

   - For General Curve Fit, the **GeneralCurveFit** element.

3. Locate the child element **Method**.

4. Inside the **Method** element, define custom fit attributes and specify their syntax.

5. Click **Apply** to save changes and then **Calculate** to generate new results.

Attributes and Syntax

You can specify Custom Fit settings with the following optional attributes:

DisplayName	A title of the fit for chart and Calculation Log.
Inverse	The inverse equation of the fit in terms of *y*. This equation is used to compute each *x* value from the curve (so make sure this is correct). If the equation is not provided, then results will be computed using an automated but slower method.

Weight	The weighting method to use.

Configuring Coefficient Estimate Heuristics

Defining a good starting point for calculating initial coefficient estimates improves the accuracy and speed of the fit. For a custom fit, you can provide the starting point estimates for any or all of the coefficients.

In addition, a range can be specified to limit or constrain the fit.

To specify an estimate, add an **Estimate** element (as a child of the **Method**) for each required estimate and set the attributes in accordance with the table below.

Expression	A numeric value or a heuristic expression to calculate.
Name	A name of a coefficient for which the estimate is for.
Min	The minimum value to limit the search range for the coefficient value. If not specified, then the range is -Infinity.
Max	The maximum value to limit the search range for the coefficient value. If not specified, then the range is +Infinity.

Heuristics expressions are used to compute starting estimates. An expression can reference aspects of the calibration data. For example, with 4PL model, the expected result for **a** coefficient might be the *y* value at the peak of the curve. In this case, you can reference *maxy* variable to define a starting estimate for an upper asymptote (**a**). It will refer to the maximum *y* value of your calibration data.

The following variables are available for reference.

Variable	Value
averagex	Average of all *x* values
averagey	Average of all *y* values
minx	Minimum *x*
miny	Minimum *y*
maxx	Maximum *x*
maxy	Maximum *y*
yatminx	*y* at the minimum *x*
yatmaxx	*y* at the maximum *x*
xatminy	*x* at minimum *y*
xatmaxy	*x* at maximum *y*
medianx	Median of all *x* values
mediany	Median of all *y* values

Variable	Value
slope	Slope of the data set
intercept	Intercept of the data set

> For more sophisticated estimates, you can use [conditional function](#). For example, if the coefficient value depends on whether the *y* increases or decreases with *x*, you can compare *yatmaxx* and *yatminx* values and adjust the estimate value accordingly.

Example Configuration

The following XML snippet shows a complete configuration of the **Method** element with:

- Custom Display Name

- Inverse Expression

- Estimate Heuristics Expressions for each coefficient

```
<Method DisplayName="4PL (from expression)" Expression="d+((a-d)/(1+(x/c)^b))"
Inverse="c*pow(((a-d)/(y-d))-1,1/b)" xmlns="http://www.myassays.com/bestfitsearch">
        <Estimate Name="a" Expression="maxy" />
        <Estimate Name="d" Expression="miny" />
        <Estimate Name="b" Expression="if(yatminx &lt; yatmaxx,-3,3)" />
        <Estimate Name="c" Expression="medianx" />
</Method>
```

These Coefficient Estimate Heuristics compute useful starting estimates for a 4PL fit for a dose response curve where the response falls with increased concentration.

Custom Flag Labels by Fit Transform Calculations

Using Custom Flag Labels by Fit Transform Calculations, you can specify when a result of Standard Curve Fit or General Curve Fit transform should be flagged and reported with a custom label rather than as a result or error.

> **ⓘ** Custom Flag Labels by Fit Transform Calculations have higher precedence and override any other defined labels. To learn more about specific labels for flagged results, see Custom Flag Label.

> **📝** The feature only applies to data points specifically flagged by the transform itself. If an input point is already flagged, then any existing custom label (or the absence of the custom label) is copied to the output.

About Custom Flag Labels by Fit Transform Calculations

You can use this advanced flagging feature to label results for fit transforms where the results cannot or should not be computed from the curve. For example, if a sample is outside the usable range of the curve, then it might be useful to flag and label the result accordingly. What is considered as the usable range of the curve is open to your own interpretation. For example, the use of the curve could be limited by:

- The defined or determined ULOQ and LLOQ values

- The mathematical limits of the curve

- Your own defined limits (defined as absolute values or using expressions with limits computed from the curve fit)

When using Standard Curve Fit or General Curve Fit transform, you can apply:

- General **CurveError** label to use if a value cannot be computed from the curve.

  You can use optional CurveError setting to specify a default custom flag label to use if the result is flagged on the input matrix or while calculating results. It simply replaces the default flagged result in the report with specified **CurveError** label.

- Custom flagging conditions—the expressions written in terms of x—based on the transform's input or output data (calculated from the curve).

  You can define any number of conditions in any order. If any of these conditions are met, then result is flagged with a specified label applied to it. If multiple labels are configured, only the first label condition to be evaluated as true is used (in the order they appear in the XML editor). These conditions take precedence over the default flagging settings and

CurveError. So, if any condition with **Type="Input"** is evaluated as true, then these will be used in place of any curve error.

Add Custom Flag Label to the Fit Transform

Assuming you have already added Standard Curve Fit or General Curve Fit transform, configure custom flag labels as follows:

In the **Assay Properties** panel, select the **XML** tab.

If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

1. Depending on the transform you're using, locate the:

   - For Standard Curve Fit, the **StandardCurveFit** element.

   - For General Curve Fit, the **GeneralCurveFit** element.

Add the **Flags** child element.

Inside the **Flags** element, optionally add a **CurveError** attribute with the following syntax:

CurveError	The custom flag label to use in place of the default ~~Flagged~~ label. When specifying custom flag text, strikethrough is not applied.

Example in the XML:

<<Flags CurveError="*My Custom Label*" >

Add a child element **Flag** for each required flagging condition and specify its attributes:

Type	The value of *x* depends on the expression type: • For Type="Input", *x* is the value of the input position. • For Type="Output", *x* is the value computed for the output position.

Condition	The condition to evaluate (typically a conditional expression). The flag condition expression can refer to: • the value of each position using the reference *x* • the computed coefficients of the fit and goodness measures • Advanced Curve Fit Evaluations • sample values of the input matrix
Label	If a flag **Condition** is satisfied (evaluated to true), then the result of the transform for the position is flagged with the associated **Label**. If you insert **{x}** in the **Label**, it inserts the value of *x* (e.g., **{x} is Below LLD** might be reported as **0.25 is Below LLD**).

Example in the XML:

<Flag Type="*Type*" Condition="*Expression*" Label="*My Custom Label*" />

Click **Apply** to save changes and then **Calculate** to generate new results.

Specifying Conditions in XML

When entering conditions in XML, there are certain symbols that must be encoded using correct XML syntax. These are listed in the table below.

Operator	Description	XML Encoding
<	Less Than	<
>	Greater Than	>
&	Ampersand	&
"	Double Quote	"
'	Apostrophe/Single Quote	'

For example, if the condition is **x<a** then this would be encoded in XML using **x < a**.

Example Configuration

With this XML snippet configuration of the **StandardCurveFit** element, any sample whose measurement response is above or below the computed asymptotes of the 4PL (the **a** and **d** coefficients of the fit) will have a label associated with it accordingly.

<StandardCurveFit StandardType="2" FitMethod="4PL" Concentrations="0.125,0.25,0.5,1,2,4" XAxisTitle="Concentration" YAxisTitle="Raw" FitToStandard="Average" CalculateFrom="Average">

```xml
<Flags CurveError="Could not calculate from curve" >

    <Flag Type="Input" Condition="x &lt; min(a,d)" Label="{x} Below
    Lower Asymptote" />

    <Flag Type="Input" Condition="x &gt; max(a,d)" Label="{x} Above
    Upper Asymptote" />

</Flags>
```
```xml
</StandardCurveFit>
```

Example Flag Conditions

XML Condition	Description
`<Flag Type="Input" Condition="x < Blank1+3*sd(Blank1)" Label="{x} Below LLD" />`	If the measurement response is less than Blank1 + 3SD, then the result is flagged and reported with the Label.
`<Flag Type="Input" Condition="x < min (a,d)" Label="Below Lower Asymptote" />`	If the measurement response is less than the lower value of the a and d coefficients (as computed from the curve), then the result is flagged and reported with the Label.
`<Flag Type="Input" Condition="x < 0.125" Label="OD < 0.125" />`	If the measurement response is less than 0.125, then the result is flagged and reported with the Label.
`<Flag Type="Output" Condition="x < 0.125" Label="Conc. < 0.125" />`	If the computed concentration is less than 0.125, then the result is flagged and reported with the Label.

Setting Numerical Formatting for Goodness Measures and Fit Coefficients

To customize how the goodness measures and fit coefficients are formatted in the report, you can set their numerical formatting in the XML editor. This topic covers the attributes to specify for configuring the format of:

- Goodness Measures and Fit Coefficient Results

- Fit Coefficient ± Errors

> This is an advanced feature that can only be configured through the XML editor.

Locating in the XML

To configure the formatting, follow these steps:

1. In the **Assay Properties** panel, select the **XML** tab.

   This opens the built-in XML editor. If the **XML** tab is not immediately visible, click **<< Show All Properties** to expand.

2. Inside the **Report** element, locate the **TransformContent Id="TransformContentStandardCurveFit1"** and:

   - For Fit Coefficients table, under the **"CoefficientsTable1"** item

   - For Goodness Measures table, under the **"GoodnessMeasuresTable1"** item

   Add child element **Setting** for each formatting setting and specify their attributes as described below.

3. Click **Apply** to save changes, and then **Calculate** to generate report with new settings.

Setting Up Format of Goodness Measures and Fit Coefficient Results

To set up the numerical formatting of these report elements, add and define numerical formatting settings according to the following example:

```
<Setting Property="ValueFormattingType" Value="Type"/>
<Setting Property="ValueFormattingPrecision" Value="Value"/>
```

Where *Type* specifies how a numerical value is formatted with regard to precision and rounding options:

- **SignificantFigures** – The value is reported to the specified number of significant figures. This accepts integer *Value* in range 1 through 14.

- **DecimalPlaces** – The number of digits to display to the right of the decimal point. This accepts integer **Value** in range 0 through 14.

For example:

```
<Content ItemId="GoodnessMeasuresTable1" Include="true">
    <Setting Property="ValueFormattingType" Value="DecimalPlaces"/>
    <Setting Property="ValueFormattingPrecision" Value="3"/>
<Content/>
```

With this configuration, the determined goodness measures will be presented to 3 decimal places.

Setting Up Format of Fit Coefficient ± Errors

For Coefficients table, you can additionally define how the ± errors are reported with **ErrorFormattingType** and **ErrorFormattingPrecision** properties. Thus, the complete configuration for this element looks like as follows:

```
<Content ItemId="CoefficientsTable1" Include="true">
    <Setting Property="ValueFormattingType" Value="SignificantFigures"/>
    <Setting Property="ValueFormattingPrecision" Value="4"/>
    <Setting Property="ErrorFormattingType" Value="SignificantFigures"/>
    <Setting Property="ErrorFormattingPrecision" Value="4"/>
<Content/>
```

This will report calculated coefficients and their ± errors to 4 significant figures.

Troubleshooting Results

What a High Blank (or Background) Means, and How to Deal with It

A high blank or background reading normally indicates a preparation error.

First, check that the plate was washed correctly and that the washer is not the source of problem. Second, consider the possibility of a reagent preparation issue. Too much labeled detector may cause this type of response in an assay. Check that the blocking step was also performed correctly, was the right amount of block used in the right buffer?

Curve Fitting with a High Blank

With data analyses that perform a Blank Correction and Standard Curve Fit, if the blank value is higher than some of the standards (e.g., the lowest standard), then a part or all of the resulting curve will be negative and fall below the x-axis.
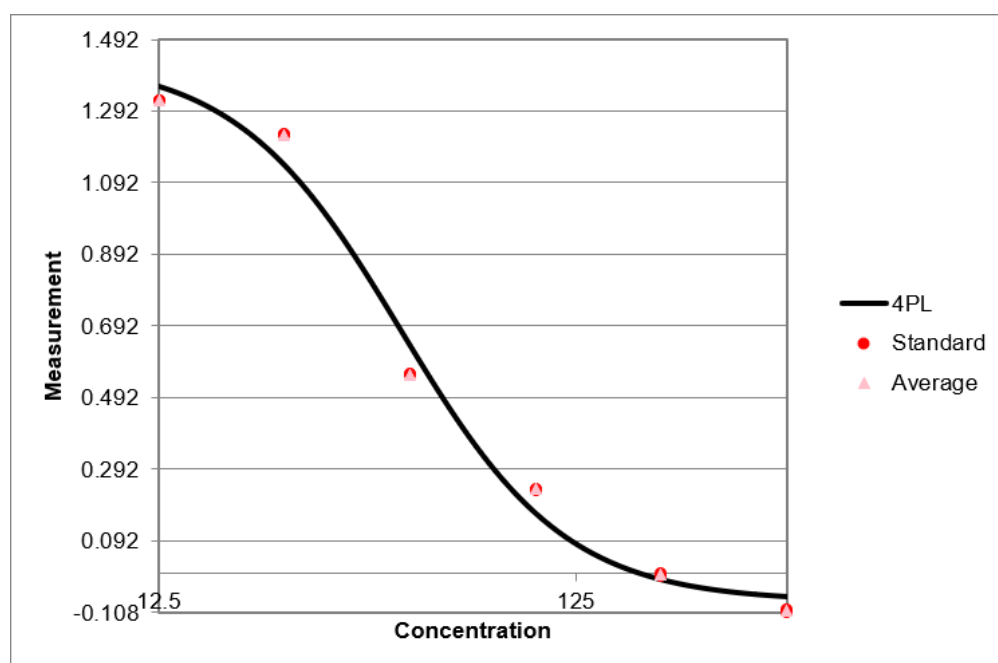
In this scenario, one point to understand is that the blank correction does not actually impact the calculated concentrations. Because all samples (standards and unknowns) are blank corrected in the same way, the whole curve shifts down the y-axis but the computed concentrations will be the same. Thus, the results will be the same if the blank is 0, small, or high. It seems counterintuitive, but this is the case. You might then wonder what is the point of performing blank correction; a blank is used in this way to simplify comparing curves across assay runs (and in the perfect situation generating a nice-looking curve through $y=0$ although that is rarely the case). The blank can also be used to identify problems with the assay run, for example a high blank may indicate preparation errors as discussed above.

With MyAssays Desktop, negative *y* values (i.e., where blank is high) are included in the curve fit, the result is that part of the curve will appear below the x-axis, but all points are included in the fit. In this case you'll get the same results, but it's clear from the chart that the blank correction is too high (causing negative standards).

Expressions

Expressions are available for use throughout MyAssays Desktop to provide flexibility in data-analysis design and configuration.

An expression is simply an operation to be computed. In the simplest case, an expression can refer to a specific numerical value, measurement, or result. For example, the expression **Control1** refers to the average of the Control1 sample replicates (that are not flagged).

> When writing expressions that refer to specific samples, in general, it is preferable to refer to a sample group, such as **Control1**, rather than specific layout positions (such as **A1**). With this approach, if your sample layout changes (perhaps you run the assay with a different sample layout), then you will not need to update your expressions.

An expression might perform mathematical or statistical operations on these values. For example, the expression **pcv(Control1)** computes the %CV of the **Control1** replicates.

An expression can be applied at various levels of the data analysis to define and compute various results. For example, matrix calculations, quantification limits, validation rules, values from fitted curves, and best fit score methods (to decide on the best fit) can all be defined using expressions.

Wherever a numerical value can be entered as a settings parameter, an expression can usually be provided to compute that parameter from other sources.

The Expressions system has been designed to:

☑ **Provide custom analysis using a familiar mathematical syntax (similar to Excel)**
☑ **Provide an easy way to reference sample data**
☑ **Take into account flagged data**

Expressions can refer to measurements or calculated results from specific layout positions (e.g., **A1**), sample groups (e.g., **Control1**), variables, and also the results of other expressions.

Culture Settings

When providing numerical values or expressions through the user interface, enter numerical values and lists using your system's regional settings. There are two settings that can vary between culture settings:

- **Decimal separator** – Typically a period (**.**) on non-European systems and a comma (**,**) on typical European system

- **List separator** – Typically a comma (**,**) on non-European systems and a semi-colon (**;**) on typical European system

For example, depending on your system's culture settings, an example expression could be entered in two forms:

mean(1.5,2.5)

mean(1,5;2,5)

> When configuring expressions directly in the XML editor, it is necessary to follow XML conventions and provide data using invariant settings; that is period decimal separator for numeric values and comma list separator.
> To learn about XML syntax and settings, see XML Editor.

Syntax and Context

The syntax of expressions is consistent throughout MyAssays Desktop. However, the application of an expression depends on the context it is being used in. For example, expressions are used in the configuration of transforms, validations, and evaluations. In each case, the application of the expression is slightly different.

Where an expression is used as a parameter to another setting, you can provide an expression that can be evaluated to a numerical result, such as **Control1*10**.

There are several situations where an expression is entered in terms of x (where x refers to an input value that will be substituted with a value for each evaluation of the expression). For example, the Expression by Matrix transform expects an expression in terms of x. In this context, you can provide an expression such as ***x*-Blank1** to subtract the mean of **Blank1** from all samples.

Where an expression is entered in terms of x, the expression is evaluated multiple times with x being substituted with different values. In the case of the Expression by Matrix transform, the expression is applied to every position on the input matrix to calculate the result of the output matrix.

There are also scenarios where a Boolean expression is expected. Validations are defined using a Boolean expression to define rules that must be satisfied for the assay to be considered valid.

For example, a validation rule can be defined with the expression **Standard1<Standard2** to check that the standard measurements are in the expected order. Similarly, a validation expression **x<15** could be used along with %CV data to validate that all samples have a %CV of less than 15.

A typical expression comprises of:

- operations (e.g., +, *, /, ^)
- operands (e.g., A1, 1.23, x, Control1, TOV1.a)
- functions (e.g. pcv, sd, median, floor)

The following table lists some examples of expressions you may use in your assay.

Example Expressions

> All expression examples provided here use a period decimal separator(.) and a comma list separator(,). Use local settings of your system when entering expressions on your own system.

Expression	Evaluated to
Unknown1	The average of the replicates of **Unknown1** (that are not flagged).
Unknown	The average of all **Unknown** samples (that are not flagged).
A1	The data for position **A1**.
A1+A2	The sum of the data at positions **A1** and **A2**.
mean(A1,A2,A3)	The average of the data at positions **A1**, **A2**, and **A3**.
pcv(Unknown1)	The percentage coefficient of variation of **Unknown1**.
Blank1+(3*sd(Blank1))	The average of the sum of **Blank1** plus 3 times the standard deviation of **Blank1** (this is often used to compute LLD).
pcv ([Unknown1,Unknown2])	The percentage coefficient of variation of all **Unknown1** and **Unknown2** replicates.
median(Standard1)	The median of the replicates of **Standard1** (that are not flagged).
x-Blank1	The value of variable x minus the average of **Blank1** position.
x>15	A Boolean expression that would evaluate to 1 (true) if the value of variable x is greater than 15; otherwise it evaluates to 0 (false).
Ifthenelse(x>15,15,x)	If the value of x is greater than 15, then the result is 15; otherwise the result is x.
x-y	The difference between x and y. Here x and y are the values of corresponding positions from two matrices of data (as used in the Expression by Matrix (Dual) transform).
median(Unknown.2.All)	The median of all Unknowns on the 2nd matrix across all

Expression	Evaluated to
	containers.
Unknown1.2.3	The average of **Unknown1** sample group on the 2nd matrix of 3rd plate.
TOV1.R2	The R^2 value of the curve fit as used in the first transform (referenced using a [Transform Output Variable](#)).
GroupValue("Blank",1)	The value of the group that is **Blank1**. (This is equivalent to the reference **Blank1**, however this method can be useful for applying calculations on group number references.)
x-GroupValue ("Blank",PosGroup())	The value of variable x minus the average of the **Blank** sample which has a group number that matches the group number of the sample at the position where the same is being evaluated. This technique can be used to write expressions that apply a calculation in accordance to a layout, such as subtracting Blanks values on 1-to-1 basis. With a layout where each Unknown group has its own **Blank** group (e.g., **Unknown1**, **Blank1**, **Unknown2**, **Blank2**, etc.) this expression will subtract the blank group associated with each sample based on the layout.

Operators

Unary Arithmetic Operator

Operator	Operation	Examples
-	Minus Sign	-1.23 $-x$

Binary Arithmetic Operators

Operator	Operation	Example
+	Addition	2+1 $x+y$ $x+1$
-	Subtraction	2-1 $x-y$ x-1
*	Multiplication	2*3 $x*y$ $y*2$
/	Division	2/2 x/y $x/2$
^	Exponentiation	2^3 x^y x^2

Binary Logical Operators

The numerical evaluation of 1 for true and 0 for false. Thus, 1>0 =1.

Operator	Operation	Examples
<	Less Than	1<2 $x<y$ $x<2$
>	Greater Than	2>1 $x>y$ $x>2$

Operator	Operation	Examples
=	Equal To	$1=1$ $x=y$ $x=2$
<=	Less Than Or Equal	$3<=9$ $3<=3$ $x<=y$ $x<=x$ $x<=3$
>=	Greater Than Or Equal	$9>=3$ $3>=3$ $y>=x$ $x>=x$ $x>=9$
<>	Not Equal	$2<>1$ $x<>y$ $x<>3$

Boolean Operations

The Boolean operations (and, or, not) are implemented as Conditional Functions.

Operands

Numbers

Number operands are simply numbers (e.g., 1.23, -100, 14).

> ℹ️ Make sure that all numerical values entered into the user interface are provided using the local settings of your system.

Variables

The *x* and *y* variables refer to the value of each position on the associated matrix. All references to these variables in expressions are equated to the associated values.

For example, in the Expression by Matrix transform, you may enter the expression ***x**100**, where the *x* variable will refer to the positions of the input matrix. In the resulting matrix, all positions will be multiplied by 100. In Expression by Matrix (Dual), the *x* and *y* variables are set to the position values of the first and second matrices. Thus, when you enter an expression ***x+y***, each position on the resulting matrix will be the sum of input matrices values.

Variable	Relevant For
None	Installed Protocols, **Certain Endpoint**: Auto Flag, Average, General Curve Fit, Matrix Difference, Median, Percentage, Percentage Coefficient of Variation, Replicate Outlier Removal, Standard Curve Fit, Standard Deviation, Variance
x	**Certain Endpoint**: Blank Correction, Dose–Response Curves, Dilution Factors, Expression by Matrix, Expression by Position, Expression by Sample Type, Factor, XY Blank Correction
x, y	Expression by Matrix (Dual), XY Expression (Dual)
y	XY Expression

Fit Transform Context Parameters

Fit Transform Context Parameters apply only within transforms that perform curve fitting as settings or in the intra-transform advanced calculations. Some of the parameters can be referenced in the general configuration of the assay (e.g., validation or evaluation tables) or in other transforms as Transform Output Variables (see subsection below).

General Fit Transform Context Parameters

These parameters can be used in configuration settings (for XY Reduction Fit Parameter, General Curve Fit, and Standard Curve Fit when using Custom Fit), flagging conditions, constraining the fit, and additional evaluations:

- Goodness of Fit Measures calculated from the fit.

Name	Expression Syntax
R^2	r2
aR^2	ar2
F	f
P	p
SE	se
AIC	aic
AICc	aicc
BIC	bic
DWS	dws
DoF	dof
RMS	rms

- **Coefficients of the Fit** – These vary depending on the selected fit method and are specified within documentation of these methods.

Specific Fit Transform Context Parameters

When using General Curve Fit and Standard Curve Fit, any defined named evaluations can be used as context parameters. You can use them in further evaluations, and custom flagging within the transform.

Also, the Dose–Response Curves transform features its own context parameters **groupnum**, **dosemin**, and **dosemax**. To learn more about their usage, see Advanced Dose–Response Curves Evaluations.

Named Evaluation Variables

Named Evaluation Variables can be referenced in any evaluation (including validation and label conditions) computed after the named evaluation. For detailed configuration and usage, see Named Evaluation Variables.

Transform Output Variables

Transform Output Variables (TOVs) can be referenced in any expression that is evaluated after the transform that produced the TOV. To learn more about their configuration and usage, see Transform Output Variables.

Layout References

When an evaluation depends on and is associated with certain layout, the expression can include references to positions, sample groups, and/or types defined on the layout. These are

defined with case-insensitive input (i.e., uppercase and lowercase letters in expressions are treated the same).

For example, **Unknown1** is the same as **unknown1**, **UNKNOWN1**, and **UnKnOWN1**.

General information on referencing the sample layout and its components is provided in the Layout References in Expressions.

Position References

A position ID refers to a specific position on the layout (e.g., **A1**, **H12**). To learn more, see Positioning on the Layout.

The available dimensions depend on the layout in use. A position on a particular matrix and/or plate can be referenced as described in sample references in multiple plate assays.

> When writing expressions, it is preferable to refer to sample groups such as **Blank1** rather than specific positions. If you have to modify your layout (perhaps because of pipetting error), you do not need to update your expressions as the group reference will refer to the correct sample on the modified layout.

Row and Column References

The Row and Column operands refer to data on a particular layout row or column (on the selected matrix). The data here refers to all non-flagged data positions with a type that is not **Unused**. Refer to these operands with the following syntax:

RowN

ColN

Where **N** is a positive integer to represent the row or column number. In microplate layouts, Row1 refers to Row A on the microplate. **Example**: **average(Row1)** will compute the mean of all non-flagged positions on Row1 for sample positions that are used (i.e., sample type is not **Unused**).

Sample References

Sample operand can contain a reference to:

- **Sample group** – It can refer to any group of any type defined on the layout. To use this operand in the expression, type in the sample type name (e.g., **Unknown**, **Blank**, **Standard**) and sample group number. **Example**: **Unknown1** refers to all non-flagged **Unknown1** sample group positions on the layout.

- **Sample type** – If no group number is specified, then it refers to all positions of that type on the layout (e.g., all **Unknowns**, **Blanks**, **Standards**). **Example**: **Unknown** refers to all non-flagged data points of **Unknown** type on the layout.

The simple sample reference usually refers to the average of non-flagged positions of the type/group. Only for group-enabled functions does it refer to the **list of values of each non-flagged position** that belong to the sample reference. **Example**: **median (Unknown1)** calculates the median of all non-flagged **Unknown1** position values defined on the layout.

If a sample reference is enclosed in square brackets (e.g., **[Unknown1]**), it refers to the **list of values of each non-flagged position**. So **[Unknown1]** is actually expanded to the list of results for the non-flagged members of **Unknown1**.

Sample References in Multiple Plate Assays

To simplify evaluation and avoid the need to write a different expression for each container, expressions use local group numbering. Thus, the **Unknown1** reference always refers to the first **Unknown** sample group on the plate being evaluated. However, the sample group, type, or position from a particular matrix or plate can be referenced.

To learn more about referencing samples, see Sample References in Multiple Container Assays topic.

Reference	Refers To
Unknown1	The average of the first **Unknown** sample group on a matrix and plate being evaluated.
A1.2	**A1** position for 2nd matrix.
A1.2.3	**A1** position for the 2nd matrix of 3rd plate.
A1..3	**A1** position for 3rd plate.
A1.2.All	The average of all **A1** positions on the 2nd matrix across all plates.
Unknown1.2	**Unknown1** sample group for 2nd matrix of data.
Unknown.2.All	The average of all **Unknown** samples on the 2nd matrix across all plates.
Unknown1.2.All	The average of all **Unknown1** replicates on the 2nd matrix across all plates.
Unknown1.2.3	**Unknown1** sample for the 2nd matrix of 3rd plate.
Unknown1..3	**Unknown1** sample on the 3rd plate.

For more information about configuring data analysis for multiple plate assays, see Multiple Plate Analysis.

Numerical Field Data Reference

Numerical Field Data values can be referenced in expressions by specifying the field data matrix letter as part of the reference. The field data matrix lettering starts from A. View the **Matrices** tab to see the lettering of any field data matrices. The following table provides examples:

Reference	Refers To
Unknown1.A	The average of the first **Unknown** sample group on the first field matrix (lettered A) and
A1.A	**A1** position for the first field matrix (lettered A).
A1.B	**A1** position for the second field matrix (lettered B).
Unknown1.A.2	The average of the first **Unknown** sample group on the first field matrix (lettered A) on the second container.
H12.C.4	**H12** position for the third field matrix (lettered C) on the fourth container.

Matrix Position References

This operand comes in handy for accessing the data on the specified matrix at the position the expression is being evaluated for. It is relevant for endpoint data only; however, it is useful for configuring how the XY (kinetic or spectral) data is treated in analysis.

For additional details and configuration examples, see the Matrix Position Reference subsection.

Matrix Position Reference

A Matrix Position Reference is a convenient way to refer to data in a specific matrix. For example, the expression:

#1-#2

can be used to compute the differences between the values on the first and second matrix (for all positions on the layout).

> A Matrix Position Reference refers to data at the associated position on a specific matrix (and optionally on a specific container/plate/analyte).

When is a Matrix Position Reference Available?

Matrix Position References are available where the expression being evaluated is associated with a position. Examples of transforms with position associated expressions are:

- Expression by Matrix
- Expression by Matrix (Dual)
- XY Expression
- XY Expression (Dual)
- XY Reduction X at Y
- XY Reduction Y at X

Also, the Range parameters (**X Minimum** and **X Maximum**) of XY transforms are position associated.

In these cases, the expression is evaluated at each and every position. The matrix position reference provides a convenient method for accessing the data on the specified matrix at the position the expression is being evaluated for.

Syntax

A Matrix Position Reference is available in two forms:

- With Matrix Number
- With Matrix Number and Container Number (e.g., plate/multiplex analyte)

The matrix number is the 1-based number of the matrix. These are listed in the **Matrices** tab.

Example References

Matrix Position Reference	Refers To
#1	Matrix 1
#1.2	Matrix 1 Container 2

> Matrix Position References are only applicable to endpoint matrices. If you mistakenly refer to a matrix that is not endpoint (e.g., XY, kinetic, or spectral) there will be an error evaluating the expression.

XY Data and Matrix Position Reference Examples

When working with XY data (e.g., kinetic or spectral), it is useful to be able to reference calculation results from the previous matrices for further analyses.

Example 1

For a kinetic data analysis, it might be useful to perform calculations only on data after a peak point has occurred. To achieve this, the first step would be to add an XY Reduction Peak Point transform that will compute the peak for each plot. To do this, use the default settings of this transform and set the result to be the *x* value at the peak for each position.

At this point we have two matrices, one Raw and one Calculated. The matrices (and their numbers) can be found under the **Assay Properties | Matrices** tab, e.g.,
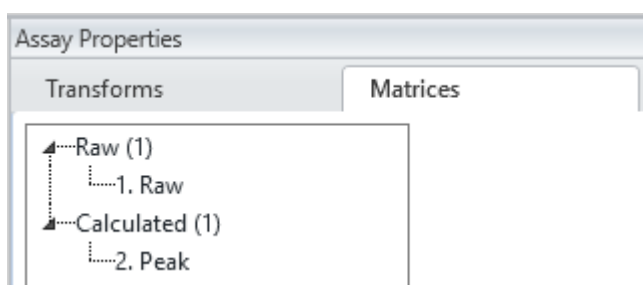
The next step would be to add another transform that uses the computed value of each sample. For example, add the XY Reduction Total transform. This simply calculates the total of the measurements. To configure the transform to only consider measurements from the peak set the **X Minimum** range option to:

#2

I.e.:
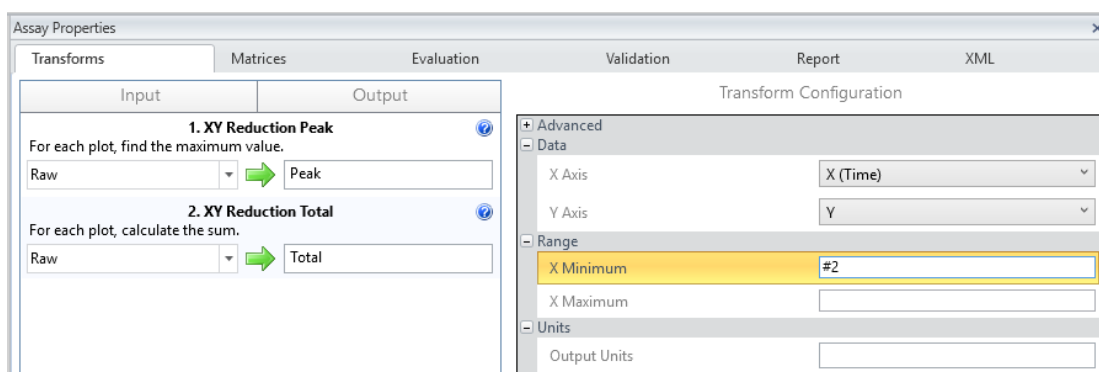
With this setting, the transforms will compute the total of the measurements for each sample but only from the peak point, e.g.:

Total is 21.2183
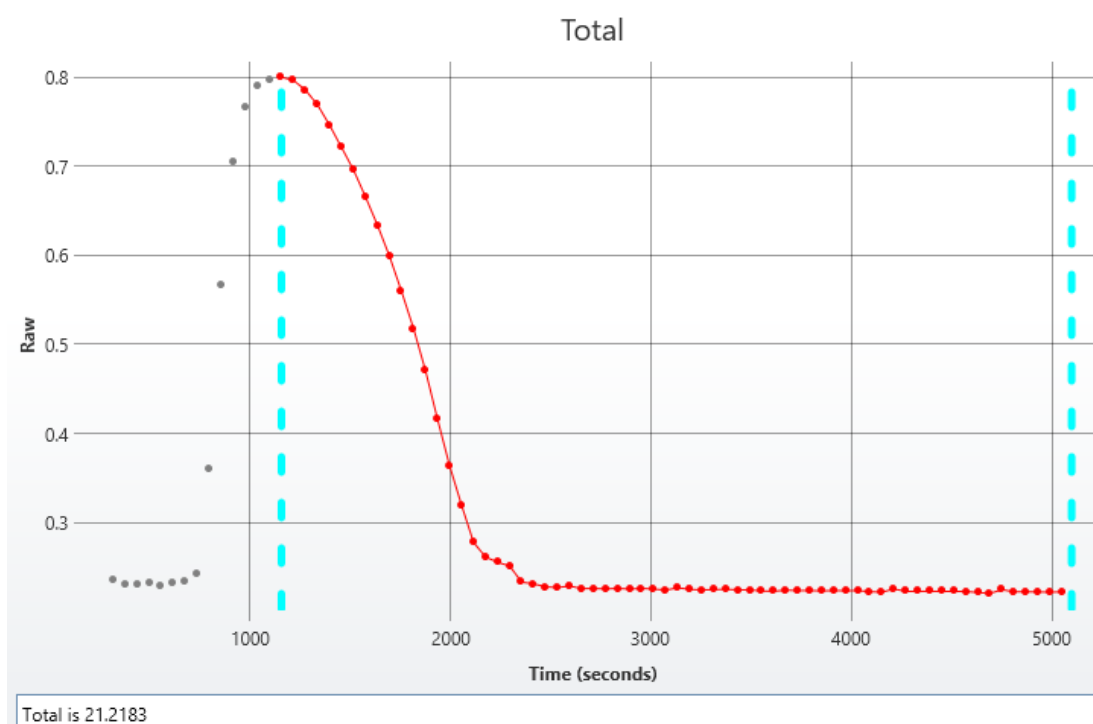
Example 2

In another kinetic example, the time taken to reach half peak can be computed. In this case:

1. The XY Reduction Peak Point can be used to compute the peak, this time with the result being set to the *y* value of the peak.

2. The Expression by Matrix transform is used to compute the *y* value at half of the peak.

3. The XY Reduction X at Y transform can be used to calculate the time (*x*) when the half-peak (*y*) is reached. In this case the Matrix Position Reference #3 is used to reference matrix 3 (the half-peak) as the Cursor for the calculation.

I.e.:

Transform Output Variables

The Transform Output Variable (TOV) feature enables a transform to expose certain calculated numerical results of the analysis as variables. TOVs can be used to reference specific quantities of interest for further analysis.

For example, if you wanted to validate that the calculated R^2 value from a Standard Curve Fit transform was greater than a specific expected value, you could create a Validation condition that references the R^2 value of the Standard Curve Fit transform. Using this feature you could validate that the R^2 value is > 0.9 with the user being alerted if the fit is below an acceptable threshold.

TOV Definition

Each TOV is a named variable with a numerical value that can be referenced in an expression.

The following evaluated values are produced as TOVs by the Standard Curve Fit transform:

- All valid calculated coefficients
- All non-matrix data (quantification limits and sum of squares)
- All valid calculated goodness measures
- All valid calculated Standard Curve Fit Named Evaluations

> 📝 Here "valid" means that result was computed successfully and has a value.

Referencing a TOV

Transform Output Variables can be referenced using expressions for:

- Any transform evaluated after the transform that produced the output variable (only where the later transform supports parameters with expression)
- The Validation expression
- The Evaluation expression
- The Label expression
- The Fit Constraint expression
- The Custom fit expression

Identifying Available TOVs

The available TOVs depend on your configured transforms. For each transform that produces TOVs, the available TOVs are added to the calculation log.

How to: Identify Available TOVs

1. [Launch an assay protocol](#) or [open a results file](#).

2. Add and configure the transforms as required.

3. After the results were calculated, open [Calculation log](#) and scroll down to the end.

4. If the transform produces TOVs, review or copy the available TOVs from the list.

The syntax of the TOV as it appears in the [Calculation log](#) is as follows:

TOV added: TOV{N}.{Name}={Value}

Where:

{N} – The number of transform in the sequence configured via **Transform** tab

{Name} – The name of a specific evaluated value

{Value} – The evaluated result of the TOV

When referenced in expression, a syntax is **TOV{N}.{Name}**, e.g., **TOV1.SE**.

> You can only reference TOVs that originate from transforms that are defined and evaluated prior to where the reference is being made. For example, the **TOV2.R2** could be referenced from the third transform onward, but not from the first. For [validations](#), [evaluations](#) and [labels](#), any TOV can be referenced as these elements are prepared after all transforms are computed.

TOVs and Multiple Plate or Multiplex Analyses

For multiple container assays (such as multiple plate or multiplex) the reference to the TOV refers to the TOV output on the container it is associated with.

For example, **TOV1.SE** would refer to the SE value of the 1st transform on the container being evaluated.

Examples:

Here are examples of TOVs along with descriptions of their behaviour.

TOV	Refers to
TOV1.ULOQ	The ULOQ value of the curve-fit as calculated in the first transform.
TOV3.m	The **m** coefficient value of [Linear Regression](#) curve fit method as calculated in the third transform.
TOV1.SE	The Standard Error value of the curve-fit as calculated in the first transform.
TOV1.SSC	The sum of squares computed from input y average and y'

TOV	Refers to
	average (flagged points not included)
TOV2.R2	The R^2 value of the curve-fit as calculated in the second transform.

Sample References in Multiple Plate Assays

This section describes how to refer to samples when defining calculations that will be performed across multiple plate assays.

MyAssays Desktop's expression system has been designed to make it easy to define calculations that apply to both single and multiple plates. Expressions can include references to sample groups.

For example, with the Expression by Matrix transform, the expression:

x-Blank1

can be used to subtract the average of the **Blank1** samples from all other samples on the plate.

This is easy to follow for a single plate assay. However, it might not be clear how to define such a calculation when running a multiple plate assay with a blank group on each plate. In this case, it might seem necessary to define an expression for each plate — this would become quite tedious if your assay is ran across many plates. Thankfully, this is not the case.

Local-Group Sample Numbering

For simplicity, MyAssays Desktop layouts and expressions use local-group numbering. This means that when you define the layout or refer to groups in an expression, the group numbers start at 1 for each plate.

Following previous example for a multiple plate assay with a single blank group on each plate, the layout definition would include **Blank1** for each plate. Thus we can continue to use the expression:

x-Blank1

to perform the blank correction for each plate, using the associated blank sample (i.e. the blank sample from plate 1 will be used to correct plate 1, while the blank sample from plate 2 will be used to correct plate 2). The software will subtract the average of the first blank group from all other samples on the same plate.

Local-group numbering extends to all samples in the layout, so an expression including **Control1** will refer to the first control group on each plate.

Regardless of how many plates you read, the same single expression can be used. If you are using more or less plates or need to change their order, there is no need to change your expression. This is sure to save your time, especially when compared to the equations you would need to use to configure this in Excel.

Global-Group Sample Numbering

Once you've calculated your results, MyAssays Desktop uses global-group numbering. Results displayed on screen or in the report will be contiguous across plates. Referring back to the same example, with global-group numbering **Blank1** is on the first plate and **Blank2** is on the second plate, etc.

This distinction between using local-group numbering for layout definition and expressions and global-group numbering for results display is the key to simplifying how to define common mathematical operations that can be applied across multiple plates.

> To learn more about group numbering in multiple plate assays, see Multiple Plate Group Numbering.

Referring to a Specific Sample on a Specific Plate

To refer to a group on a specific plate, append the group reference with two dots followed by the plate number. For example, to refer to the **Blank1** group on the first plate, use:

x-**Blank1..1**

With this expression applied to the Expression by Matrix transform, every sample on every plate would be corrected by the **Blank1** group measured on the first plate. In this case, it would only be necessary to perform a blank measurement on the first plate.

Referencing Samples on the Specific Plate and/or Matrix

You can also reference samples on the specific matrix and plate as follows:

[Reference].[Matrix].[Plate]

Where:

- **Reference** – Sample type, group, or a position you want to refer to, e.g., **Blank**, **Unknown1**, **A5**.

- **Matrix** – The 1-based sequential number of the matrix. Matrix 1 will always be the first set of measurement data. Depending on your assay, subsequent matrices might be further measurements or the results of any transforms.
  To learn more about the matrix numbering, see Viewing Available Matrices and Configuring Their Settings.

- **Plate** – The plate number on the **Measurements** tab, in the **Plate IDs** subtab. Add **All** instead of a plate number to reference samples across all plates.

If you omit **[Plate]**, then this will reference sample on the specific matrix of corresponding plate. For example, **Blank1.2** refers to the first blank group on the second matrix of the plate being evaluated.

> ℹ If your assay contains one matrix of data, and you configured the Expression by Matrix transform, then **Blank1.2** refers to transform result for **Blank1** sample.

The reference of transform results can be included in the expressions for any transform downward to the referenced one (only where the later transform supports parameters with expression), validation, evaluation, and labels.

To reference samples from a specific plate, append the **[Reference]** with **..** and plate number, e.g., **Blank1..1** refers to the first blank group of the selected matrix on the first plate.

Functions

This section provides reference information for various functions available to perform calculations on data.

Syntax

These take the form of a function name followed by a comma-separated list of values in brackets. The function data can refer to any operand type.

1. If the function refers to a single operand of any type:

   function(operand)

2. If the function refers to a list of operands:

   - If operands do NOT include sample references:

   function(operand1,operand2,...,operandN)

   - If operands include ONLY sample references:

   function([operand1,operand2,...,operandN])

   - If operands include any operand type AND sample references:

   function ([samplereference1,samplereference2,...,samplereferenceN],operand1,operand2,...,operandN)

3. If the function requires vector operands:

   - **function({list of *y*s},{list of *x*s})**

   - **function({(samplereference1),(samplereference2),...,(samplereferenceN)}, {operand1,operand2,...,operandN})**

Calculation Functions

This section describes functions that calculate the result of mathematical operations on an argument or a list of arguments. Calculation functions use general syntax for functions and perform an operation on a list of 1 or more operands. The evaluation of these functions results in a single numeric value.

Name	Description	Example
abs	Returns the absolute value of argument. The absolute value of a non-negative argument is the argument itself. The absolute value of a negative argument is -1 times the argument.	**abs(-1.23)** =1.23 **abs(1.23)** =1.23
average	Described in group-enabled functions.	**average(1,2)** =1.5 **average(-3,0.25,5)** =0.75
auc	*Syntax:* **auc (method,xmin,xmax,number,coefficients...)** Calculates the area under the plotted 4PL or 5PL curve using the sum of trapezia method. The area under the curve is the area between the curve and the x-axis. Areas below the x-axis are considered negative. Input parameters: • **method** – This is either 4PL or 5PL fit method. Specify within single or double quotes: **"4PL"** or **'4PL'**; **"5PL"** or **'5PL'**. • **xmin** – The minimum numerical value of the area on the x-axis. • **xmax** – The maximum numerical value of the area on the x-axis. • **number** – The number of trapezium intervals for computing the area under the curve. Higher number of intervals gives more accurate results. We recommend to use value of 1000.	**auc ('4PL',0.023, 22.727,1000, 12.648,2.499,0.151, 73.746)** =1663.5 **auc ("5PL",0.125,4,100, 0.226,1.956,2538, 1.648,2439570)** =1663.5

Name	Description	Example
	• **coefficients** – The coefficients of the selected **method** that must be specified in the following order: For 4PL: **a**, **b**, **c**, **d** For 5PL: **a**, **b**, **c**, **d**, **m** When calculating area under curve (AUC) for Dose–Response Curves, replace **xmin** with **dosemin** and **xmax** with **dosemax** context variables. These are set to the minimum and maximum numerical values in the **Doses**. For more information, see Advanced Dose–Response Curves Evaluations.	
ceiling	*Syntax:* **ceiling(argument,multiple)** Returns argument rounded up, away from zero, to the nearest multiple of significance. If it is an exact multiple, no rounding occurs. Input parameters: • **argument** – The value you want to round off. • **multiple** – The multiple to which you want to round. If both parameters are negative, the value is rounded down, away from zero. If argument is negative, and multiple is positive, the value is rounded up towards zero.	**ceiling(1.23,0.05)** =1.25 **ceiling(-1.23,0.05)** =-1.2
count	Described in group-enabled functions.	**count(1,2,3)** =3 **count(-2.44,2,5,98,6)** =5
exp	*Syntax:* **exp(argument)** Returns **e** raised to the power of the given number. It	**exp(2)** =7.389056…

Name	Description	Example
	accepts only a single argument. For example, **exp (A1+A2)** but not **exp(A1,A2)**. Input parameter: • **argument** – The exponent applied to the base **e**.	**exp(-1)** =0.367879…
floor	*Syntax:* **floor(argument,multiple)** Returns argument rounded down, toward zero, to the nearest multiple of significance. Input parameters: • **argument** – The value you want to round off. • **multiple** – The multiple to which you want to round. ⓘ With a positive **argument**, the value is rounded down toward zero. With a negative **argument**, the value is rounded down away from zero. If the **argument** is an exact multiple of **multiple**, no rounding occurs.	**floor(1.23,0.05)** =1.2 **floor(-1.23,0.05)** =-1.25
intercept	Calculates the point at which the least square's fit line will intersect the y-axis by using existing x values and y values. The intercept point is based on a best fit regression line plotted through the known x values (independent set of arguments) and known y values (dependent set of arguments). ⓘ Requires a vector of arguments as parameters. The number of y and x operands is required to be the same and greater than 2. In other words, {$y1,y2,y3$} and {$x1,x2,x3$}; {$y1,y2, … yN$} and {$x1, x2, … xN$}.	**intercept({1,2},{3,2})** =4 **intercept({-2.44,2,5,98,6}, {0.1,0.2,0.3,0.4,0.5})** =-12.152
ln	Returns the natural logarithm of an argument. Natural logarithms are based on the constant **e** (2.718281828459…). The argument is supposed to be positive. ⓘ **ln** is the inverse of the **exp** function.	**ln(10)** =2.302585… **ln(1.23)** =0.207014…

Name	Description	Example
log	*Syntax:* **log(argument,base)** Calculates the logarithm of an argument to the base that you specify. Input parameters: - **argument** – Positive real numerical value or [expression](#) for which you want the logarithm. - **base**– Base of the logarithm. If the base is omitted, it defaults to 10.	**log(2,4)** =0.5 **log(1.23,2)** =0.298658…
log10	Returns the base-10 logarithm of a positive argument.	**log10(1.23)** =0.089905… **log10(0.1)** =-1
max	Returns the largest value in a set of values. To determine the maximum of positions in a sample group or sample type, type in the argument it square brackets (i.e., **max ([Unknown1])**). Otherwise the reference is treated as the average of positions.	**max(1,2,3)** =3 **max(-2.44,2,5,98,6)** =98
median	Described in [group-enabled functions](#).	**median(1,2,3,4)** =2.5 **median(-2.44,2,5,98,6)** =5
min	Inversely to **max** function, returns the smallest number in a set of values. All requirements of the **max** apply to **min**.	**min(1,2,3)** =1 **min(-2.44,2,5,98,6)** =-2.44
mod	*Syntax:* **mod(number,divisor)** Returns the remainder after the number is divided by a divisor. The result has the same sign as the divisor.	**mod(2,0.3)** =0.2 **mod(1.23,5)**

Name	Description	Example
	Input parameters: • **number** – The argument for which you want to find the remainder. • **divisor** – The value to divide the **number** with.	=1.23
pow	*Syntax:* **power(argument,power)** Raises the argument to the given power. Input parameters: • **argument** – Numeric value or an expression to raise to a power. • **power** – Exponent to raise power to.	**power(2,3)** =8 **power(1.23,5)** =2.815305…
slope	Returns the slope of the linear regression line through data points in *x*s and *y*s. The slope is the vertical distance divided by the horizontal distance between any two points on the line, which is the rate of change along the regression line. ⓘ Requires a vector of arguments as parameters. The number of *y* and *x* operands is required to be the same and greater than 2 (i.e., {*y1,y2,y3*} and {*x1,x2,x3*}; {*y1,y2, … yN*} and {*x1, x2, … xN*}).	**slope({1,2},{3,2})** =-1 **slope({-2.44,2,5,98,6}, {0.1,0.2,0.3,0.4,0.5})** =112.88
stdev	The same as **sd** in group-enabled functions.	**stdev(1,2,3)** =1 **stdev(-2.44,2,5,98,6)** =42.772359…
sum	Described in group-enabled functions.	**sum(1,2,3)** =6 **sum(-2.44,2,5,98,6)** =108.56
var	Described in group-enabled functions.	**var(1,2,6)** =7

Name	Description	Example
		var(-2.44,2,5,98,6)
		=1829.47472

Conditional Functions

This section describes Boolean logical and conditional operations.

> As with all expression elements, these functions can be used in conjunction with other expression operands, operators and functions. Where a sample reference is used as an input parameter to a conditional function, it refers to the average of the non-flagged data points.

Boolean Logical Functions

These are particularly useful for defining validation, flagging, and label conditions.

Name	Description	Example
and	*Syntax:* **and(a,b)** Tests a number of input conditions and returns 1 if all of the conditions evaluate to true, or 0 otherwise.	**and (Unknown>0,Unknown<10)** Tests if the mean of the Unknowns is within the range of 0 to 10.
or	*Syntax:* **or(a,b)** Tests a number of input conditions and returns 1 if any of the conditions evaluate to true, or 0 otherwise.	**or(*x*<5,*x*>10)** Tests if the value of *x* is less than 5 or greater than 10.
not	*Syntax:* **not(a)** Returns a logical value that is the opposite of an input logical value or expression (i.e., returns 0 if the supplied argument is true and returns 1 if the supplied argument is false).	**not(Blank>1)** Tests if the mean of the Blanks is less than or equal to 1.

Conditional Function

Name	Description	Example
if **ifthenelse**	*Syntax:* **ifthenelse(1,2,3)** or **if(1,2,3)** > The **if** and **ifthenelse** perform the same function. Requires 3 parameters: 1. The Boolean condition to evaluate (which will evaluate to true or false). 2. The result if the condition is true.	**ifthenelse (Unknown1>10,10,Unknown1)** **if(Unknown1>10,10,Unknown1)** If the value of **Unknown1** is greater than 10 then the result is 10, otherwise the value equals **Unknown1**'s value.

Name	Description	Example
	3. The result if the condition is false.	
	If the value of the first condition is true, then the result is the second argument otherwise the third.	**ifthenelse(PosReplicate ()=1,_x_*0.5,_x_*0.125)**
		if(PosReplicate ()=1,_x_*0.5,_x_*0.125)
	When using the Expression by Matrix transform to define a calculation to perform on all samples, this can be used to concisely define different calculations to perform on different sample types or replicates by Position Functions to query the sample at each position.	Where the sample is the first replicate the value is multiplied by a factor of 1/2 and other replicates by 1/8. (Here the position function **PosReplicate()** is used to reference the replicate number.)

Group-Enabled Functions

This section describes functions that operate on list of values with an open-ended length.

Where a sample reference is used as a parameter to a group-enabled function, any sample group/type reference inside a Group-Enabled Function's parameter list refers to the non-flagged values of that group/type.

Syntax

These functions are specified with the following syntaxes:

- **function(Sample type or group reference)** – If there is 1 input sample group/type reference.

- **function([Sample type or group reference, Sample type or group reference, ... , Sample type or group reference])** – If there are 2 or more input sample group/type references.

> When there are 2 or more sample group/type references inside a parameter list, insert each group reference inside square brackets (e.g., **pcv ([Standard1,Unknown2]**) to access the values of non-flagged data points.

> With Group-Enabled functions, care should be taken when providing a list of groups to the function. MyAssays Desktop will not accept a list of groups i.e. **sd (Unknown1,Unknown2)** as this is ambiguous. This example could refer to the SD of all replicates of Unknown1 and Unknown2, or it could be the SD of the average of Unknown1 and Unknown2. In these cases, either use **[ ]** to enclose the sample groups, or use another function such as **average**. For example, to calculate the SD of all replicates of Unknown1 and Unknown2, the following expression should be used: **sd([Unknown1,Unkonwn2])**. To calculate the SD of the average of the replicates of Unknown1 and Unknown2, the following expression should be used: **sd(average (Unknown1),average(Unknown2))**.

The following table lists group-enabled functions in alphabetical order:

Name	Description	Minimum number of parameters	Example
average	The same as **mean**.	1	**Unknown1** Returns the mean of all replicates in the

Name	Description	Minimum number of parameters	Example
			Unknown1 sample.
			average([Unknown, Blank])
			Returns the mean of the Unknowns and Blanks.
choose	Reference the value at the specified position in a list. This can be used to access a specific replicate within a sample group.	2	**choose(1,[Unknown1])**
count	Counts the number of non-flagged values.	1	**count(Unknown)**
mad	Calculates the [median absolute deviation](#) of the non-flagged positions. The median absolute deviation is the median of the absolute values of the deviation of each observation from the mean of the variable.	1	**mad(Control1)** Returns the median absolute deviation of all replicates in the **Control1** sample. **mean([Unknown, Blank])** Returns the median absolute deviation of the Unknowns and Blanks.
mean	Calculates the mean of the non-flagged positions.	1	**mean(Unknown1)** Returns the mean of all replicates in the **Unknown1** sample. **mean([Unknown, Blank])** Returns the mean of the Unknowns and Blanks.
median	Calculates the median of a finite list of non-flagged positions. If there is an even number of arguments in the set, then median calculates the average of the two positions in the middle.	1	**median(Unknown1)** Returns the median of the **Unknown1** replicates. **median([Standard2, Unknown4])**

Name	Description	Minimum number of parameters	Example
			Returns the median replicate of **Standard2** and **Unknown4** samples.
pcv	Calculates the percentage coefficient of variance (**%CV**) of a finite list of non-flagged positions.	2	**pcv(Unknown)** Calculates the %CV of all Unknowns. **pcv([Unknown1, Unknown1.2])** Calculates the %CV of the **Unknown1** replicates in the first and the second matrix of data.
rsd	Calculates the robust standard deviation of a finite list of non-flagged positions. The robust standard deviation is the median average deviation (mad) * 1.4826.	2	**rsd(Standard2)** Calculates the robust standard deviation of the **Standard2** sample replicates. **rsd([Unknown1, Unknown3])** Calculates the robust standard deviation of the **Unknown1** and **Unknown3** sample replicates.
sd	Calculates the standard deviation of a finite list of non-flagged positions. The standard deviation is a measure of how widely values are dispersed from the average value (the **mean**). This function uses the "sample of population" method, equivalent to **stdev.s**	2	**sd(Standard2)** Calculates the standard deviation of the **Standard2** sample replicates. **sd([Unknown1, Unknown3])** Calculates the standard deviation of the

Name	Description	Minimum number of parameters	Example
	Square brackets specify to extract all replicate values of the groups contained therein. The following expression: **sd ([Unknown1,Unknown3])** will extract values for each sample replicate. In this example if there are 2 replicates of each sample group, the n value will be 4. This is true regardless of the input matrix - so if an Average matrix is selected, each replicate will be included in the calculation. To calculate the Standard Deviation of the Averages, instead use the following syntax: **sd(average (Unknown1),average (Unknown3))**		**Unknown1** and **Unknown3** sample replicates.
se	Calculates the standard error of a finite list of non-flagged positions.	2	**se(Unknown1)** Calculates the standard error of the **Unknown1** sample replicates. **se([Unknown, Control])** Calculates the standard error of all**Unknown** and **Control** sample replicates.
sum	Returns the total of all items in the finite list of non-flagged positions.	1	**sum(Unknown)**

Name	Description	Minimum number of parameters	Example
			Returns the sum of all samples of the **Unknown** type. **sum([Unknown1, Unknown1.2, Unknown1.3])** Returns the sum of all replicates of the **Unknown1** samples on the containers from 1 to 3.
var	Calculates the variance of a finite list of non-flagged positions. Variance is a measurement of the spread between positions in a data set. The variance measures how far each number in the set is from the mean.	2	**var(Unknown4)** Calculates the variance of the replicates in the **Unknown4** sample. **var([Unknown1, Unknown1.2])** Calculates the variance of the **Unknown1** sample replicates in the first and the second container of data.
head	Returns a subset of the provided list, the *n* elements from the start of the list. The final parameter is the number of elements *n* in the new list. The last argument is the number of elements to get from head. This function is useful for working with **obs** for QC rules. For more information see Quality Control	1	**head(3,2,1)** Returns the result 3 from the provided list **3,2** **head([Unknown1],1)** Returns the value of the first replicate of **Unknown1** **average(head(3,2,2))** Returns the result 2.5
tail	Returns a subset of the provided list, the *n* elements from the end of the list.	1	**tail(3,2,1)** Returns the result 2 from

Name	Description	Minimum number of parameters	Example
	The final parameter is the number of elements *n* in the new list. The last argument is the number of elements to get from tail. This function is useful for working with **obs** for QC rules. For more information see Quality Control		the provided list **3,2** **tail([Unknown1],1)** Returns the value of the last replicate of **Unknown1**

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to find medium value for **Unknown1** and **Unknown2** positions.

The example uses a layout with 16 **Unknown** sample groups, where **Unknown1** at **A1**, **A2** **A3**, **A4**, **A5**, and **A6**, **Unknown2** at **A7**, **A8**, **A9**, **A10**, **A11**, **A12**, etc.). I.e.:

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	1	1	1	1	2	2	2	2	2	2
B	3	3	3	3	3	3	4	4	4	4	4	4
C	5	5	5	5	5	5	6	6	6	6	6	6
D	7	7	7	7	7	7	8	8	8	8	8	8
E	9	9	9	9	9	9	10	10	10	10	10	10
F	11	11	11	11	11	11	12	12	12	12	12	12
G	13	13	13	13	13	13	14	14	14	14	14	14
H	15	15	15	15	15	15	16	16	16	16	16	16

⬤ Unknown

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

We use the expression:

median([Unknown1,Unknown2])

Unknown1 and **Unknown2** refer to the lists of non-flagged data points for the **Unknown1** and **Unknown2** sample groups. From this list the median is calculated.

The result will be (also displayed here to 3 decimal places):

1.202

Layout Analysis Functions

Layout Analysis Functions are available only if the evaluation is associated with a layout. Otherwise an error message will be displayed.

Position Functions

Position Functions are only available when there is a position associated with the expression being evaluated. They do not use input parameters.

> Position functions can be used in conjunction with conditional function in the Expression by Matrix transform to perform different calculations on different sample types, positions, or replicates.

The following table lists the position functions:

Name	Description	Example
PosValueByIndex	*Syntax:* **PosValueByIndex (PositionNum)** Returns the value at the specified (1-based) position number (in accordance with position numbering). The valid range of PositionNum depends on the layout. For a 12x8 plate this will be 1-96. For rack layouts, this depends on the number of samples measured.	**PosValueByIndex (1)** Value of position A1 **PosValueByIndex (13)** Value of position B1 (on a 12x8 layout) **PosValueByIndex(PosNum()+2)** Value at the position two to the right of the current position.
PosValueBySampleReplicate	*Syntax:* **PosValueBySampleReplicate (Type , GroupNum ,ReplicateNum)** Returns the value of the position occupied by the specified replicate of the	**PosValueBySampleReplicate("Unknown",1,2)** Returns the value of the position occupied by the second replicate of Unknown1.

Name	Description	Example
	specified group of the specified type. The valid range of ReplicateNum and GroupNum depends on the layout. This depends on the number of replicates of each sample group, and the number of groups of the specified sample type.	
PosNum	*Syntax:* **PosNum()** Returns the 1-based position number of each position, which is assigned in accordance with position numbering.	**ifthenelse(mod(PosNum (),2)=0,*x*,0)** Sets the values of odd positions to zero.
PosContainerNum	*Syntax:* **PosContainerNum ()** Returns the 1-based container number for the given context. For example, if the **PosContainerNum()** is used in an expression on a multiple plate assay, this would return the number of the plate.	**ifthenelse (PosContainerNum ()=1,4*x,x)** Multiplies the values on the first container by 4.
PosGroup	*Syntax:* **PosGroup()** Returns the 1-based group number of the sample group at the position, using Local Numbering. For example, if the position contains **Unknown3**, then the group is 3.	**ifthenelse(PosGroup ()=1,2*x,x)** Doubles the values of the first replicates in each sample group.
PosType	*Syntax:* **PosType()** Returns the sample type number associated with the position.	**ifthenelse(PosType ()=LayoutType ("Blank"),0,*x*)** Sets the values of all **Blank**

Name	Description	Example
	This can be used in conjunction with the LayoutType function to compare the associated position with a particular named sample type.	positions to 0.
PosReplicate	*Syntax:* **PosReplicate()** Returns the 1-based replicate number of the specified in the argument position. Replicate numbers are assigned in accordance with position numbering. This function is based purely on the layout and does not take flagging into account.	**ifthenelse(PosReplicate ()=1,x,0)** Returns the values of the first replicate for each sample; sets the values of all other replicates to zero.
PosXValuesByIndex	*Syntax:***PosXValuesByIndex (PositionNum)** For XY data matrices, returns the non-flagged X values of the specified position. The valid range of PositionNum depends on the layout. For a 12x8 plate this will be 1-96. For rack layouts, this depends on the number of samples measured.	**mean(PosXValuesByIndex (1))** Returns the average of all non-flagged X values of position A1.
PosYValuesByIndex	*Syntax:***PosYValuexByIndex (PositionNum)** For XY data matrices, returns the non-flagged Y values of the specified position.	**mean(PosYValuesByIndex (2))** Returns the average of all non-flagged Y values of position A2.

Name	Description	Example
	The valid range of PositionNum depends on the layout. For a 12x8 plate this will be 1-96. For rack layouts, this depends on the number of samples measured.	**sd(PosYValuesByIndex (PosNum(),1))** Returns the standard deviation of all non-flagged Y values of each position on the first container. Note XY Reduction Function simplifies this calculation. **pcv(PosYValuesByIndex (PosNum(),1))** Returns the %CV of all non-flagged Y values of each position on the first container. Note XY Reduction Function simplifies this calculation.
PosZValuesByIndex	*Syntax:***PosZValuexByIndex (PositionNum)** For XYZ data matrices, returns the non-flagged Z values of the specified position. The valid range of PositionNum depends on the layout. For a 12x8 plate this will be 1-96. For rack layouts, this depends on the number of samples measured.	**mean(PosZValuesByIndex (3))** Returns the average of all non-flagged Z values of position A3
PosYValuesByType	*Syntax:***PosYValuesByType (Type)** For XY data matrices, returns the non-flagged Y values of all non-flagged positions of the specified type.	**PosYValuesByType ("Unknown")** Returns the non-flagged Y values of all non-flagged Unknown samples.
PosYValuesByGroup	*Syntax:* **PosYValuesByGroup (Type,GroupNum)**	**PosYValuesByGroup ("Unknown",1)** Returns the non-flagged

Name	Description	Example
	For XY data matrices, returns the non-flagged Y values of all non-flagged positions of the specified group.	Y values of Unknown1
PosYValuesAll	*Syntax:***PosYValuesAll (MatrixNumber)** For XY data matrices, returns the non-flagged Y values of all non-flagged used positions on the specified matrix.	**mean(PosYValuesAll(1))** Returns the average of all non-flagged Y values of data matrix 1.

Layout Functions

These functions require an associated layout.

Layout Functions Parameters

PositionNum

To simplify performing analyses based on sample positions, numerical position references are used in various functions. Positions are numbered from 1, left-to-right row-wise. For example, on a 12x8 microplate layout, position number 1 is well A1, position 2 is well A2 and B1 is position number 13.

For rack-based layouts the same numbering convention is used with the upper limit being dependant on the number of samples measured.

Type

Type can be specified as a sample type number or case-insensitive sample type name in quotes:

- **LayoutNumGroups**(3)
- **LayoutNumGroups**("Blank")
- **LayoutNumGroups**("blank")
- **LayoutNumGroups**("bLaNK")

> ℹ️ "**Unused**" type is not supported.

ContainerNum

Where a layout function accepts the **ContainerNum** argument:

- If **ContainerNum** is 0 (or not specified), then the function will be evaluated for all containers in the layout.

- If **ContainerNum** is specified (as a 1-based container number), then only the layout for that container is considered.

GroupNum

This is the 1-based group number of a sample group.

Layout Evaluation Functions

Layout Evaluation functions enable sample group references to be more flexible (e.g., for applying calculations on group number references).

Name	Description	Example
GroupValue	*Syntax:* **GroupValue(Type,GroupNum)** Returns the value of the sample group with the specified type and group number.	**GroupValue ("Unknown",1)** The value of the group that is **Unknown1**.

> The **GroupValue** function can be used in conjunction with **PosGroup()** to obtain the group of a specified type that matches the group number of the position being evaluated. For example, if you want to reference the **Unknown** group that has the same number as the current position, use: **GroupValue("Unknown", PosGroup())**

The following table lists the layout functions in alphabetical order:

Name	Description
LayoutCommonNumReplicatesType	*Syntax:* **LayoutCommonNumReplicatesType (Type)** If all groups of the specified Type on all containers have the same number of replicates, then it returns that number. Otherwise -1 is returned. For example: **LayoutCommonNumReplicatesType ("Unknown")** Tests if all **Unknown** sample groups on all containers have the same number of replicates. Returns this number if it is the same; otherwise,

Name	Description
	returns -1.
LayoutHeight	*Syntax:* **LayoutHeight()** The number of rows in the layout (note, this is same value for all containers). It is useful for specifying column-based expressions.
LayoutNumContainers	*Syntax:* **LayoutNumContainers()** The number of containers in the layout. It is useful for specifying expressions for a certain container of data.
LayoutNumGroups	*Syntax:* **LayoutNumGroups (Type,ContainerNum)** The number of groups with the specified type. For example: **LayoutNumGroups("Blank", 1)** Returns the number of **Blank** sample group on the 1st container.
LayoutNumGroupsTotal	*Syntax:***LayoutNumGroupsTotal(Type)** The total number of groups of the specified type on all containers.
LayoutNumGroupsAcrossContainers	*Syntax:* **LayoutNumGroupsAcrossContainers (Type)** Determines the number of groups of the specified Type parameter on each of the containers. If this is the same number on every container (including 0), then this value is returned. Otherwise -1 is returned. For example: **LayoutNumGroupsAcrossContainers ("Unknown")** Tests if there is the same number of **Unknown** sample groups on all containers.
LayoutNumPositions	*Syntax:* **LayoutNumPositions**

Name	Description
	(Type,**GroupNum**,**ContainerNum)**
	The number of positions with the specified type and group number.
	For example:
	LayoutNumPositions("Standard", 3, 1)
	Returns the number of **Standard3** replicates on the 1st container.
LayoutNumUsedPositions	*Syntax:* **LayoutNumUsedPositions (ContainerNum)**
	The number of positions that have a type that is not **Unused** (i.e., Type ≠ 1).
	For example:
	LayoutNumUsedPositions(2)
	For the 2nd container, returns the number of positions that are not **Unused**.
LayoutPositions	*Syntax:* **LayoutPositions()**
	The total number of positions (note, this is same value for all containers).
	It is useful for specifying position-based expressions.
LayoutType	*Syntax:* **LayoutType(Type)**
	The sample type number that represents this type.
	ⓘ Each sample type is identified by a unique integer value.
	For example:
	LayoutType("Blank")
	Is useful for writing expression-based conditions for a particular type.
LayoutWidth	*Syntax:* **LayoutWidth()**
	The number of columns in the layout (note, this is same value for all containers).

Name	Description
	It is useful for specifying row-based expressions (e.g., By-Row Blank Correction).

Flagged Status Functions

Flagged Status Functions query the flagged status of sample positions and sample groups. If all replicates of a group are flagged, the group is considered to be flagged.

These functions can count flagged statuses on a specific container or to all measured containers. Use the ContainerNum parameter to specify which container(s).

These functions are only applicable to endpoint matrices.

Name	Description	Example
NumFlaggedGroups	*Syntax:***NumFlaggedGroups (Type,ContainerNum)** The total number of flagged groups for the specified sample type. (If all replicates of a group are flagged, the group is considered to be flagged.)	**NumFlaggedGroups ("Standard",1)** Returns the total number of flagged groups for the Standard sample type on container 1. **NumFlaggedGroups ("Standard")** Returns the total number of flagged groups for the Standard sample type across all containers.
NumFlaggedPositions	*Syntax:***NumFlaggedPositions (ContainerNum)** The total number of flagged positions for used sample types on the specified container.	**NumFlaggedPositions (1)** Returns the total number of flagged positions for used sample types on container 1. **NumFlaggedPositions()** Returns the total number of flagged positions for used sample types across all containers.

Probability Functions

This section describes syntax and usage of probability functions in MyAssays Desktop.

Overview

The probability functions can be used to examine variability between two sets of data.

Syntax and Parameters

Name	Description	Example
chisq.dist.rt	*Syntax:* **chisq.dist.rt(x,df)** Returns the right-tailed probability of the chi-squared distribution. Requires 2 parameters: • **x** – The value that evaluates the function. • **df** – An integer numerical value or an expression (with integer numeric result), that specifies degrees of freedom.	**chisq.dist.rt (0.0034,8)** Calculates the right tailed probability of the chi-squared distribution for 0.0034 with degrees of freedom set to 8.
f.dist	*Syntax:* **f.dist(*x*,df1,df2,Cumulative)** Evaluates the value of F probability distribution (degrees of diversity) for two data sets. Requires the following parameters: • ***x*** – Positive numerical value at which to evaluate the function • **df1** – An integer numerical value or an expression (with integer numeric result), that specifies numerator degrees of freedom. • **df2** – An integer numerical value or an expression (with integer numeric result), that specifies denominator degrees of freedom. • **Cumulative** – A logical value that determines the form of the function. If set to **true**, then **f.dist** returns the cumulative distribution ; if **false**, it returns the probability density function.	**f.dist (5.7,5,10,true)** Calculates a cumulative F probability for 5.7 with degrees of freedom specified as 5 and 10.
f.dist.rt	*Syntax:* **f.dist.rt(x,df1,df2)**	**f.dist.rt**

Name	Description	Example
	Calculates the F Probability Distribution measuring the degree of diversity between two data sets. Requires 3 parameters: • **x** – the value that evaluates the function • **df1** – An integer numerical value or an expression (with integer numeric result), that specifies numerator degrees of freedom. • **df2** – An integer numerical value or an expression (with integer numeric result), that specifies denominator degrees of freedom.	**(0.2291,3,8)** Calculates the F Probability Distribution for 0.2291 with degrees of freedom specified as 3 and 8.
f.inv	*Syntax:***f.inv(p,df1,df2)** Returns the inverse of the F probability distribution (the inverse of the **fdist**) for a given probability. Requires 3 parameters: • **p** – A probability (between 0 and 1) at which to evaluate the inverse of the **fdist**. • **df1** – An integer numerical value or an expression (with integer numeric result), that specifies numerator degrees of freedom. • **df2** – An integer numerical value or an expression (with integer numeric result), that specifies denominator degrees of freedom.	**f.inv(0.9,6,96)** Finds a numerical value for which the F probability equals 0.9 with degrees of freedom specified as 6 and 96.

Typically, when specifying degrees of freedom with an expression, you may find the Layout Analysis Functions in conjunction with **count function** useful to refer to the number of non-flagged positions of a certain sample type.

Example Expressions

Expression	Evaluated to
f.inv(0.95,2,10)	A numerical value for which the F probability equals 0.95 and degrees of freedom specified as 2 and 10.
f.inv(0.95,LayoutNumGroups ("Standard"),count ([Standard,Unknown]))	A numerical value for which the F probability equals 0.95 and degrees of freedom specified as the number of **Standards** and the number of all

Expression	Evaluated to
	non-flagged **Standard** and **Unknown** samples' replicates.
f.dist(0.5667,2,10,false)	The F probability density value for 0.5667 and degrees of freedom specified as 2 and 10.
f.dist(0.5667,count([Stand-ard,Test]),LayoutNumGroups("Stand-ard"),true)	The cumulative F distribution value for 0.5667. The degrees of freedom here are specified as the num-ber of all non-flagged **Standard** and **Unknown** samples' replicates and the number of **Standards**.
f.dist(Lay-outCommonNumReplicatesType ("Standard")* (tov1.ssr),LayoutNumGroups("Stand-ard"),count([Stand-ard,Unknown]),true)	The cumulative F distribution value for the num-ber of **Standard** replicates multiplied by the [Sum of Squares TOV](#) from the first configured trans-form. The degrees of freedom are specified as number of **Standards** and the number of all non-flagged **Standard** and **Unknown** samples' rep-licates.

Statistical Functions

This section describes statistical functions that operate on list of values with open-ended length.

Where a [sample reference](#) is used as a parameter to a function, any sample group/type reference inside a Statistical Function's parameter list refers to the non-flagged values of that group/type.

Syntax

These functions are specified with the following syntaxes:

- **function([Sample type or group reference])** – If there is 1 input sample group/type reference.

- **function([Sample type or group reference, Sample type or group reference, ... , Sample type or group reference])** – If there are 2 or more input sample group/type references.

> Because Statistical Functions are not group enabled functions, insert each group reference inside square brackets (e.g., **stdev.s([Standard1,Unknown2])** to access the values of non-flagged data points.

The following table lists statistical functions in alphabetical order:

Name	Description	Minimum number of parameters	Example
stdev.p	Calculates the standard deviation of a supplied set of values, using the "entire population" method. ⓘ Use stdev.p function when the data represents the entire population.	1	**stdev.p([Unknown])** Returns the standard deviation of all replicates in the **Unknown** sample type. **stdev.p([Unknown, Blank])** Returns the standard deviation of the Unknowns and Blanks.
stdev.s	Calculates the sample standard deviation of a supplied set of values, using the "sample of the entire population" method. The same as **sd**. ⓘ Use stdev.s function when the data is a sample of the entire population	1	**stdev.s([Unknown1])** Returns the standard deviation of the replicates of the **Unknown1** sample.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to find the standard deviation value for the **Unknown**sample type.

The example uses a layout with 16 **Unknown** sample groups, where **Unknown1** at **A1**, **A2 A3**, **A4**, **A5**, and **A6**, **Unknown2** at **A7**, **A8**, **A9**, **A10**, **A11**, **A12**, etc.). I.e.:

● Unknown

Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

We use the expression:

stdev.p([Unknown])

Unknown refers to the list of non-flagged data points for the **Unknown** sample type. From this list the standard deviation is calculated.

The result will be (also displayed here to 3 decimal places):

0.540

Evaluating Z Factor/Z Prime (Z')

Z Factor/Z Prime (Z') (as defined by: *Zhang JH, Chung TD, Oldenburg KR, A Simple Statistical Parameter for Use in Evaluation and Validation of High Throughput Screening Assays. J Biomol Screen. 1999;4(2):67-73*) is used to assess quality of:

- HTS assay

- Population of tested sample compounds

The commonly used equation is

$$Z = 1 - \frac{3SD \ of \ sample + 3SD \ of \ control}{|mean \ of \ sample - mean \ of \ control|}$$

It represents how well separated the positive and negative controls are, and indicates whether an assay is likely to contain false positives/negatives.

This statistic can be added to an assay using the Evaluation option with the expression:

1-((3*sd(Neg Control)+3*sd(Pos Control))/abs(Neg Control-Pos Control))

Where **Neg Control** and **Pos Control** are the sample/control groups to test.

Integration with Readers

EnSight (Kaleido) Integration

The latest documentation relating to working with MyAssays Desktop Pro and EnSight (via Kaleido software):

Kaleido 3.0

MyAssays Desktop Pro for Kaleido 3.0 (Installation Notes).pdf

Using MyAssays Desktop with Kaleido 3.0.pdf

Video tutorials for using MyAssays Desktop and Folder Poll with Kaleido 3.0:

https://www.myassays.com/introduction-to-kaleido-3-0-and-myassays-desktop.video

https://www.myassays.com/kaleido-3-0-data-export-and-import-into-myassays-desktop.video

https://www.myassays.com/create-a-new-protocol-with-kaleido-3-0-xml-data-in-myassays-desktop.video

https://www.myassays.com/kaleido-3-0-data-analysis-automation-with-myassays-desktop.video

Kaleido 2.0

MAD R3.2 and Folder Poll Configuration for Kaleido 2.0.pdf

Video tutorials for using MyAssays Desktop and Folder Poll with Kaleido 2.0:

https://www.myassays.com/folder-poll-with-myassays-desktop-pro-and-kaleido-2-0-(1-of-2).video

https://www.myassays.com/folder-poll-with-myassays-desktop-pro-and-kaleido-2-0-(2-of-2).video

EnVision Integration

The EnVision manager software can output data in many possible export configurations.

If using EnVision Manager v14.xxx or later, then select **Export format** option as **CSV for MyAssays Desktop** option:
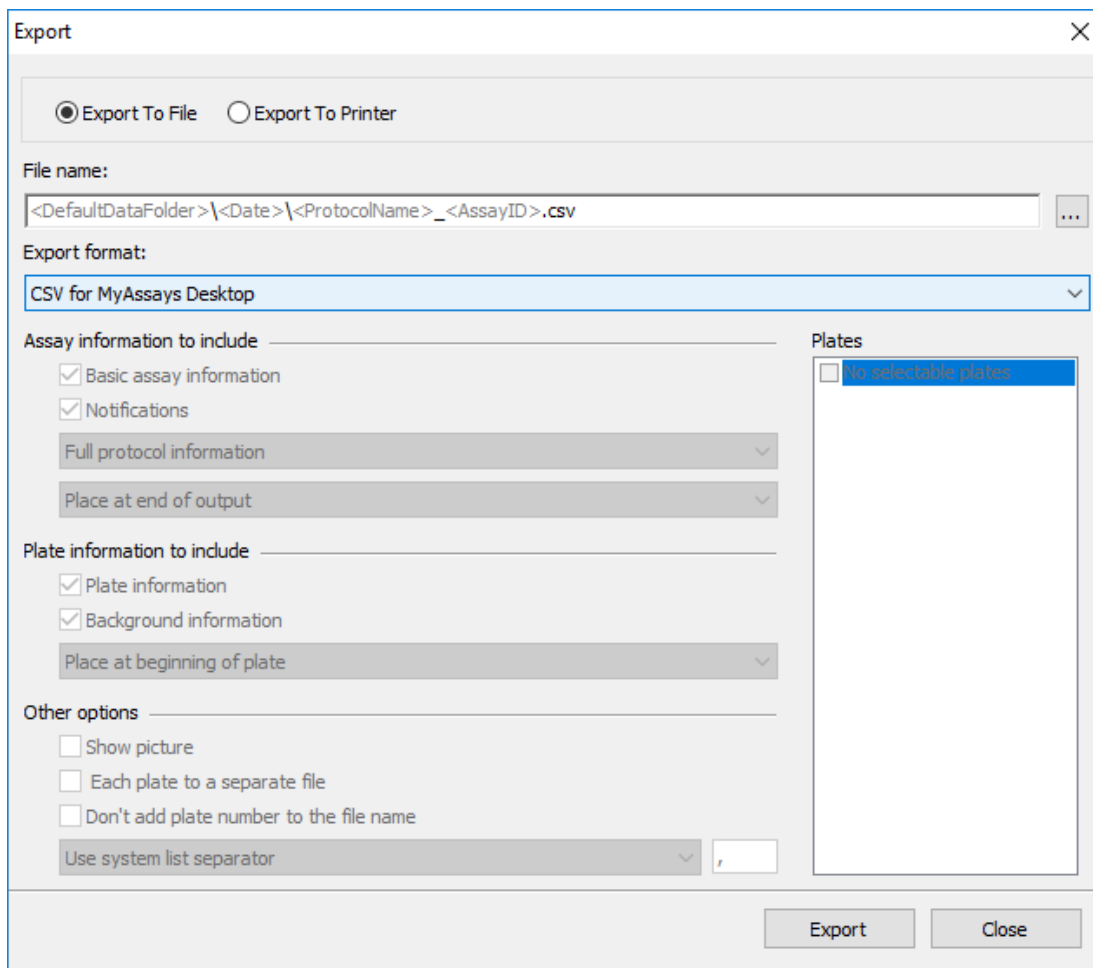
To configure earlier EnVision Manager versions to output data in a format compatible with MyAssays Desktop EnVision import scripts, use the default CSV **Export format: Plate 2 (with well headers)** option, e.g.:

MyAssays Desktop supports EnVision's most commonly used measurement and export methods. If you are working with a currently unsupported measurement configuration, we can provide an import script to support it. To request a new import method, please email us your requirements and an example measurement file to support@myassays.com.

If you are working with the Enhanced Security Edition of MyAssays Desktop:

To ensure a secure hand-off of data using data certification, then EnVision Manager v14.xxx or later is required. MyAssays Desktop Enhanced Security can work with earlier EnVision versions, but data certificate generation is not available from the EnVision software.

INTELLIFLEX Integration

MyAssays Desktop Pro provides first class data analysis tools that can be integrated with measurement data files created by the Luminex INTELLIFLEX.

If you are working in a 21CFR11 or GxP environment the Enhanced Security functions provide a secure and tracked integration when working with the INTELLIFLEX.

For a walk-through of working with INTELLIFLEX data files, please review these video resources:

- INTELLIFLEX Data File Export

- INTELLIFLEX Field Data Import

- Quantitative Data Analysis Protocol Creation

- Quantitative Data Analysis Protocol Use

- Qualitative Data Analysis Protocol Creation

- Qualitative Data Analysis Protocol Use

INTELLIFLEX Data Export

This section describes the appropriate settings in the INTELLIFLEX user interface for exporting CSV data files. Video Walkthrough...

To export data from the INTELLIFLEX user interface for import into MyAssays Desktop, follow the below steps:

1. Select **RESULTS** from the menu.
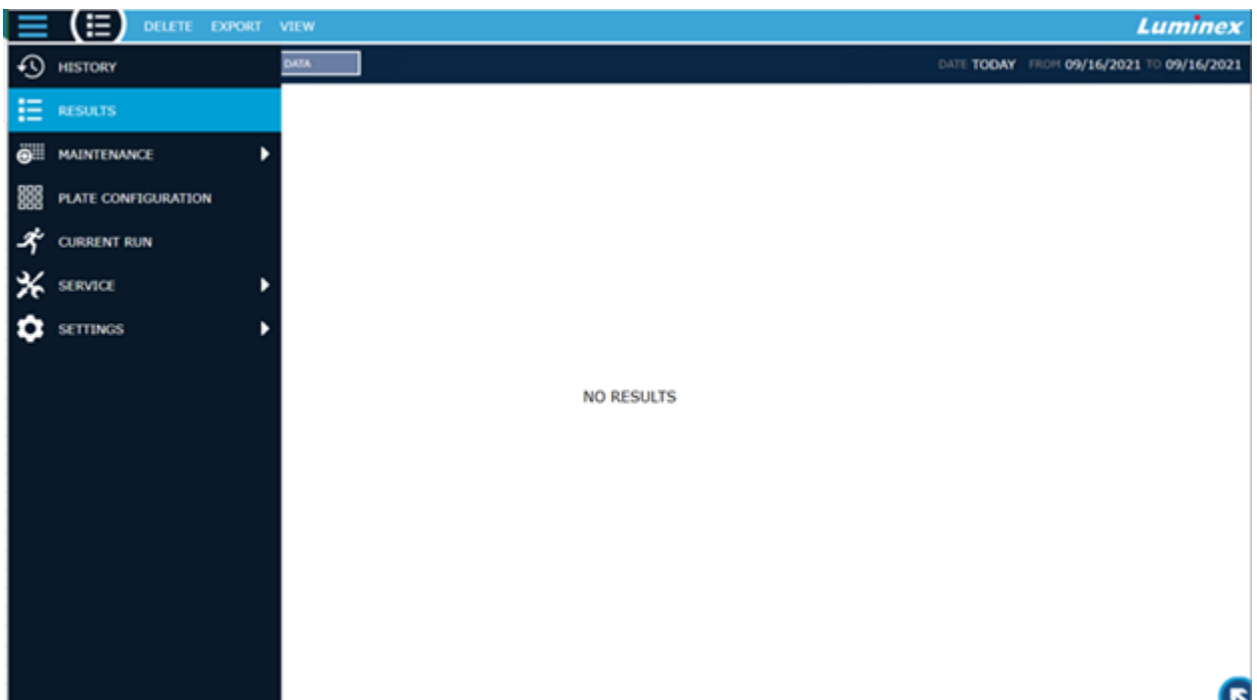
2. Select **VIEW | FILTER**, select appropriate parameters, and press **APPLY**.
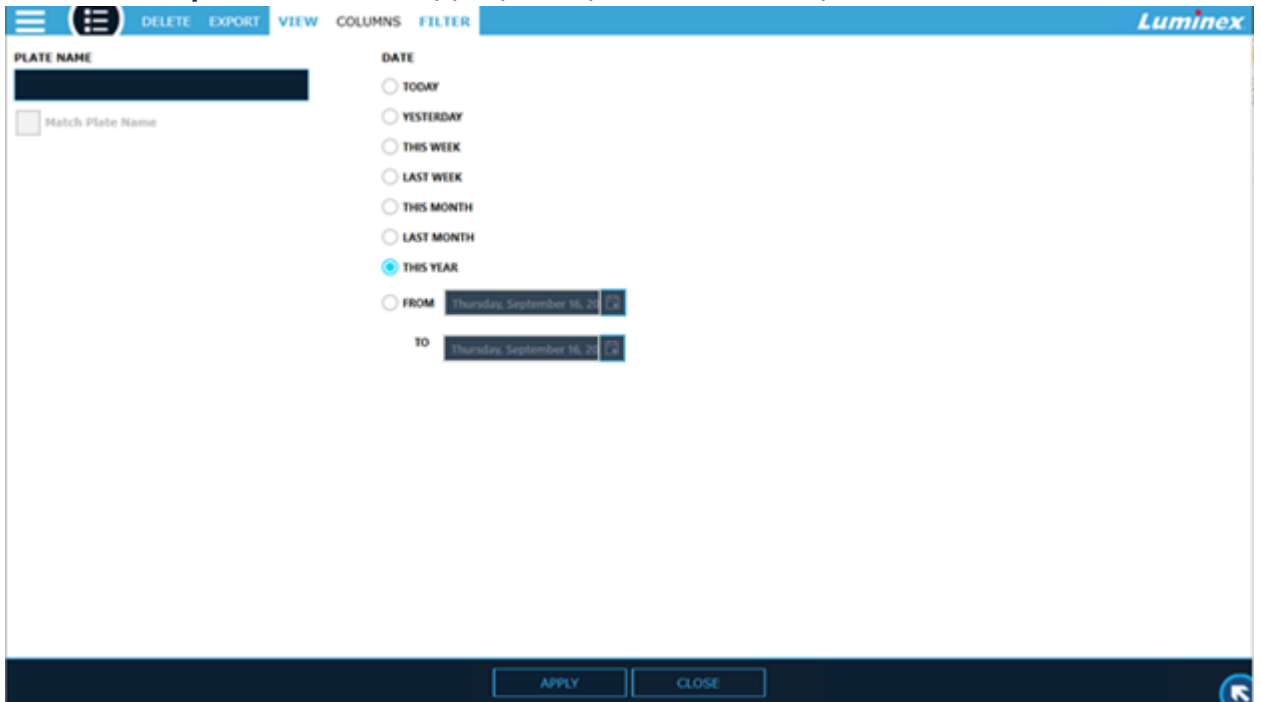
3. Select **EXPORT | SETTINGS**. Select the required columns for import into MyAssays Desktop. These columns must at least include: **PLATE GEOMETRY**, **WELL LOCATION**, **MEDIAN**, and **COUNT**. Press **APPLY**.
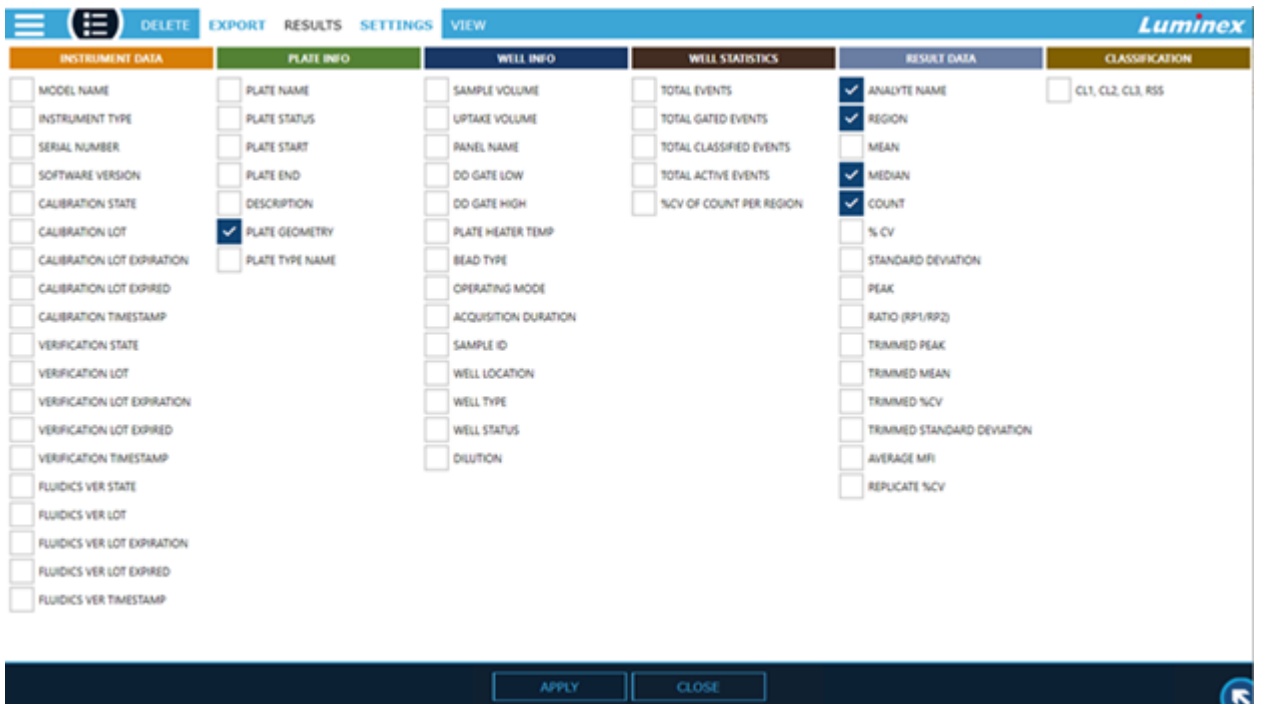
4. Select **EXPORT | RESULTS | EXPORT** (button at the bottom of the screen).
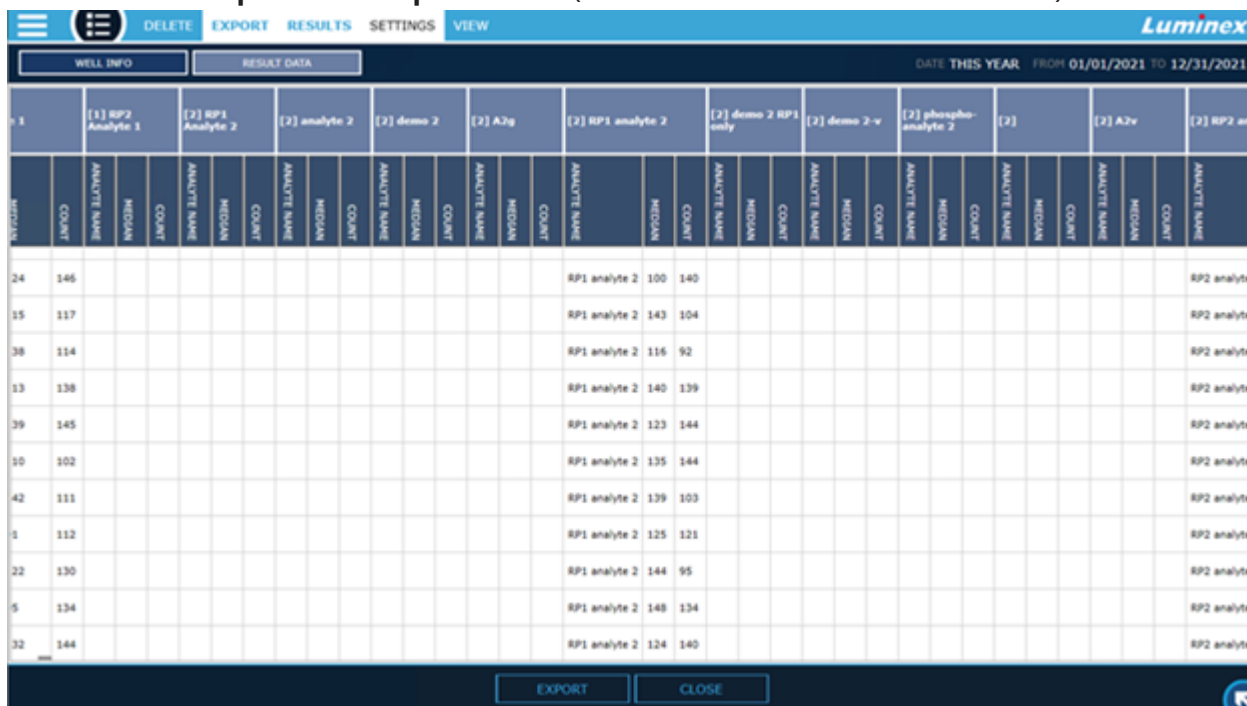
5. Confirm Report Type (in drop-down) is set to **INTELLIFLEX**, and save to USB or accessible network folder.
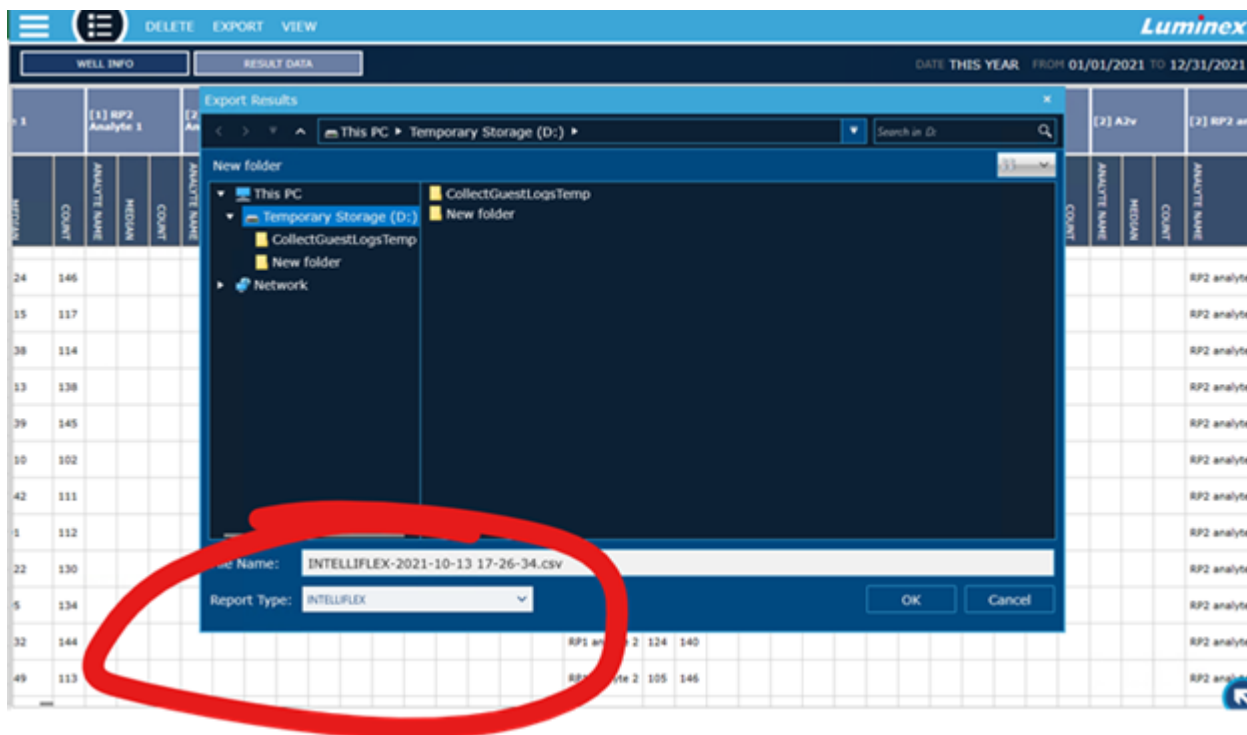
Creating a New Protocol with INTELLIFLEX Data Files

To create a new protocol using an INTELLIFLEX CSV data file:

1. Open **MyAssays Desktop Explorer**, and click **New Protocol**.
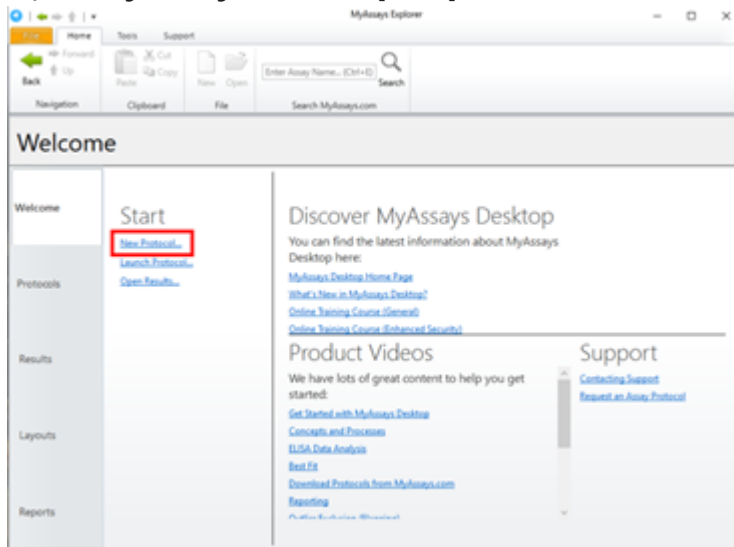
2. Select the **My data is in a file or spread across multiple files**, and the **Create multiplex assay** options.
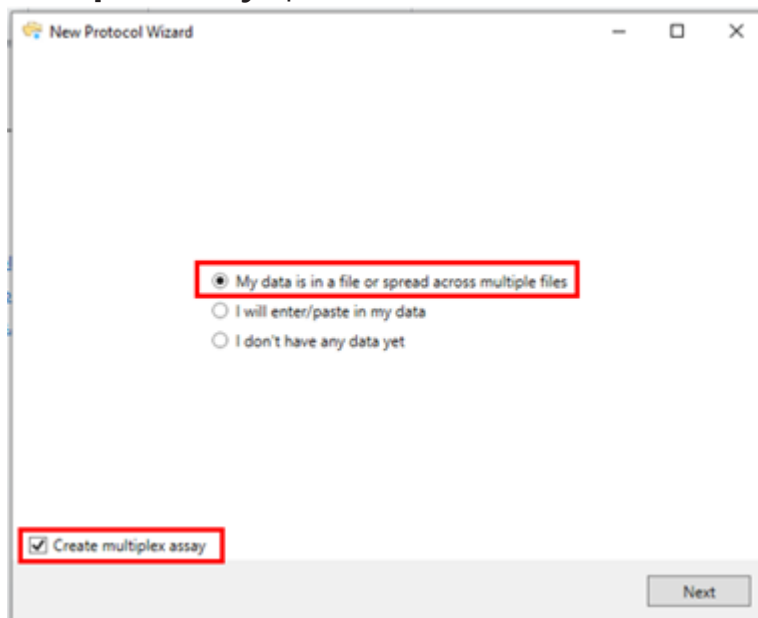
3. Browse for and select the measurement data file, and leave the **Automatically import measurement data** checkbox selected.
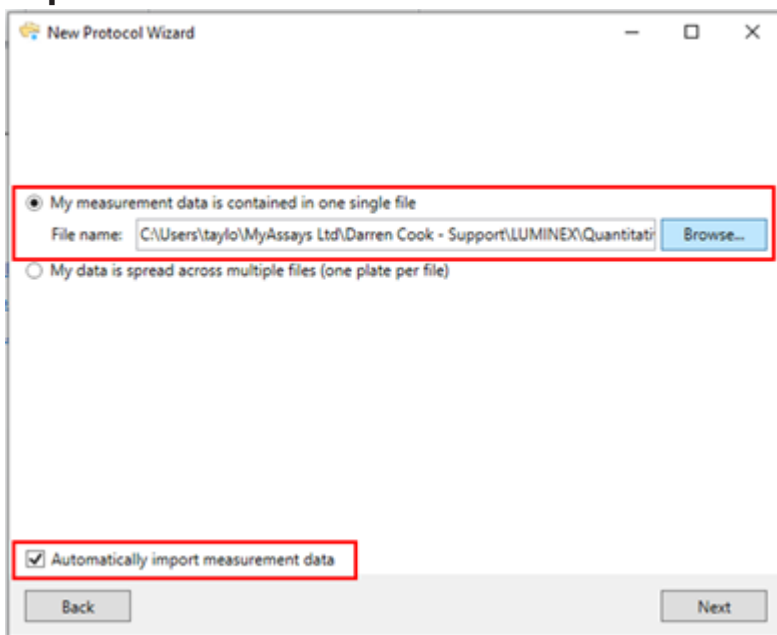
4. Select the import method required, LuminexIntelliflex.All will import all measurement and field data, while LuminexIntelliflex.MedianCount will import only the median and count data for each analyte.

5. Review imported data.

6. Specify the sample types used in your assay.

7. Specify the plate layout used for your assay.
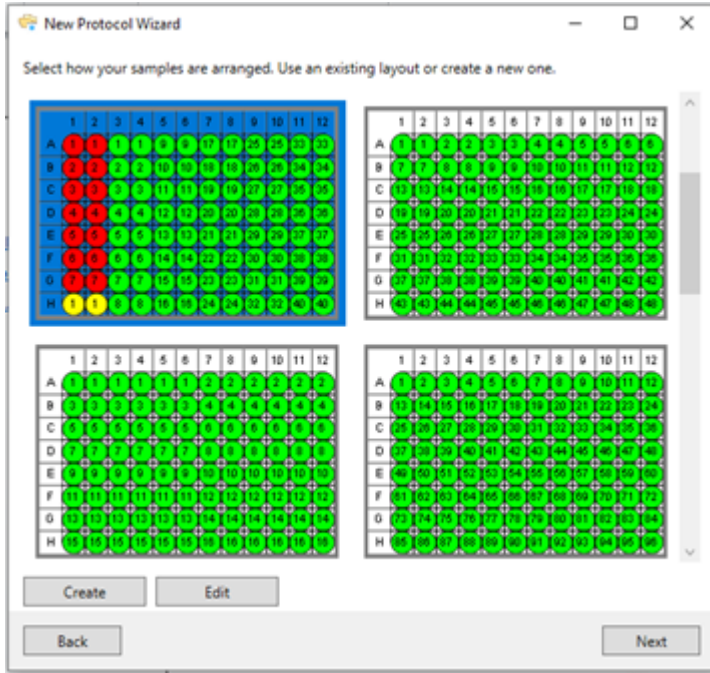
8. Review imported data with plate overlay.
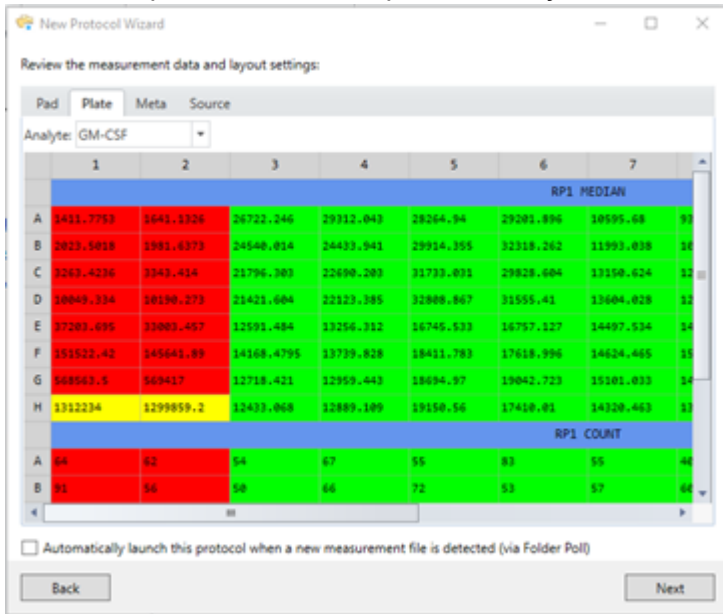
9. Specify protocol name, and optionally include a description.
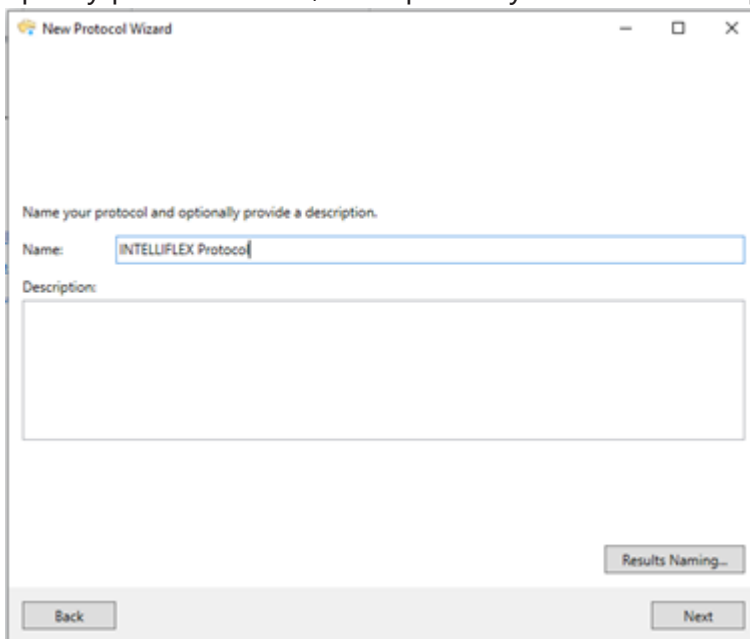
10. Review protocol configuration and press **Finish** to launch the protocol.
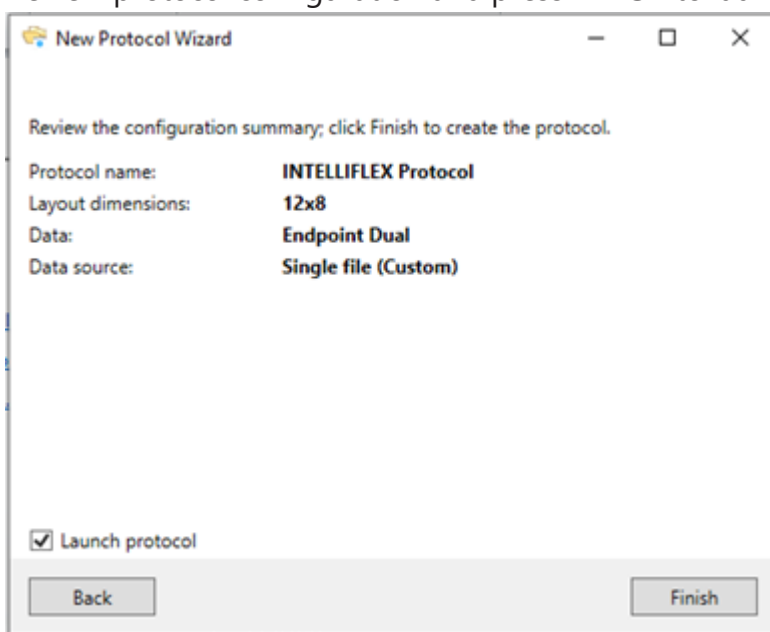
Configure a Quantitative INTELLIFLEX Protocol

This section describes how to create a common configuration for quantitative multiplex analysis consisting of a blank correction, standard curve fit, dilution factors, and percentage coefficient of variation calculations. Video Walkthrough...

Blank Correction

The blank correction transform will subtract the average of the specified blank group from all other samples on the plate. Follow the steps below to add the blank correction transform. If your assay does not include a blank correction step, this transform can be omitted from the analysis.

1. Open the **Properties | Transforms** tab, select **Add**.
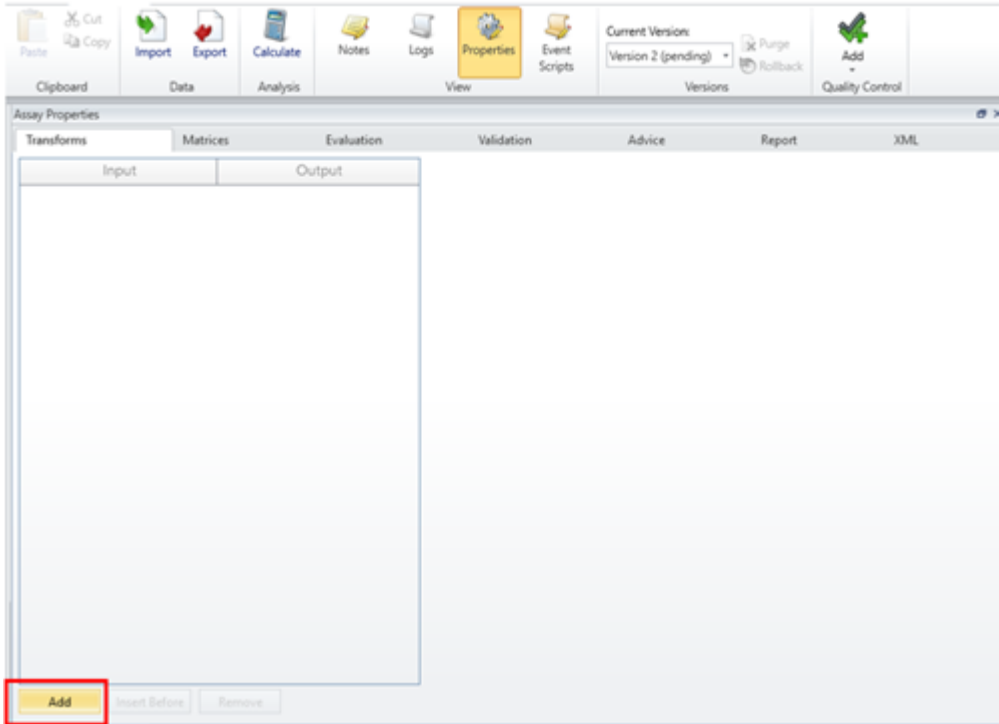
2. Select **Blank Correction** and press **Create**.
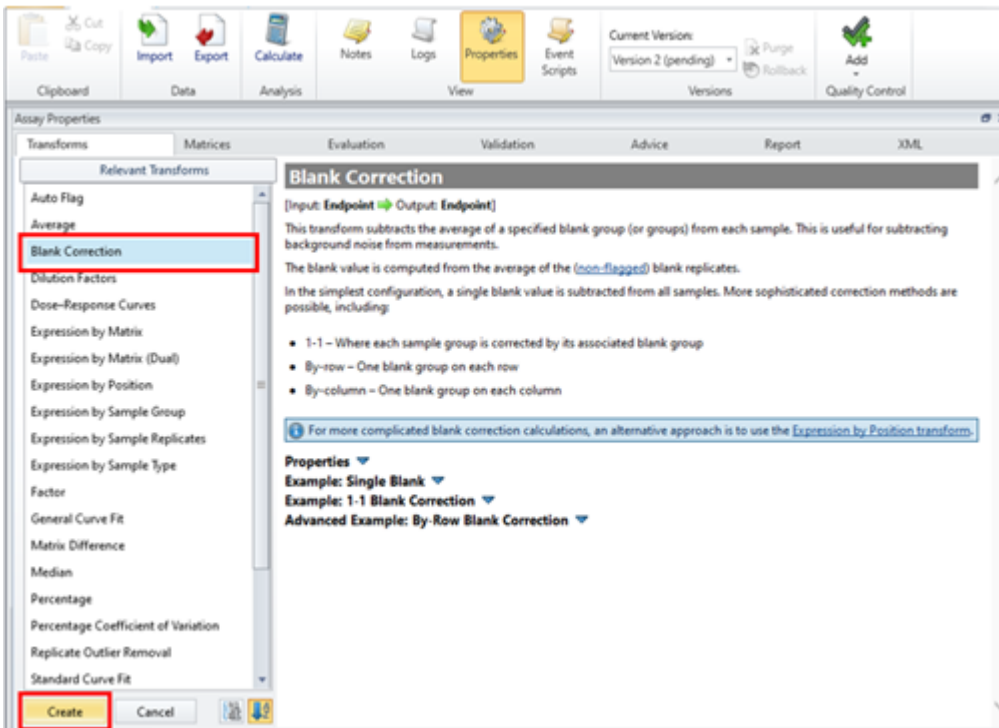
3. Specify the input data matrix using the dropdown box, and the blank type to be used for the blank correction.
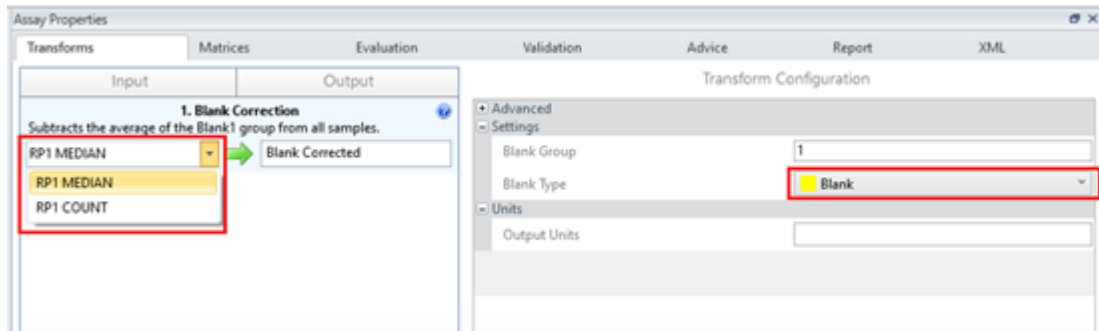
Standard Curve Fit

The Standard Curve Fit transform will apply a standard curve fit to each analyte's standard samples, plotting the specified input data matrix on the y-axis against the entered concentrations, and fitting the curve using the selected fit method. The Unknown sample concentrations are calculated using the resulting fit equation for each analyte.

1. On the **Properties | Transforms** tab, select **Add**.
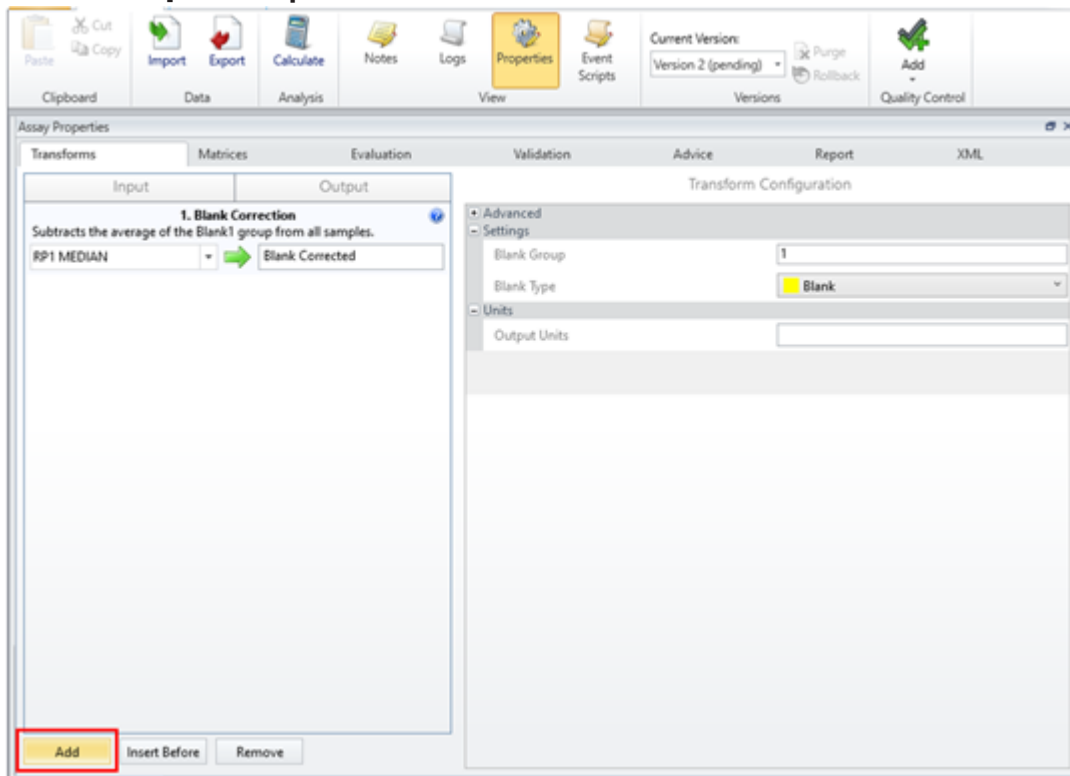
2. Select **Standard Curve Fit** and press **Create**.
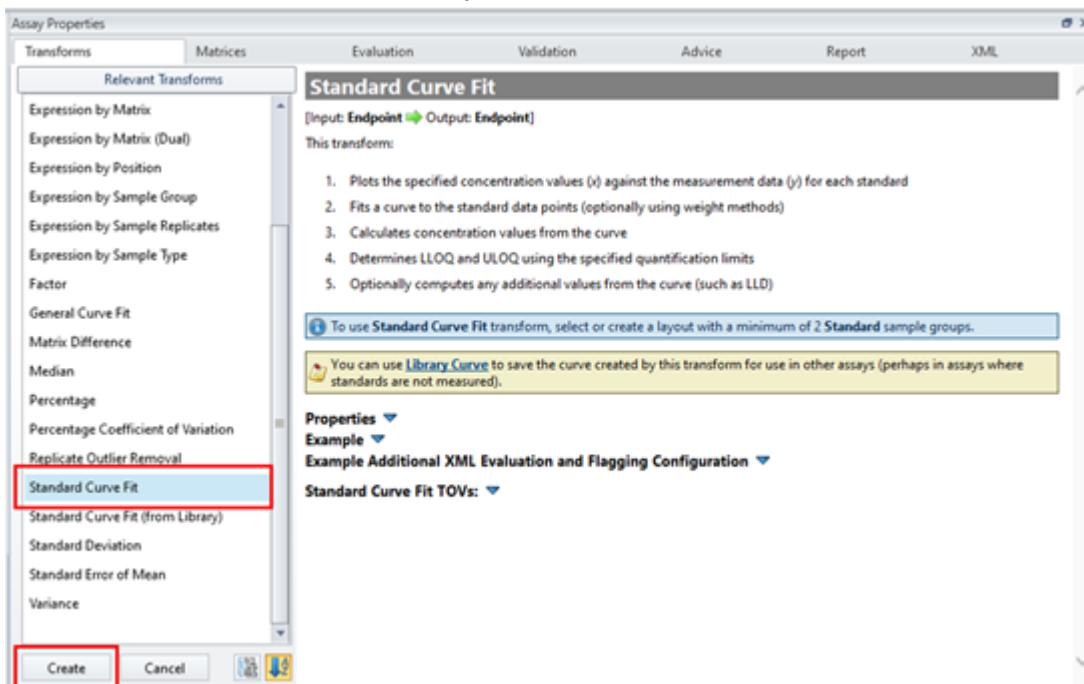
3. Select the input data matrix from the dropdown box.
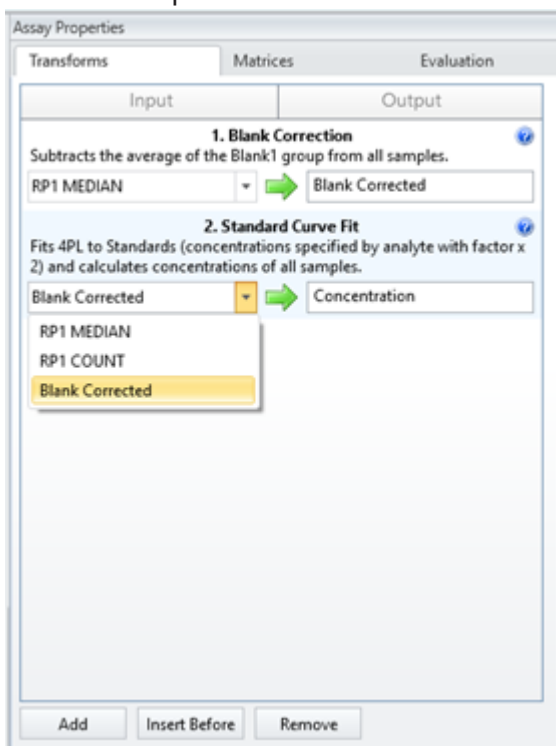
4. Specify standard concentrations for each analyte using the **Concentrations** dropdown box.
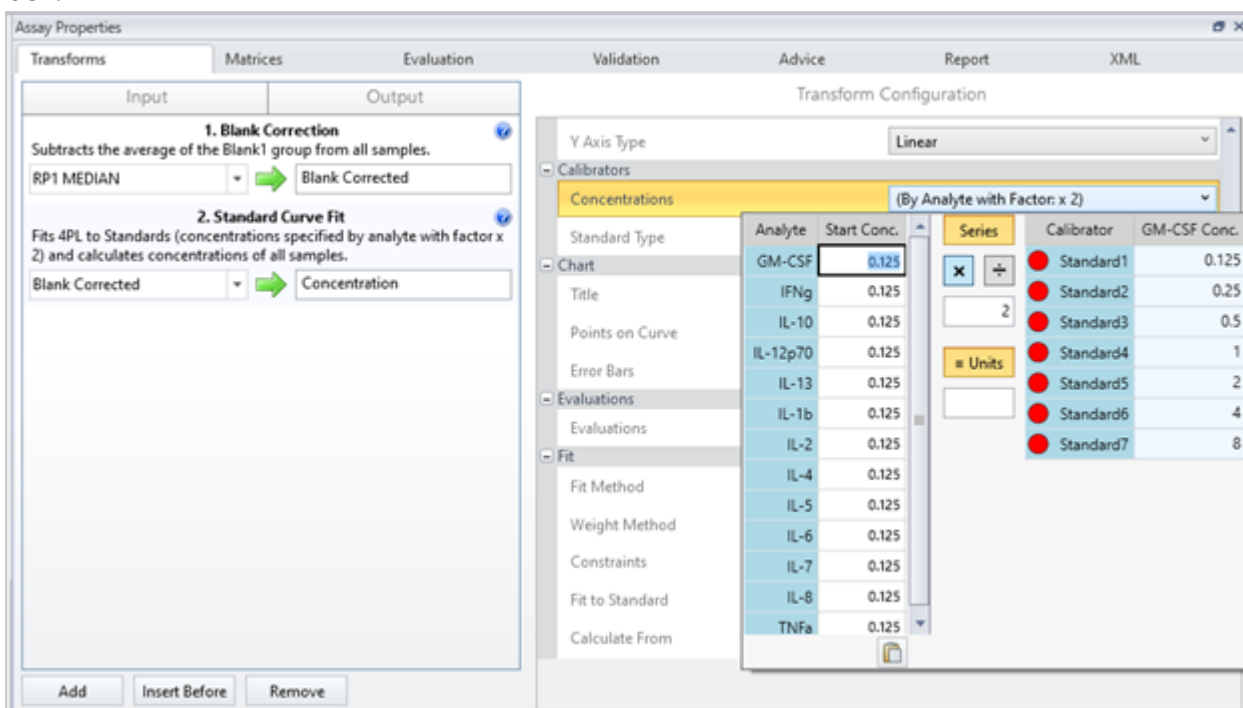
5. Specify fit method using the **Fit Method** dropdown box.
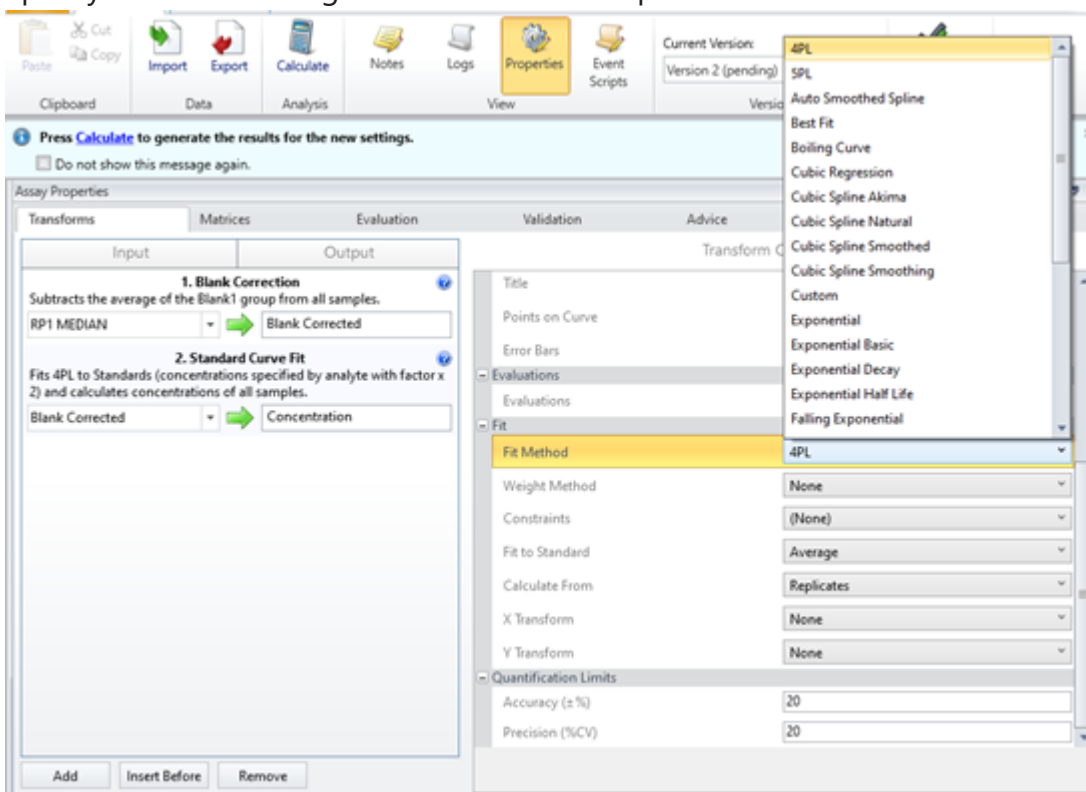
Dilution Factors

The dilution factors transform multiplies the sample group by a specified factor. This can be particularly useful in situations where Unknown samples have been diluted prior to addition to the plate. If for example the sample was diluted 1 part sample to 1 part diluent, the dilution factor should be entered as 2. If a sample has not been diluted, a dilution factor of 1 should be entered. To add the dilution factors transform, follow the below steps. If your assay does not include dilution factors, this transform can be omitted.

1. On the **Properties | Transforms** tab, select **Add**.
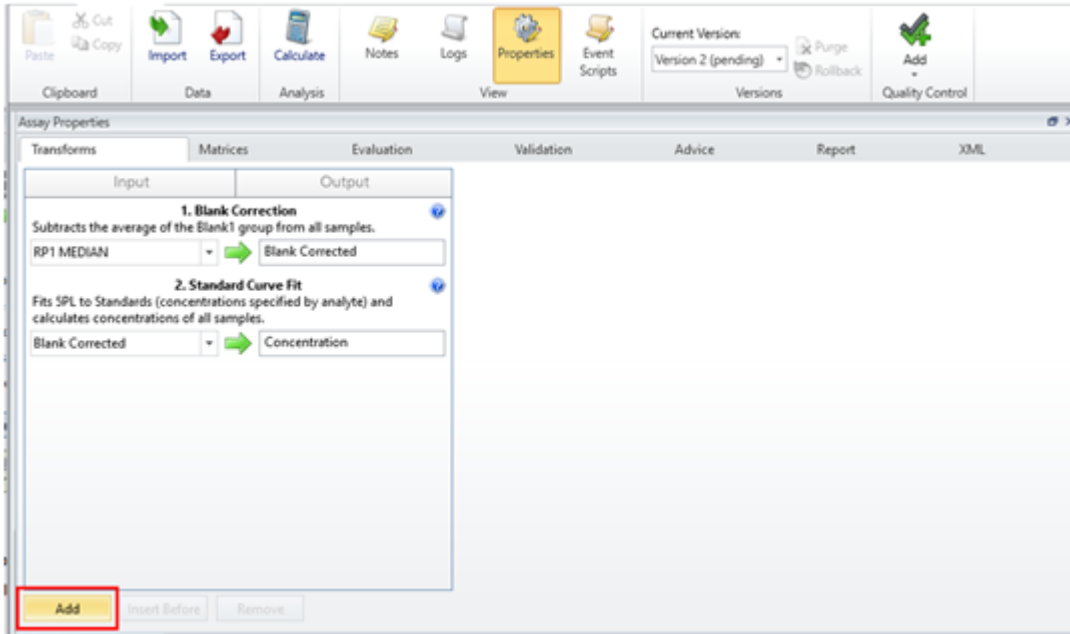
2. Select **Dilution Factors**, and press **Create**.
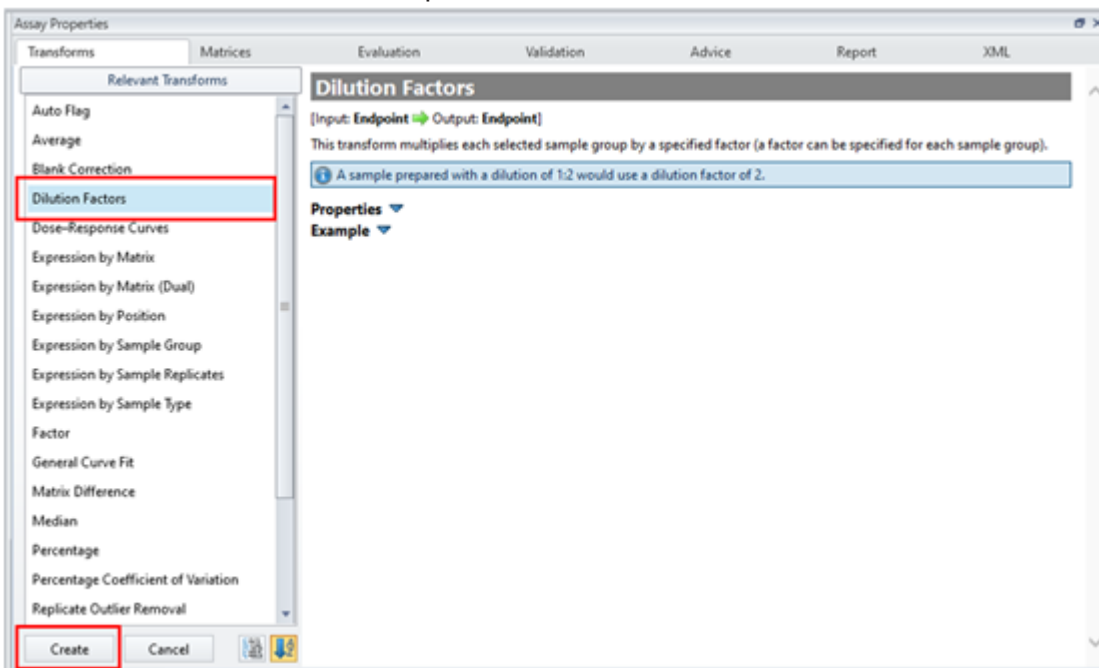
3. Specify the input data matrix using the dropdown box, and enter any applicable dilution factors in the **Factors** dropdown box.
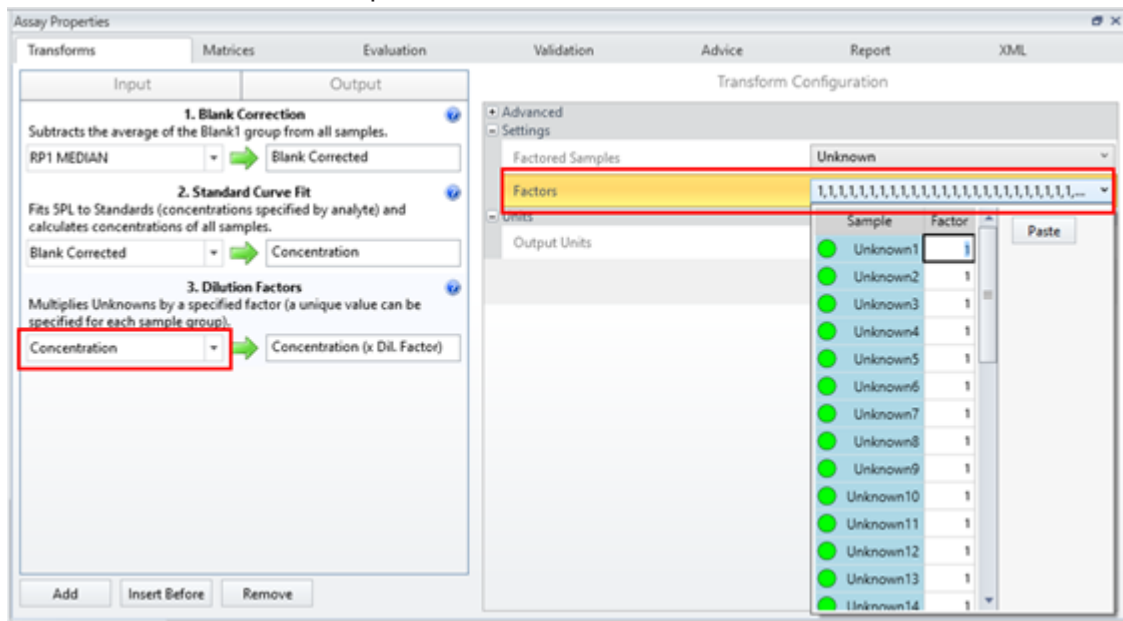
Percentage Coefficient of Variation

The Percentage Coefficient of Variation transform calculates the %CV of the replicates in each sample group. This is the standard deviation divided by the sample group mean and multiplied by 100. Follow the directions below to add the Percentage Coefficient of Variation transform. If your assay is not run with multiple replicates per sample group, this transform can be omitted.

1. On the **Properties | Transforms** tab, select **Add**.
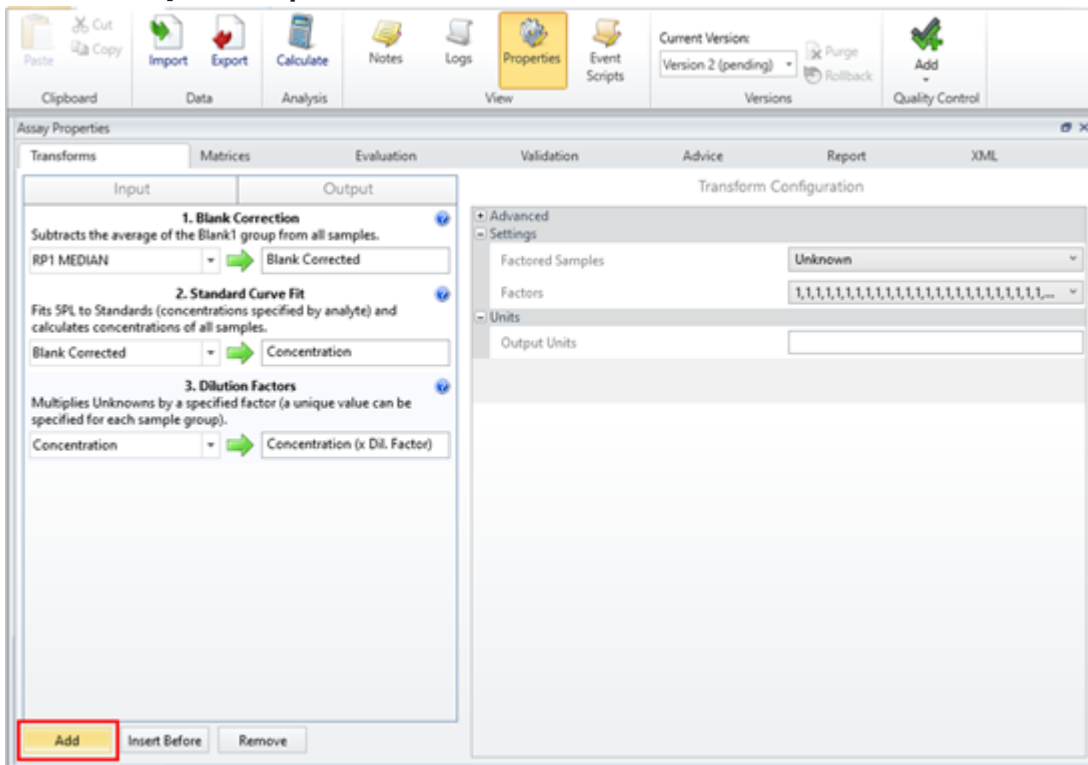
2. Select the **Percentage Coefficient of Variation** transform and press **Create**.
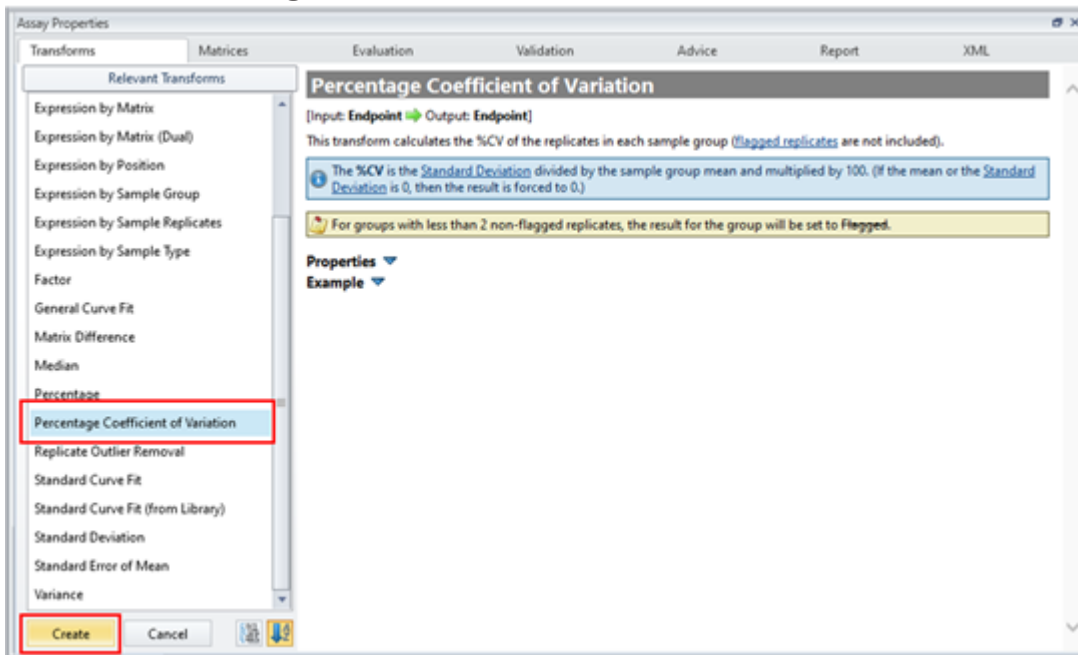
3. Select the input data matrix from the dropdown box.
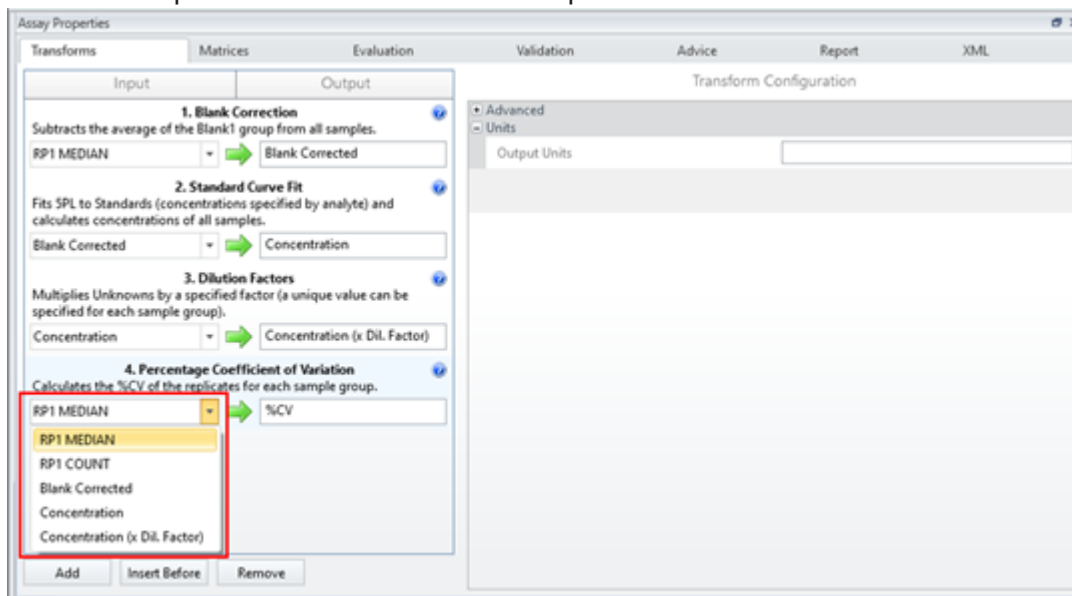
Report Format

Using the Matrices and Report tab, settings can be added to improve the report formatting.

Matrices Tab

Open Properties | Matrices to view all imported and calculated data matrices. This includes raw data, field data, and calculated data matrices. By selecting a matrix, we can define numerical formatting settings, apply sample labels, select sample table replicates, and apply value bars or color scale. Include or exclude the data from sample tables by toggling the Include in Sample Tables checkbox. For more information on the settings available please see Matrices Video Walkthrough...

Report Tab

Open Properties | Report to see the currently included report elements. Your report can be separated into different sheets displaying related information. Report elements can be reordered by using the Arrows to the right of the report tree:

Recommended Settings for Multiplex Assays:

1. Add the Sheet Name **{AnalyteName}** to the **SampleTable1** report element to separate each analyte's sample table on a separate sheet named with the imported Analyte Name.

2. Add the Sheet Name **{AnalyteName} Fit Details** to the **TransformContentStandardCurveFit1** report element to add the curve fit and corresponding information to a separate sheet named with the imported Analyte Name

followed by "Fit Details".
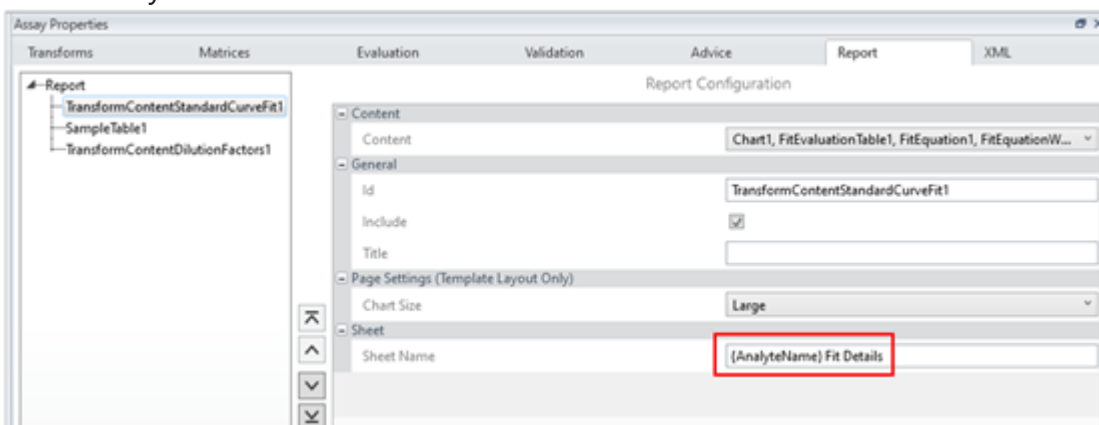
3. If you would like the curve chart and curve data table (displaying information about the standard samples) to appear on the Analyte Name sheets, make the following changes to the Report section of the **Properties | XML** tab and press **Apply** to apply changes.
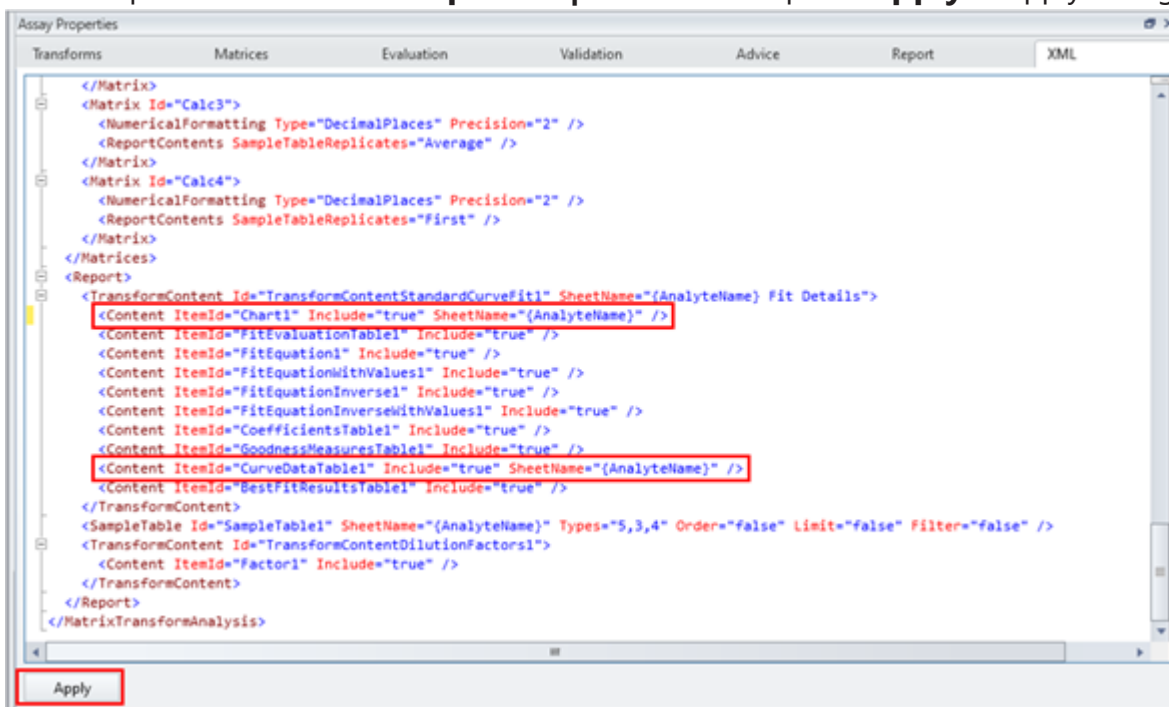
Add **SheetName="{AnalyteName}"** to the **Chart1** and **CurveDataTable1** elements.

Configure a Qualitative INTELLIFLEX Protocol

This section describes how to configure qualitative multiplex analysis using INTELLIFLEX data files. This example follows the Luminex SARS-CoV-2 Multi-Antigen IgG Assay Kit insert. Video Walkthrough...

Count > 75

The first requirement for this assay is to ensure the Count is > 75. To do this, we will add an Expression by Matrix Transforms and add sample labels.

1. Open the **Properties | Transforms** tab, select **Add**.
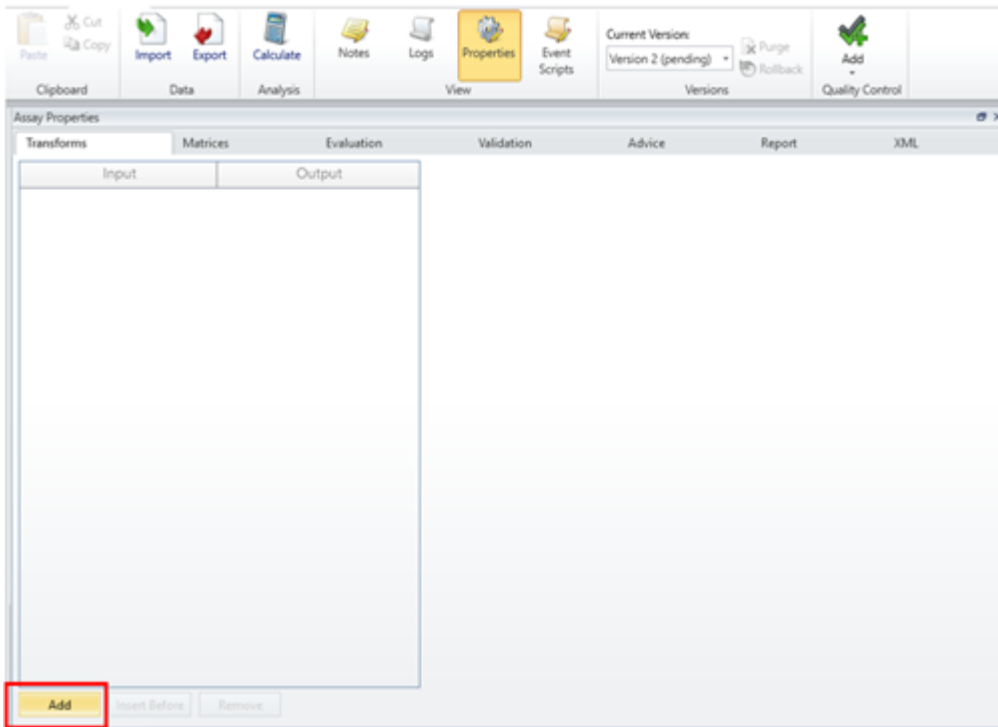
2. Select **Expression by Matrix** and press **Create**.
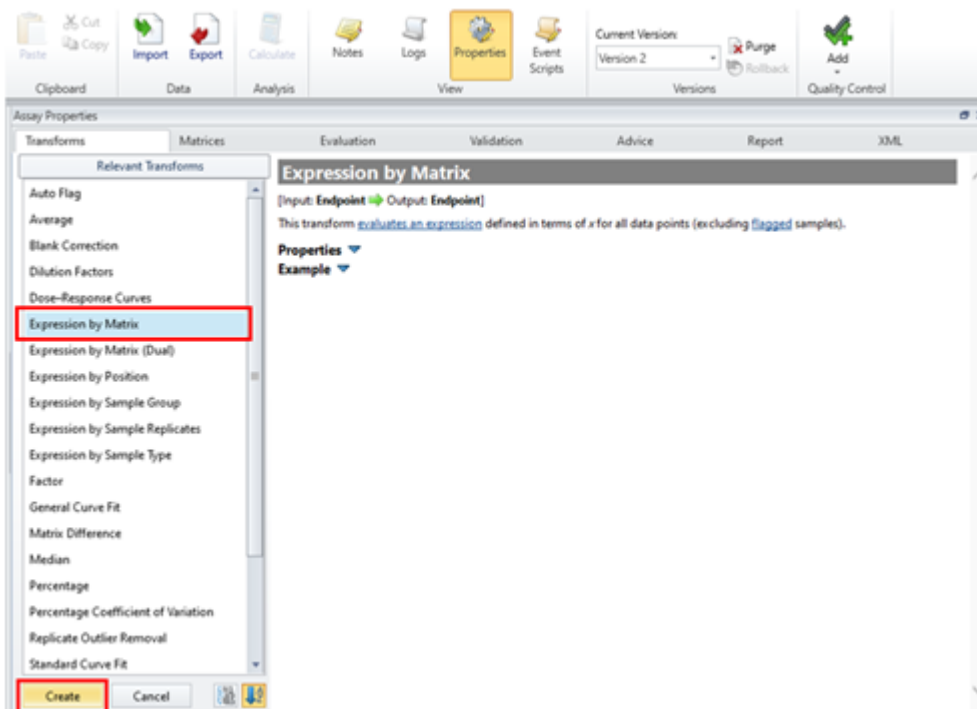
3. Select the appropriate input matrix for the Expression by Matrix Tranform, in this example: RP1 COUNT, with the output matrix named Count > 75. The matrix expression

should be set to x.
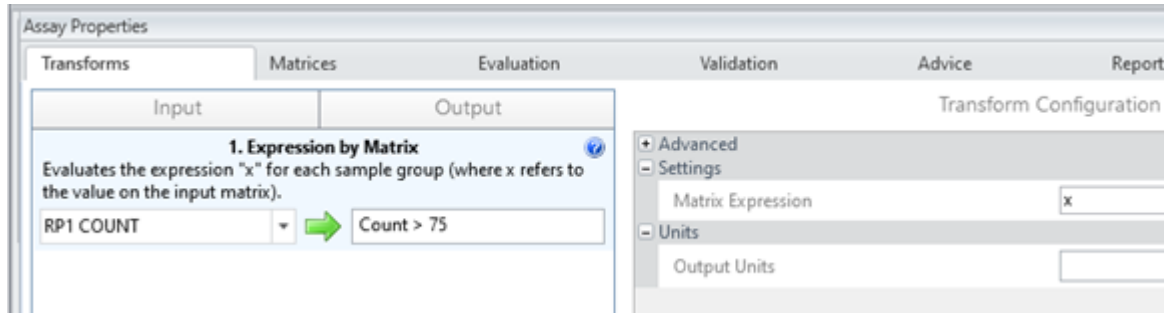
Configure Sample Labels

For the Count > 75 column of the sample table, add sample labels to report if the criteria is met. To do this, open the **Properties | Matrices** tab.

1. Select the Count > 75 matrix.

2. Open the Sample Labels dropdown box and select **Add**.
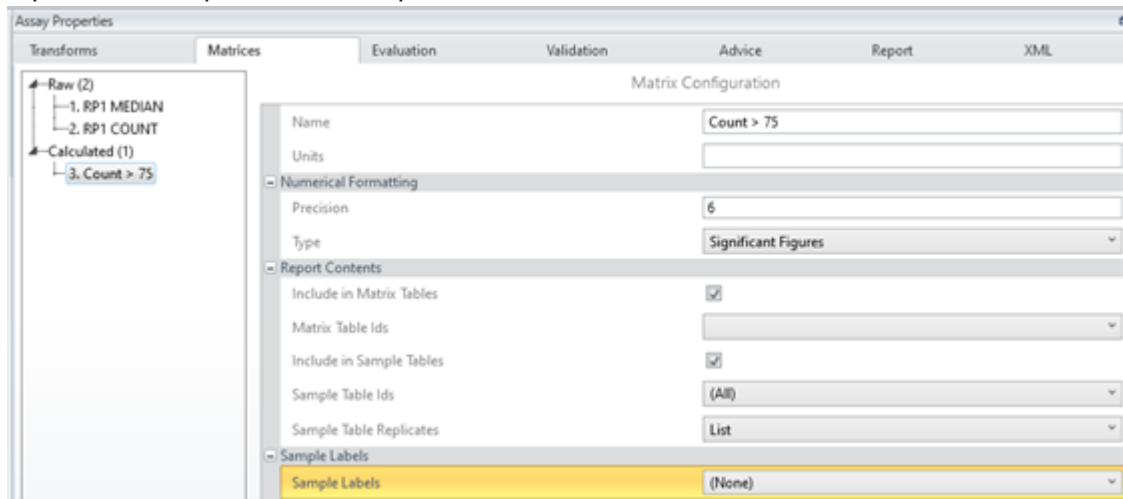
3. Configure the sample label conditions. The label conditions will be x > 75 with the label OK, and x <= 75 with the label Insufficient Count.
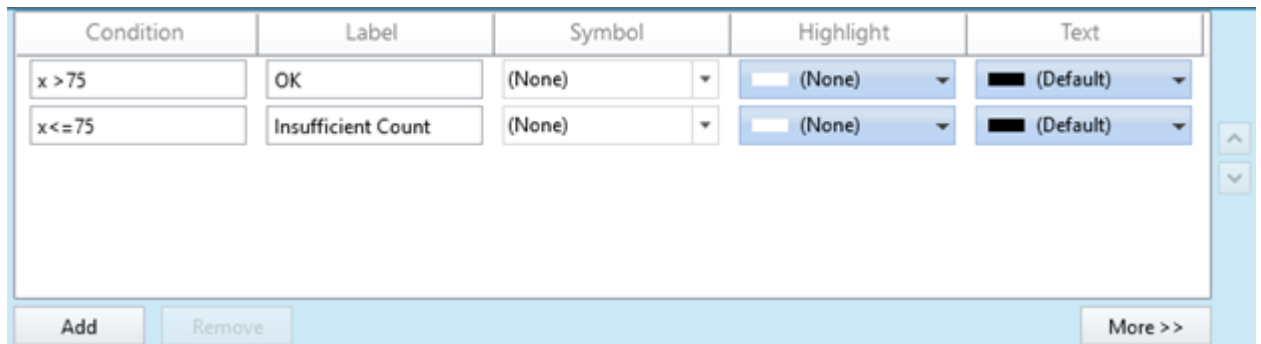
Sample Table Custom Columns

Configure each analyte's positive/negative designations in a custom column reporting the overall results. To do this, first navigate to the **Properties | Report** tab.

1. Select **Add Element**, and choose **Sample Table (Custom Columns)**
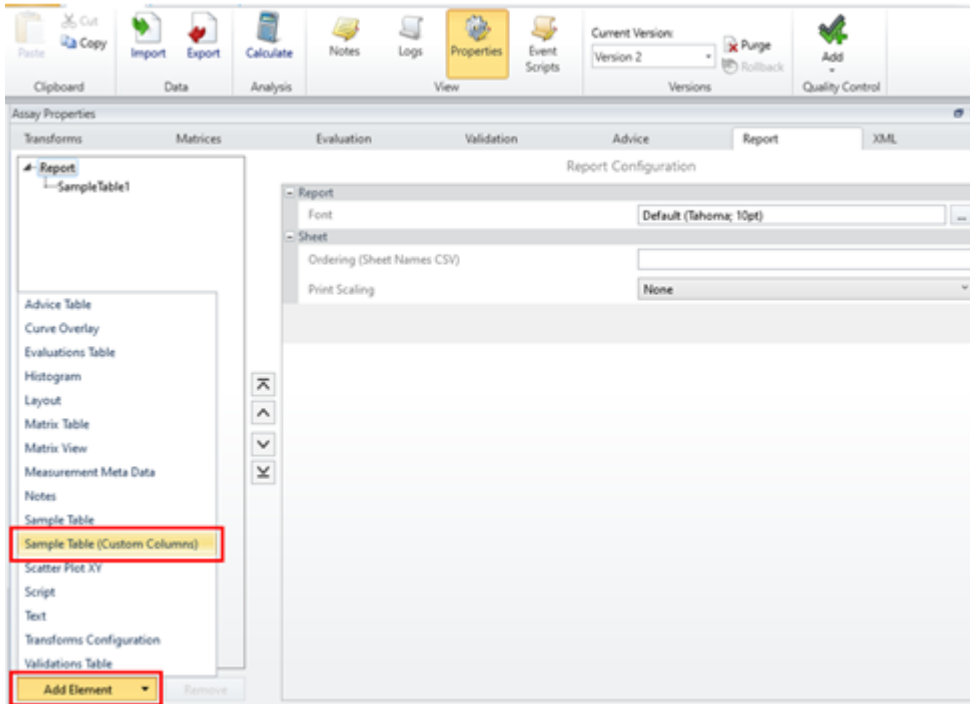
2. Using the arrows to the right of the report element tree, move the SampleTableCustomColumn1 report element to the top so it will appear first in the report. Add the Sheet Name **Overall Results** to allow the new sample table to appear on its own sheet:
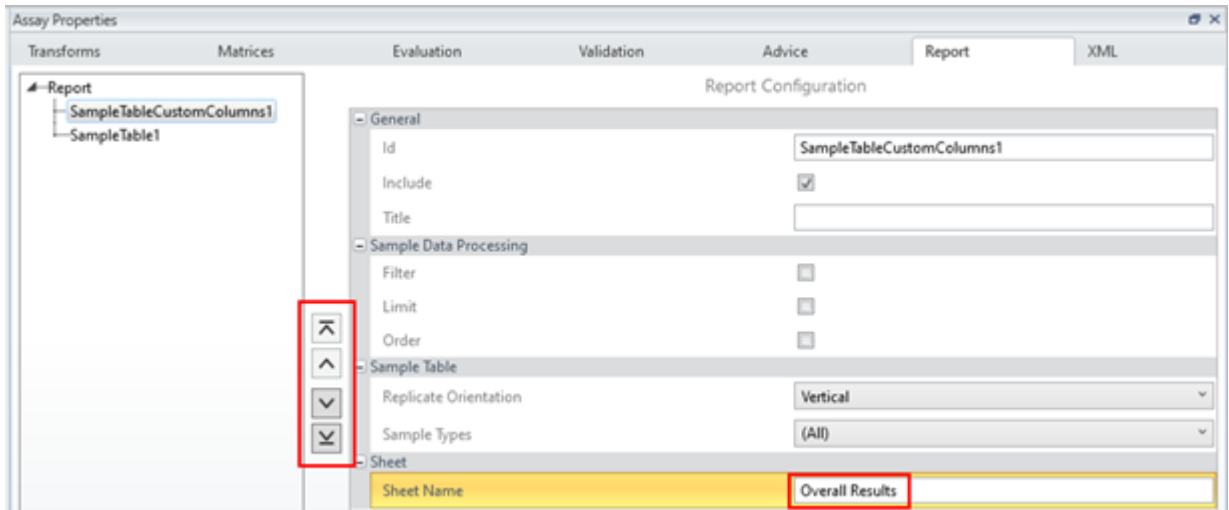
3. To include this sample table only once in the report, select **First Analyte** from the **Include For** dropdown box.
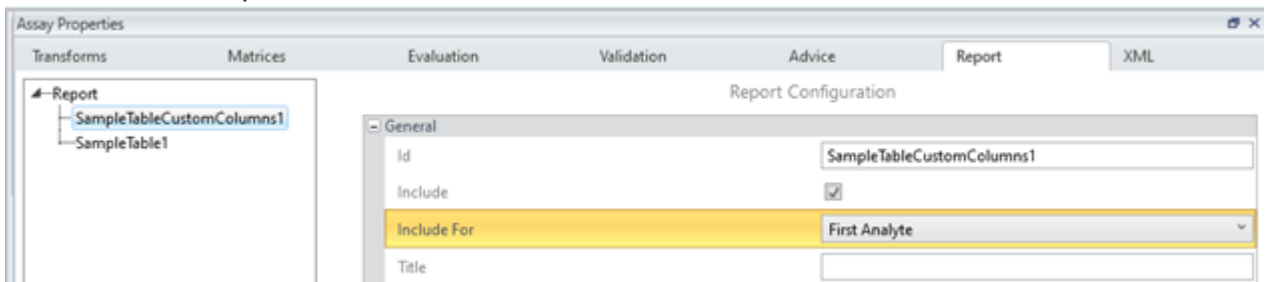
4. Select the **Edit** button to the right of the column field to begin configuring the columns of the sample table.
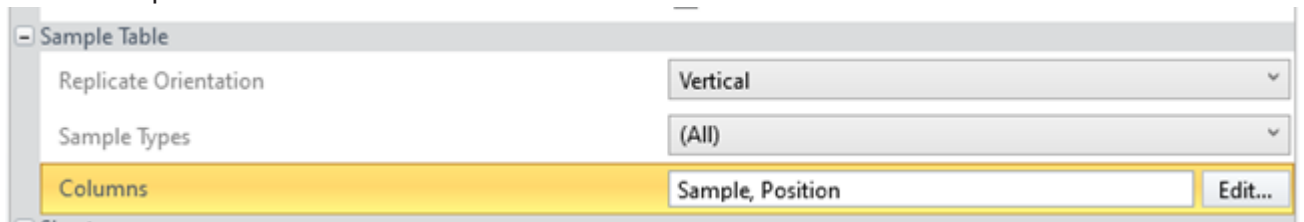
5. The new sample table will report results based on the additional criteria outlined in the kit insert:
   a. The Background MFI should be < 300
   b. The IgG MFI should be > 2500
   c. The IgA MFI should be <= 0.8 when divided by the MFI of the IgG control
   d. The IgM MFI should be <= 0.5 when divided by the MFI of the IgG control
   e. The analytes should be designated as positive if the MFI is > threshold (in this example, the threshold is set to 100)

6. This will be accomplished by adding 7 qualification columns to the sample table. First, we'll add a qualification column to report a Pass designation if the IgG MFI > 2500. For more information on the requirements for adding qualification columns, see Sample Table Custom Columns.

7. Select the **Add Column** option and select to add a **Quantification** column. Specify the **Custom Name** Background < 300. To display the results for each replicates, select the **List** option from the **Replicates** dropdown box. To display the results for the average, select the **Average** option from the Replicates dropdown box.
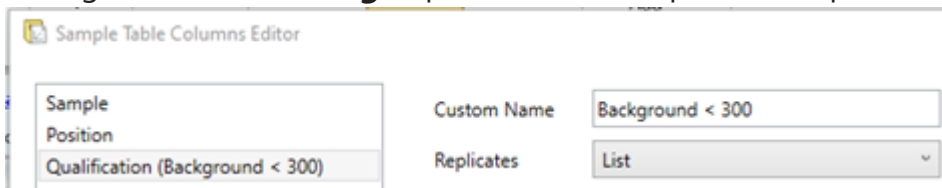
8. Specify the **Reference**, **Matrix**, and **Analyte**. For this column, add the reference name a, RP1 MEDIAN matrix, and B001 analyte.

References		
Name	Matrix	Analyte
a	RP1 MEDIAN	B001

9. Specify the sample report labels. The rule conditions will reference the Reference ID specified. The rule conditions and labels should be configured as:

Rules

Condition	Label	Highlight	Highlight Row	Text	Symbol
a < 300	OK		☐		(None)
a >= 300	High Backgrou		☐		(None)

10. Select the **Add Column** option, and select to add another **Qualification** column. Specify the **Custom Name** IgG Control. To display the results for each replicates, select the **List** option from the **Replicates** dropdown box. To display the results for the average, select the **Average** option from the Replicates dropdown box.

Sample Table Columns Editor

Sample	Custom Name	IgG Control
Position		
Qualification (IgG Control)	Replicates	Average

11. Specify the **Reference**, **Matrix**, and **Analyte**. For this column, add the reference name a, RP1 MEDIAN matrix, and G001 analyte.

Custom Name	IgG Control
Replicates	Average

References

Name	Matrix	Analyte
a	RP1 MEDIAN	G001

12. Specify the sample report labels. The rule conditions will reference the Reference ID specified. The rule conditions and labels should be configured as:

Condition	Label	Highlight	Highlight Row	Text	Symbol
a>2500	Pass	▾	☐	▾	(None) ▾
a<=2500	Fail	▾	☐	▾	(None) ▾

Add   Remove

13. Add an additional **Qualification** column for the IgA control to report a Pass designation if the IgA MFI <=0.8 when divided by the MFI of the IgG Control. This will be added in a similar manner to the previous qualification, however two references will be specified, RP1 Median matrix for G001 and A001 containers.

Custom Name   IgA Control

Replicates   Average ▾

References

Name	Matrix	Analyte	
a	RP1 MEDIAN ▾	G001 ▾	
b	RP1 MEDIAN ▾	A001 ▾	

Add   Remove

14. The rule conditions will reference both containers:

Condition	Label	Highlight	Highlight Row	Text	Symbol
b/a<=0.8	Pass	▾	☐	▾	(None) ▾
b/a>0.8	Fail	▾	☐	▾	(None) ▾

Add   Remove

15. Add a third Qualification column for the IgM control to report a Pass designation if the IgM MFI is <=0.5 when divided by the MFI of the IgG Control. Again specify two

references - RP1 Median matrix for G001 and M001.

Custom Name	IgM Control
Replicates	Average

References

Name	Matrix	Analyte	
a	RP1 MEDIAN	G001	
b	RP1 MEDIAN	M001	

Add   Remove

16. The rule conditions will reference both containers:

Rules

Condition	Label	Highlight	Highlight Row	Text	Symbol
b/a<=0.5	Pass	☐		▬	(None)
b/a>0.5	Fail	☐		▬	(None)

Add   Remove

17. With these qualifications added for the controls, next three additional Qualification columns should be added to report positive/negative results for the last three analytes, N001, R001, and S001. These will be reported as positive if the MFI values are greater than the threshold (in this case 100). Use the Highlight and Text controls to optionally change the cell highlighting and font color. To report results for both replicates, use the

List option from the **Replicates** dropdown box.

18. With these settings added, a new sample table appearing on a sheet named Overall Results will appear in the report.

Sample	Positions	Background < 300	IgG Control	IgA Control	IgM Control	N001	R001	S001
Unknown1	A1	OK	Pass	Pass	Pass	Negative	Positive	Positive
	B1	OK				Negative	Positive	Positive
Unknown2	C1	OK	Pass	Pass	Pass	Negative	Positive	Negative
	D1	OK				Negative	Positive	Positive
Unknown3	E1	OK	Pass	Pass	Pass	Negative	Negative	Negative
	F1	OK				Negative	Negative	Negative
Unknown4	G1	OK	Pass	Pass	Pass	Negative	Positive	Positive
	H1	OK				Negative	Positive	Positive
Unknown5	A2	OK	Pass	Pass	Pass	Negative	Positive	Negative
	B2	OK				Negative	Positive	Negative
Unknown6	C2	OK	Pass	Pass	Pass	Negative	Positive	Positive
	D2	OK				Negative	Positive	Positive
Unknown7	E2	OK	Pass	Pass	Pass	Positive	Positive	Negative
	H2	OK				Positive	Negative	Negative
Unknown8	F2	OK	Pass	Pass	Pass	Negative	Positive	Positive
	G2	OK				Negative	Positive	Positive
Unknown9	A3	OK	Pass	Pass	Pass	Negative	Negative	Negative
	B3	OK				Negative	Negative	Negative
Unknown10	C3	OK	Pass	Pass	Pass	Positive	Negative	Negative
	D3	OK				Positive	Negative	Negative
Unknown11	E3	OK	Pass	Pass	Pass	Positive	Negative	Negative
	F3	OK				Positive	Negative	Negative
Blank1	G3	OK	Fail	Fail	Fail	Negative	Negative	Negative
	H3	OK				Negative	Negative	Negative

Report Format

Using the **Matrices** and **Report** tab, settings can improve the report formatting.

Matrices Tab

Open Properties | Matrices to view all imported and calculated data matrices. This includes raw data, field data, and calculated data matrices. By selecting a matrix, we can define numerical formatting settings, apply sample labels, select sample table replicates, and apply value bars or color scale. Include or exclude the data from sample tables by toggling the Include in Sample Tables checkbox. For more information on the settings available please see Matrices Video Walkthrough...

Report Tab

Open Properties | Report to see the currently included report elements. Your report can be separated into different sheets displaying related information. Report elements can be reordered by using the Arrows to the right of the report tree.

Recommended Settings for Multiplex Assays:

1. Add the Sheet Name **{AnalyteName}** to the **SampleTable1** report element to separate each analyte's sample table on a separate sheet named with the imported Analyte Name.


Using an Existing INTLLIFLEX Protocol

This section describes how to use an existing INTELLIFLEX multiplex analysis protocol in MyAssays Desktop. Quantitative Video Walkthrough... Qualitative Video Walkthrough...

Locating and Opening Protocols

Protocol files can be saved to any location (like other Windows files). For preconfigured protocol files, please open the **MyAssays Desktop Explorer | Protocol**s tab.
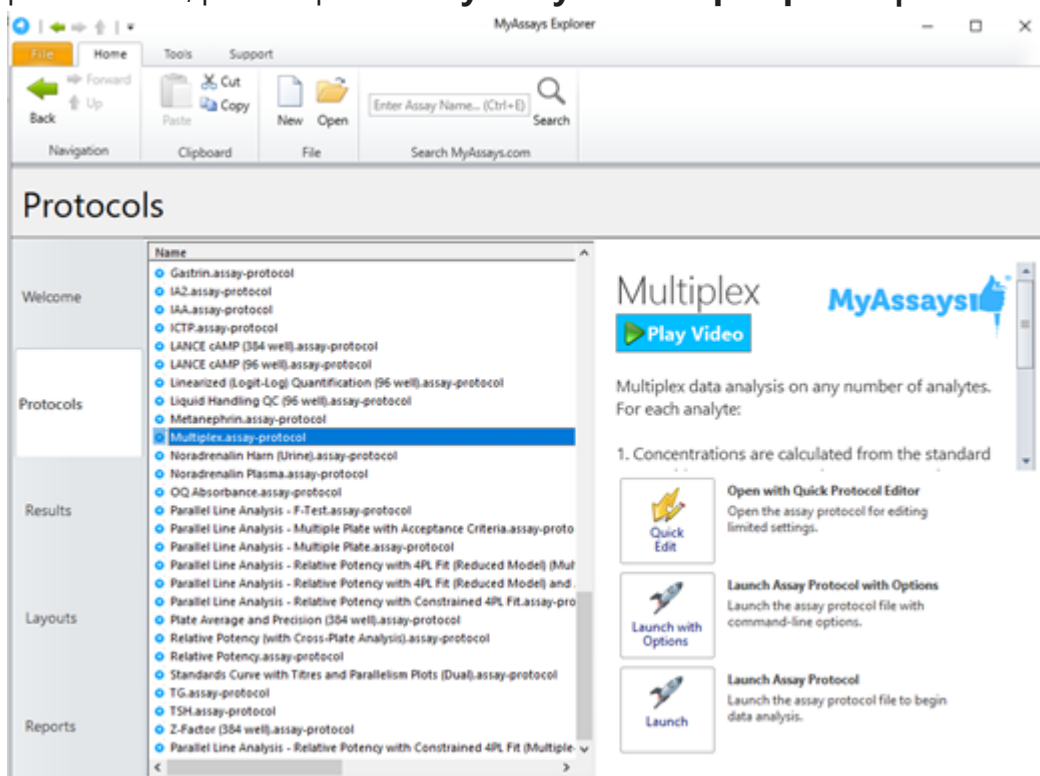
Double click on the protocol file or press **Launch** to open the protocol file. If your protocol is stored in a different location, double click to open the file.

Data Import

To improt your data into the MyAssays Desktop Protocol:

1. Press **Import**to open the Import Wizard.
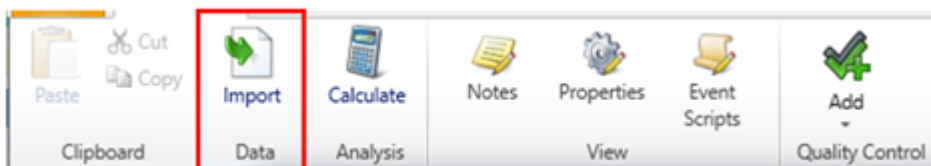
2. Select **Measurements** and press **Next**.
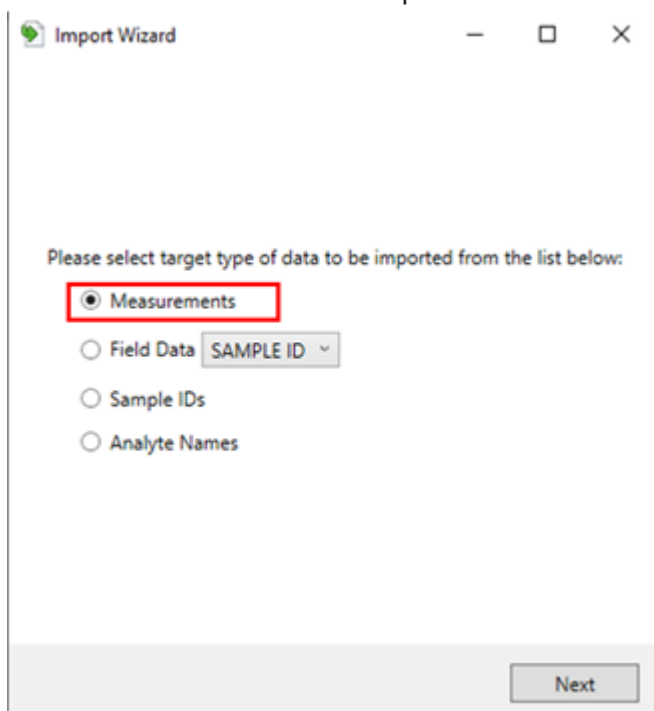
3. Select **My measurement data is contained in one single file**, browse for and select the measurement data file, and leave the **Use existing measurement import configuration** checkbox selected.
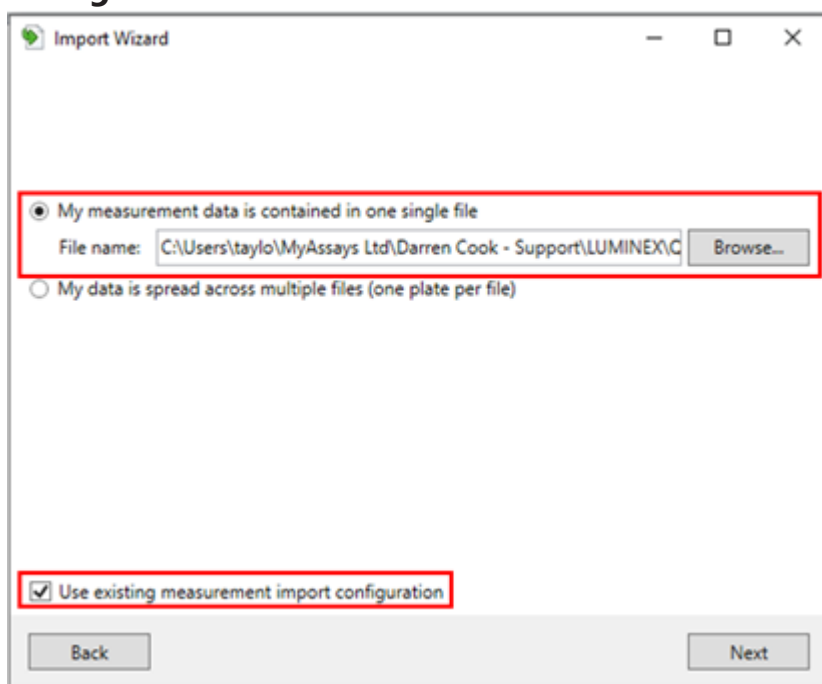
4. Review the data to be imported and press **Finish**. By leaving the **Calculate results** checkbox selected your results will be calculated, however if there are additional

changes required, deselect this checkbox to import the data without calculating results.
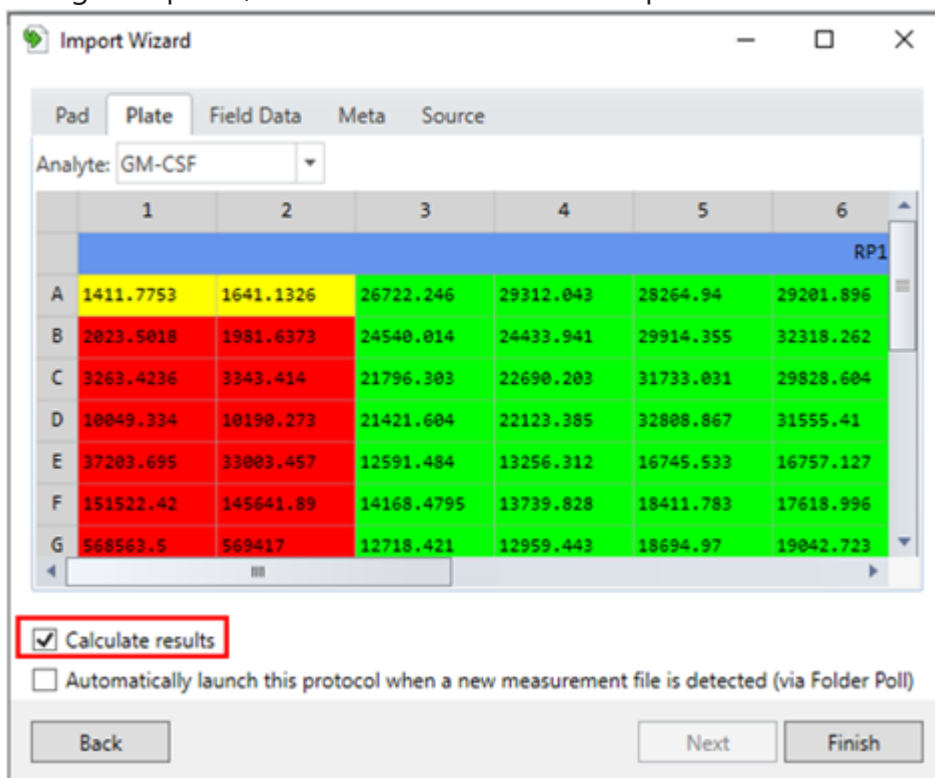
Microplate Settings

Ensure the microplate settings match those used in your assay. Within the protocol, on the **Microplate** tab, select the correct plate layout, **Edit** an existing layout, or **Create** a new

layout to match your assay. [Video Walkthrough...](#)
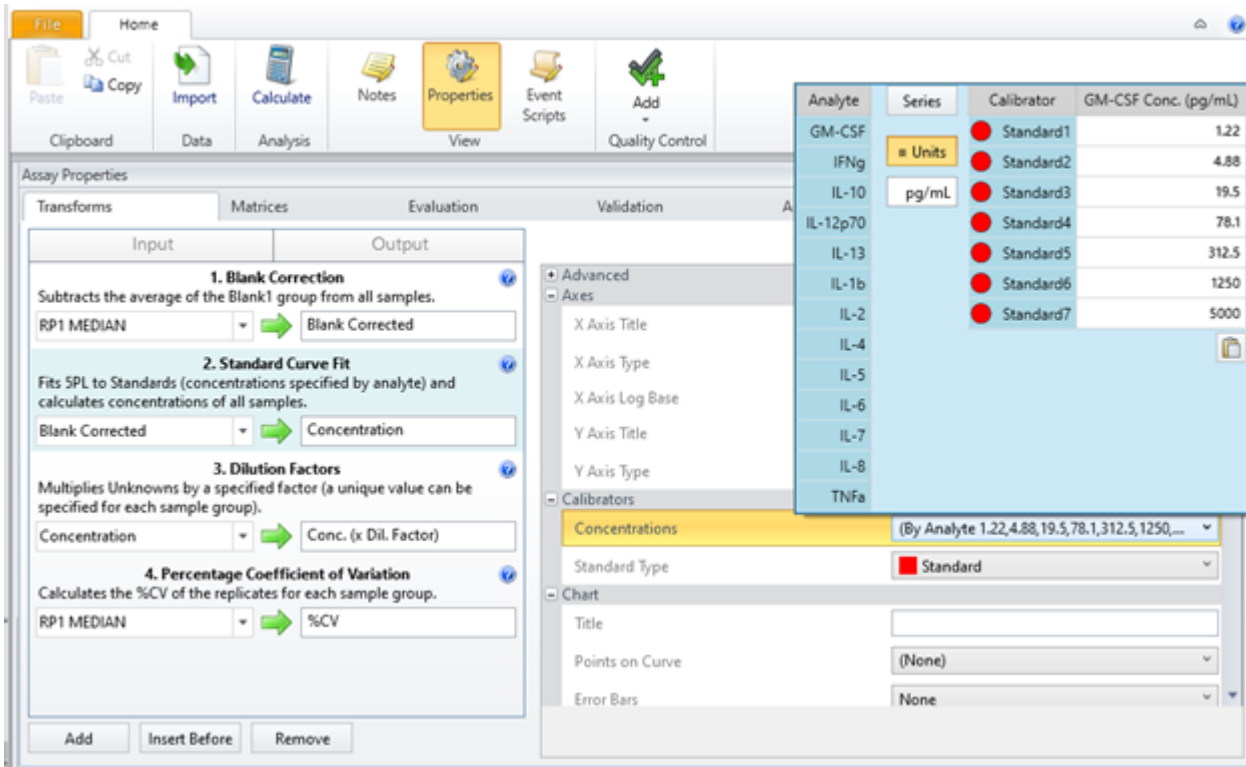
Sample IDs

Within the protocol, on the **Sample ID**s tab you can manually enter or copy and paste in Sample IDs for your assay. You can also use the Import Wizard (described above for importing measurement data) to import Sample IDs.
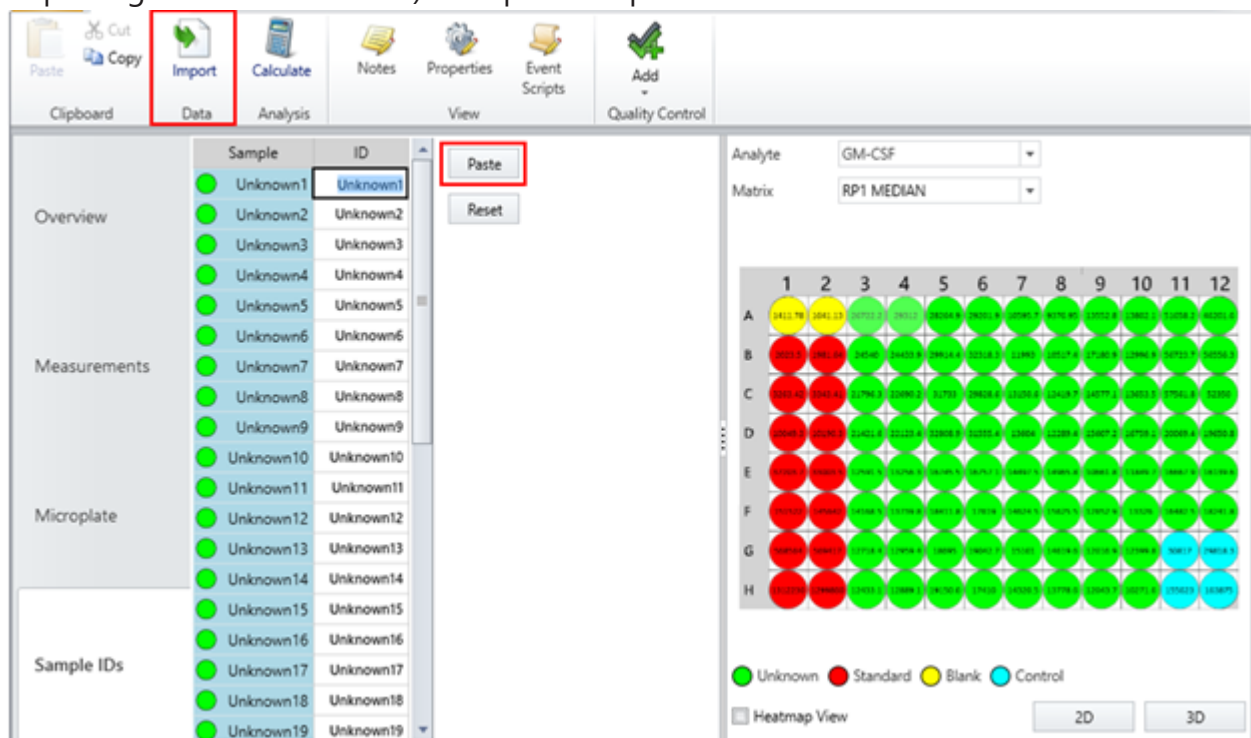
Standard Concentrations

For Quantitative assays, the standard concentration values can be updated using the **Properties | Transform** tab, selecting **Standard Curve Fit**, and updating the **Concentrations** dropdown box.
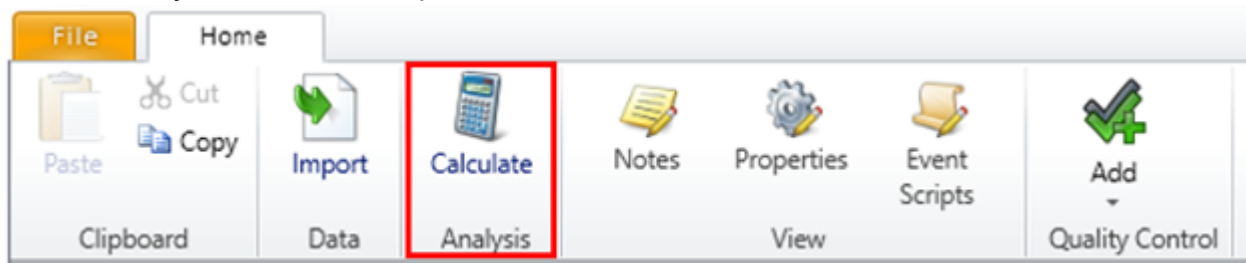
Calculate

To calculate your new results, press the **Calculate** button:

VICTOR Manager Integration with MyAssays Desktop

Overview

This topic describes how to configure the PerkinElmer VICTOR manager software to automatically launch a MyAssays Desktop protocol for analysis of the measured data.

> If you are working with the newer VICTOR Nivo reader, see the VICTOR Nivo Integration topic.

With this configuration in place, data analysis can be performed automatically as soon as VICTOR measurements are completed with little or no user intervention is required. In addition, results can be automatically saved/printed/exported as required to provide a seamless integrated measurement and analysis solution.

Terminology

Between the separate VICTOR manager software and MyAssays Desktop software, there is some overlap in terms used. Both systems use the term "protocol", for clarity in this section we refer to a VICTOR protocol as the *VICTOR measurements protocol* and a MyAssays Desktop protocol as the *MyAssays Desktop protocol*.

Integration Workflow

The general workflow is to:

1. Use the VICTOR manager software to create and configure the required measurement settings (the VICTOR measurements protocol).

2. Export the measurement data to a TXT file.

3. Create a MyAssays Desktop protocol to perform the required analysis.

4. Configure the VICTOR measurements protocol to launch the MyAssays Desktop along with the MyAssays Desktop protocol when the measurements are completed and provide the path to the exported TXT file (using the command line).

The creation of a VICTOR measurement protocol and a MyAssays Desktop protocol are not covered here. It is assumed that you already have these in place and are ready to integrate them.

MyAssays Analysis Launcher

MyAssays Desktop data analysis can be initiated from the command line. MyAssays Desktop offers many options and settings for complete control over the data analysis process.

Writing command line arguments is typically a complicated error-prone process. To simplify this task, MyAssays Desktop includes the MyAssays Analysis Launcher tool. This provides a point-and-click user interface for building a command line to launch MyAssays Desktop analysis. The resulting command line argument is displayed within the tool and can be easily copied and pasted into other applications.

To get started, we recommend familiarising yourself with the MyAssays Analysis Launcher tool. This can be found in MyAssays Desktop Explorer under the **Tools** tab. Select the **Analysis Launcher** option to launch it.

Using Analysis Launcher

To use Analysis Launcher, select a MyAssays Desktop protocol file to launch and use the user interface to configure the operations required.

If you have a compatible VICTOR TXT file to hand, use the **Import Measurements** option and select the file.

If you would like the results to be calculated automatically, select the **Calculate** option.

Notice, in the lower part of the Analysis Launcher the tool that as settings are made the command line argument is updated accordingly.
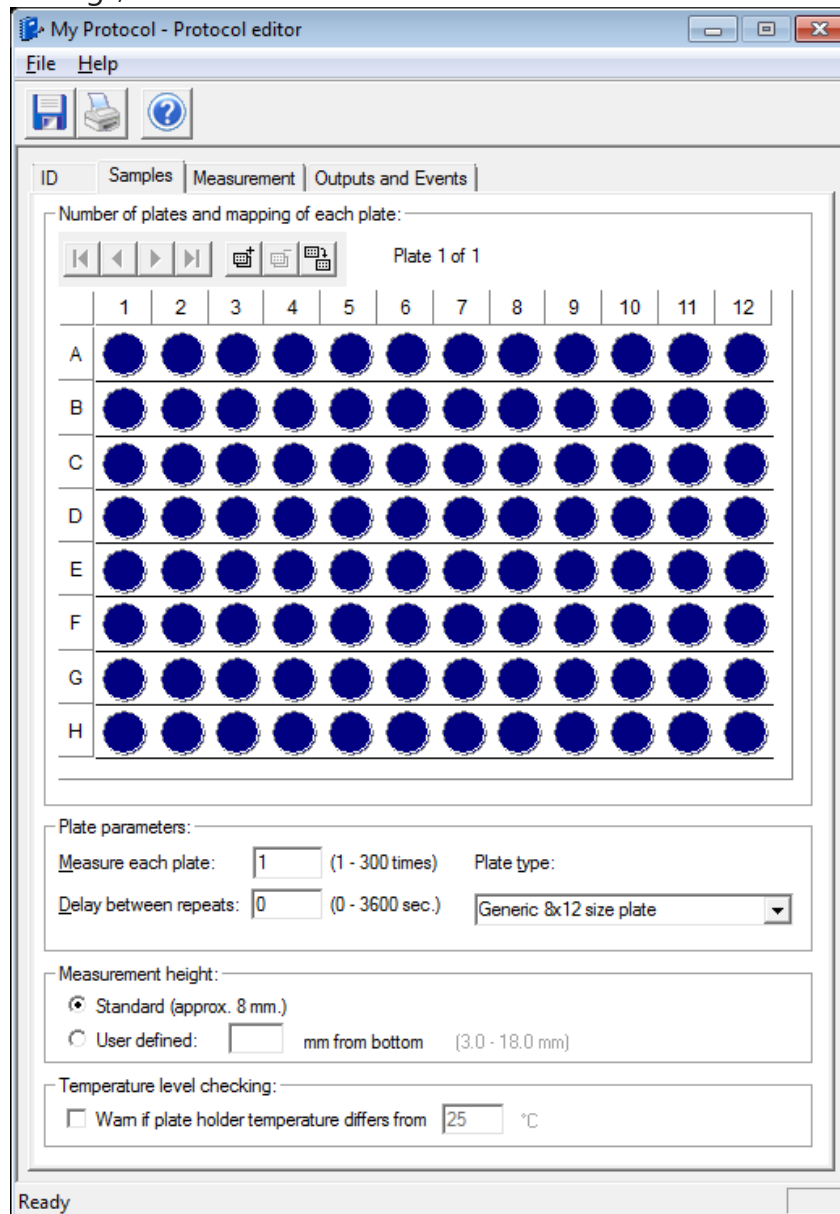
To launch the analysis, click **Launch**.

Example Integration

This section describes how to modify a VICTOR measurement protocol to launch MyAssays Desktop:

1. Launch the PerkinElmer VICTOR Manager Explorer.

2. Select and open the VICTOR measurements protocol to edit.

   You should see a window displaying the measurement configuration settings, similar to this:

3. Select the **Outputs and Events** tab

4. Select the **File output** check box

5. Select **File type** as **Text**

6. Specify the **Filename** as required (this could be made up of the various macros)

> For example, in this configuration the file is output to the Documents folder with a name created from the Protocol Name and Run ID:

With this setting in place, the results are exported to a text file when measurements are completed. You can try this now (perhaps with an empty plate) to check that the settings are expected.

You can then test importing this data into a MyAssays Desktop protocol "manually" by launching the MyAssays Desktop protocol and using the **Import Wizard** to import the text file.

The final part is to configure the VICTOR measurement protocol's **Assay end system command** setting. This is used to issue the command line.

1. Return to the VICTOR measurements protocol editor.

2. In the first edit box, enter the full path to the MyAssays Desktop Analysis exe, this is typically:

> **C:\Program Files\MyAssays\MyAssays Desktop\MyAssays.Desktop.Analysis.exe**

> If you have installed MyAssays Desktop to another location, then you will need to enter the correct path. If you are not, use the MyAssays Analysis Launcher application and inspect the command line:

3. In the second edit box, enter the MyAssays Desktop protocol filename to use followed by:

   /import-raw:<OutputFileName>

   This setting passes the filename generated by the VICTOR manager software to MyAssays Desktop so that the new measurement data file can be imported. The **<OutputFileName>** is a macro used by VICTOR manager software to refer to the new measurement data file.

   For example, to use the MyAssays Desktop protocol: **My Endpoint 12x8 Protocol (1)** in my documents folder I use:

   "C:\Users\Darren Cook\Documents\MyAssays\Protocols\My Endpoint 12x8 Protocol (1).assay-protocol" /import-raw:<OutputFileName>

   This would appear in the VICTOR measurements protocol editor as follows:
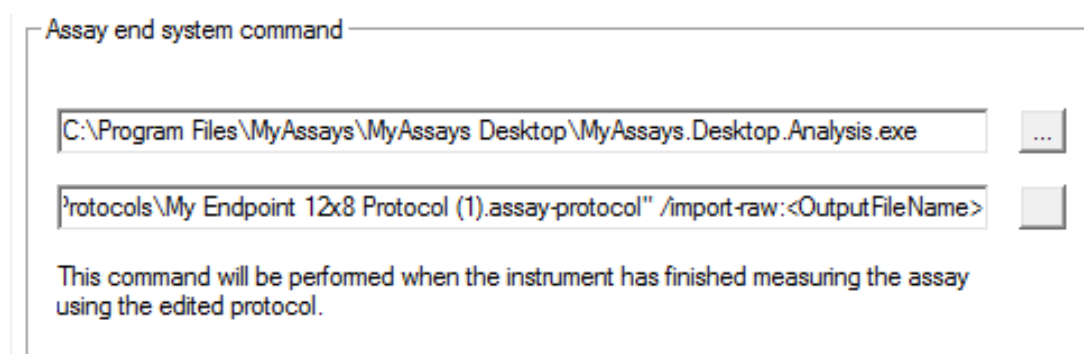
4. Save these changes to the VICTOR measurements protocol.

   Similarly, if you are not sure, use the MyAssays Analysis Launcher application and inspect the command line.

   With this setting in place, the results will be exported to a text file when measurements are completed and then imported into MyAssays Desktop. You can try this now (perhaps with an empty plate) to check that the integration is working.

   With these basic settings, the calculations are automatically performed. This gives the user an opportunity to review the settings and perhaps make some changes (such as a different layout or marking outliers to exclude) before pressing the **Calculate** button.

   If you would like calculations to be performed automatically, add:

   /calc

To the end of the command line argument in the VICTOR **Assay end system command**, e.g.:

You can also add further command line arguments to automatically print, export, etc. Use the Analysis Launcher tool or refer to the Command Line Arguments section for more information.

VICTOR Nivo Integration

To process the readings produced by the Victor Nivo reader, we suggest exporting data in the .XLSX format. Since VICTOR Nivo reader control software is a browser-based application, use your browser to configure readings.

MyAssays Desktop supports automatic import of VICTOR Nivo 2.5.0 XLSX files (and most files from v2.0.2). The import includes:

- **Measurements data**

    The readings output by the VICTOR Nivo reader control software. This also includes two technologies combined in a single protocol and data read from partial plates.

- **Metadata**

    Any information included in the **Parameters** worksheet of your Victor Nivo XLSX file. You can include this information in the report via Measurement Meta Data report element.

> 📝 If you are working with the older VICTOR Manager software, see VICTOR Manager Integration with MyAssays Desktop.

Importing Data from VICTOR Nivo 2.5.0 XLSX Files

The integration includes automatic processing of:

- New <INTEGER><SPACE>OPERATION naming convention.

- List and plate formats for kinetic measurements.

- Export of two technologies, such as Abs Kinetics and FI Endpoint, combined in one protocol in a single Excel sheet one below the other.
  The previous version (v2.0.2) exported each of them to a different sheet.

- Data measured on partial plates.
  If the imported VICTOR Nivo data contains positions that were not measured, then these values are imported as excluded and will not be included in the data analysis. Endpoint empty cells are indicated and reported with a dash "-"; not measured XY cells are simply not included.

Automating Import of VICTOR Nivo Files

You can use Folder Poll to automatically launch MyAssays Desktop protocol as soon as a new .XLSX file has been saved to a folder. The easiest way to configure the Folder Poll integration is using MyAssays Desktop; MyAssays Desktop can automatically configure folder polls

directly from your MyAssays Desktop protocol. For a video walk-through, see [Folder Poll with MyAssays Desktop](#).

> A folder poll can be created either using MyAssays Desktop when creating new protocol, importing data into existing protocol, or via the Folder Poll Manager. Refer to **Folder Poll User's Guide** to learn more.

> If you are using the Enhanced Security edition, you can automate the integration using the Autologin account. For a detailed description of this feature, see [Configuring Autologin Account](#).

Unsupported Imports

- Scan well area measurements are not currently supported.

- The unit values are not automatically imported.
  You can add the output units later when configuring the transform settings.

WIZARD² Integration

Play Video

MyAssays Desktop Pro provides first class data analysis tools that can be integrated directly with the WIZARD² gamma counter. MyAssays Desktop Pro can be installed and used on the WIZARD²'s own PC for a seamless integration with the counting process. In this way, data analysis can be performed automatically each time counting is completed. Data analysis results can be printed, exported and archived automatically with no user-intervention required after counting.

Also, MyAssays Desktop Pro can be installed and used on a PC separate from the WIZARD². Perhaps at a PC in your office and away from the lab. In this way you can build data analysis protocols and process results at the comfort of your own desk, freeing up access to the WIZARD².

If you are working in a 21CFR11 or GxP environment the Enhanced Security functions provide a secure and tracked integration when working with the WIZARD².

For a walk-through of working with WIZARD² please review these video resources:

- WIZARD² Gamma Counter Integration
- WIZARD² Gamma Counter Integration with Enhanced Security
- WIZARD² Gamma Counter Data Import Support (CSV and XML)

WIZARD² Data Import

The WIZARD² manager software can output measurement data (including as CPM) in either CSV or XML format. The XML format is recommended because it provides a richer set of data including:

- **Metadata**

  Any metadata associated with the imported measurements. It can then be included in the report via Measurement Meta Data report element.

- **Field Data**

  All associated textual or numerical data is automatically imported and stored alongside measurements. See Adding Field Data Alongside Measurements for more details.

- **Spectrum Channel Counts**

- **Sample Bar Code**

Importing XML Data from WIZARD²

You can select which XML data to import into MyAssays Desktop:

Custom
WIZARD² (All Data)
WIZARD² (CPM)
WIZARD² (Spectral and CPM)
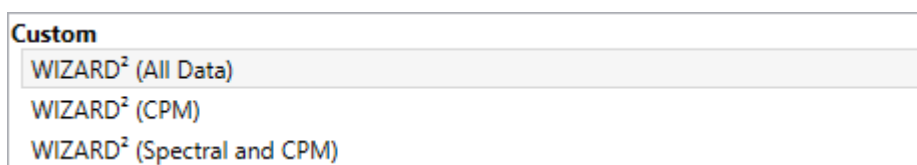
The resulting protocol will import only the selected data items.

If you select the **All Data** option for the measurement files that contain more than 10 matrices of data, MyAssays Desktop will include only the first matrix of the imported data in the report's Sample Table. In this case, MyAssays Desktop will notify you accordingly:
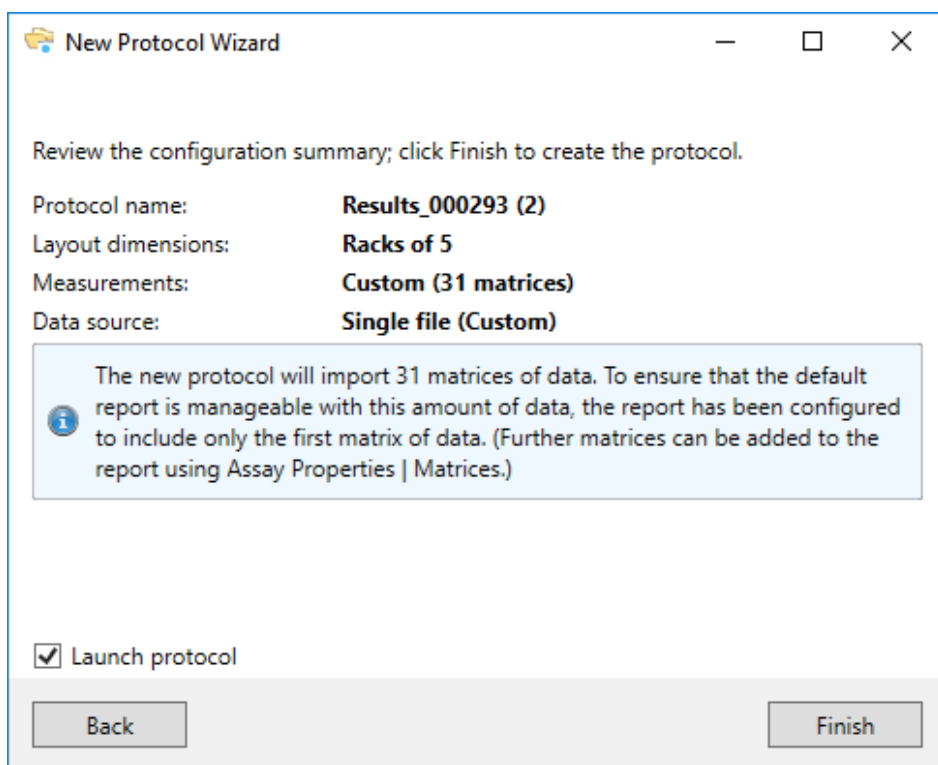
Including Additional Matrices in the Sample Table

All of the imported data will be available for analyses and processing. Using **Matrices** tab of the **Assay Properties** panel, you can select the matrices of data to include in the Sample Tables. Choose the matrix to include and set the **Include in Sample Tables** check box:
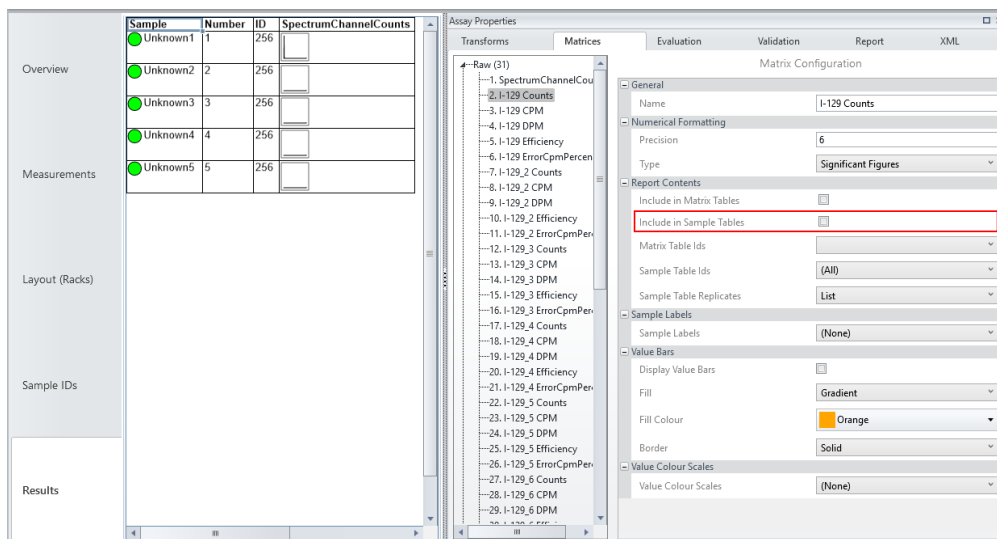
To learn more about the applicable settings, see [Viewing Available Matrices and Configuring Their Settings](#).

Unsupported Data Imports

MyAssays Desktop WIZARD² XML Import does not support importing XML files that contain measurements with:

- Repeat values > 1.
  Only measurements where **Repeat="1"** will be imported.
- Combination of rack sizes.

XSLT

How to Use XSLT for Custom Export

In most cases, you will probably export your reports in one of the provided formats. For special circumstances (such as a specific output for a LIMS system), you may need to save the results of your data analysis in another file format, with specific column or decimal separators, or both. For these purposes, you can use XSLT export settings.

XSLT and Report Files

When you apply XSLT to transform the report, it converts the report.xml file. This XML file is used to define how to generate the actual report file with the exported data.

For example, the **Txt (tab column separator, period decimal separator).xslt** transform will convert the report to a text file format as described, whereas the same report could be transformed to HTML using the **Html Tables.xslt** format.

For more information about XSLT, see https://www.w3.org/TR/xslt-10.

> MyAssays Desktop currently only supports **XSLT 1.0** format.

Applying XSLT File to Report

MyAssays Desktop provides some example XSLT files at MyAssays\XSLT. These are already used for some of the predefined export options but you can apply them using the Export Wizard. By using these files, you can specify both the XSLT transformation and the file format your laboratory works with.

How to Apply XSLT File to Report

1. Open a results file.

2. On the **Home** ribbon tab, in the **Data** group, select **Export**.
   This launches Export Wizard.

3. Select **Custom** export format from the list.

4. Select **XML Transform (via XSLT 1.0)**.

5. Select a destination to export the report to (optionally using macros).

6. Select a file extension from the drop-down or type another file extension to export your file with.
   XSLT does not imply any particular file extension because the output file may be of any type.

7. Specify the XSLT file to transform your report with.
   For example, select a predefined file from **MyAssays\XSLT**.

> If you select **Copy XSLT file to protocol**, then the selected XSLT file will be stored inside the protocol. It will be available as **Protocol Content** option on the next runs of Export Wizard even if you will transfer the assay to another source.

   Optionally select how to preview the output file from the **Preview Transformed Export** drop-down.

8. To apply the selected export settings on the future runs, select **Configure protocol to automatically export**.
   To launch the results with the default associated application after each calculation, select **Open with default viewer**.

9. Click **Finish**.

> The Export Wizard is available only in the results mode. If you want to save the export configuration to an assay-protocol, then after you configured the export apply Save command for this operation.

Creating Custom XSLT Files

XSLT converts the report.xml to generate the final output. So, if you want to develop your own XSLT, note that actual content of the report.xml depends on the assay protocol configuration.

> We recommend making sure that the protocol you want to transform is complete and you do not plan to change it significantly (e.g., change order or add transforms, add other report elements, etc.). Major changes to the protocol can impact the report.xml, which, in turn, may impact the XSLT transform.

To get started with building your own XSLT file, first generate the report.xml file as follows:

1. Launch an assay protocol, review or edit its settings, and then click **Calculate** to generate results.

2. On the **Home** ribbon tab, in the **Data** group, select **Export**.
   This launches Export Wizard.

3. Select **Custom** export format from the list and then select **XML**.

4. Complete the wizard to generate the report.xml content for the data.

It is possible to use the existing XSLT files stored in your MyAssays/XSLT folder as a starting point. Copy and paste their content to a new file to experiment and tweak the provided examples. Then you also can apply your XSLT via Export Wizard to test your XSLT files.

> To develop XSLT solutions for more demanding requirements, contact support@myassays.com.

Using Other Scripting Tools

If you prefer to use other scripting tools instead of XSLT, then:

1. Export a report.
   Generate a report.xml file or one of the other formats such as TXT.

2. Launch a scripting tool and convert the exported report with it.

You can automate this by launching MAA from command line with the export parameter and launching the report with your scripting tool.

> For further automation of this process, use Folder Poll.

XSLT Encoding

When exporting via XSLT, the output encoding can be changed within each XSLT file or using a global setting to apply to all export files. Values set in XSLT will override the global value.

- XSLT encoding can be specified by adding an encoding attribute of the XSLT file itself, e.g. **<xsl:output encoding="ISO-8859-1"/>**

- To apply globally, use **DefaultEncoding** attribute in **ews.config.xml** file (under **Settings**), e.g. **<ExportWizardSettings xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:xsd="http://www.w3.org/2001/XMLSchema" DefaultEncoding="Windows-1252">**

Common encoding values include:

- ISO-8859-1
- UTF-8
- UTF-16
- UTF-32
- ASCII
- US-ASCII
- Windows-1252

Calculation Log

The Calculation Log stores all details of the calculations performed.

How to: Open Calculation Log

1. Launch an assay protocol or open a results file.

2. Press the **Logs** button to open **Logs** panel with **Calculation Log** tab.

3. Review as required.

Logged Calculations

The content included in the Calculation Log depends on the configuration of each of the following settings:

- **Transforms** – Run and results of each transform (in the sequence they are configured).

- **Evaluation** – Run and results of the computed evaluations.

- **Validation** – Run and results (pass or fail) of the computed validations.

- **Transform Output Variables** – Non-matrix calculations produced by the transforms

Additionally, it might also produce fit transform context parameters and a variety of transform-specific calculations. For example, if a Standard Curve Fit transform is configured, then the log also contains coefficient constraints, weighting infinity resolution, custom flag label for Standard Curve Fit and more.

Level of Details

The Calculation Log can be viewed in the following modes:

- **Detailed** – Lists all logged calculations in great depth (e.g., transform calculations for each position)

- **Summary** – Contains overview of performed calculations

- **None** – No data is displayed in the log

By default, the log is displayed in **Detailed** mode.

> To change the level of details, in the XML editor, add the **CalculationLog** element as a child of the **MatrixTransformAnalysis** and select preferable view mode.

Saving Log to a File

Press the **Save Log** button to save the log for the current assay run to your preferred destination in a .TXT file.

Error Log

If any errors occurred during an assay run, they are stored and described in the Error log in similar to the Calculation Log level of details. To view the log, select **Error Log** subpane of **Logs** pane.

Command Line Arguments

MAA can be launched via **MyAssays.Desktop.Analysis.exe** (the executable responsible for data analysis) along with command line arguments to automate common tasks. This technique can be used to initiate protocol execution from a third-party application. This includes:

- Launching a protocol
- Importing data
- Calculating results
- Exporting data
- Printing report
- Creating new protocol (requires Pro version)

> To assist with creating the command line, use the Analysis Launcher tool.

MyAssays Desktop Analysis with Command Line Arguments

Access MyAssays Desktop Analysis Executable

The **MyAssays.Desktop.Analysis.exe** executable can be found in MyAssays Desktop's installation folder. This is typically:

- `"C:\Program Files (x86)\MyAssays\MyAssays Desktop\MyAssays.Desktop.Analysis.exe"` – For 32-bit version of Windows
- `"C:\Program Files\MyAssays\MyAssays Desktop\MyAssays.Desktop.Analysis.exe"` – For 64-bit version of Windows

How to: Access Installation Folder from Registry

To simplify integration with 3rd party applications, the installation folder of MyAssays Desktop can also be obtained from the registry:

- `Computer\HKEY_LOCAL_MACHINE\SOFTWARE\MyAssays\MyAssays Desktop\@InstallLocation` – For 32-bit version of Windows
- `Computer\HKEY_LOCAL_MACHINE\SOFTWARE\WOW6432Node\MyAssays\MyAssays Desktop\@InstallLocation` – For 64-bit version of Windows

Launch Protocol or Results

In the simplest case, **MyAssays.Desktop.Analysis.exe** can be launched with an assay-protocol or assay-results file:

```
"C:\Program Files\MyAssays\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe"
"C:\Users\UserName\Documents\MyAssays\Protocols\ELISA
(96 well).assay-protocol"
```

```
"C:\Program Files\MyAssays\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe"
"C:\Users\UserName\Documents\MyAssays\Results\ELISA (96
well) (1).assay-results"
```

Importing Measurements

When launching an existing assay-protocol file, or creating a new one, you can specify the raw data file to launch it with. For example, the MyAssays.Desktop.Analysis.exe can be launched with:

/import-raw:"*{filename}***"**

Where *{filename}* is the full path to the data file to import. For example:

```
/import-
raw:"C:\Users\UserName\Documents\MyAssays\Measurements\E
xamples\12x8 Endpoint.txt"
```

In this case, the MyAssays Desktop will launch its New Protocol Wizard with the data file automatically imported (assuming it is a file that can be imported) and ready for the user to build a new protocol for their measurement data.

In addition, a protocol file can also be specified:

"*{protocol}***" /import-raw:"***{filename}***"**

Where *{protocol}* is either a MyAssays Desktop assay-protocol file (e.g., ELISA (96 well).assay-protocol) or a name to create an assay-protocol file to.

In case the protocol does not yet exist, the MyAssays Desktop will launch the New Protocol Wizard as above and save the new protocol to the specified name. For example:

```
"C:\Program Files\MyAssays\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe"
"C:\Users\UserName\Documents\MyAssays\Protocols\NEW
ELISA.assay-protocol" /import-
raw:"C:\Users\UserName\Documents\MyAssays\Measurements\E
xamples\12x8 Endpoint.txt"
```

If the protocol already exists, then MyAssays Desktop will launch the protocol and import the data. In addition, there are further command-line options that will perform the analysis and export the report (to XLSX, PDF, DOCX). For example, with:

"{protocol}" /import-raw:"{filename}" /calc /export-report:xlsx /exit

MyAssays Desktop will launch the protocol, import the data, calculate the results, and export the results to Excel then exit.

Command Line Arguments

When the **MyAssays.Desktop.Analysis.exe** is launched with a protocol file (with .assay-protocol extension), a number of arguments can be included to automate various functions:

> Arguments with values that include spaces must be put in quotes.

Argument	Use to
/autologin	Perform operations permitted under MyAssays Desktop Enhanced Security Autologin account.
/calc	Compute data analysis operations configured in the protocol automatically. ℹ️ Use this option in conjunction with **/import-raw** to perform calculations on the imported raw data.
/calc-log:" {log}"	Save calculation log in a file. The *{log}* is the full path to the file, including its name and extension. For example: **/calc-log:"C:\Users\UserName\Documents\MyAssays\Logs\calculation .log"**
/error-log:" {filename}"	Save error log in a file. The *{log}* is the full path to the file, including its name and extension. For example: **/error-log:"C:\Users\UserName\Documents\MyAssays\Logs\error.log"**
/exit	Exit the program automatically after calculations are completed or printed.
/export-report: {filetype}	Export the report in XLSX, PDF, or XML *{filetype}*format and then save in \MyAssays\Reports\ folder. For example: **/export-report:pdf** ℹ️ Add **:nolaunch** at the end to prevent the report from launching immediately after export.
/export-report:xslt1 {filetype}:"	Convert the report using the specified XSLT template where *{filename}* is the full path to the template file in the \MyAssays\XSLT folder. This report is then exported and saved in HTML, TXT, CSV or XML *{filetype}*format

Argument	Use to
{filename}"	(\MyAssays\Reports\ folder). For example: **/export-report:xslt1***csv:***"C:\Users\UserName\Documents\MyAssays\XSLT\Csv Tables (by Data).xslt"** ℹ️ Add **:nolaunch** at the end to prevent the report from launching immediately after export. 📝 Configure the protocol to use **Custom (including text/XML/CSV/LIMS compatible, etc.)** Export Wizard's option (requires Pro license) and save the export settings to the protocol (rather than using **/export-report**).
/import-containerids: {filename}	Import a file with container (plate, analyte, or batch) identifiers from the *{filename}* full path. 📝 Overrides **Import Wizard**'s previously configured setting.
/import-raw:" {filename}"	Import the raw data file to the protocol; *{filename}* is the full path to the data file to import. ℹ️ If **{protocol}** is not specified, then New Protocol Wizard is launched automatically to create assay-protocol with imported measurements. In this case, all other import options are not supported.
/import-sampleids:" {filename}"	Import a table-based Sample IDs data contained in text file of any format from the *{filename}* full path. 📝 Overrides **Import Wizard**'s previously configured setting.
/import-tweaks:" {filename}"	Specify a protocol tweaks file that defines changes to the protocol configuration. ℹ️ Add **:saveprotocol** at the end to save the protocol file with tweaks automatically. 📝 If the Save changes to protocol option is selected (under **File | Save** in the MAA), then changes are saved to the protocol

Argument	Use to
	📋 irrespective of this option (e.g., when calculations are performed).
/noappwin	Do not display the application window.
/notopmost	By default, the application window is brought to the top when it is loaded. Use this setting to override this default behaviour and to disable bringing the window to the top.
/performance-report:"{filename}"	Output an XML performance report of MyAssays Desktop Analysis. The report includes system information and timings useful for evaluating system performance and troubleshooting. This performance data is collected during the run of the launched process with the report being exported when the MyAssays Desktop Analysis application exits. For example: **/performance-report:"C:\Users\UserName\Documents\MyAssays\Logs\performance.log"**
/print	Print the report (if the calculations succeeded) with the default printer (if available).
"{protocol}"	Launch an existing file or create new assay-protocol via New Protocol Wizard (requires Pro version). The "*{protocol}*" argument can be specified as: - Full path to an assay-protocol file to create or launch: **"C:\MyAssayData\Protocols\NEW ELISA.assay-protocol"** **"C:\Users\Username\Documents\MyAssays\Protocols\ELISA (96 well).assay-protocol"** - Protocol name without specifying its folder. In this case, the protocol is created in or launched from the default Protocols folder (i.e., as configured by Assay Data Folder Root setting): **"NEW ELISA.assay-protocol"** **"ELISA (96 well).assay-protocol"**
/tab:{tab}	Select the tab to launch MAA with; *{tab}* is zero-based **tab number**: Overview = 0; Measurements =1; Microplate = 2; Sample IDs = 3; Results = 4.

How to Use Long Command Line Argument

The maximum number of characters in the command line is > 255. If the command line argument exceeds this length, you can either:

- Use shorter file and folder names where possible

- Store the argument list in a text file and execute it with @ syntax. For example:

```
"C:\Program Files\MyAssays\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe" @
"C:\Users\UserName\Documents\MyAssays\arguments.txt"
```

To easily build and configure command line, use the Analysis Launcher.

Examples of Command Line Usage

```
"C:\Program Files\MyAssays\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe"
"C:\Users\UserName\Documents\MyAssays\Protocols\ELISA
(96 well).assay-protocol" /import-
raw:"C:\Users\UserName\Documents\MyAssays\Measurements\E
lisa-Absorbance.txt" /import-
sampleids:"C:\Users\UserName\SampleID\DemoScanFile.csv"
/calc /export-report:xlsx:nolaunch
```

In this example, the ELISA (96 well).assay-protocol is launched and executed in MAA with Elisa-Absorbance.txt measurements and DemoScanFile.csv file with Sample IDs ; calculated results are exported in XLSX report (and not automatically launched) under \MyAssays\Reports\ folder.

```
"C:\Program Files\MyAssays\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe"
"C:\Users\UserName\Documents\MyAssays\Protocols\ELISA
(96 well).assay-protocol" /import-
raw:"C:\Users\UserName\Documents\MyAssays\Measurements\E
lisa-Absorbance.txt" /import-
sampleids:"C:\Users\UserName\SampleID\DemoScanFile.csv"
/calc /export-report:xlsx:nolaunch /print /noappwin
```

As with previous example, the protocol with specified measurements and Sample IDs is computed and the results are exported to XLSX file, but without displaying MAA window. Additionally, the report is printed with default printer.

```
"C:\Program Files\MyAssays\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe" "NEW ELISA.assay-
protocol" /import-
raw:"C:\Users\UserName\Documents\MyAssays\Measurements\E
lisa-Absorbance.txt"
```

In this case, New Protocol Wizard launches with Elisa-Absorbance.txt measurements imported to create a new protocol with the specified name (NEW ELISA).

```
"C:\Program Files (x86)\MyAssays\MyAssays
```

```
Desktop\MyAssays.Desktop.Analysis.exe"
"C:\Users\UserName\Documents\MyAssays\Protocols\ELISA
(96 well).assay-protocol" /calc /exit /performance-
report:"C:\Users\UserName\Desktop\Performance
Report.xml"
```

In this example, the ELISA (96 well).assay-protocol is launched and executed in MAA, results are calculated and a performance report is created and stored on the User's Desktop.

Tweak Files

This section provides information about the protocol tweaks feature. This feature enables an external application to change and apply specific settings of the data analysis.

> This is an advanced feature and misuse of it could cause problems.

Overview

Protocol tweaks are used to define changes to the data analysis parameters of an existing protocol. Any of the assay protocol parameters can be tweaked. This is useful to control the analysis process by other software such as instrument-control software or LIMS.

For example, a LIMS could initiate execution of data analysis and specify customizations (such as standard concentrations or layout); the customisations are merged with the existing protocol, the analysis performed, and results generated with data exported as required.

Protocol tweaks are defined in an XML file and can be applied by launching the protocol and specifying the tweak file to apply.

> Any data analysis parameter can be modified.

Tweak Syntax

A protocol-tweak.xml file is an XML with the following syntax:

<?xml version="1.0" encoding="utf-8"?>

<ProtocolTweaks>

<Tweak XPath="*Full assay setting to tweak path*">*Substitute data*</Tweak>

</ProtocolTweaks>

> You can insert any number of tweaks under <ProtocolTweaks> section.

Using the Feature

To use the protocol tweak feature, it is recommend to developing a protocol-tweak file as follows:

1. Build or obtain an assay-protocol file that meets your data analysis requirements.
2. Identify which analysis parameters should be tweaked.
3. Develop a protocol-tweak.xml file.
4. Test the protocol-tweak.xml file.

With your working protocol-tweak.xml file, use your instrument control or LIMS software to insert relevant content into the protocol-tweak.xml file.

How to: Apply Protocol Tweaks

The easiest way to apply a protocol tweak file is to use the Analysis Launcher. Use this tool to select the protocol and tweak file and launch the application.

The Analysis Launcher tool will also generate and display the command line argument to use. You can use this command line setting to launch the operation yourself (perhaps calling it from another software application that prepares the tweak file's contents). More information about command-line arguments is available here.

When the protocol is launched and tweak file applied, the system will perform various checks on the incorporated tweaks to detect any report any possible configuration errors in common usage scenarios.

If the protocol is successfully tweaked the analysis operations will continue as specified. The actual behaviour will depend on any further command line settings (such as automatic calculation, export, etc.)

> Tweak changes are not automatically saved to the incorporated assay file. A tweaked protocol appears as modified and not saved (with ***** in title). If you save the protocol, the tweaks will be saved to the protocol file.

Changing the Default Matrix Limit for Including Raw and Field Matrices

When creating a new protocol for a large amount of data, MyAssays limits the number of matrices included in the report. This topic explains how to change the default matrix limit settings for both measurements and field data.

> 📝 This is an advanced configuration setting that can only be changed via XML.

For general principles of working with a lot of readings, see Handling a Large Number of Raw and Field Matrices. To learn more about accompanying the measurements with related information, see Adding Field Data Alongside Measurements.

Where the Matrix Limit Settings Are Stored

The common settings for handling large amount of measurements are stored in the **pws.config.xml** file. This file is located in your **Precanned\Settings** subfolder in your MyAssays Desktop's installation folder. This is typically:

- `"C:\Program Files (x86)\MyAssays\MyAssays Desktop\Precanned\Settings\pws.config.xml"` – For 32-bit version of Windows
- `"C:\Program Files\MyAssays\MyAssays Desktop\Precanned\Settings\pws.config.xml"` – For 64-bit version of Windows

Using this file, you can edit the default matrix limit settings for raw data, field data, or both.

Changing Matrix Limit

To change the default limit settings for measurements, follow these steps:

1. Launch the **pws.config.xml** file with your default XML editor.
2. Locate the **Report** element.
3. Depending on the data you're changing the limit for, edit:

   - **MatrixLimit** value to alter the default setting for raw measurements data.
   - **FieldLimit** value to alter the default limit for field data matrices.

4. Save the changes to the file.

This change will not affect the application of the limit. Refer to How the Matrix Limit Is Applied to learn more.

Installing MyAssays Desktop Alongside WorkOut

MyAssays Desktop can be installed and used alongside an existing WorkOut installation (including WorkOut versions 1.x, 2.x, Plus, and Plus MMD). This is referred to as a Side-By-Side installation.

Certain modules (relating to data import and analysis) are shared between the applications. If you plan to use both WorkOut and MyAssays Desktop on the same system, then please follow these points to avoid known conflict issues:

- Always install MyAssays Desktop **after** installing WorkOut (i.e., do not install, update, patch, or repair a WorkOut installation after installing MyAssays Desktop).
- If WorkOut is uninstalled leaving a MyAssays Desktop installation, then it will be necessary to also uninstall MyAssays Desktop and then reinstall MyAssays Desktop.

If MyAssays Desktop has been installed with a Side-By-Side WorkOut installation, then this will be reported in the **File** | **Information** tab of MyAssays Desktop Explorer.

Known Issues

If the points above are not followed, then you may see the following problems with MyAssays Desktop:

- Unable to import data
- Unable to produce a valid report (on data calculation)

To resolve these issues, please uninstall MyAssays Desktop and then reinstall MyAssays Desktop to update the shared component files to the newest version.

Referencing MyAssays Desktop

You can refer to MyAssays Desktop in your paper, thesis or publication.

To refer to the data analysis tool include the text:

"MyAssays Desktop *Product Version* from MyAssays Ltd., https://www.myassays.com"

> To obtain current *Product Version* open **Information** screen of **File** tab in the MADE. You can either click the **Copy** icon or enter it manually to your publication.

Tips for Repairing a Corrupted System

If MAD suddenly or unexpectedly stops working and is unable to successfully launch then it is likely that the system has somehow been corrupted. Guidance for diagnosing and resolving possible causes of system corruption are provided here.
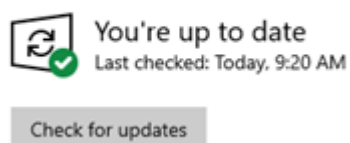
Check if any Windows updates are pending

1. Open Settings

2. Select **Update & Security**
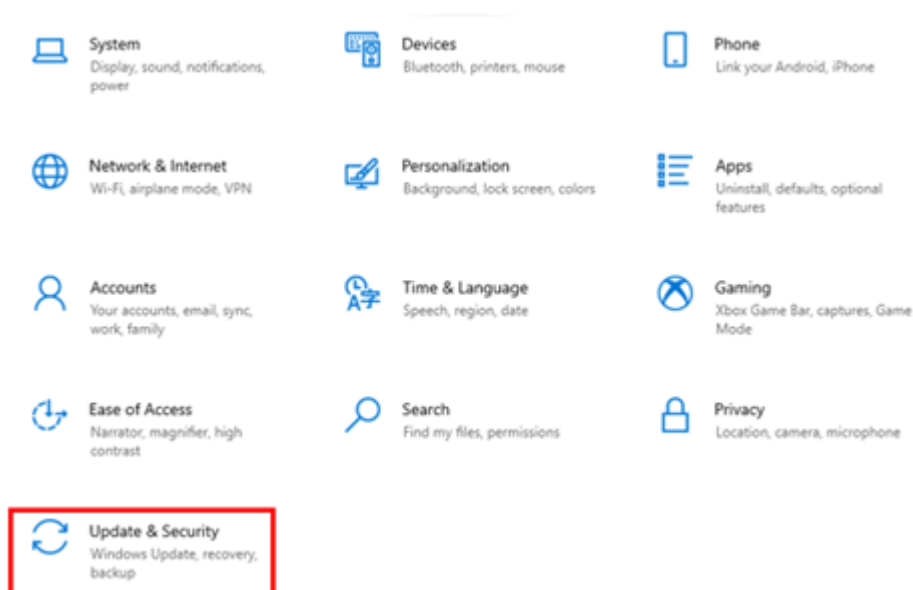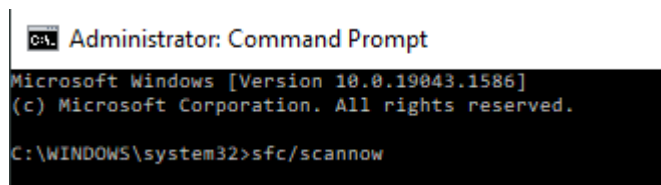

3. Check update status

4. If updates are pending, select to install and restart the system. During system restart, any pending updates will be applied.

Run Windows System File Checker

Start | type **cmd** and press **Ctrl + Shift + Enter** to launch a command prompt with administrator rights. When prompted, type the following:

sfc / scannow

This process may take several minutes to complete.

Repair a Windows Image

Run the following commands (in the same way as SFC) for further tests:

Dism /Online /Cleanup-Image /ScanHealth

Dism /Online /Cleanup-Image /CheckHealth

If any issues are detected, use the following to restore:

Dism /Online /Cleanup-Image /RestoreHealth

For more information, see the following link from Microsoft. More...

View Recently Installed Windows Updates

Check for recent Windows updates that were applied at the time the issue started and remove any that might be the cause.

To review recently installed Windows updates:

1. Open **Settings | Updates & Security**

2. Select **View update history**
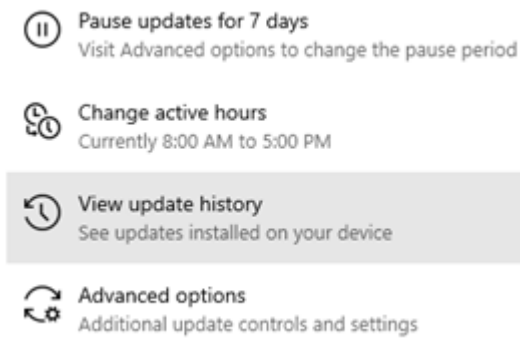
For example, on this system the MyAssays Desktop Explorer could not open. The issue started on 16th March, 2021. By uninstalling the latest update, the issue was resolved.
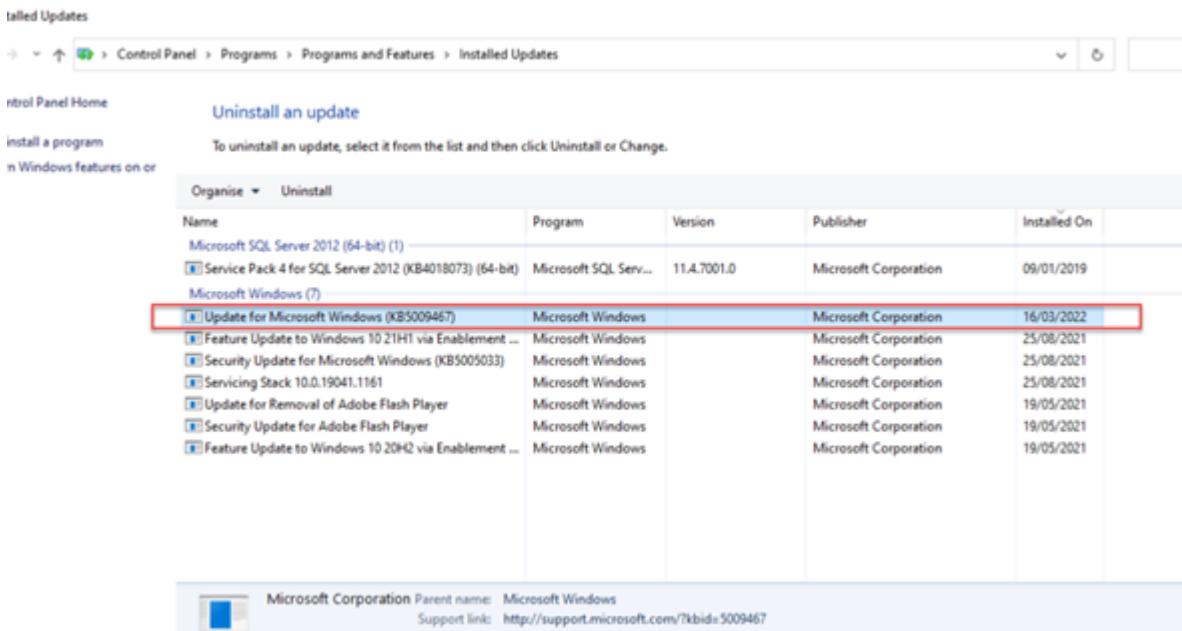
Enable MAD Logging

To enable MyAssays Desktop Logging:

1. Open the **MyAssays Desktop Explorer**

2. Open **File | Data**
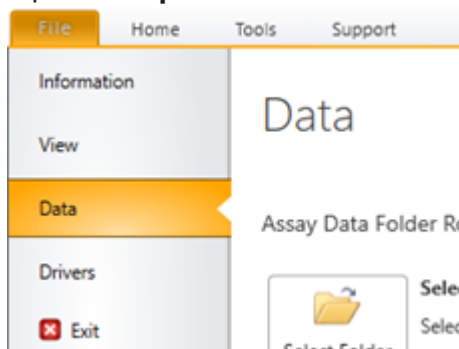
3. Select the **Collect Diagnostic Logs** checkbox:
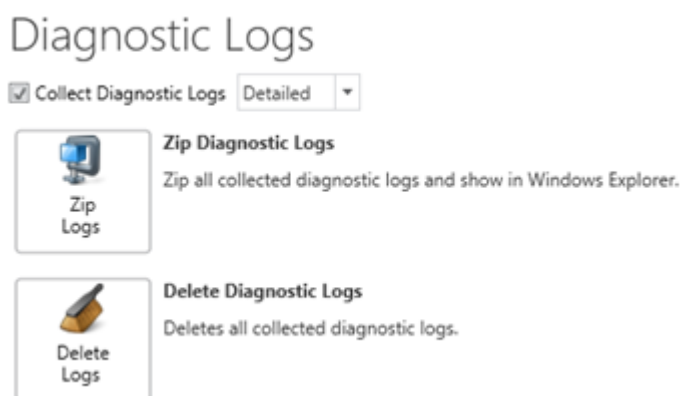
4. Perform the steps to recreate the issue

5. In **MyAssays Desktop Explorer | File | Data**, select **Zip Diagnostic Logs**
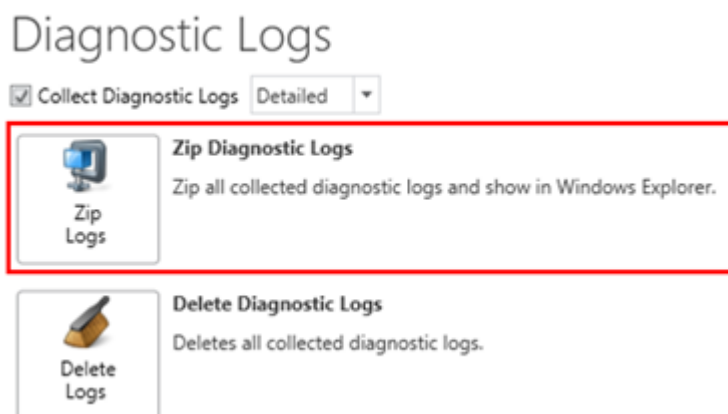
6. This will open the Windows Explorer to the file location. Provide the .zip file to support@myassays.com.

Check Event Viewer

Launch **eventvwr**

Check for any unexpected system events under **Windows Logs**, paying close attention to **System** and **Application** logs.
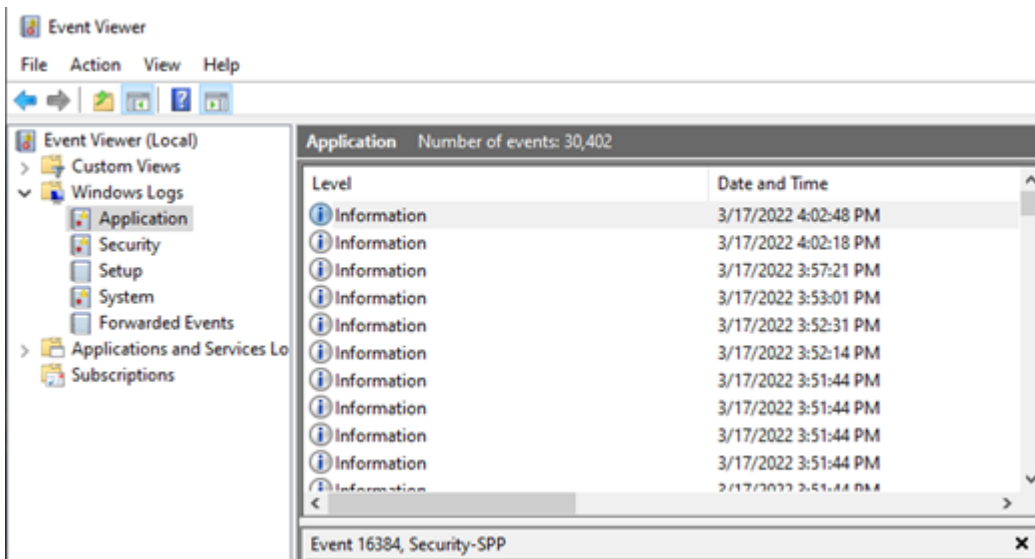
System Restore Point

If any system restore points have been created, consider reverting to an earlier version.

To do this:

1. Launch Control Panel, in the Control Panel search box, type **recovery**.
2. Select **Recovery | Open System Restore**.
3. Use the tools to apply system restore.

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