# MyAssays Desktop User's Guide 

MyAssaysı

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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 rackbased 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

Data can be collected and processed together in any combination. For example, dual endpoint measurements read at both 665 nm and 620 nm 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 meta data (data accompanying the read such as measurement date/time, barcode, etc.) are imported automatically. (For the latest list of currently support format, 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 meta data (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 color
- By graphical value bars


## Data Analysis

Beyond the online database of ready-to-use preconfigured protocol, 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 - $R^{2}, a R^{2}, ~ S E, F-$ statistic, P-value (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 usercustomizable 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 preinstalled 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.

## Product Editions

MyAssays Desktop is available in various configurations to suit different budgets and needs:

Basic: Operates with preconfigured protocols (either those included in the installation package or as downloaded from MyAssays.com). The Basic edition allows tweaking limited protocol parameters (such as fit method, sample concentrations, layout, etc.).

Pro: Includes all of the features of the Basic edition plus functionality for creating new custom protocols. This edition provides full access to the Matrix-Transform data analysis model, offering a wealth of easy-to-use tools for building data analysis solutions tailored to your lab.

## Pro Add-Ons:

Optional add-on functionality is available for the Pro edition:

## 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 ${ }^{\circledR}$ xPONENT and Meso Scale Discovery Workbench ${ }^{\circledR}$ CSV and TXT formats.


## QC

The QC option provides a range of inter-assay analysis features to support the continuousmonitoring 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 and CUSUM 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.


## Enhanced Security Add-On

For those users working under GxP or 21CFR11, the Enhanced Security edition offers the features 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/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 log-in 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 outputs).


## Licensing

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

## Edition Comparison

| Feature | Basic | Pro |
| :---: | :---: | :---: |
| Downloadable Protocols (from myassays.com) | $\checkmark$ | $\checkmark$ |
| Preconfigured Protocols (96/384 versions): | $\checkmark$ | $\checkmark$ |
| - ELISA | $\checkmark$ | $\checkmark$ |
| - DNA/Protein Quantification | $\checkmark$ | $\checkmark$ |
| - ATP lite protocol | $\checkmark$ | $\checkmark$ |
| - Generic DELFIA | $\checkmark$ | $\checkmark$ |
| - Generic LANCE | $\checkmark$ | $\checkmark$ |
| - Generic Fluorescence Polarization protocol | $\checkmark$ | $\checkmark$ |
| - Monochromator Spectral | $\checkmark$ | $\checkmark$ |
| - Kinetic for $\mathrm{Ca} 2+$ | $\checkmark$ | $\checkmark$ |
| - Bacterial growth | ص | $\checkmark$ |
| Import Script Support | $\checkmark$ | $\checkmark$ |
| Excel Import | $\checkmark$ | $\checkmark$ |
| Worklist Import | $\checkmark$ | $\checkmark$ |
| Data Visualization (3D View/Heatmap/Kinetic Overlay/Spectral Plot) | $\checkmark$ | $\checkmark$ |
| Versioned Analysis | $\checkmark$ | $\checkmark$ |
| Export to XLSX/DOCX/PDF | $\checkmark$ | $\checkmark$ |
| Edit Protocols | Limited | $\checkmark$ |
| Report Customization | Limited | $\checkmark$ |
| Custom Export (e.g., for LIS/LIMS) | $\square$ | $\checkmark$ |
| Multiple Plate Support | ص | $\checkmark$ |
| Create New Protocols (New Protocol Wizard) | $\square$ | $\checkmark$ |
| Matrix-Transform Data Analysis | $\square$ | $\checkmark$ |
| Custom Validation Rules | $\square$ | $\checkmark$ |
| Custom Evaluation Expressions | = | $\checkmark$ |
| Best Fit | $\square$ | $\checkmark$ |
| Folder Poll | $\square$ | $\checkmark$ |
| PLA | $\square$ | $\checkmark$ |

## 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:

Memory:
Available disk space:
Operating systems:
Other software:
Display:

Intel/AMD 2 GHz or faster processor (32-
bit or 64-bit)
2GB RAM
300MB
Windows 10, Windows 8.x, Windows 7,
Windows Vista, Windows XP SP3
Microsoft .NET 4.0.3 or later
$1024 \times 768$ or higher resolution

## Installation Process

The latest version of MyAssays Desktop can be downloaded here.

## Upon downloading the installation package:

1. Double-click on 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 and then check I accept the terms of the license agreement box and press Next to continue.
If you do not agree with terms of the license agreement, click Cancel to exit the setup wizard.
3. If you are content with the default path, press Next to continue. To pick another destination folder, press Change... and set preferable root.
4. Check the choices you made and press Install. The process will take a few moments.
5. Click Finish to complete the installation. Check 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.
[^0]
## Launching

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

## On Windows 10:

Choose Start, then scroll down to and click on 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 on the desktop icon and select Pin to Start or Pin to Taskbar.

## Product Licensing

To use MyAssays Desktop, you must provide and activate a valid license.
You can obtain a trial, temporary, or permanent license from MyAssays Ltd.
A serial code represents your license or licenses (for multi-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.

An administrator account is required to activate (or deactivate) a license.
If you have a serial code, select the I have a serial code to activate button and press 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 press Next.

Your email address is required for administrating 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. Check the Use internet connection for activation checkbox and press Continue to proceed.
2. Fill in your personal details and press 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. Press 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. Uncheck Use internet connection for activation checkbox and press 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. Press Close to exit License Activation Wizard and start the application.

## 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. Select the File tab and select the Information option:

The availability of licensed features is marked with the following icons:
d for active features.
$\mathbb{X}$ 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 on 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, Iaunch the Deactivation Wizard as follows:

1. Launch MyAssays Desktop Explorer.
2. Set File tab and select Information section.
3. Click on the Deactivate License button.

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 checkbox checked and press Continue to proceed with deactivation.
2. Check the checkbox to confirm deactivation and press 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. Press 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. Uncheck the Use internet connection for deactivation checkbox and press

Continue to proceed with deactivation.
2. Check the checkbox to confirm deactivation and press 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 press 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

If you have been provided with a new serial code to replace an existing license (perhaps as the result of a purchased upgrade or support extension), then it will be necessary to activate your new license to replace the existing one.

1. Launch MyAssays Desktop Explorer.
2. Select the File tab and select the Information option.
3. Select Activate New License.
4. Press 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. Select the File tab and select the Information option.
3. Select 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 short-cut 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-hand 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 preinstalled 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 the launched assay name and any description. It might also include a link to online content (such as kit manufacturer's product insert).

Along the left-hand 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 meta-data). 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.

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 press the Calculate button 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.

Pressing the Calculate button:

- performs the calculations
- generates the report
- and 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 select 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 meta-data 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

Press 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 pressed 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. Press the 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).

(1)
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

Online videos are provided to help you get started and walk through features in detail:

## Getting Started

- http://www.myassays.com/myassays-desktop-fundamentals.video
- http://www.myassays.com/download-and-use-protocols-from-myassays.video


## Importing Data

- http://www.myassays.com/import-measurement-data-from-excel-files-with-myassaysdesktop.video
- http://www.myassays.com/import-measurement-data-from-multiple-excel-files-with-myassays-desktop.video


## ELISA

- http://www.myassays.com/elisa-data-analysis-with-myassays-desktop.video
- http://www.myassays.com/multiple-plate-elisa-with-myassays-desktop.video


## Excluding Outliers (Flagging)

- https://www.myassays.com/myassays-desktop-flagging-outliers.video


## Worklists

- https://www.myassays.com/myassays-desktop-sample-ids-and-worklists.video


## Export

- https://www.myassays.com/myassays-desktop-custom-export-for-lims.video


## Multiplex

- https://www.myassays.com/myassays-desktop-introducing-the-multiplex-protocol.video
- https://www.myassays.com/myassays-desktop-automatic-launching-of-multiplexanalysis.video


## Folder Poll

- https://www.myassays.com/folder-poll-with-myassays-desktop.video


## Inter-Assay Quality Control

- https://www.myassays.com/myassays-desktop-inter-assay-quality-control.video


## 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.

An assay will contain different types of samples such as:

- Unknown - Samples to quantify or qualify
- Standard - Samples with a known quantity used for preparing a calibration or standard curve
- Control - Samples used for control purposes such as inter-assay or inter-assay quality control
- Blank - A sample without any expected response, used to remove background noise

Other sample types are possible; you can create and name your own sample types as you require.

With MyAssays Desktop, we use a color to indicate sample type:
Standard $\bigcirc$ Blank $\bigcirc$ Control Unknown
Typically assay samples will be replicated. To identify replication, each sample is given a number. Thus a sample type and number uniquely identifies a sample. All positions on a layout with the same type and number are replicates of the same sample.
For example, 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.). l.e.:

|  | 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 |

The use of a sample layout introduces a convenient layer of abstraction over the measurement data. For example, being able to refer to, for example, Control 1 to reference all Control1 replicates is much simpler than having to remember or decode the measurement data. Also, MyAssays Desktop calculations are based around the sample layout, therefore you can easily change the sample layout (perhaps because you need to use a different positioning of your samples on a different run of your assay) without needing to make any changes to your calculation settings. If you have ever had to change an Excel spreadsheet because of a change in layout, then you will appreciate that this abstraction is a valuable time saver.

## 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

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.

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 textbox 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 on 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 on Show Quick Access Toolbar Below/Above the Ribbon (depending on its current location), Minimize the Ribbon, and change the Quick Access Toolbars view by adding or excluding some options in More Commands pop-up menu.

## Folder Side Bar

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 subdirectories 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 thatyou 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.

## Folder Side Bar 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 ( ${ }^{*}$. $T X T$, *.CSV, <br>  |
| Results | Assay results files with .assay-results extension |
| Layouts | Layout files with .assay-samplelayout extension |
| Reports | Report files with supported report extension (*.DOC, *PPT, ${ }^{*} . X L S$, *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 on 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 on 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 on 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 in 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 | A summary of assay protocols, including the name, the instrument <br> settings, the position used and layout, and any configured transformations |
| Protocols | Measurements |
| Pre-canned and custom raw-data files |  |
| Results | Two assets: <br> • Overview with the assay protocol summary <br> - Latest Report with the latest report of the results |
| $\underline{\text { Layouts }}$ | A microplate control showing each plate layout in the layout |

## 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 Side Bar 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 MyAssays.com

## How to: Find an Assay Protocol from MyAssays.com Knowledge Base

First, in MADE, enter an assay title or keyword (i.e., Cortisol, Human, ELISA):

- In the MADE Menu Bar, Search MyAssays.com panel

OR

- Use a keyboard shortcut (CTRL + E), which automatically redirects you to a search textbox

Next, press the Search button or Enter on keyboard.
When you have performed a search, the Search Results tab is displayed on Folder Side Bar.

## Using the Search Results

Upon performing a search, you will see the list of assay protocols that contain a keyword you have entered.

To specify the search results and ensure finding the protocol you're looking for, each protocol contains a detailed summary. To see further information on a particular position, single-click on its title. Some of the assays contain Kit Booklet from the manufacturer. To read it, click on View Assay PDF link under the assay summary.
For every assay protocol in the list, the following actions are available on the Preview pane:

- Download and Launch - Persists a single assay protocol to your Protocols tab and automatically launches it in MAA.

You can also double-click on a file from the list to download it to your PC and launch it in MAA automatically.

- Download - Stores a single or multiple assay protocols to your Protocols tab.

If you select multiple items from the list, only this option is available and
(1) displayed. To select multiple protocols from the search results, use the (Ctrl+Shift+Arrow Keys) keyboard shortcut and Ctrl + A to select all search results.

- Launch Assay Protocol - Appears if you have downloaded a particular assay protocol previously. The above actions are then not displayed. To enable re-downloading, click on 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.


## No Results Found

If the assay you are looking for is not yet in the MyAssays database, an Information dialog box appears.
Click Yes to proceed to a Request Protocol form.

## Search + Download from MyAssays.com

Download and use preconfigured assay protocols from the MyAssays.com knowledge base on your PC.
Submit a Search and explore search results options of the constantly evolving protocols database.

## Protocols Tab

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

(1)
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:

## How to: Create New Assay Protocol

In the MADE Welcome Screen, click on New Protocol....

## OR

In the Folder Side Bar, select the Protocols tab and click on the New button on the MADE Ribbon.

When this option is selected, a New Protocol Wizard will be displayed.

## How to: Launch Assay Protocol File

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

- double-click on its title
- right-click on the title and choose Run with MyAssays Desktop Analysis
- click on the Launch Assay Protocol button 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

Launch an assay protocol with command-line options for more control over the analysis. This feature will open the Launcher tool with the selected protocol.

If you press the Launch Assay Protocol with Options button, the dialog window with a visual representation of supported command-line options will appear.

## How to: Launch Assay Protocol with Command Line Options

1. Launch MADE.
2. Select the File tab of MADE Ribbon.
3. Select the View screen.
4. Check the Show Launch Assay Protocol with Options button checkbox.

(1)
The Show Launch Assay Protocol with Options button state (checked/unchecked) persists between sessions.

If it is checked, 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:

- Click on the Request an Assay protocol on a Support subpane of the Welcome Screen.


## OR

- On the MADE Ribbon, select the Support tab and press the Request an Assay protocol button.

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, press 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. Check the View Measurements checkbox.
(1) The View Measurements state (checked/unchecked) persists between sessions.

If it is checked, an additional tab is displayed on the Folder Side Bar.
The measurements tab contains a default Examples folder with a $12 \times 8$ 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-fileformats.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.).

(1)
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
Navigate to the Results tab, select a single assay result file to open, and do one of the following:

- double-click on its title
- check the Open icon on the MADE Ribbons File group
- check the Open icon in Latest Report inset of the Preview pane

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.

(1)
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 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 on a 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. Rightclick on 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, press the Add to Quick Access Toolbar command. 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 on 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 on Customize Quick Access Toolbar on the context menu.
- Click on the Advanced option on the Quick Access Toolbar and click on 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, press the OK button to save changes or Cancel to undo them.

To return the toolbar to its default configuration, click on 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 on any spot on the Ribbon and check Minimize Ribbon in the drop-down list. To undo minimizing, repeat these actions and uncheck the command.

## Layout Editor

## Layout Editor

## Overview

Most assays allow you to specify your own layout for processing and distinguishing various types of measurement data.

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. Create new or modify existing layouts after analysis and easily recalculate results to correct for preparation errors.

## Using the Layout Editor

The Layout Editor is displayed when you press the Create button 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 setup 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 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. 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

## 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, press the Fill button. 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
- Snake 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, press the Save + Close button. This will save the new layout to your Layouts tab 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 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).

## Multiplex Options

For multiplex assays, only single layouts can be applied.

## Layout Configuration

The 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)


## 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 Group Numbering

When defining the layout (in the Layout Editor), the numbering for each sample group on each and 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.

When the analysis is performed, the software will apply the group numbers across plates contiguously. 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 Unknowns110 and plate 2 would include Unknowns11-20.

## Analysis

## Versioned Analysis

## Overview

When you launch an assay protocol and press the Calculate button, 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.

(1)
Each time the Calculate button is pressed, 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. Hover to a Versions Group on the Home tab of the MAA Ribbon.
3. Select the Version you need from Current version drop-down list.

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.

Pressing 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 press 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.

(1)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 pressed again, the Version $\{\mathbf{n}\}$ (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 assayresults 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 checkbox 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.

(1)
The Save Changes to Protocol state (checked/unchecked) 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
- File | Save BSA

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 checkbox is checked.

## - Save Results As

With this command you can save the assay results with all changes to a new .assay-results file. When you press the Save Results As button, a dialog box appears. You can provide a new file name 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 press the Save Protocol As button, a dialog box appears. You can provide a new file name 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 the Results Naming button is pressed, 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 textboxes 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 textbox (manually or from clipboard).
- Click the Browse... button to provide the full path to the folder in Browse for Folder tree view. Press 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. Press 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. Press 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.

(1)
If the Test settings when OK is clicked checkbox is enabled, MAA checks the accessibility of specified target path and verifies if the file can be created.

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

## New Protocol Wizard

## How to: Launch New Protocol Wizard

1. Launch the MADE and do one of the following:
2. Select the New Protocol... option on MADE Welcome Screen.
3. Select the Protocols tab and click on the New button of File group.

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 buttons to configure the following assay parameters:

- Measurement data specifics
- Layout and sample types settings
- Administrative properties (meta data)
- A name and (optionally) a description for the protocol

At any step, you can click on 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 textbox 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:

- Press the Analysis Launcher button on the Tools tab in the Utilities group of the MADE Ribbon.
- Enable the Launch Assay Protocol with Options feature and press the Launch Assay Protocol with Options button.
- 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.

## 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

In the MADE Ribbon, select Backstage File Screen| Data. Press the Select
Folder Root button 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

## Visualizing Data

## Heatmap Plate View

The Heatmap View displays a plate layout colored 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 tab. Check
2. Check the Heatmap View option in the lower left corner of the right pane.

Heatmap view is relevant for endpoint data only.

## Structure

Heatmap View comprises:

- Plate preview with the color of each position based on its numerical value converted to a color 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



## Heatmap View Settings

## Minimum and Maximum Controls

These settings allow you to set the color scheme range displayed on the heatmap plate preview. Each position on the layout is colored according to its numerical value and the color scale (using the color range $\mathrm{min} / \mathrm{max}$ values). Values outside the range are rounded to the nearest min or max color.

## How to: Change the Minimum Value

1. Hover and click on the minimum value on the left side of the color bar to edit the heatmap minimum value.
2. Type in a minimum value for the heatmap (e.g., 0.05).
3. Click on the check icon to save your changes or on 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 and click on the maximum value (right side of the color bar) to edit the max value.
2. Type in a maximum value for the heatmap (e.g., 2.00).
3. Click on the check icon to save your changes or on the cross icon to cancel them.

For multiple plate multiplex assays, consider all used positions before you type in min and max 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 on the Log10 scale button (right one). The heatmap is refreshed to display a Log10 color scale.
- Linear scale - Click on the Linear scale button (left one). The heatmap is refreshed to display a linear color 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 $\mathrm{min} / \mathrm{max}$, then the heatmap scale is updated accordingly.

## How to: Access the Auto Scale

1. With the Heatmap View turned on, click on the Auto Scale button (on the right side of the heatmap maximum control).
2. Click on the Auto Scale button.

You can toggle the Auto Scale setting on and off by clicking on 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 Measurementsor Microplate tab.
2. Check the Heatmap View option in the lower left corner of right pane.
3. Click the 3D button.

You can toggle between the 2D and 3D view using the corresponding buttons.

## 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 Standard $\mathbf{1}$ comprises of 3 replicates measured at position $\mathbf{A 1}, \mathbf{A} \mathbf{2}$, and $\mathbf{A 3}$, if position A1 is flagged, Standard1 would refer to only the not-flagged values (i.e., the average of the data at positions $\mathbf{A} \mathbf{2}$ and $\mathbf{A 3}$ ).

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 $\mathbf{A 1}$ 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 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.
(1.) 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, press the Properties button to open it.
3. Press the Add button.
4. Select the Standard Curve Fit transform.
5. Press 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. Press the Calculate button.
9. 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.
10. Select the sample type on the legend to view how the points are spread on the curve.
11. Position the mouse pointer over the point to flag and left-click.
12. Press the Calculate button to perform the calculations with the new settings and to see the results.
(1) 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.

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).

| Flags |  |  |  |  | $\times$ |
| :---: | :--- | :--- | :--- | :--- | :--- |
| Status | Type | Position | Point | Plate | Matrix |
| $\square$ | Point | A5 | 7 | Plate 1 | Raw |
| $\square$ | Point | A5 | 6 | Plate 1 | Raw |
| $\square$ | Point | A5 | 5 | Plate 1 | Raw |
| $\square$ | Position | A1 | - | Plate 1 | Raw |
| $\square$ | Position | A2 | - | Plate 1 | Raw |
| $\square$ | Position | A3 | - | Plate 1 | Raw |

Toggle 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 $\mathbf{4 . 2 3}$ 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 $\mathbf{A} 4$ 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 |
| :--- | :--- | :--- | :--- |
| OUnknown1 | 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 $\mathbf{1 . 2 3}$ 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.

To label sample results that satisfy specified conditions without flagging them, please refer to the Sample Labels topic.

## 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).

## 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. Select the XML tab in the Assay Properties panel (If the XML tab is not immediately visible, press the << Show All Properties button 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, press 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 transform is the only transform that provides custom flag settings by calculation. For more details, see Standard Curve Fit Custom Flag Labels.

## 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.

## Matrices

Generally, all data in MyAssays is stored in matrices. Each matrix can contain one or more replicates, and for each matrix certain relevant transforms can be applied. In the Matrices Tab, the settings for each of these matrices can be configured.

## How to: View Matrices Tab

1. Launch an assay protocol or open a results file.
2. If you cannot see the Assay Properties panel, press the Properties button to open it.
3. Select the Matrices tab (If the Matrices tab is not immediately visible, press the << Show All Properties button to expand).

## Matrix Selection Pane

This pane includes available matrices in a tree list. This list contains two basic branches: Raw and Calculated.

## Raw

This is input data that is stored in the Measurements Tab. The quantity and type of Raw matrices depends on the assay type and configuration.

Click here to learn more about measurement data.

## Calculated

This consists of all new matrices that are created and added to output by transforms.

## Matrix Configuration Pane

Each input and each output matrix of a newly added transform is automatically included in both Sample and Matrix Tables. With the following settings, you can configure whether and how they are displayed.

## General

| Name | A title to be used for a matrix in the headers of the Sample Table and Matrix <br> Table. 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 <br> of Precision depends on the Type setting. |
| :--- | :--- |


| Type | Specifies how a numerical value is formatted with regard to precision and <br> rounding options: <br> - Significant Figures - The value is reported to the specified number of <br> significant figures. This accepts Precision values in range 1 through 14. <br> - Decimal Places - The number of digits to display to the right of the <br> decimal point. This accepts Precision values in range 0 through 14. |
| :--- | :--- |

## Report Contents

| Include in <br> Matrix <br> Tables | Defines whether the associated matrix should be included in the Matrix Tables |
| :--- | :--- |
| Include in <br> Sample <br> Tables | Defines whether associated matrix should be included in the Sample Tables |
| Matrix <br> Table Ids | Defines in which Matrix Table(s) the associated matrix should be included. |
| Sample <br> Table Ids | Defines in which Sample Table(s) the associated matrix should be included. |
| Sample | Determines how replicates of each sample group are included in the Sample <br> table: <br> - Average - The average value of all replicates is displayed. This applies to <br> Endpoint data only. <br> licates |
| - List - All replicate values are included in the table. <br> - First - Only the first value is displayed. This simplifies the view of <br> transforms that result in the same values for all replicates of each sample <br> group (e.g., Average, XY Replicates Average). |  |

## Configuration of Endpoint Matrices

For endpoint data you can additionally configure the following settings to apply on the report.

## Sample Labels

If this is specified, the Condition is evaluated for each position of the associated matrix and Label is displayed in place of the value for the position. For further details on this feature see Sample Labels topic.

## Value Bars

Within this category you can configure whether and how to fill replicate values with color for any Raw or Calculated endpoint matrix.

The value bars are created using the minimum and maximum replicate values of the matrix. These are treated as $0 \%$ and $100 \%$, respectively, and filled in accordingly.

| Display <br> Value Bars | Defines whether this feature is used in the Sample Tables. |
| :--- | :--- |
| Fill | Defines how to fill in the value bar. Select one of the following types: <br> Solid - To fill value bars self-colored with Fill Colour. <br> Gradient - To fill value bars with the gradation from Fill Color in the left to <br> white on the right. |
| Fill Colour | Click on the drop-down to open a color picker. |
| Border | It defines how to fill in the value bar's border. Select one of the following <br> types: <br> Solid - To fill value bars self-colored with Fill Colour. <br> None - To not display the Border. |

## Sample Labels

The Sample Labels feature can be used add your own text in-place or alongside measurement or computed numerical values. Also, your data or labels can be highlighted to visually enhance the report output; this is useful to draw the reader's eye to specific areas of interest or to color code your report content.

Samples are reported with label and/or colour in accordance with the rules that you specify.
You can define as many rules as you need. If a data point satisfies multiple conditions, then all corresponding labels are displayed in the report.

The rules for sample labels are applied to the corresponding data included in the report. In the Matrix Table report element, the label or coloring would apply to each position. In the Sample Table report element, this might be each individual replicate value or each sample's average; it depends on how the data is configured in the report output.

For example, here is a Matrix Table output highlighting all sample measurements > 1.5 in yellow.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | 9 | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 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 |

With the Sample Table report element, each matrix can be configured 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.) In either case the sample label will be applied to the selected data.

For 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 average 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 |  |

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.

Applying label, unlike flagging, does not exclude data from calculations, nor does it

©change the actual value used in subsequent calculations. It simply replaces their reported values with a specified Label and applies any colouring.

## How to: Apply a Sample Label

1. Launch an assay protocol or open a results file.
2. If you cannot see the Assay Properties panel, press the Properties button to open it.
3. Select the Matrices tab (If the Matrices tab is not immediately visible, press the << Show All Properties button to expand).
4. Select one of the numbered matrices from under either the Raw or Calculated branch, which contains the data to label.
5. Click on the drop-down Label property of the Matrix Configuration pane to view Matrix Sample Label Editor.
6. Enter the condition (in terms of $x$ ) along with the label and any highlight or text coloring to apply.
7. Press Add to add further rules. Click outside the Editor when you have finished.
8. Press the Calculate button to perform calculations with the new settings and to see the results.

In the Matrix Sample Label Editor, you can add and remove any number of rules and move them up or down with the corresponding arrow buttons.

| Label | The rules are specified with the following editable text box properties: <br> - Condition - A Boolean condition to evaluate (typically a conditional <br> expression) in terms of $\mathbf{x}$. The $\mathbf{x}$ value specified in the expression refers to <br> the sample. <br> - Label - The label to be displayed in the Sample Table and Matrix Table, if <br> the Condition is satisfied. Use $\{\mathbf{x}\}$ <br> in the refer to the data value that was used <br> - Highlight - This sets the background color for the cell when Condition is <br> satisfied. Where there are multiple Conditions satisfied, the color of the <br> first satisfied Condition is applied. |
| :---: | :---: |
| - Text - This sets the text color for the cell when Condition is satisfied. |  |
| Where there are multiple Conditions satisfied, the color of the first |  |
| satisfied Condition is applied. |  |

If the Condition is satisfied, the replicate will be reported with the corresponding Label in place of its value.

## Reporting Data with Labels

The results with labels appear in associated matrix's Sample Table and Matrix Table.
For example,

| Sample | Positions | Raw | Concentration |
| :--- | :--- | :--- | :--- |
| OUnknown1 | A3 | 1.694 | $>1$ |
|  | A4 | 1.766 | $>1$ |

Here the Condition $\mathbf{x}>\mathbf{1}$ and Label $\mathbf{> 1}$ are specified for Concentration matrix. In this case the calculation of the concentration for positions $\mathbf{A 3}$ and $\mathbf{A} 4$ is reported as $\mathbf{> 1}$.

Where label has been applied on the data and there is a $\{\mathbf{x}\}$ reference associated with the Label, the numeric value appears in the Label, i.e.:

| Sample | Positions | Raw | Concentration |
| :--- | :--- | :--- | :--- |
| OUnknown1 | A3 | 1.694 | $2.153>1$ |
|  | A4 | 1.766 | $3.857>1$ |

## Sample Labels Examples

| Condition | Label Applied If |
| :--- | :--- |
| $\mathbf{x < 1}$ | The value is greater than 1. |
| and $(\mathbf{x}>\mathbf{0}$, <br> $\mathbf{x}<\mathbf{1})$ | The value is in the 0-1 range. |
| $\mathbf{x}<$ Control1 | The value is greater than mean of Control1 sample group. |
| $\mathbf{x >}$ TOV1.d | The value is greater than the d coefficient of the 4PL curve-fit (assuming that <br> the 1st transform is a Standard Curve Fit transform using the 4PL curve-fit). <br> See Transform Output Variables for more details of how to refer to such <br> results. |

## Validation

MyAssays Desktop's Validation features can automatically check that measurements and results are within expected ranges. Any configured validation tests are performed as part of each assay run with the results (pass or fail) being clearly presented as part of the output report.

For example, a validation can test that the \%CV of the replicates of all sample groups is less than 15.

## Validation Definition

A validation is defined using a Boolean validation condition. If the condition evaluates to true, then the validation rule is considered to be satisfied and the result for the validation is Pass. If the condition evaluates to false, the validation test result is Fail.

The validation condition is specified using an expression along with a matrix reference and type. For example, the validation condition expression:

## x < 15

When associated with the \%CV matrix and evaluated on all groups will check that the \%CV of all sample groups is $<15$.

Validation rules are arranged by validations tables. You can add as many validations rules as you need to each validation table. You can create as many validations tables as you need. It is useful to group related validations into validations table accordingly.

Each validation table is a separate report element so can be configured separately. For example, you might want each validation table to appear on a different sheet in the report.

## Working with Validations

The following sections explain how to add, define, and review validation rules. Also, example validation expressions are provided:

## How to: Add Validation to an Assay

1. Launch an assay protocol or open a results file.
2. If you cannot see the Assay Properties panel, press the Properties button to open it.
3. Select the Validation tab (If the Validation tab is not immediately visible, press the << Show All Properties button to expand.)
4. Press the Add button on Tables pane.
5. Review and edit the validation's properties as required.

## Validation Configuration

The Validation tab consists of three panes:

- Tables - For managing the validation tables.
- Conditions - For managing the validation conditions.
- Condition Configuration - For specifying a validation condition.


## Tables

The Tables pane defines the validation tables that are available for inclusion in the report. Each validation table is given a unique identifier (e.g., ValidationsTable1).

Use the Add and Remove buttons to define the number of tables required.
You may prefer to include all conditions in one single table or arrange conditions between multiple tables.

The ordering, settings, and inclusion of each Validation Table is controlled via the
Report contents.

## Conditions

The Conditions pane defines each validation condition for the selected validations table.
Use the Add or Remove buttons to add conditions as required. Use the Up and Down buttons to set the order in which the conditions will appear in the table.

For each condition, a description can be specified under the Description column. Use this to provide a clear textual description; this will be used in the report to convey what has been validated.

For each condition, select which Matrix the condition applies to.

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. Also, it is possible to validate non-matrix data (such as transform output variables).

(1)
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.

## Conditions Configuration

The Conditions Configuration pane is used to specify the selected validation's condition.
The Expression setting is used to define the validation expression Boolean condition. This will typically be an expression with a logical operator and perhaps a conditional function.
The interpretation of the expression depends on the Type setting:

- Position - The expression is evaluated for every position on the matrix of every container.
- Group - The expression is evaluated for every sample group on the matrix of every container. (A sample group refers to the average of the replicates that belong to the group that are not flagged).
- Single - the expression is evaluated once (useful for checking specific sample groups).

Single type expressions are the simplest; they define a single expression that is evaluated once on the specified matrix of each container.

For example, Standard1 < Standard2 is an example of a Single type expression that validates that the value of Standard1 is less than Standard2 on the specified matrix. (For multiple plate assays, this condition will be evaluated on every plate.)

For Position or Group expressions, the expression will include an $\mathbf{x}$ reference, and in these cases the $x$ variable refers to each position or each group. For example, if you wanted to check that the value at every measured position in a matrix is greater than 0.5 , then use the Position setting with the expression: $\mathbf{x} \boldsymbol{>} \mathbf{0 . 5}$. In this case every data point (on the selected matrix) is validated.

Similarly, if you wanted to check that the average value of each group in a matrix is less than 3, use the Group setting with the expression $\mathbf{x}<\mathbf{3}$. In this case the average of every sample group (on the selected matrix) is validated.

The Types setting is used to specify which sample types a Position or Group expression will be evaluated 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 to select which types to validate.

## Validating 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 Single type and referring to the data to validate within the expression. This will typically be using a Transform Output Variable (TOV). The TOVs that are available will depend on your configured transforms.

For example, the expression TOV1.R2 $\boldsymbol{>} \mathbf{0 . 9}$ will check 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).

To apply any new or modified settings, press the Calculate button and inspect the report to see the results. Each validation test verifies the result in terms of the specified Boolean condition.

For Position and Group validations, the result is only Pass if all evaluations evaluate to true.

The results will appear in the associated validation table in the report and will be marked as Pass, Fail, or Inconclusive accordingly:

## Pass

If the validation condition is evaluated as true (the numerical result not equal 0 ).
Fail

If the validation condition is evaluated as false (the numerical result equals 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).

All validations are evaluated (irrespective of whether they are included in the report). You may configure how and if the Validation Tables are reported. In any case, the results of each validation test are listed in the Calculation log.

## Examples

Here are examples of validation rules along with descriptions of their behavior. They apply the validation on the selected data matrix.

| Type | Condition | Validates |
| :---: | :---: | :---: |
| Position | x < 2.5 | All positions (that are not flagged) have a value less than 2.5. |
| Position | and ( $\mathrm{x}>0, \mathrm{x}<2.5$ ) | All positions (that are not flagged) have a value less than 2.5. |
| Group | x < 2.5 | The average of the replicates (that are not flagged) of all sample groups is less than 2.5. |
| Position | and ( $\mathrm{x}>0, \mathrm{x}<2.5$ ) | The average of the replicates (that are not flagged) of all sample groups is greater than 0 and less than 2.5. |
| Single | Control1 < 1.5 | The average of Control 1 replicates (that are not flagged) is less than 1.5. |
| Single | sd(Control1) < 10 | The standard deviation of the Control 1 replicates (that are not flagged) is less than 10. |
| Single | pcv(Control 1 ) <15 | The \%CV of the Control 1 replicates (that are not flagged) is less than 15. |
| Single | median(Control 1 ) $>0.75$ | The median of the Control 1 replicates (that are not flagged) is greater than 1.5 . |
| Single | TOV1.R2 > 0.9 | The $R^{2}$ value of the curve fit (as used in the first |


| Type | Condition | Validates |
| :--- | :--- | :--- |
|  | transform) is greater than 0.9. (The $R^{2}$ value is <br> referenced using a Transform Output Variable). |  |

## Evaluation

MyAssays Desktop's Evaluation feature can be used to calculate and present specific quantities of interest in the report. For example, the limits of detection of an assay could be computed and reported using an evaluation.

Evaluations are expression-based calculations arranged as Evaluation Tables for inclusion in the report. Any value that can be referenced or computed can be included in an Evaluation table.

Unlike the Sample Table or Matrix Table report elements (which display the results of a calculation performed on each sample), an Evaluation Table reports calculations that are not computed for every sample.

If you want to perform a calculation with a result for every sample, instead of using

(1)an evaluation, use a transform with the results for each sample displayed in the Sample Table or Matrix Table.

## Evaluation Definition

A single evaluation is defined using an expression and can be given a description to accompany its result.

Evaluations are arranged by Evaluation Tables. You can add as many evaluations as you need to each Evaluation Table. You can create as many tables as you need. It is useful to group related evaluations into Evaluation Tables accordingly.

## Working with Evaluations

The following sections explain how to add, define, and review evaluations. Also, example evaluations expressions are provided.

## How to: Add an Evaluation to an Assay

1. Launch an assay protocol or open a results file.
2. If you cannot see the Assay Properties panel, press the Properties button to open it.
3. Select the Evaluation tab (If the Evaluation tab is not immediately visible, press the << Show All Properties button to expand).
4. Press the Add button on Tables pane.
5. Review and edit the evaluation's properties as required.

## Evaluation Configuration

The Evaluation tab consists of three panes:

- Tables - For managing the evaluation tables
- Evaluations - For managing the evaluations
- Expression Configuration - For specifying the evaluation expression


## Tables

The Tables pane defines the Evaluation Tables that are available for inclusion in the report. Each table is given a unique identifier (e.g., EvaluationsTable1).

Use the Add and Remove buttons to define the number of tables required.

You may prefer to include all evaluations in a single table or arrange evaluations between multiple tables.

The ordering, settings, and inclusion of each Evaluation Table is controlled via the Report contents.

## Evaluations

The Evaluations pane defines each evaluation for the selected evaluations table.
Use the Add or Remove buttons to add evaluations as required. Use the Up and Down buttons to set the order in which the evaluations will appear in the table.

For each evaluation, a description can be specified under the Description column. Use this to provide a clear textual description; this will be used in the report to convey what has been evaluated.

For each condition, select which Matrix the condition applies to. 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 validate non-matrix data (such as transform output variables).

If there are no available matrices, then the (NA) label appears. In this case evaluations can still be created that do not refer to endpoint matrix data.

Evaluations are not applicable to $X Y$ data matrices. To perform an evaluation on XY data, first use an XY reduction transform and evaluate the endpoint result.

## Expression Configuration

The Expression Configuration pane is used to specify the selected evaluation's expression.
The Expression setting is used to define the expression to evaluate. This might reference a specific sample group or position on the selected matrix. It might also perform a calculation or function. Refer to the expression section for a complete description of available expression functionality.

The Numerical Formatting options are used to specify how the computed value is presented:

## Numerical Formatting

| Precision | The number of digits to be displayed for a numerical value. The interpretation <br> of Precision depends on the Type setting. |
| :--- | :--- |
| Type | Specifies how a numerical value is formatted with regard to precision and <br> rounding options: |
| - Significant Figures - The value is reported to the specified number of |  |
| significant figures. This accepts Precision values in range 1 through 14. |  |
| - Decimal Places - The number of digits to display to the right of the |  |
| decimal point. This accepts Precision values in range 0 through 14. |  |

## Evaluation Results

Evaluations are computed when the data analysis is performed (after all transform calculations). To apply any new or modified settings, press the Calculate button and inspect the report to see the results.

Each evaluated expression results in a single numeric value. If there is an error in evaluating the expression, then the error message is reported (in red) as the result.

All evaluations are performed (irrespective of whether they are included in the report). You may configure how and if the Evaluation Tables are reported. In any case, the results of each evaluation test are listed in the Calculation log.

## Examples

Here are examples of evaluations along with descriptions of their behavior. They apply the evaluation on the selected data matrix.

| Evaluates | Computes |
| :--- | :--- |
| Control1 | The average of all Control1 replicates (that are not flagged) |
| Control1/Control2 | The ratio of Control1 and Control2 |
| sd(Control1) | The standard deviation of the Control1 replicates (that are not <br> flagged) |
| pcv(Control1) | The \%CV of the Control1 replicates (that are not flagged) |
| Unknown | The average of all replicates of all Unknown samples (that are <br> not flagged) |
| median <br> (Unknown) | The median of all Unknown sample measurement (that are not <br> flagged) |
| TOV1.R2 | The R |
| (referenced using a Transform Output Variable) |  |,

## Report Content

## Overview

The primary output of the data analysis process is the report. MyAssays Desktop provides comprehensive functionality to configure the report's:

- content
- presentation
- export

This section describes how to configure the content that is included in the report.

> Within the MyAssays Desktop Application, the report can be displayed as Sheet View or Page View; these settings are available in the 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).

## Report Content Definition

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 colored value bars.
- Evaluation - Any configured evaluation settings will result in one or more evaluation tables, each listing the results of the computed evaluations.
- Validation - Any configured validation settings will result in one or more validation 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 Standard Curve Fit transform is configured, then the calculated concentrations will be available for
inclusion in a Sample Table and/or Matrix Table, along with details of the fit (including standards chart and equations), each of which can be further configured.

The configuration and ordering of each report element is defined in the Report tab.

## How to: View Report Tab

1. Launch an assay protocol or open a results file.
2. If you cannot see the Assay Properties panel, press the Properties button to open it.
3. Select the Report tab (If the Report tab is not immediately visible, press the << Show All Properties button to expand).
4. Review and edit the report's elements as required.

## Report Element Configuration

The Report tab consists of two panes:

- Reports - This pane manages the report elements and their ordering.
- Report Configuration - This displays the available settings for the selected report element.


## Reports Pane

The Reports pane lists the report elements that will be included in the report. Their ordering reflects the order in which they will be added to the report.

Use the Add Element button 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.

Use the Remove button 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 elements:

## General

| Id | Each report element is automatically given a unique identifier (Id). This <br> identifier is used to identify the report element when configuring custom |
| :--- | :--- |

\(\left.$$
\begin{array}{|l|l|}\hline & \begin{array}{l}\text { report templates (It is also used for advanced settings such as custom export } \\
\text { and XML configuration). }\end{array} \\
\hline \text { Include } & \begin{array}{l}\text { This checkbox can be used to exclude the report element (without deleting the } \\
\text { settings). }\end{array}
$$ <br>

\hline The identifier.\end{array}\right\}\)| 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\} and |
| \{AnalyteName\}) to automatically refer to the data that it is associated with. |
| If a title is not specified, then the element is displayed without any title. |

## Sheet

| Sheet | This setting defines the name of a sheet to insert the contents into. This is only <br> applicable to sheet-based content such as Excel output or data in the Sheet <br> View. <br> Name <br> Each report element can be included on its own separate sheet or elements <br> can be added together on the same sheet. Where a common sheet name is <br> used across report elements, the elements are added in the order as defined <br> in the Reports pane. <br> This property can refer to report macros (such as \{PlateNum\} and <br> \{AnalyteName\}) to automatically group associated content into a sheet of <br> the same name. <br> Note, if Sheet Name is defined for one report element, then the report <br> 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 comprises 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, it is recommended to use the Sheet Name setting; this can be used 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 sheet tab named on by the plate number (i.e., Plate 1, Plate 2, Plate 3, etc.).

## 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 <br> number; for multiplex, this is the analyte number) |
| \{PlateName\} | The plate name (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 <br> analyte name |

These macros can be used in conjunction with other text (e.g., Plate \{PlateNum\} would be expanded to Plate $\mathbf{1}$ 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 Reports 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 be automatically removed too.

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. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the required report element from the Add Element drop-down list in the Reports pane.
3. Review and edit the element's settings as required.
4. Press the Calculate button to perform calculations with the new settings.

The following table describes each report element in more detail along with any applicable settings.

| Report <br> Element | Description | Settings |
| :--- | :--- | :--- |
| Evaluations <br> Table | The details and results of any configured <br> evaluations arranged in a table. | Include Description - <br> Include the description <br> column. <br> Include Expression - Include <br> the expression column. <br> Include Header - Include the |
| $\underline{\text { Histogram }}$ | The Histogram represents the data by <br> displaying the average of each sample in | Matrix - The matrix of data to <br> plot. |


| Report <br> Element | Description <br> vertical columns. Each sample is denoted <br> by a bar of the color of its sample type. <br> In addition, to indicate the error or <br> uncertainty in a reported measurement or <br> calculated data, the variability of data can <br> be represented with optional error bars. | Error Bars - Use this setting to <br> convey accurate range of +/- <br> data error. <br> Title - The title for a <br> histogram chart. <br> Types - Which sample types <br> to include in the histogram. |
| :--- | :--- | :--- |
| Layout | A graphical representation of the sample <br> layout. | Size - Small, Medium, or <br> Large (medium size will fit on |
| a page-width). |  |  |


| Report <br> Element | Description | Settings |
| :---: | :---: | :---: |
| Measurement <br> 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. | (No additional settings.) |
|  | Any notes associated with the assay run. | Exclude if Empty - If this option is set, then this element is only included if notes are entered. |
| Notes | 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, LeveyJennings, or CUSUM charts reporting the latest results along with historical results. | (No additional settings.) |
| 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. <br> For endpoint data, a numerical value is reported. For XY data, a thumbnail plot is displayed. <br> 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. | Include Positions - Include the Positions column to report the sample positions where the sample was measured. <br> Replicate Orientation - How the replicates appear in the table. <br> Types - Which sample types to include in the sample table. <br> Thumb Plot - For XY data, various options for defining the inclusion and sizing of XY thumb plot charts. <br> Thumb Scale - For XY data, various options for defining how XY thumb plot charts are scaled. |
| Transform | Various report elements generated as a | Content - Use this setting to |


| Report <br> Element | Description | Settings |
| :--- | :--- | :--- |
| $\underline{\text { Content }}$ | consequence of a specific transform. <br> For example, a Standard Curve Fit <br> transform adds a concentration table, a <br> chart, and equations to the report as <br> Transform Content report elements. | specify which sub-elements to <br> include (or exclude) and their <br> ordering. The available sub- <br> elements depend on the <br> associated transform. |
| $\underline{\text { Validations }}$ | The details and results of any configured <br> validations arranged in a table. Each <br> validation result is reported as a pass or <br> fail. | Include Description - <br> Include the description <br> column. <br> Include Expression - Include <br> the expression column. |

## 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.

## 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 corresponding Sample Table or Matrix Id (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.

## Evaluations Table

## How to: Add Evaluations Table Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Evaluations Table element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new 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 unchecking corresponding checkboxes.

| 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.

The Evaluation Table 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 the description if specified (e.g., on the third row in this example) or Expression\#\{index\} if it is not. The Expression column contains the evaluated expression and the Results display the computed result of each configured Evaluation.

## Histogram

A histogram can be use to graphically present the spread of measurements or results. This can be useful for spotting outliers.

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).

For example, the following Histogram was generated using a configuration to plot the Average values of Control, Unknown and Standards with error-bars indicating the standard deviation and a custom title.


## How to: Add Histogram Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Histogram element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

The Histogram is configured with the common report settings as covered in the Report Content section plus the Histogram specific settings described below.

## General

| Matrix | The matrix of data to plot. Select the relevant matrix name from a drop-down <br> list. |
| :--- | :--- |

## Histogram

| Error Bars | Use this setting to select the type of error bars to use (or none). <br> Error bars can display the Standard Error, \%CV, or Standard Deviation of <br> the (not-flagged) replicates of the group. If the Replicates option is selected <br> the error bars reflect the minimum and maximum value of the replicates of <br> the sample. <br> With the None selection, the error bars are not shown. |
| :--- | :--- |
|  | The title for a histogram chart. |
|  | Which sample types to include in the histogram. |

## Layout

## How to: Add Layout Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Layout element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

As with other Report Elements, you can configure how it appears in the report using common report settings.

In addition, Layout has a configurable Size setting. You can select Small, Medium, or Large option (medium size will fit on a page-width). If multiple layouts are defined in the assay protocol, then all of them will be included in the report.

The Layout report element adds an image of the sample layout used in the assay to the report. This includes a layout itself and a legend with the sample types that are included in the layout. I.e.:

|  | 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 $\bigcirc$ Blank $\bigcirc$ Control $\bigcirc$ Unknown

## Matrix Table

## How to: Add Matrix Table Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Matrix Table element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

Matrix Table lists the results of the performed analysis in a matrix-table structure. 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.

The Matrix Table is configured with specific to this report element and with general report configuration settings.

## Matrix Table

The matrix table(s) 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 <br> matrices (per plate/analyte). In this case, the final row of the table will <br> contain a key that explains ordering of the matrices. <br> Or select Separate for a separate table for each included matrix. |
| :--- | :--- |

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.

| Include <br> Thumb <br> Plots | Defines whether thumb plots are included in the report. |
| :--- | :--- |
| Thumb Plot <br> Height | This specifies the height to use for all thumbs in the report. |
| Thumb Plot | This specifies the width to use for all thumbs in the report. |

## Width

For XY data, various options for defining how XY thumb plot charts are scaled. These can be fixed values (or determined for each position). The plot lines are plotted within this scan.

## Thumb Scale

| Thumb <br> Auto Scale <br> Max X | Specifies whether the maximum $\mathbf{X}$ scale of each plot is: <br> - Fixed - The scale limit of the thumb plots used in the table is specified by the associated Thumb Scale Max X value. <br> - Plot - The scale limit of each thumb plot is automatically determined by the maximum $\mathbf{X}$ data in each plot (i.e., each plot may have a different maximum $\mathbf{X}$ limit). <br> - Table - The scale limit of every thumb plot in the table is the same. This is determined from the maximum $\mathbf{X}$ of all plots data points in the table. |
| :---: | :---: |
| Thumb <br> Auto Scale <br> Max Y | Specifies whether the maximum $\mathbf{Y}$ scale of each plot is: <br> - Fixed - The scale limit of the thumb plots used in the table is specified by the associated Thumb Scale Max Y value; <br> - Plot - The scale limit of each thumb plot is automatically determined by the maximum $\mathbf{Y}$ data in each plot (i.e., each plot may have a different maximum $\mathbf{Y}$ limit). <br> - Table - The scale limit of every thumb plot in the table is the same. This is determined from the maximum $\mathbf{Y}$ of all plots data points in the table. |
| Thumb <br> Auto Scale <br> Min X | Specifies whether the minimum $\mathbf{X}$ scale of each plot is: <br> - Fixed - The scale limit of the thumb plots used in the table is specified by the associated Thumb Scale Min X value. <br> - Plot - The scale limit of each thumb plot is automatically determined by the minimum $\mathbf{X}$ data in each plot (i.e., each plot may have a different minimum $\mathbf{X}$ limit). <br> - Table - The scale limit of every thumb plot in the table is the same. This is determined from the minimum $\mathbf{X}$ of all plots data points in the table. |
| Thumb | Specifies whether the minimum $\mathbf{Y}$ scale of each plot is: |

$\left.\begin{array}{|l|l|}\hline & \begin{array}{l}\text { - Fixed - The scale limit of the thumb plots used in the table is specified by } \\ \text { the associated Thumb Scale Min } \mathbf{Y} \text { value. }\end{array} \\ \text { Auto Scale } \\ \text { Min } \mathbf{Y}\end{array} \quad \begin{array}{l}\text { - Plot - The scale limit of each thumb plot is automatically determined by } \\ \text { the minimum } \mathbf{Y} \text { data in each plot (i.e., each plot may have a different } \\ \text { minimum } \mathbf{Y} \text { limit). } \\ \text { - Table - The scale limit of every thumb plot in the table is the same. This is } \\ \text { determined from the minimum } \mathbf{Y} \text { of all plots data points in the table. }\end{array}\right\}$

For example,

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 0.253 | 0.270 | 0.463 | 0.470 | 1.214 | 1.261 | 0.115 | 0.116 | 0.115 | 0.115 | 0.490 | 0.477 |

This is how 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 Matrix Table for each included matrix) or in a combined arrangement. For example, here is a snippet of a Matrix Table for the XY Reduction Average raw and calculated data:

|  | 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 | - | - | $\sqrt{ }$ | $\checkmark$ | - | - |
|  | 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 Averag |  |  |  |  |  |

Each cell contains the thumbnail plot for corresponding input XY position and the calculated numerical result.

## 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.

## Matrix View

## How to: Add Matrix View Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Matrix View element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

Matrix View displays the data of a specified matrix, using coloring as either Layout or Heatmap. 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 includes the following configurable settings:

## General

| Matrix | The matrix of data to plot. Select the relevant matrix name from a drop-down <br> 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.

Matrix view can be configured with coloring 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. E.g.:

- Heatmap - Each position displays the numeric value with respect to the default or custom heatmap scale. The scale legend is also included. This setting is relevant for endpoint data only. E.g.:



## Measurement Meta Data

## How to: Add Measurement Meta Data Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Measurement Meta Data element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

The Measurement Meta Data is configured with common report settings that are covered in the Report Content section.

If there is any meta data associated with your measurement data, then it can also be added to the generated report. This data is reported in a two-column table with the name of each entry and its value. For example,

| Data Filename | C: $\backslash . . . \backslash$ Documents <br> ance.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 ver- <br> sion | 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 meta data table features details about the measurements data file and the details obtained from the VICTOR plate reader.

## Notes

## How to: Add Notes to the Analysis

1. Launch an assay protocol or open a results file.
2. In the MAA Ribbon click on the Notes button of the Home tab's View group.
3. The Notes panel will appear down-most of the screen.
4. Enter or paste any Notes as required.

For a particular assay run you may optionally provide notes to store alongside results in the report (e.g., preparation notes, Lot ID, etc.). This can be used to reference the peculiarities of this data analysis.

## How to: Add Notes Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Notes element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

Entered Notes will appear under Notes: title.

## Notes

Notes element includes the following checkbox setting:

$$
\begin{array}{l|l}
\hline \text { Exclude If } & \begin{array}{l}
\text { This setting automatically excludes Notes from the results, if it contains no } \\
\text { Empty }
\end{array} \\
\text { information. }
\end{array}
$$

The Notes element is also configured with common report settings that are covered in the Report Content section.

## Sample Table

## How to: Add Sample Table Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Sample Table element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

Sample Table lists the results of the performed data analysis by sample groups. Flagged data is displayed as defined by the associated transform and matrix configuration. Each row in the table corresponds to a sample.

The Sample Table is configured with general report and specific to this element settings. The former are described in general report configuration settings and the latter are covered below.

## Sample Table

| Include Pos- <br> itions | Include the Positions column to report the sample positions where the sample <br> was measured. |
| :--- | :--- |
| Replicate | How the replicates appear in the table: |
| Orientation | - Vertical - Each position is listed in a new line of the column. <br> - Horizontal - All positions are listed in the same line. |
| Types | Which sample types to include in the sample table. |

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.

| Include <br> Thumb <br> Plots | Defines whether thumb plots are included in the report. |
| :--- | :--- |
| Thumb Plot | This specifies the height to use for all thumbs in the report. |


| Height |  |
| :--- | :--- |
| Thumb Plot <br> Width | This specifies the width to use for all thumbs in the report. |

For XY data, various options for defining how XY thumb plot charts are scaled. These can be fixed values (or determined for each position). The plot lines are plotted within this scan.

## Thumb Scale

| Thumb <br> Auto Scale <br> Max X | Specifies whether the maximum $\mathbf{X}$ scale of each plot is: <br> - Fixed - The scale limit of the thumb plots used in the table is specified by the associated Thumb Scale Max X value. <br> - Plot - The scale limit of each thumb plot is automatically determined by the maximum $\mathbf{X}$ data in each plot (i.e., each plot may have a different maximum $\mathbf{X}$ limit). <br> - Table - The scale limit of every thumb plot in the table is the same. This is determined from the maximum $\mathbf{X}$ of all plots data points in the table. |
| :---: | :---: |
| Thumb <br> Auto Scale <br> Max Y | Specifies whether the maximum $\mathbf{Y}$ scale of each plot is: <br> - Fixed - The scale limit of the thumb plots used in the table is specified by the associated Thumb Scale Max Y value; <br> - Plot - The scale limit of each thumb plot is automatically determined by the maximum $\mathbf{Y}$ data in each plot (i.e., each plot may have a different maximum $\mathbf{Y}$ limit). <br> - Table - The scale limit of every thumb plot in the table is the same. This is determined from the maximum $\mathbf{Y}$ of all plots data points in the table. |
| Thumb <br> Auto Scale <br> Min X | Specifies whether the minimum $\mathbf{X}$ scale of each plot is: <br> - Fixed - The scale limit of the thumb plots used in the table is specified by the associated Thumb Scale Min X value. <br> - Plot - The scale limit of each thumb plot is automatically determined by the minimum $\mathbf{X}$ data in each plot (i.e., each plot may have a different minimum $\mathbf{X}$ limit). <br> - Table - The scale limit of every thumb plot in the table is the same. This is |


|  | determined from the minimum $\mathbf{X}$ of all plots data points in the table. |
| :---: | :---: |
| Thumb <br> Auto Scale <br> Min Y | Specifies whether the minimum $\mathbf{Y}$ scale of each plot is: <br> - Fixed - The scale limit of the thumb plots used in the table is specified by the associated Thumb Scale Min Y value. <br> - Plot - The scale limit of each thumb plot is automatically determined by the minimum $\mathbf{Y}$ data in each plot (i.e., each plot may have a different minimum $\mathbf{Y}$ limit). <br> - Table - The scale limit of every thumb plot in the table is the same. This is determined from the minimum $\mathbf{Y}$ of all plots data points in the table. |
| Thumb Scale Max X | Determines custom maximum $\mathbf{X}$ scale for thumb plots if Thumb Auto Scale Max X is Fixed. |
| Thumb <br> Scale Max <br> Y | Determines custom maximum $\mathbf{Y}$ scale for thumb plots if Thumb Auto Scale Max $\mathbf{Y}$ is Fixed. |
| Thumb Scale Min X | Determines custom minimum $\mathbf{X}$ scale for thumb plots if Thumb Auto Scale Min X is Fixed. |
| Thumb Scale Min Y | Determines custom minimum $\mathbf{Y}$ scale for thumb plots if Thumb Auto Scale Min $\mathbf{Y}$ is Fixed. |

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 snippet of five Standard samples and the positions they are designated to. Also, the raw values (My Raw Data column) for each replicate and the calculated results per sample
for the Percentage Coefficient of Variation transform (\%CV column) are included. Each row contains replicates of the corresponding sample in the Vertical orientation.

For XY data, the Sample Table contains Thumb Plots that is simply a thumbnail graphical representation of each kinetic/spectral data plot at a position.


Here the replicates for each sample group, XY Raw data and calculated results for XY Replicates Average transform are displayed in Horizontal orientation.

## Transform Content

Some transforms can output additional items in the report. 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, the Dilution Factors transform outputs optional report content named Factor Column.

| 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 |
|  | E3 | 2 | 0.279 | 0.558 |
|  | E4 | 0.367 | 0.734 |  |

- 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, Dilutions Table, Curve Data Table, etc.
- Equation - The formula of a fit method that was used to plot a curve. E.g., the formula for Linear Regression:
$y=m x+c$

A report can contain one or more Transform Content sub-elements.

## How to: Configure Transform Content in the Report

1. Open the Report tab.
2. Select Transform Content element, which contains transform name in the title, e.g.

TransformContentDilutionCurves1.
3. Click on a drop-down of Content option of the Report Configuration pane.
4. Review and edit content items as required.
5. Press Calculate button to perform calculations with the new settings.

The Histogram is configured with common report settings that are covered in the Report Content section and the setting described below.

| Content | Use this setting to specify which sub-elements to include (or exclude) and <br> their ordering. The available sub-elements depend on the associated <br> transform. |
| :--- | :--- |

You can configure which optional items are actually included in report with the Content Editor. Select the sub-element, move in to the Included/Excluded pane with right/left arrow buttons, or change its' positioning with the Up and Down buttons on the right of the Included pane.

To include or exclude all transform content from the report, use the Add All or Remove All buttons, respectively.

## Validation Table

## How to: Add Validations Table Element to the Report

1. Open the Report tab (If the Report tab is not immediately visible, press the $\ll$ Show All Properties button to expand).
2. Select the Validations Table element from the Add Element drop-down list in the Reports pane.
3. Review and edit the settings as required.
4. Press the Calculate button to perform calculations with the new settings.

Validations Table indicates whether each validation has passed or failed and, when Validations are defined, is added to the report automatically.

By default Validation table in Report is displayed as three-column table with the number of rows corresponding to the number of Conditions added. The columns are Results,
Expression and Description.
While the Results are definitely included to the report, you might prefer to hide former properties by unticking corresponding checkboxes.

| Include <br> Description | When checked, the column contains Description if specified or Condition\# <br> \{index\} if it was not. |
| :--- | :--- |
| Include <br> Expression | If included, this outputs the Condition defined for each Validation. |

The Validation Table is also configured with common report settings that are covered in the Report Content section.

The Validation Table typically consists of three columns. For example,

| Results | Expression | Description |
| :--- | :--- | :--- |
| ${\hline \multirow{10}{}}{ } }$ | $x<2.5$ | All non-flagged positions have a value less than 2.5 (Pos- <br> ition type) |
| Pass | $x<2.5$ | The average of the replicates (that are not flagged) of all <br> sample groups is less than 2.5 (Group type) |
| $\approx$ Pass | Unknown1 <br> $>1.5$ | Condition \#3 |



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 color, 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.

## Report Template

## Overview

The report template enables presenting your analysis results tailored to your laboratory's standards and requirements. This feature merges together report elements with a preconfigured template. Full power of MS Word or WordPad features is available to customise page-based reporting of the results.

For example, you can define custom sequence and/or inclusion of report elements, insert relevant images or textual descriptions for a printed document. Moreover, simply apply styling settings and include the results you require for your current purpose.

Report template affects Page View and page-based outputs (DOC, DOCX, PDF) of the analysis results only.

## Report Template Configuration

## How to: Add New Report Template for Page-Based Reporting

1. Launch an assay protocol or open a results file.
2. Select the Ribbon's Report tab and switch to the Page View of the results (If the Report tab is not immediately visible press the << Show All Properties button to expand).
3. Hover to Template group and press New button. This launches the Template.DOCX file with 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 press Calculate to generate a new 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 braces.

Report templates have no restrictions with regard to 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/etc., add textual information, macros etc. In fact, any change is possible provided it is supported in the editor.

## How to: Add Report Element Id to the Report Template

1. Launch an assay protocol or open a results file.
2. Open 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 (e.g., \{SampleTable1\}).
5. Save changes to the report template and press Calculate to generate a new report with the new settings.

When you have made changes to the template file and saved them, you can switch back to MAA and press Calculate to generate a new report with the new settings while keeping the editor open. This way you can review modified report in Page View and make further changes if needed.

The defined template will be applied for all page-based reports for this assay results.
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:

- Press Edit button to modify you template file's content according to freshly added report elements or updated requirements. It will launch your default .DOCX editor with the existing template file.
- Press Delete button to remove the existing template file (a warning message will prompt for confirmation before this action is completed).


## Reference

## Transforms

Transforms can be described as a set 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.

## Transform Manager

Transforms are added and configured via the Transform Manager. The Transform Manager occupies the full width and height available for the transform tab's contents.

## How to: Add the Transform

1. Launch an assay protocol or open a results file.
2. If you cannot see the Assay Properties panel, press the Properties button to open it.
3. Press the Add button.
4. Select the transform.
5. Press 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 Properties section above).
8. Press the Calculate button 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 are required to be executed for a particular data type.
- 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.

On top of that, all transforms share the following common settings:

## Advanced

| Included <br> Samples | The sample types to be computed by this transform. |
| :--- | :--- |
|  | Sample types not selected in the Included Samples option will not be <br> computed by this transform; for those cases, this setting specifies what the <br> result will be for those excluded samples: |
| Excluded | - Flagged With Value - The result is flagged with the input value reported. <br> Results |
| This will appear in the report with the value with strikethrough, e.g., 4.23. <br> will appear in the report as Flagged. |  |
| - Equal Input - The result is set to match the value of the input. |  |

## Units

|  | The measurement units to be included in the header of the Sample Table. <br> If the output units of the transform are the same as the input, then use "ditto" |
| :--- | :--- |
| Output |  |
| 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. With MyAssays Desktop, you can layer as many transforms as you require 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 not-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 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, the Advanced settings of each transform can be used 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 | Flag all data points that satisfy the specified Boolean expression. |
| Average | Calculate the average of replicates for each sample group. |
| Blank <br> Correction | Subtract the specified blank value from each input data point. |
| Dilution Curves | Create a dilutions chart for each group of the specified sample type, fit selected curve-fitting method, and calculate the specified titer from the curve. |
| Dilution <br> Factors | Multiply sample groups of the selected type(s) by a specified factor (a unique value can be specified for each group). |
| Expression <br> by Matrix (Dual) | Evaluate the expression in terms of $\mathbf{x}$ and $\mathbf{y}$ for each sample group. The $\mathbf{x}$ and $\mathbf{y}$ variables refer to the values on the first and on the second input matrix, respectively. |
| Expression <br> by Matrix | Evaluate the expression in terms of $\mathbf{x}$. |
| Expression by Position | Evaluates an expression in terms of $\mathbf{x}$ for each specified position. |
| Factor | Multiply all input data points of the specified sample type(s) by a specified factor. |
| Matrix <br> Difference | Calculate the difference between values on the first matrix and the second for each sample group. |
| Median | Calculate the median of the replicates for each sample group. |
| Percentage <br> Coefficient of <br> Variation | Calculate 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 <br> Outlier <br> Removal | Flags the specified number of replicates for each sample group, in which \%CV of its replicates is greater than specified threshold. |
| Standard <br> Curve Fit | Constructs a standard curve by plotting the standard input concentration values vs data points. |


| Transform | Operation |
| :--- | :--- |
| Standard <br> Deviation | Calculate the standard deviation of the replicates for each sample group. |
| Standard <br> Error of | Calculate the standard error of the mean for replicates of each sample group. |
| Mean |  |

## Auto Flag

## [Input: Endpoint $\Rightarrow$ 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.

## Properties

## Settings

## Auto Flag <br> The expression to evaluate, where a single $\mathbf{x}$ 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 $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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 $\mathbf{x}>\mathbf{1}$.

## 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 | 7.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.487 |
| 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 | 1.214 | 1.244 | 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 | 7.196 | 1.206 | 1.226 | 7.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| G | 1.797 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 7.308 | 7.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| H | 0.253 | 0.270 | 0.463 | 0.470 | 1.214 | 1.267 | 0.115 | 0.116 | 0.115 | 0.115 | 0.490 | 0.477 |

## Average

## [Input: Endpoint $\Rightarrow$ Output: Endpoint]

This transform calculates the average of the replicates in each sample group (flagged replicates are not included).

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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.). l.e.:

|  | 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 |

## Onknown

## 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 |
| :--- | :--- | :--- | :--- |
| OUnknown1 | A1 | 0.364 | 0.344 |
|  | A2 | 0.323 |  |
| OUnknown2 | A3 | 2.105 | 2.115 |
|  | A4 | 2.124 |  |
| Unknown3 | A5 | 1.213 | 1.220 |
|  | A6 | 1.226 |  |
| Unknown4 | A7 | 1.159 | 1.175 |
|  | A8 | 1.190 |  |
| OUnknown5 | A9 | 0.110 | 0.113 |
|  | A10 | 0.116 |  |

## - Matrix Table

Here all calculated data is displayed in a Matrix Table.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.344 | 0.344 | 2.115 | 2.115 | 1.220 | 1.220 | 1.175 | 1.175 | 0.113 | 0.113 | 1.472 | 1.472 |
| $\mathbf{B}$ | 0.448 | 0.448 | 1.879 | 1.879 | 1.211 | 1.211 | 1.193 | 1.193 | 0.131 | 0.131 | 0.777 | 0.777 |
| $\mathbf{C}$ | 0.581 | 0.581 | 0.494 | 0.494 | 1.223 | 1.223 | 1.207 | 1.207 | 0.115 | 0.115 | 0.620 | 0.620 |
| $\mathbf{D}$ | 0.790 | 0.790 | 0.371 | 0.371 | 1.177 | 1.177 | 1.226 | 1.226 | 0.104 | 0.104 | 0.490 | 0.490 |
| $\mathbf{E}$ | 1.085 | 1.085 | 0.323 | 0.323 | 1.220 | 1.220 | 1.248 | 1.248 | 0.113 | 0.113 | 1.564 | 1.564 |
| $\mathbf{F}$ | 1.435 | 1.435 | 0.395 | 0.395 | 1.201 | 1.201 | 1.213 | 1.213 | 0.109 | 0.109 | 0.784 | 0.784 |
| $\mathbf{G}$ | 1.797 | 1.797 | 0.579 | 0.579 | 1.217 | 1.217 | 1.307 | 1.307 | 0.127 | 0.127 | 0.656 | 0.656 |
| $\mathbf{H}$ | 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 $\Rightarrow$ 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 (not-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

For more complicated blank correction calculations, an alternative approach is to use the Expression by Position transform.

## Properties

## Settings

| Blank | The group number of the sample to use for correction. This can be defined as <br> a number or as an expression. The expression can refer to $\mathbf{x}$, which is the <br> Group number of the sample to be corrected. For example, set this to $\mathbf{x}$ to <br> perform a 1-to-1 correction where each group is corrected by the sample of <br> 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 $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.192 | 0.199 | 0.347 | 0.346 | 0.325 | 0.321 | 0.803 | 0.797 | 1.589 | 1.593 | 0.241 | 0.246 |
| $\mathbf{B}$ | 0.293 | 0.300 | 0.586 | 0.584 | 0.800 | 0.793 | 0.402 | 0.401 | 0.839 | 0.837 | 0.562 | 0.564 |
| $\mathbf{C}$ | 0.537 | 0.534 | 0.549 | 0.547 | 0.878 | 0.875 | 0.471 | 0.471 | 0.759 | 0.756 | 1.039 | 1.043 |
| $\mathbf{D}$ | 0.858 | 0.855 | 0.320 | 0.325 | 0.531 | 0.530 | 1.552 | 1.551 | 0.429 | 0.427 | 0.424 | 0.424 |
| $\mathbf{E}$ | 1.523 | 1.527 | 0.486 | 0.490 | 1.289 | 1.283 | 1.430 | 1.438 | 1.494 | 1.501 | 1.427 | 1.429 |
| $\mathbf{F}$ | 1.622 | 1.621 | 0.621 | 0.626 | 0.667 | 0.663 | 1.350 | 1.347 | 0.631 | 0.634 | 1.695 | 1.694 |
| $\mathbf{G}$ | 0.001 | 0.001 | 0.356 | 0.352 | 0.418 | 0.412 | 1.172 | 1.174 | 1.572 | 1.570 | 0.595 | 0.590 |
| $\mathbf{H}$ | 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.). l.e.:

|  | 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 $\bigcirc$ Blank $\bigcirc$ Control $\bigcirc$ 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.191 | 0.198 | 0.346 | 0.345 | 0.324 | 0.320 | 0.802 | 0.796 | 1.588 | 1.592 | 0.240 | 0.245 |
| $\mathbf{B}$ | 0.292 | 0.299 | 0.585 | 0.583 | 0.799 | 0.792 | 0.401 | 0.400 | 0.838 | 0.836 | 0.561 | 0.563 |
| $\mathbf{C}$ | 0.536 | 0.533 | 0.548 | 0.546 | 0.877 | 0.874 | 0.470 | 0.470 | 0.758 | 0.755 | 1.038 | 1.042 |
| $\mathbf{D}$ | 0.857 | 0.854 | 0.319 | 0.324 | 0.530 | 0.529 | 1.551 | 1.550 | 0.428 | 0.426 | 0.423 | 0.423 |
| $\mathbf{E}$ | 1.522 | 1.526 | 0.485 | 0.489 | 1.288 | 1.282 | 1.429 | 1.437 | 1.493 | 1.500 | 1.426 | 1.428 |
| $\mathbf{F}$ | 1.621 | 1.620 | 0.620 | 0.625 | 0.666 | 0.662 | 1.349 | 1.346 | 0.630 | 0.633 | 1.694 | 1.693 |
| $\mathbf{G}$ | 0.000 | 0.000 | 0.355 | 0.351 | 0.417 | 0.411 | 1.171 | 1.173 | 1.571 | 1.569 | 0.594 | 0.589 |
| $\mathbf{H}$ | 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 $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 1.962 | 1.999 | 2.038 | 1.922 | 1.995 | 0.002 | 1.628 | 1.670 | 1.624 | 1.554 | 1.701 | 0.000 |
| $\mathbf{B}$ | 0.784 | 0.760 | 0.754 | 0.751 | 0.797 | 0.002 | 1.124 | 1.104 | 1.072 | 1.077 | 1.106 | 0.002 |
| $\mathbf{C}$ | 0.586 | 0.575 | 0.582 | 0.590 | 0.576 | 0.001 | 0.724 | 0.737 | 0.690 | 0.711 | 0.717 | 0.002 |
| $\mathbf{D}$ | 0.441 | 0.441 | 0.427 | 0.419 | 0.439 | 0.002 | 0.095 | 0.095 | 0.093 | 0.096 | 0.096 | 0.001 |
| $\mathbf{E}$ | 1.956 | 1.970 | 1.875 | 2.043 | 1.959 | 0.001 | 1.449 | 1.479 | 1.428 | 1.395 | 1.385 | 0.001 |
| $\mathbf{F}$ | 1.416 | 1.358 | 1.407 | 1.352 | 1.452 | 0.001 | 0.242 | 0.230 | 0.249 | 0.235 | 0.251 | 0.000 |
| $\mathbf{G}$ | 1.438 | 1.429 | 1.488 | 1.401 | 1.372 | 0.002 | 0.943 | 0.952 | 0.956 | 0.912 | 0.969 | 0.002 |
| $\mathbf{H}$ | 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 I.e.:

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| A | 1 | 1 | 1 | 1 | 1 | 1 | 9 | 9 | 9 | 9 | 9 | 9 |
| B | 2 | 2 | 2 | 2 | 2 | 2 | 10 | 10 | 10 | 10 | 10 | 10 |
| C | 3 | 3 | 3 | 3 | 3 | 3 | 11 | 11 | 11 | 11 | 11 | 11 |
| D | 4 | 4 | 4 | 4 | 4 | 4 | 12 | 12 | 12 | 12 | 12 | 12 |
| E | 5 | 5 | 5 | 5 | 5 | 5 | 13 | 13 | 13 | 13 | 13 | 13 |
| F | 6 | 6 | 6 | 6 | 6 | 6 | 14 | 14 | 14 | 14 | 14 | 14 |
| G | 7 | 7 | 7 | 7 | 7 | 7 | 15 | 15 | 15 | 15 | 15 | 15 |
| H | 8 | 8 | 8 | 8 | 8 | 8 | 16 | 16 | 16 | 16 | 16 | 16 |

To perform 1-1 correction, specify Blank Group to $\mathbf{x}$ 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 1.960 | 1.997 | 2.035 | 1.919 | 1.992 | 0.000 | 1.628 | 1.670 | 1.623 | 1.554 | 1.701 | 0.000 |
| $\mathbf{B}$ | 0.783 | 0.758 | 0.752 | 0.750 | 0.796 | 0.000 | 1.122 | 1.102 | 1.070 | 1.075 | 1.104 | 0.000 |
| $\mathbf{C}$ | 0.585 | 0.574 | 0.581 | 0.589 | 0.575 | 0.000 | 0.722 | 0.735 | 0.688 | 0.709 | 0.714 | 0.000 |
| $\mathbf{D}$ | 0.439 | 0.439 | 0.425 | 0.417 | 0.437 | 0.000 | 0.094 | 0.094 | 0.093 | 0.095 | 0.095 | 0.000 |
| $\mathbf{E}$ | 1.955 | 1.969 | 1.873 | 2.042 | 1.958 | 0.000 | 1.448 | 1.478 | 1.427 | 1.394 | 1.384 | 0.000 |
| $\mathbf{F}$ | 1.415 | 1.358 | 1.406 | 1.352 | 1.451 | 0.000 | 0.241 | 0.229 | 0.249 | 0.235 | 0.251 | 0.000 |
| $\mathbf{G}$ | 1.436 | 1.427 | 1.486 | 1.399 | 1.369 | 0.000 | 0.941 | 0.950 | 0.955 | 0.910 | 0.967 | 0.000 |
| $\mathbf{H}$ | 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 $12 \times 8$ microplate:

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathbf{A}$ | 1 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 1 |
| $\mathbf{B}$ | 2 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 2 |
| $\mathbf{C}$ | 3 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 3 |
| $\mathbf{D}$ | 4 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 4 |
| $\mathbf{E}$ | 5 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 5 |
| $\mathbf{F}$ | 6 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 6 |
| $\mathbf{G}$ | 7 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 7 |
| $\mathbf{H}$ | 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.) l.e.:

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| A |  | 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 |  | 27 |  |  | 30 | 3 |
| D | 4 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |  | 40 | 4 |
| E | 5 |  | 42 | 43 | 44 |  |  | 47 | 48 | 49 | 50 | 5 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| F | 6 | 51 | 52 |  |  | 55 |  |  | 58 |  | 60 | 6 |
| G | 7 | 61 |  |  |  |  |  |  | 68 |  | 70 | 7 |
| H | 8 | $71$ | $72$ | 73 | 74 | 75 | $76$ | 77 | 78 |  | 80 | 8 |

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 $\mathbf{x}=\mathbf{1}$, this means $\mathbf{1 + f l o o r ( ( 1 - 1 ) / 1 0 ) , 1 ) , ~ f l o o r = 0 ~ a n d ~ t h e ~ B l a n k ~ G r o u p ~}$ is taken as 1 . For the first row, $\mathbf{x}$ 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, $\mathbf{x}$ is from 11 to 20, floor=1, so the Blank2 group is subtracted from
Unknowns11-20, etc.

## Blank Corrected

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathbf{A}$ | 0 | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 0 |
| $\mathbf{B}$ | 1 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 1 |
| $\mathbf{C}$ | 2 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 2 |
| $\mathbf{D}$ | 3 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 3 |
| $\mathbf{E}$ | 4 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 4 |
| $\mathbf{F}$ | 5 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 5 |
| $\mathbf{G}$ | 6 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 6 |
| $\mathbf{H}$ | 7 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 7 |

## Dilution Curves

## [Input: Endpoint $\Rightarrow$ Output: Endpoint]

This transform creates a curve fit and calculates, in respect of this curve, a titer value for each sample group of the specified dilution type.

## Properties

## Settings

| Dilution <br> Type | The sample type to use for the dilution. |
| :---: | :---: |
| Dilutions | This specifies standard concentration values. You can Enter or Paste the values into the edit box. If the values are in a sequence, select the Series button to define the series. The series is calculated from the value specified in the first row and the sequence settings with arithmetic operators and a factor (either even or fractional). Also, you can press the $\mathbf{r}$ button to set a number to repeat sequence with in the edit box. |
|  | All sample groups are assumed to have the same number of <br> 1. positions defined on the layout (e.g., if Unknown1 has 10 samples, then all Unknowns on the layout must also have 10 samples). |
| Fit Method | The curve fitting method to construct a curve for your data based on the specified Dilution Type. |
| Titer To Calculate | An expression representing the titer value to calculate. |
| Weight <br> Method | Specifies the weight function for the transform. |
| X Axis Type | A type to plot an $\mathbf{X}$ axis in a chart: <br> - Logarithmic <br> - Linear |
| Transform | Function for $\mathbf{X}$ values transform. |
| Y Axis Type | A type to plot an $\mathbf{Y}$ axis in a chart: |


|  | • Logarithmic <br> • Linear |
| :--- | :--- |
| $\mathbf{Y}$ | Function for $\mathbf{Y}$ values transform. |

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ microplate stored in the Raw matrix. In this example we would like to create a curve fit for each sample group of the Unknown type.

Here is some example raw data displayed here to 3 decimal places:

## Raw

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.000 | 2.682 | 2.345 | 2.612 | 2.732 | 2.675 | 2.664 | 2.574 | 2.580 | 2.361 | 0.871 | 2.839 |
| $\mathbf{B}$ | 0.000 | 2.577 | 1.735 | 2.518 | 2.701 | 2.537 | 2.571 | 2.450 | 2.453 | 2.171 | 0.437 | 2.809 |
| $\mathbf{C}$ | 0.000 | 2.537 | 1.290 | 2.497 | 2.683 | 2.447 | 2.490 | 2.273 | 2.344 | 1.695 | 0.222 | 2.783 |
| $\mathbf{D}$ | 0.000 | 2.358 | 0.793 | 2.318 | 2.585 | 2.195 | 2.205 | 1.856 | 2.069 | 1.070 | 0.094 | 2.658 |
| $\mathbf{E}$ | 0.000 | 1.958 | 0.369 | 1.799 | 2.224 | 1.636 | 1.661 | 1.192 | 1.485 | 0.550 | 0.037 | 2.322 |
| $\mathbf{F}$ | 0.000 | 1.352 | 0.151 | 1.118 | 1.517 | 0.909 | 0.947 | 0.638 | 0.868 | 0.257 | 0.013 | 1.495 |
| $\mathbf{G}$ | 0.000 | 0.745 | 0.053 | 0.540 | 0.872 | 0.425 | 0.485 | 0.282 | 0.417 | 0.094 | 0.002 | 0.862 |
| $\mathbf{H}$ | 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.). l.e.:

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| A | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |
| B | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |
| C | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |
| D | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |
| E | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |
| F | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |
| G | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |
| H | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |  |Unused Unknown

To create a curve and calculate concentrations for this matrix, specify following settings:

1. Dilution Type to Unknown.
2. Dilutions count is equal to maximum number (8) of replicates in sample group of the Unknown. Set this parameter to 0.01 and series to divide by 3.
3. Set Fit Method of 4PL.
4. Set a Titer To Calculate to 1.5.
5. Select a Weight Method of None.
6. Set an $\mathbf{X}$ Axis Type to Logarithmic.
7. Set a X Transform to None.
8. Set an X Axis Type to Linear.
9. Set a X Transform to None.

The transform generates a Dilutions Table and a Chart by default. Other elements such as Matrix table and Notes can be added to report optionally.

## Dilutions Table

This table lists coefficients calculated from the selected Fit Method and a resulting value for each sample. With the example data provided above, the results are as follows:

| Sample | $\mathbf{a}$ | $\mathbf{b}$ | $\mathbf{c}$ | $\mathbf{d}$ | $\mathbf{R}^{\mathbf{2}}$ | Result |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Ounknown1 | -0.0584816 | 0.875198 | 0.0000376679 | 2.67099 | 0.999497 | 0.0000522186 |
| Ounknown2 | -0.0901615 | 0.606878 | 0.00226574 | 3.29931 | 0.997736 | 0.00184835 |
| Ounknown3 | 0.103291 | 1.07281 | 0.0000588689 | 2.59484 | 0.999371 | 0.0000738691 |
| Ounknown4 | 0.176798 | 1.10415 | 0.000035979 | 2.73875 | 0.999281 | 0.0000381935 |
| Ounknown5 | 0.0355624 | 0.998377 | 0.0000794665 | 2.64392 | 0.999147 | 0.000101774 |
| Ounknown6 | 0.0581275 | 0.980399 | 0.000077654 | 2.66458 | 0.999619 | 0.0000965551 |
| Ounknown7 | 0.0190159 | 0.929062 | 0.000146444 | 2.60957 | 0.999764 | 0.000199822 |
| Ounknown8 | 0.0468791 | 0.936045 | 0.000090142 | 2.57555 | 0.999425 | 0.000124316 |
| Ounknown9 | 0.0138517 | 0.919968 | 0.000515222 | 2.53025 | 0.999769 | 0.000767282 |
| Ounknown10 | -0.00938083 | 0.681115 | 0.135122 | 6.05263 | 0.999738 | 0.0267169 |
| Ounknown11 | 0.298789 | 1.20751 | 0.0000424681 | 2.83485 | 0.999004 | 0.0000389155 |

## Chart

The chart contains a curve fit plotted with 4PL for titer and for each sample group.


## Titer

The output matrix named Titer can be optionally added to the report. It contains the calculated titer value for each data point. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |
| $\mathbf{B}$ | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |
| $\mathbf{C}$ | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |
| $\mathbf{D}$ | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |
| $\mathbf{E}$ | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |
| F | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |
| $\mathbf{G}$ | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |
| H | Flagged | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.027 | 0.000 |

## Dilution Factors

## [Input: Endpoint $\Rightarrow$ Output: Endpoint]

This transform multiplies each selected sample group by a specified factor (a factor can be specified for each sample group).

A sample prepared with a dilution of 1:2 would use a dilution factor of 2 .

## Properties

## Settings

| Factored <br> 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 $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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.). I.e.:

|  | 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 $\bigcirc$ Blank $\bigcirc$ Control $\bigcirc$ Unknown
To multiply selected sample types in this matrix by specified factors, set Factored Samples to Unknown and specify Factors as $\mathbf{2}$ for every odd sample group and as $\mathbf{5}$ 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) |
| :--- | :--- | :--- | :--- | :--- |
| OUnknown1 | 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. Select the XML tab in the Assay Properties panel (If the XML tab is not immediately visible, press the << Show All Properties button 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.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 4.210 | 4.248 | 2.426 | 2.452 | 2.318 | 2.380 | 0.220 | 0.232 | 2.926 | 2.962 |
| $\mathbf{B}$ | 0.455 | 0.441 | 9.345 | 9.440 | 6.015 | 6.090 | 5.900 | 6.030 | 0.660 | 0.650 | 3.930 | 3.840 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.948 | 1.028 | 2.412 | 2.478 | 2.406 | 2.420 | 0.226 | 0.232 | 1.226 | 1.252 |
| $\mathbf{D}$ | 0.806 | 0.774 | 1.820 | 1.890 | 5.835 | 5.935 | 6.055 | 6.205 | 0.505 | 0.530 | 2.445 | 2.450 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.558 | 0.734 | 2.430 | 2.450 | 2.466 | 2.524 | 0.222 | 0.228 | 3.158 | 3.098 |
| $\mathbf{F}$ | 1.425 | 1.445 | 1.890 | 2.055 | 5.980 | 6.030 | 6.130 | 5.995 | 0.545 | 0.540 | 3.960 | 3.875 |
| $\mathbf{G}$ | 1.791 | 1.803 | 1.120 | 1.194 | 2.410 | 2.456 | 2.616 | 2.612 | 0.252 | 0.254 | 1.304 | 1.318 |
| $\mathbf{H}$ | 0.253 | 0.270 | 2.315 | 2.350 | 6.070 | 6.305 | 0.575 | 0.580 | 0.575 | 0.575 | 2.450 | 2.385 |

## Expression by Matrix (Dual)

## Input: Dual Endpoint $\Rightarrow$ Output: Endpoint

This transform evaluates an expression defined in terms of $\mathbf{x}$ and $\mathbf{y}$ for all data points (excluding flagged samples). $\mathbf{x}$ refers to the data for the sample on the first input matrix, and $\mathbf{y}$ refers to the data for the same sample on the second input matrix.

## Properties

## Settings

| Dual Matrix <br> Expression | The expression to evaluate, where $\mathbf{x}$ and $\mathbf{y}$ variables are set to value of each <br> position of the input matrices |
| :--- | :--- |

If the expression does not contain the $\mathbf{x}$ and $\mathbf{y}$ variables, the transform will output the

(1)same evaluation result for all positions. For example, if you enter $\left\{\mathbf{2}^{\wedge} \mathbf{3 + 4 \}}\right.$, the resulting matrix will contain 12 in each position.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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)

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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)

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.204 | 0.201 | 0.213 | 0.209 | 0.206 | 0.208 | 0.216 | 0.217 | 0.216 | 0.213 | 0.205 | 0.218 |
| $\mathbf{B}$ | 0.216 | 0.200 | 0.214 | 0.214 | 0.204 | 0.201 | 0.215 | 0.216 | 0.203 | 0.219 | 0.207 | 0.204 |
| $\mathbf{C}$ | 0.206 | 0.210 | 0.208 | 0.203 | 0.201 | 0.218 | 0.212 | 0.217 | 0.216 | 0.213 | 0.208 | 0.204 |
| $\mathbf{D}$ | 0.215 | 0.215 | 0.214 | 0.203 | 0.214 | 0.213 | 0.219 | 0.219 | 0.213 | 0.201 | 0.202 | 0.219 |
| $\mathbf{E}$ | 0.215 | 0.220 | 0.219 | 0.212 | 0.210 | 0.211 | 0.214 | 0.214 | 0.201 | 0.202 | 0.202 | 0.207 |
| $\mathbf{F}$ | 0.214 | 0.212 | 0.202 | 0.200 | 0.201 | 0.217 | 0.213 | 0.209 | 0.218 | 0.207 | 0.216 | 0.216 |
| $\mathbf{G}$ | 0.211 | 0.211 | 0.218 | 0.209 | 0.214 | 0.213 | 0.201 | 0.211 | 0.205 | 0.210 | 0.201 | 0.212 |
| $\mathbf{H}$ | 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 $\mathbf{x}+$ $y$.

## 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.568 | 0.524 | 2.318 | 2.333 | 1.419 | 1.434 | 1.375 | 1.407 | 0.326 | 0.329 | 1.668 | 1.699 |
| $\mathbf{B}$ | 0.671 | 0.641 | 2.083 | 2.102 | 1.407 | 1.419 | 1.395 | 1.422 | 0.335 | 0.349 | 0.993 | 0.972 |
| $\mathbf{C}$ | 0.793 | 0.785 | 0.682 | 0.717 | 1.407 | 1.457 | 1.415 | 1.427 | 0.329 | 0.329 | 0.821 | 0.830 |
| $\mathbf{D}$ | 1.021 | 0.989 | 0.578 | 0.581 | 1.381 | 1.400 | 1.430 | 1.460 | 0.314 | 0.307 | 0.691 | 0.709 |
| $\mathbf{E}$ | 1.320 | 1.285 | 0.498 | 0.579 | 1.425 | 1.436 | 1.447 | 1.476 | 0.312 | 0.316 | 1.781 | 1.756 |
| $\mathbf{F}$ | 1.639 | 1.657 | 0.580 | 0.611 | 1.397 | 1.423 | 1.439 | 1.408 | 0.327 | 0.315 | 1.008 | 0.991 |
| $\mathbf{G}$ | 2.002 | 2.014 | 0.778 | 0.806 | 1.419 | 1.441 | 1.509 | 1.517 | 0.331 | 0.337 | 0.853 | 0.871 |
| $\mathbf{H}$ | 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 $\Rightarrow$ Output: Endpoint]

This transform evaluates an expression defined in terms of $\mathbf{x}$ for all data points (excluding flagged samples).

## Properties

## Settings

| Matrix <br> Expression | The expression to evaluate, where a single $\mathbf{x}$ variable is set to value of each |
| :--- | :--- |
| position of the input matrix |  | If the expression does not contain the $\mathbf{x}$ variable, the transform will output the same

(1)evaluation result for all positions. For example, if you enter $\left\{\mathbf{2}^{\wedge} \mathbf{3 + 4 \}}\right.$, the resulting matrix will contain 12 in each position.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ microplate stored in the Raw matrix. In this example we would like to square each measurement.

Here is some example raw data displayed here to 3 decimal places:
Raw

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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 $\mathbf{x}^{*} \mathbf{x}$.

## 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.132 | 0.104 | 4.431 | 4.511 | 1.471 | 1.503 | 1.343 | 1.416 | 0.012 | 0.013 | 2.140 | 2.193 |
| $\mathbf{B}$ | 0.207 | 0.194 | 3.493 | 3.565 | 1.447 | 1.484 | 1.392 | 1.454 | 0.017 | 0.017 | 0.618 | 0.590 |
| $\mathbf{C}$ | 0.345 | 0.331 | 0.225 | 0.264 | 1.454 | 1.535 | 1.447 | 1.464 | 0.013 | 0.013 | 0.376 | 0.392 |
| $\mathbf{D}$ | 0.650 | 0.599 | 0.132 | 0.143 | 1.362 | 1.409 | 1.467 | 1.540 | 0.010 | 0.011 | 0.239 | 0.240 |
| $\mathbf{E}$ | 1.221 | 1.134 | 0.078 | 0.135 | 1.476 | 1.501 | 1.520 | 1.593 | 0.012 | 0.013 | 2.493 | 2.399 |
| $\mathbf{F}$ | 2.031 | 2.088 | 0.143 | 0.169 | 1.430 | 1.454 | 1.503 | 1.438 | 0.012 | 0.012 | 0.627 | 0.601 |
| $\mathbf{G}$ | 3.208 | 3.251 | 0.314 | 0.356 | 1.452 | 1.508 | 1.711 | 1.706 | 0.016 | 0.016 | 0.425 | 0.434 |
| $\mathbf{H}$ | 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 $\Rightarrow$ Output: Endpoint]

This transform enables an expression to be defined for each position in terms of $\mathbf{x}$ (where $\mathbf{x}$ refers to the value of position on the input matrix). This is useful for applying various tests to different samples simultaneously.

## 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 on a 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 colored to match its sample type.

|  | If the protocol contains $>1$ plate/analyte, select the one to specify expressions <br> for from a drop-down list in the upper right corner of the Editor. To maximize <br> its view, click on the arrow button in the lower left corner of the Editor. <br> Within each grid you can select and specify an expression in terms of $\mathbf{x}$ for: |
| :--- | :--- |
| - a single position. |  |
| - multiple positions (within a single plate) to set to a same expression. |  |
| Position |  |
| Expressions |  | | - 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 $\mathbf{x}$ ) 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 $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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 $\mathbf{x}$ *10
- A10 and H12 with the expression $\mathbf{x}$ *100
- E2 with the expression $\mathbf{x * 2}$


## 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 3.640 | 3.230 | 21.050 | 21.240 | 12.130 | 1.226 | 1.159 | 1.190 | 0.110 | 11.600 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 2.130 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 0.253 | 0.270 | 0.463 | 0.470 | 1.214 | 1.261 | 0.115 | 0.116 | 0.115 | 0.115 | 0.490 | 47.700 |

## Factor

## [Input: Endpoint $\Rightarrow$ 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.

## Properties

## Settings

| Factor | The value to multiply all data points by. This can be specified as a number or <br> an expression to evaluate. |
| :--- | :--- |

## Example:

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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 here to 3 decimal places:

## Raw

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.728 | 0.646 | 4.210 | 4.248 | 2.426 | 2.452 | 2.318 | 2.380 | 0.220 | 0.232 | 2.926 | 2.962 |
| $\mathbf{B}$ | 0.910 | 0.882 | 3.738 | 3.776 | 2.406 | 2.436 | 2.360 | 2.412 | 0.264 | 0.260 | 1.572 | 1.536 |
| $\mathbf{C}$ | 1.174 | 1.150 | 0.948 | 1.028 | 2.412 | 2.478 | 2.406 | 2.420 | 0.226 | 0.232 | 1.226 | 1.252 |
| $\mathbf{D}$ | 1.612 | 1.548 | 0.728 | 0.756 | 2.334 | 2.374 | 2.422 | 2.482 | 0.202 | 0.212 | 0.978 | 0.980 |
| $\mathbf{E}$ | 2.210 | 2.130 | 0.558 | 0.734 | 2.430 | 2.450 | 2.466 | 2.524 | 0.222 | 0.228 | 3.158 | 3.098 |
| $\mathbf{F}$ | 2.850 | 2.890 | 0.756 | 0.822 | 2.392 | 2.412 | 2.452 | 2.398 | 0.218 | 0.216 | 1.584 | 1.550 |
| $\mathbf{G}$ | 3.582 | 3.606 | 1.120 | 1.194 | 2.410 | 2.456 | 2.616 | 2.612 | 0.252 | 0.254 | 1.304 | 1.318 |
| $\mathbf{H}$ | 0.506 | 0.540 | 0.926 | 0.940 | 2.428 | 2.522 | 0.230 | 0.232 | 0.230 | 0.230 | 0.980 | 0.954 |

## Matrix Difference

## Input: Dual Endpoint $\Rightarrow$ 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.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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 here to 3 decimal places:

## Raw (1)

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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)

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.204 | 0.201 | 0.213 | 0.209 | 0.206 | 0.208 | 0.216 | 0.217 | 0.216 | 0.213 | 0.205 | 0.218 |
| $\mathbf{B}$ | 0.216 | 0.200 | 0.214 | 0.214 | 0.204 | 0.201 | 0.215 | 0.216 | 0.203 | 0.219 | 0.207 | 0.204 |
| $\mathbf{C}$ | 0.206 | 0.210 | 0.208 | 0.203 | 0.201 | 0.218 | 0.212 | 0.217 | 0.216 | 0.213 | 0.208 | 0.204 |
| $\mathbf{D}$ | 0.215 | 0.215 | 0.214 | 0.203 | 0.214 | 0.213 | 0.219 | 0.219 | 0.213 | 0.201 | 0.202 | 0.219 |
| $\mathbf{E}$ | 0.215 | 0.220 | 0.219 | 0.212 | 0.210 | 0.211 | 0.214 | 0.214 | 0.201 | 0.202 | 0.202 | 0.207 |
| $\mathbf{F}$ | 0.214 | 0.212 | 0.202 | 0.200 | 0.201 | 0.217 | 0.213 | 0.209 | 0.218 | 0.207 | 0.216 | 0.216 |
| $\mathbf{G}$ | 0.211 | 0.211 | 0.218 | 0.209 | 0.214 | 0.213 | 0.201 | 0.211 | 0.205 | 0.210 | 0.201 | 0.212 |
| $\mathbf{H}$ | 0.216 | 0.209 | 0.215 | 0.206 | 0.218 | 0.206 | 0.209 | 0.219 | 0.215 | 0.219 | 0.216 | 0.217 |

(1)
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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.160 | 0.122 | 1.892 | 1.915 | 1.007 | 1.018 | 0.944 | 0.973 | -0.106 | -0.097 | 1.258 | 1.263 |
| $\mathbf{B}$ | 0.239 | 0.241 | 1.656 | 1.674 | 0.999 | 1.017 | 0.965 | 0.990 | -0.071 | -0.089 | 0.579 | 0.564 |
| $\mathbf{C}$ | 0.381 | 0.365 | 0.266 | 0.311 | 1.005 | 1.021 | 0.991 | 0.993 | -0.103 | -0.097 | 0.405 | 0.422 |
| $\mathbf{D}$ | 0.591 | 0.559 | 0.150 | 0.175 | 0.953 | 0.974 | 0.992 | 1.023 | -0.112 | -0.095 | 0.287 | 0.271 |
| $\mathbf{E}$ | 0.890 | 0.845 | 0.060 | 0.155 | 1.005 | 1.014 | 1.019 | 1.048 | -0.090 | -0.088 | 1.377 | 1.342 |
| $\mathbf{F}$ | 1.211 | 1.234 | 0.176 | 0.211 | 0.995 | 0.989 | 1.013 | 0.990 | -0.109 | -0.099 | 0.576 | 0.559 |
| $\mathbf{G}$ | 1.580 | 1.592 | 0.342 | 0.389 | 0.991 | 1.016 | 1.107 | 1.095 | -0.079 | -0.083 | 0.451 | 0.447 |
| $\mathbf{H}$ | 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 $\Rightarrow$ Output: Endpoint]

This transform calculates the median of the replicates in each sample group (flagged replicates are not included).

(1)
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.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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 here to 3 decimal places:
Raw

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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.). l.e.:

|  | 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 |  |
|  | B1 | 0.455 | 0.455 |
|  | B2 | 0.441 |  |
|  | B3 | 1.869 |  |

## - Matrix Table

Here all calculated data is displayed in a Matrix Table.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.364 | 0.364 | 1.226 | 1.226 | 1.226 | 1.159 | 1.159 | 1.159 | 1.463 | 1.463 | 1.463 |
| $\mathbf{B}$ | 0.455 | 0.455 | 0.455 | 1.218 | 1.218 | 1.218 | 1.180 | 1.180 | 1.180 | 0.768 | 0.768 | 0.768 |
| $\mathbf{C}$ | 0.575 | 0.575 | 0.575 | 1.206 | 1.206 | 1.206 | 1.203 | 1.203 | 1.203 | 0.613 | 0.613 | 0.613 |
| $\mathbf{D}$ | 0.774 | 0.774 | 0.774 | 1.167 | 1.167 | 1.167 | 1.211 | 1.211 | 1.211 | 0.489 | 0.489 | 0.489 |
| $\mathbf{E}$ | 1.065 | 1.065 | 1.065 | 1.215 | 1.215 | 1.215 | 1.233 | 1.233 | 1.233 | 1.549 | 1.549 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.425 | 1.425 | 1.196 | 1.196 | 1.196 | 1.199 | 1.199 | 1.199 | 0.775 | 0.775 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.791 | 1.791 | 1.205 | 1.205 | 1.205 | 1.306 | 1.306 | 1.306 | 0.652 | 0.652 | 0.652 |
| $\mathbf{H}$ | 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 $\Rightarrow$ Output: Endpoint]

This transform calculates the \%CV of the replicates in each sample group (flagged replicates are not included).

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 not-flagged replicates, the result for the group will be set to Flagged.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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 here to 3 decimal places:

## Raw

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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.). l.e.:

|  | 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 $\bigcirc$ Blank $\bigcirc$ Control $\bigcirc$ 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.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 8.440 | 8.440 | 0.635 | 0.635 | 0.754 | 0.754 | 1.866 | 1.866 | 3.755 | 3.755 | 0.865 | 0.865 |
| $\mathbf{B}$ | 2.210 | 2.210 | 0.715 | 0.715 | 0.876 | 0.876 | 1.541 | 1.541 | 1.080 | 1.080 | 1.638 | 1.638 |
| $\mathbf{C}$ | 1.460 | 1.460 | 5.726 | 5.726 | 1.909 | 1.909 | 0.410 | 0.410 | 1.853 | 1.853 | 1.484 | 1.484 |
| $\mathbf{D}$ | 2.864 | 2.864 | 2.668 | 2.668 | 1.202 | 1.202 | 1.730 | 1.730 | 3.416 | 3.416 | 0.144 | 0.144 |
| $\mathbf{E}$ | 2.607 | 2.607 | 19.265 | 19.265 | 0.580 | 0.580 | 1.644 | 1.644 | 1.886 | 1.886 | 1.356 | 1.356 |
| $\mathbf{F}$ | 0.986 | 0.986 | 5.915 | 5.915 | 0.589 | 0.589 | 1.575 | 1.575 | 0.652 | 0.652 | 1.534 | 1.534 |
| $\mathbf{G}$ | 0.472 | 0.472 | 4.523 | 4.523 | 1.337 | 1.337 | 0.108 | 0.108 | 0.559 | 0.559 | 0.755 | 0.755 |
| $\mathbf{H}$ | 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 $\Rightarrow$ Output: Endpoint]

This transform calculates a percentage value for each sample with respect to the specified 0\% and $100 \%$ values.

## Properties

## Settings

$\mathbf{P 0}$ and $\mathbf{P 1 0 0}$ 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 Control $\mathbf{1}$ and $\mathbf{P 1 0 0}$ is Control2, then when the analysis is performed, the \%s for container 1 will be calculated using Control 1 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 <br> expression. All values less than P0 will have negative value in resulting matrix. |
| :--- | :--- |
| $\mathbf{P 1 0 0}$ | The value treated as "100\%." This can be defined as a number or as an <br> expression. All values greater than P100 will have values greater than 100 in <br> resulting matrix. |

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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 here to 3 decimal places:

## Raw

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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 $\mathbf{P 1 0 0}$ 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 12.13 | 10.77 | 70.17 | 70.80 | 40.43 | 40.87 | 38.63 | 39.67 | 3.67 | 3.87 | 48.77 | 49.37 |
| $\mathbf{B}$ | 15.17 | 14.70 | 62.30 | 62.93 | 40.10 | 40.60 | 39.33 | 40.20 | 4.40 | 4.33 | 26.20 | 25.60 |
| $\mathbf{C}$ | 19.57 | 19.17 | 15.80 | 17.13 | 40.20 | 41.30 | 40.10 | 40.33 | 3.77 | 3.87 | 20.43 | 20.87 |
| $\mathbf{D}$ | 26.87 | 25.80 | 12.13 | 12.60 | 38.90 | 39.57 | 40.37 | 41.37 | 3.37 | 3.53 | 16.30 | 16.33 |
| $\mathbf{E}$ | 36.83 | 35.50 | 9.30 | 12.23 | 40.50 | 40.83 | 41.10 | 42.07 | 3.70 | 3.80 | 52.63 | 51.63 |
| $\mathbf{F}$ | 47.50 | 48.17 | 12.60 | 13.70 | 39.87 | 40.20 | 40.87 | 39.97 | 3.63 | 3.60 | 26.40 | 25.83 |
| $\mathbf{G}$ | 59.70 | 60.10 | 18.67 | 19.90 | 40.17 | 40.93 | 43.60 | 43.53 | 4.20 | 4.23 | 21.73 | 21.97 |
| $\mathbf{H}$ | 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 $\Rightarrow$ 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.

This transform can be used to perform automatic outlier rejection (useful when samples are measured in replicate groups of 3 or more).

## Properties

## Settings

| Outliers To <br> Remove | Specifies the maximum number of outliers to remove. The minimum and <br> default value for this setting is 1. |
| :--- | :--- |
| \%CV | Defines threshold percentage coefficient of variance. Data point with superior <br> Threshold <br> or inferior values will be flagged. The default value is $15 \%$. |

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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 $\mathbf{A 1}$ to $\mathbf{H} 1$, Unknown2 from $\mathbf{B 2}$ to $\mathbf{H} 2$, etc.). l.e.:

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | 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 |

[^1]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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | $z .105$ | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.797 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 0.253 | 0.270 | 0.463 | 0.470 | 1.214 | 1.261 | 0.115 | 0.116 | 0.115 | 0.115 | 0.490 | 0.477 |

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 $\Rightarrow$ Output: Endpoint]
This transform:

1. Plots the specified concentration values ( $\mathbf{X}$ ) against the measurement data ( $\mathbf{Y}$ ) 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)

To use Standard Curve Fit transform select or create a layout with a minimum of 2 Standard sample groups.

## Properties

Axes

| $\mathbf{X}$ Axis Title | A name of the $\mathbf{X}$ axis on the chart |
| :--- | :--- |
| X Axis Type | A type to plot an $\mathbf{X}$ axis in a chart: <br> - Logarithmic <br> - Linear |
| $\mathbf{Y}$ Axis Title | A name of the $\mathbf{Y}$ axis on the chart |
|  | A type to plot an $\mathbf{Y}$ axis in a chart: <br> • Logarithmic <br> Y Axis Type |

## Calibrators

| Concentrations | Defines the $\mathbf{X}$ value for each point of the chart. |
| :--- | :--- |
| Standard Type | Defines a sample type to treat as a standard. |

Fit

| Calculate <br> 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?). The options are: <br> - Replicates - Every position will contain the result of $\mathbf{X}$, calculated from value of every replicate ( $\mathbf{Y}$ ). <br> - Average - Replicates from the same sample contain the result of $\mathbf{X}$, calculated from averaged value of replicates ( $\mathbf{Y}$ ). |
| :---: | :---: |
|  | (1) Any flagged positions on the input are also flagged in the output. |
| Fit Method | The curve-fitting method to construct a curve for your data based on the specified Standard Type. <br> You can also use the Best Fit feature to plot the most appropriate fit for your data automatically. |
| 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. I.e.: <br> - $R^{2}$ <br> - $R^{2}$ with Low-End Accuracy <br> - $R^{2}$ with High-End Accuracy <br> - $R^{2}$ with Low-End and High-End Accuracy <br> - 1/Standard-Error <br> - 1/P-Value |
| Fit To Standard | Defines which points are used as the calibrators to fit the curve to: <br> - Replicates - All replicate points from each Standard sample group are used as calibrators. <br> - 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 $\mathbf{X}$ values are interpreted in the transform: <br> - None - The $\mathbf{X}$ values remain as they are. <br> - Log10 - Each $\mathbf{X}$ point is taken as a common logarithm of $\mathbf{X}$. <br> - Log2 - Each $\mathbf{X}$ point is taken as a binary logarithm of $\mathbf{X}$. <br> - $\mathbf{L o g} \mathbf{N}$ - Each $\mathbf{X}$ point is taken as a natural logarithm of $\mathbf{X}$. |
| :---: | :---: |
| Y <br> Transform | Determines how the $\mathbf{Y}$ values are interpreted in the transform: <br> - None - The $\mathbf{Y}$ values remain as they are. <br> - Log10 - Each $\mathbf{Y}$ point is taken as a common logarithm of $\mathbf{Y}$. <br> - Log2 - Each $\mathbf{Y}$ point is taken as a binary logarithm of $\mathbf{Y}$. <br> - LogN - Each $\mathbf{Y}$ point is taken as a natural logarithm of $\mathbf{Y}$. |

## Quantification Limits

| Accuracy <br> $( \pm \%)$ | Defines a percentage limit of accuracy for Standard Type sample groups. <br> This is used to verify whether the accuracy of the calibrators' fits in required <br> limits. The default value is 20\%. |
| :--- | :--- |
| Precision <br> $(\% C V)$ | Defines a \%CV precision limit. This is used to verify whether \%CV for each <br> Standard Type sample group is lower than required limit. The default value <br> 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 $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.192 | 0.199 | 0.347 | 0.346 | 0.325 | 0.321 | 0.803 | 0.797 | 1.589 | 1.593 | 0.241 | 0.246 |
| $\mathbf{B}$ | 0.293 | 0.300 | 0.586 | 0.584 | 0.800 | 0.793 | 0.402 | 0.401 | 0.839 | 0.837 | 0.562 | 0.564 |
| $\mathbf{C}$ | 0.537 | 0.534 | 0.549 | 0.547 | 0.878 | 0.875 | 0.471 | 0.471 | 0.759 | 0.756 | 1.039 | 1.043 |
| $\mathbf{D}$ | 0.858 | 0.855 | 0.320 | 0.325 | 0.531 | 0.530 | 1.552 | 1.551 | 0.429 | 0.427 | 0.424 | 0.424 |
| $\mathbf{E}$ | 1.523 | 1.527 | 0.486 | 0.490 | 1.289 | 1.283 | 1.430 | 1.438 | 1.494 | 1.501 | 1.427 | 1.429 |
| $\mathbf{F}$ | 1.622 | 1.621 | 0.621 | 0.626 | 0.667 | 0.663 | 1.350 | 1.347 | 0.631 | 0.634 | 1.695 | 1.694 |
| $\mathbf{G}$ | 0.001 | 0.001 | 0.356 | 0.352 | 0.418 | 0.412 | 1.172 | 1.174 | 1.572 | 1.570 | 0.595 | 0.590 |
| $\mathbf{H}$ | 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.). l.e.:

|  | 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 |

To configure a Standard Curve Fit for this matrix, provide following settings:

1. Set $\mathbf{X}$ Axis Title to Concentration.
2. Set $\mathbf{X}$ Axis Type to Logarithmic.
3. Set $\mathbf{Y}$ Axis Title to Raw.
4. Set $\mathbf{X}$ Axis Type to Linear.
5. Set Concentrations in Standard 1 to 0.125 and a Series to multiply by 2.
6. Set Standard Type to Standard.
7. Set Calculate From to Average.
8. Select a Fit Method of 4PL.
9. Set Fit To Standard to Average.
10. Select a Weight Method of None.
11. Set a X Transform to None.
12. Set a X Transform to None.
13. Set Accuracy ( $\pm \%$ ) to $20 \%$.
14. Set Precision (\%CV) to $20 \%$.

## Concentration

The transform will generate an output matrix named Concentration with concentrations ( $\mathbf{X}$ ) 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):

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | Flagged | Flagged | 0.352 | 0.352 | 0.318 | 0.318 | 0.844 | 0.844 | 2.890 | 2.890 | 0.153 | 0.153 |
| $\mathbf{B}$ | 0.274 | 0.274 | 0.623 | 0.623 | 0.841 | 0.841 | 0.423 | 0.423 | 0.886 | 0.886 | 0.600 | 0.600 |
| $\mathbf{C}$ | 0.572 | 0.572 | 0.585 | 0.585 | 0.928 | 0.928 | 0.503 | 0.503 | 0.799 | 0.799 | 1.131 | 1.131 |
| $\mathbf{D}$ | 0.906 | 0.906 | 0.317 | 0.317 | 0.566 | 0.566 | 2.561 | 2.561 | 0.454 | 0.454 | 0.450 | 0.450 |
| $\mathbf{E}$ | 2.390 | 2.390 | 0.521 | 0.521 | 1.550 | 1.550 | 1.969 | 1.969 | 2.240 | 2.240 | 1.947 | 1.947 |
| $\mathbf{F}$ | 3.243 | 3.243 | 0.662 | 0.662 | 0.704 | 0.704 | 1.702 | 1.702 | 0.671 | 0.671 | 5.174 | 5.174 |
| $\mathbf{G}$ | Flagged | Flaged | 0.362 | 0.362 | 0.439 | 0.439 | 1.332 | 1.332 | 2.710 | 2.710 | 0.630 | 0.630 |
| $\mathbf{H}$ | 0.275 | 0.275 | 0.843 | 0.843 | 2.338 | 2.338 | 1.030 | 1.030 | 0.566 | 0.566 | 0.622 | 0.622 |

Click here to learn about 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 Standard Curve Evaluations. Moreover, with Standard Curve Custom Flag Labels, 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>
```

<StandardCurveFitStandardType="2" FitMethod="4PL" Concentrations="0.25,0.5,1,2,4,8"
XAxisTitle="Concentration" YAxisTitle="OD" FitToStandard="Average"
CalculateFrom="Average">
<Evaluations>
<EvaluationType="CalcY" Expression="Blank + (3 * sd(Blank))"
Description="My LLD"Name="LLD" />
</Evaluations>
<Flags>
<FlagType="Input"Condition="x \< 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 downward to 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:

|  | $\mathbf{1}$ |  | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :--- | :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | Below <br> LLD | Below <br> LLD | 0.352 | 0.352 | 0.318 | 0.318 | 0.844 | 0.844 | 2.890 | 2.890 | 0.153 | 0.153 |
| $\mathbf{B}$ | 0.274 | 0.274 | 0.623 | 0.623 | 0.841 | 0.841 | 0.423 | 0.423 | 0.886 | 0.886 | 0.600 | 0.600 |
| $\mathbf{C}$ | 0.572 | 0.572 | 0.585 | 0.585 | 0.928 | 0.928 | 0.503 | 0.503 | 0.799 | 0.799 | 1.131 | 1.131 |
| $\mathbf{D}$ | 0.906 | 0.906 | 0.317 | 0.317 | 0.566 | 0.566 | 2.561 | 2.561 | 0.454 | 0.454 | 0.450 | 0.450 |
| $\mathbf{E}$ | 2.390 | 2.390 | 0.521 | 0.521 | 1.550 | 1.550 | 1.969 | 1.969 | 2.240 | 2.240 | 1.947 | 1.947 |
| $\mathbf{F}$ | 3.243 | 3.243 | 0.662 | 0.662 | 0.704 | 0.704 | 1.702 | 1.702 | 0.671 | 0.671 | 5.174 | 5.174 |
| $\mathbf{G}$ | Below <br> LLD | Below <br> LLD | 0.362 | 0.362 | 0.439 | 0.439 | 1.332 | 1.332 | 2.710 | 2.710 | 0.630 | 0.630 |
| $\mathbf{H}$ | 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 Deviation

## [Input: Endpoint $\Rightarrow$ 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.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 not-flagged replicates, the result for the group will be set to Flagged.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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.). l.e.:

|  | 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 $\bigcirc$ Blank $\bigcirc$ Control $\bigcirc$ 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.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.029 | 0.029 | 0.013 | 0.013 | 0.009 | 0.009 | 0.022 | 0.022 | 0.004 | 0.004 | 0.013 | 0.013 |
| $\mathbf{B}$ | 0.010 | 0.010 | 0.013 | 0.013 | 0.011 | 0.011 | 0.018 | 0.018 | 0.001 | 0.001 | 0.013 | 0.013 |
| $\mathbf{C}$ | 0.008 | 0.008 | 0.028 | 0.028 | 0.023 | 0.023 | 0.005 | 0.005 | 0.002 | 0.002 | 0.009 | 0.009 |
| $\mathbf{D}$ | 0.023 | 0.023 | 0.010 | 0.010 | 0.014 | 0.014 | 0.021 | 0.021 | 0.004 | 0.004 | 0.001 | 0.001 |
| $\mathbf{E}$ | 0.028 | 0.028 | 0.062 | 0.062 | 0.007 | 0.007 | 0.021 | 0.021 | 0.002 | 0.002 | 0.021 | 0.021 |
| $\mathbf{F}$ | 0.014 | 0.014 | 0.023 | 0.023 | 0.007 | 0.007 | 0.019 | 0.019 | 0.001 | 0.001 | 0.012 | 0.012 |
| $\mathbf{G}$ | 0.008 | 0.008 | 0.026 | 0.026 | 0.016 | 0.016 | 0.001 | 0.001 | 0.001 | 0.001 | 0.005 | 0.005 |
| $\mathbf{H}$ | 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 $\Rightarrow$ 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.

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 not-flagged replicates, the result for the group will be set to Flagged.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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 $\mathbf{A 3}$, Unknown2 in from $\mathbf{A 4}$ to $\mathbf{A 6}$, etc.). I.e.:

|  | 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 |
| :--- | :--- | :--- | :--- |
| OUnknown1 | 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.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.587 | 0.587 | 0.587 | 0.302 | 0.302 | 0.302 | 0.355 | 0.355 | 0.355 | 0.452 | 0.452 | 0.452 |
| $\mathbf{B}$ | 0.474 | 0.474 | 0.474 | 0.226 | 0.226 | 0.226 | 0.354 | 0.354 | 0.354 | 0.216 | 0.216 | 0.216 |
| $\mathbf{C}$ | 0.036 | 0.036 | 0.036 | 0.236 | 0.236 | 0.236 | 0.365 | 0.365 | 0.365 | 0.168 | 0.168 | 0.168 |
| $\mathbf{D}$ | 0.142 | 0.142 | 0.142 | 0.266 | 0.266 | 0.266 | 0.375 | 0.375 | 0.375 | 0.128 | 0.128 | 0.128 |
| $\mathbf{E}$ | 0.269 | 0.269 | 0.269 | 0.284 | 0.284 | 0.284 | 0.379 | 0.379 | 0.379 | 0.483 | 0.483 | 0.483 |
| $\mathbf{F}$ | 0.352 | 0.352 | 0.352 | 0.263 | 0.263 | 0.263 | 0.368 | 0.368 | 0.368 | 0.225 | 0.225 | 0.225 |
| $\mathbf{G}$ | 0.412 | 0.412 | 0.412 | 0.207 | 0.207 | 0.207 | 0.394 | 0.394 | 0.394 | 0.176 | 0.176 | 0.176 |
| $\mathbf{H}$ | 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 $\Rightarrow$ 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.

- 

The variance is the sum of the squares of the difference of each replicate and the mean divided by $\mathbf{n - 1}$ (where $\mathbf{n}$ is the number of the replicates).

For groups with less than 2 not-flagged replicates, the result for the group will be set to Flagged.

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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.). I.e.:

|  | 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 $\bigcirc$ Blank $\bigcirc$ Control $\bigcirc$ 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.

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\mathbf{B}$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\mathbf{C}$ | 0.000 | 0.000 | 0.001 | 0.001 | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\mathbf{D}$ | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\mathbf{E}$ | 0.001 | 0.001 | 0.004 | 0.004 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\mathbf{F}$ | 0.000 | 0.000 | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\mathbf{G}$ | 0.000 | 0.000 | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\mathbf{H}$ | 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 $\mathbf{X}$ chart axis and for evaluations: <br> - Index - The 1-based position number of the data point in the collection. <br> - X - Depending on the measurements data type, this option is displayed as: <br> - X (Cycle) - For kinetic data with no time values, $\mathbf{X}$ equals the Index. <br> - X (Time) - For kinetic data, if time values are stored, then this is the time stamp associated with the data point. <br> - X (Wavelength) - For spectral data, if wavelength values are stored, then this is the wavelength of the data point. <br> - $\mathbf{Y}$ - Each value is set to a $\mathbf{Y}$ value of the corresponding input matrix's data point. |
| :---: | :---: |
| Y Axis | This setting determines which values to consider in the $\mathbf{Y}$ chart axis and for evaluations: <br> - Index - The 1-based position number of the data point in the collection. <br> - X-Depending on the measurements data type, this option is displayed as: <br> - X (Cycle) - For kinetic data with no time values, $\mathbf{X}$ equals the Index. <br> - X (Time) - For kinetic data, if time values are stored, then this is the time stamp associated with the data point. <br> - X (Wavelength) - For spectral data, if wavelength values are stored, then this is the wavelength of the data point. |


|  | - $\mathbf{Y}$ - Eeach value is set to a $\mathbf{Y}$ value of the corresponding input matrix's data <br> 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 (that are also not flagged) are processed by the transform.

The range can be defined by setting the $\mathbf{X}$ Minimum and $\mathbf{X}$ Maximum properties to a value or expression:

| $\mathbf{X}$ Minimum | A numerical value or expression that defines the minimum $\mathbf{X}$ data point to <br> include within the subset. If this is not specified, then all data points less than <br> $\mathbf{X}$ Maximum are included. |
| :--- | :--- |
| $\mathbf{X}$ | A numerical value or expression that defines the maximum $\mathbf{X}$ data point to <br> include within the subset. If this is not specified, then all data points greater <br> than $\mathbf{X}$ Minimum are included. |
| $\mathbf{M a x i m u m ~}$ |  |

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 on 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 $Y$ axes. 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 axis settings specify what data should be processed by the transform. For further details you can refer to the 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 for Flagged Endpoint.

## XY Range

By default, XY data transform calculations are performed on all $X Y$ 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 <br> Correction | Subtracts the average of specified Blank group(s) from each input position. |
| Expression (Dual) | Evaluates an expression in terms of $\mathbf{x}$ and $\mathbf{y}$, where variables are set to the value of each position of the first ( $\mathbf{x}$ ) and second ( $\mathbf{y}$ ) 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 <br> 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). |
| Replicates <br> Average | Calculates the XY average plot for each sample group. |

## XY Baseline Correction

[Input: XY $\Rightarrow$ 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.

## Properties

## Settings

| Method | The method for a baseline correction: |
| :---: | :---: |
|  | - Average Between X1 And X2 - Correct points by the average $\mathbf{Y}$ of the not-flagged points between and including points $\mathbf{X}$ Index $\mathbf{1}$ and $\mathbf{X}$ Index 2. |
|  | - Average Of N Lowest - Correct points by the average Y of the lowest not-flagged $\mathbf{N}$. |
|  | - Proportional N1 Lowest and N2 Highest - Proportional percentage between average of the $\mathbf{N} 1$ lowest and $\mathbf{N} \mathbf{2}$ highest not-flagged points. |

The visibility of the following settings depend on the selected Method. For example, if you choose the Average Of $\mathbf{N}$ Lowest, then only the $\mathbf{N}$ setting will be displayed.

| X Index 1 <br> X Index 2 | These settings are used in the Average Between X1 And X2 method. <br> These are 1-based index numbers and apply to the data sets with or without time values. Only not-flagged points that are $<=\mathbf{X}$ Index $\mathbf{1}$ and $>=\mathbf{X}$ Index $\mathbf{2}$ are used. $\mathbf{X}$ Index $\mathbf{1}$ and $\mathbf{X}$ Index $\mathbf{2}$ must be >=1 and $\mathbf{X}$ Index $\mathbf{2}$ must be $>=X$ Index 1. <br> If there are no included points between $\mathbf{X} \operatorname{Index} \mathbf{1}$ and $\mathbf{X} \operatorname{Index} \mathbf{2}$, 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. <br> It is the number of lowest not-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 $=\mathbf{N}$, then the result is that all points are corrected |


|  | by the average of all points. |
| :--- | :--- |
| $\mathbf{N 1}$ | These settings are used in the Proportional $\mathbf{N} 1$ Lowest and $\mathbf{N} 2$ Highest <br> method. <br> $\mathbf{N} 1$ is the number of the lowest points, $\mathbf{N} 2$ <br> to is the number of the highest points <br> is computed. Then each $\mathbf{Y}$ value is scaled between these points (e.g., if a point <br> equals the average of the lowest, then it is set to 0; or if a point equals the <br> average of the highest, it is set to 100). |
| Also, note results here are clipped. In other words, all results will fall within <br> the range 0 and 100, so values which are calculated to < 0 or > 100 will be set <br> to 0 and 100, respectively. <br> If the average of the lowest values is equal to the average of the highest <br> values, then this cannot be calculated and the output position will be flagged. <br> If there are less than $\mathbf{N 1}$ or $\mathbf{N} \mathbf{2}$ valid readings, then the output position will be <br> flagged. |  |

## XY Blank Correction

[Input: XY $\Rightarrow$ 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.

## Properties

## Settings

This transform requires a layout with at least 1 Blank group.

| Blank | The group number of the sample to use for correction. This can be defined as <br> a number or as an expression. The expression can refer to $\mathbf{x}$ which is the <br> Group number of the sample to be corrected. |
| :--- | :--- |
| Blank Type | For example, set this to $\mathbf{x}$ to perform a 1-to-1 correction where each group is <br> corrected by the sample of the specified blank type with the same group <br> number. |

## Example: Single Blank

Let's assume that we have some $\mathbf{X Y}$ measurement data for a $12 \times 8$ 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.). l.e.:

|  | 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 $\bigcirc$ Blank $\bigcirc$ Control $\bigcirc$ 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 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 $12 \times 8$ 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. I.e.:

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | 1 | 1 | 1 | 1 | 1 | 1 | 9 | 9 | 9 | 9 | 9 | 9 |
| B | 2 | 2 | 2 | 2 | 2 | 2 | 10 | 10 | 10 | 10 | 10 | 10 |
| C | 3 | 3 | 3 | 3 | 3 | 3 | 11 | 11 | 11 | 11 | 11 | 11 |
| D | 4 | 4 | 4 | 4 | 4 | 4 | 12 | 12 | 12 | 12 | 12 | 12 |
| E | 5 | 5 | 5 | 5 | 5 | 5 | 13 | 13 | 13 | 13 | 13 | 13 |
| F | 6 | 6 | 6 | 6 | 6 | 6 | 14 | 14 | 14 | 14 | 14 | 14 |
| G | 7 | 7 | 7 | 7 | 7 | 7 | 15 | 15 | 15 | 15 | 15 | 15 |
| H | 8 | 8 | 8 | 8 | 8 | 8 | 16 | 16 | 16 | 16 | 16 | 16 |

Specify Blank Group to $\mathbf{x}$ 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 $12 \times 8$ 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.) l.e.:

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 1 |
| B | 1 | 2 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |Blank $\square$ 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 ( $\mathbf{x}$ ) to the blank number on its row. In other words, for $\mathbf{x}=\mathbf{1}$ this means $\mathbf{1 + f l o o r ( ( 1 - 1 ) / 1 0 ) , 1 ) , ~ f l o o r = 0 ~ a n d ~ t h e ~ B l a n k ~ G r o u p ~}$ is taken as 1 . For the first row, $\mathbf{x}$ 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, $\mathbf{x}$ 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 $\Rightarrow$ Output: XY]

This transform evaluates an expression defined in terms of $\mathbf{x}$ and $\mathbf{y}$ for each not-flagged input XY data point within the specified range. In this case $\mathbf{x}$ refers to the data for the sample on the first input matrix and $\mathbf{y}$ refers to the data for the same sample on the second input matrix.

This transform is useful when it is necessary to perform a common operation on twosets 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 $X Y$ measurements.

## Properties

## Settings

| Expression | The expression to evaluate, where variables are set to the value of each position of the first ( $\mathbf{x}$ ) and second $(\mathbf{y})$ input matrices. Default expression value is $\mathbf{x}-\mathbf{y}$. |
| :---: | :---: |
|  | 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 checkbox is checked, the chart includes both the input and the calculated plot. If it is unchecked, the chart shows the calculated plot only. |

## XY Expression

## [Input: XY $\Rightarrow$ 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.

This transform is useful when it is necessary to perform an operation on all inputpoints 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.

## Properties

## Settings

| Expression | The expression to evaluate, where the $\mathbf{y}$ variable is set to the value of each <br> position of the input matrix. |
| :--- | :--- |
|  | To refer to the position's corresponding data on an endpoint matrix, <br> use a Matrix Position Reference (e.g., \#2) to refer to the data on the <br> second matrix. |
|  | When the checkbox is ticked, the chart includes both the input and the <br> calculated plot. If it is unchecked, the chart shows the calculated plot only. |

## XY Fit

[Input: XY $\Rightarrow$ 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.

## Properties

## Settings

Fit Method The curve fitting method to construct the curve (from each XY plot)

## XY Join

## [Input: Dual XY $\Rightarrow$ 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).

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.

## Properties

Advanced, Units and Range settings do not apply to this transform.

If $\mathbf{X}$ is set as Index, then the first index of the joined matrix is 1 plus the last used

If $\mathbf{X}$ is set as $\mathbf{X}$, then the $\mathbf{X}$ values specified in each input matrix are used (unchanged) in the output matrix.

When using this transform, consider the $\mathbf{X}$ Axis Data setting. The joined data will use the data from both input matrices. To ensure that the resulting joined contents has sequential $x$ values, set the X Axis Data setting to Index.

## XY Outlier Removal

## [Input: XY $\Rightarrow$ 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.
This transform can be used to automatically remove outlier points in XY data.

## Properties

## Settings

| Num <br> Regression <br> Points | The number of regression points used for each linear regression segment <br> when determining the maximum slope. The default and minimum value is 2. |
| :--- | :--- |
| Threshold | Defines the threshold \% accuracy to flag outliers. <br> It calculates absolute \% difference between back fit value and the original $\mathbf{y}$ <br> value. The back fit is computed from slope and intercept for each $\mathbf{x}$ value in <br> the regression set. If this \% difference is > the specified Threshold, then the <br> data point is flagged on the output matrix. |

## XY Replicates Average

[Input: XY $\Rightarrow$ Output: XY]
This transform calculates the average XY (kinetic/spectral) plot for each sample group. 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.

## 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 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 $Y$ axes. 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 axis settings specify what data should be processed by the transform. For further details you can refer to the 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 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 |
| :--- | :--- |


| $\underline{\text { Average }}$ | 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 <br> each position. |
| $\underline{\text { Maximum }}$ | Determined maximum slope between two adjacent points within specified <br> range at each position. |
| $\underline{\text { Peak }}$ | Determined peak (minimum or maximum) data point within the specified <br> range of the non-flagged points at each position. |
| $\underline{\underline{\text { Total }}}$ | The sum of non-flagged data points within specified range at each position. <br> $\underline{X A t Y}$ |
| The $\mathbf{X}$ value at which the specified $\mathbf{Y}$ value crosses the evaluated plot of non- <br> flagged points within the specified range at each position. |  |
| $\underline{Y \text { Between } Y}$ | The difference between the first two $\mathbf{X}$ points that equal or cross specified $\mathbf{Y}$ <br> value at each position. |
| Determined $\mathbf{Y}$ value for a specified $\mathbf{X}$ value within the specified range of the <br> not-flagged points at each position. |  |

## XY Reduction Average

## [Input: XY data $\Rightarrow$ 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.

## Example

Let's assume that we have some $\mathbf{X Y}$ measurement data for a $12 \times 8$ 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 $\mathbf{X Y}$ data to an average endpoint value:

1. Specify Data: $\mathbf{X}$ Axis as $\mathbf{X}$ (Time), $\mathbf{Y}$ Axis as $\mathbf{Y}$.
2. Leave $\mathbf{X}$ Minimum and $\mathbf{X}$ Maximum blank.
3. Press Calculate.

## Average

The transform will generate an endpoint matrix named Average with the value at each position being the averaged value of the $\mathbf{Y}$ input data points. With the example data provided above, the resulting averaged value for the $\mathbf{A 1}$ plot is as follows (also displayed here to 3 decimal places):
2.857


## XY Reduction Fit Parameter

## [Input: XY data $\Rightarrow$ 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.


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 4 PL ).

## 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 |

## XY Reduction Maximum Slope

## [Input: XY data $\Rightarrow$ 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 ).

(1)
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 regression of adjacent points (using the specified number of linear regressions points) and determining the slope with the maximum (upward or downward) value.

Flagged positions or points or those outside specified ranges are not included in the calculations.

## Properties

## Settings

|  | Determines the type of slope to be found by this transform. The settings <br> are: |
| :--- | :--- |
| Max is | Auto - The maximum slope is determined from the general direction of <br> each plot by using the linear regression. If the slope of the plot is <br> positive, the Fastest Increase is used; if negative, the Fastest Decrease <br> is used. <br> - Fastest Increase - The maximum slope is the slope with the highest <br> positive value. |
| - Fastest decrease - The maximum slope is the slope with the greatest |  |
| negative value. |  |


|  | - X At Centre Absolute - The result is the $\mathbf{X}$ at the center of the determined maximum slope. <br> - Y At Centre Absolute - The result is the $\mathbf{Y}$ at the center of the determined maximum slope. <br> - X At Centre Relative - The result is the $\mathbf{X}$ at the center of the determined maximum slope relative to the first not-flagged data point that is greater than $\mathbf{X}$ Minimum. <br> - Y At Centre Relative - The result is the $\mathbf{Y}$ at the center of the determined maximum slope relative to the first not-flagged data point that is greater than $\mathbf{X}$ Minimum. <br> - Extrapolated $\mathbf{Y}$ - A value of $\mathbf{Y}$ is calculated from the determined maximum slope using the $\mathbf{X}$ value specified with $\mathbf{X}$ For Extrapolation. |
| :---: | :---: |
| X for <br> Extrapolation | When Extrapolated $\mathbf{Y}$ option in the Result Is setting is chosen, then this can be used to specify an expression used to determine the $\mathbf{X}$ value to calculate $\mathbf{Y}$ for. |

## XY Reduction Peak

[Input: XY data $\Rightarrow$ 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.

## Properties

## Settings

| Peak | This setting determines which data point is considered as the peak: <br> - Max - The point with the maximum $\mathbf{Y}$ value <br> - Min - The point with the minimum $\mathbf{Y}$ value |
| :--- | :--- |
| Result | This setting determines which axis's coordinate is stored in resulting matrix: <br> - $\mathbf{X}$ - Projection of Peak value on X axis <br> - $\mathbf{Y}$ - Projection of Peak value on Y axis |

## XY Reduction Total

[Input: XY data $\Rightarrow$ Output: Endpoint]
This reduction transform computes the sum of all $Y$ values for each $X Y$ plot (within the specified range of points to consider). Flagged positions or points are not included in the calculations.

## XY Reduction X At Y

## [Input: XY data $\Rightarrow$ Output: Endpoint]

This reduction transform finds the $\mathbf{X}$ value at which the specified $\mathbf{Y}$ value (Cursor) crosses the plot (within the specified range). If the $\mathbf{Y}$ position is in between two adjacent data points, then an interpolated value is calculated from the bounding points.
$\mathbf{X}$ and $\mathbf{Y}$ 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.

(1)
This transform can be used to determine the $X$ value at the point where the horizontal (defined by Y ) value crosses each plot.

## Properties

## Settings

| Cursor | The expression evaluated for each position that represents the target in $\mathbf{Y}$ 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 <br> Type | This defines how the Cursor is treated for each position. The settings are: <br> - Absolute - The value specified by Cursor is the value to use in the calculation of $\mathbf{X}$. <br> - Relative From First Measured - The value of Cursor is added to the $\mathbf{Y}$ value of the first point for the position (even if the first point is Flagged or outside the range). <br> - Relative From First In Range - The value of Cursor is added to the $\mathbf{Y}$ value of the first non-flagged data point within the range. |
| Result is | Specifies the result of the analysis. The settings are: <br> - Absolute - The computed $\mathbf{X}$ value. <br> - Relative From First Measured - The computed $\mathbf{X}$ value minus the $\mathbf{X}$ |


|  | value of the first point for the position (even if the first point is Flagged or <br> out of range). |
| :--- | :--- |
| - Relative From First In Range - The computed $\mathbf{X}$ value minus the $\mathbf{X}$ value |  |
| of the first non-flagged data point within the range. |  |

## XY Reduction X Between Y

[Input: XY data $\Rightarrow$ Output: Endpoint]
This reduction transform computes the difference between the first two $\mathbf{X}$ points at which the specified $\mathbf{Y}$ value (Cursor) crosses or equals the plot.
$\mathbf{Y}$ 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.

## Properties

## Settings

| Cursor | The expression evaluated for each position that represents the target in $\mathbf{Y}$ 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 <br> Type | This defines how the Cursor is treated for each position. The settings are: <br> - Absolute - The value specified by Cursor is the value to use in the calculation of $\mathbf{X}$. <br> - Relative From First Measured - The value of Cursor is added to the $\mathbf{Y}$ value of the first point for the position (even if the first point is Flagged or outside the range). <br> - Relative From First In Range - The value of Cursor is added to the $\mathbf{Y}$ 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 $12 \times 8$ microplate stored in the Raw matrix. In this example we would like to calculate the difference between first two $\mathbf{X}$ points that equal or cross the specified Cursor and then reduce data to the difference between these 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 $\mathbf{X}$ value when crossing/equaling specified Cursor:

1. Specify Data: $\mathbf{X}$ Axis as $\mathbf{X}$ (Time), $\mathbf{Y}$ Axis as $\mathbf{Y}$.
2. Leave $\mathbf{X}$ Minimum and $\mathbf{X}$ Maximum blank.
3. Specify Settings: Cursor as 0.7, Cursor Type as Absolute.
4. Press 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 $\mathbf{A 1}$ plot is as follows (also displayed here to 3 decimal places):
591.737


Plot crosses $\mathrm{y}=0.7$ at $\mathrm{X} 1=914.729$ and $\mathrm{X} 2=1506.466$, difference $=591.737$

## XY Reduction Y At X

## [Input: XY data $\Rightarrow$ Output: Endpoint]

This reduction transform finds the $\mathbf{Y}$ value at which the specified $\mathbf{X}$ value (Cursor) crosses the plot (within the specified range). If the $\mathbf{X}$ position is in between two adjacent data points, then an interpolated value is calculated from the bounding points.

The $\mathbf{X}$ 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.

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 ).

## Properties

## Settings

|  | The expression evaluated for $\mathbf{X}$ value of each position. |
| :---: | :---: |
| Cursor | 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 <br> Type | This defines how the Cursor is treated for each position. These settings are used to handle scenarios where $\mathbf{X}$ values for each position may be out of sync by adding an offset to the cursor. The settings are: <br> - Absolute - The value specified by the Cursor is the value to use in the calculation of $\mathbf{Y}$. <br> - Relative From First Measured - The Cursor value is added to the $\mathbf{X}$ value of the first point for the position (even if the first point is Flagged or out of range). <br> - Relative From First In Range - The Cursor value is added to the $\mathbf{X}$ value of the first non-flagged data point within the range |

## Curve Fitting

## 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:
$\mathbf{y}=$ the dependent variable (i.e., what you measure as the signal)
$\mathbf{x}=$ the independent variable (i.e., what you control, such as dose, concentration, etc.)

## Coefficients of the Fit

The 4 parameters consist of the following:

- $\mathbf{a}=$ the minimum value that can be obtained (i.e., what happens at 0 dose).
- $\mathbf{d}=$ the maximum value that can be obtained (i.e., what happens at infinite dose).
- $\mathbf{c}=$ the point of inflection (i.e., the value of $x$ at the point on the $S$-shaped curve halfway between $a$ and d).
- $\mathbf{b}=$ 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 $\mathbf{d}$ will always define the upper and lower asymptotes (horizontals) of the curve. $\mathbf{a}$ and $\mathbf{d}$ are the same units at $\mathbf{y}$. The curve can only be used to calculate concentrations for signals within a and d. Samples outside the range of the determined $\mathbf{a}$ and $\mathbf{d}$ 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 4 PL is equal to the $\mathbf{c}$ coefficient of the 4 PL . In this case you can simply look at the calculated 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 $\mathbf{x}$ 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 $\mathbf{y}=50$, then you can calculate where $\mathbf{y}=50$ using the equation to solve $\mathbf{x}$ (above), substituting in the calculated coefficients.


## Linear Regression

It is a basic and easy regression model that fits data in a linear way.
Linear regression sets the linear relationship between the dependent variable (y) and a single independent variable ( $\mathbf{x}$ ). 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:
$y=m x+c$

## Variables

In this model we have the following:
$\mathbf{y}=$ the dependent variable (i.e., what you measure as the signal)
$\mathbf{x}=$ the independent variable (i.e., what you control, such as dose, concentration, etc.)

## Coefficients of the Fit

$\mathbf{m}=$ the slope of the fitted line
$\mathbf{c}=$ 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 $\mathbf{m}$ and $\mathbf{c}$ 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.

Fitted plot may show the nonlinear character of data. In this case you may and are advised to consider setting other methods.

## Goodness of Fit Measures

$\mathbf{R}^{\mathbf{2}}, \mathbf{a} \mathbf{R}^{\mathbf{2}}, \mathbf{P}, \mathbf{S E}, \mathbf{F}$ are calculated when each fit method is used. These measures are indicators as to how position the data fits the curve fit model.

The following table describes these measures and how they can be used to assess the fit.

| Name | Description <br> $R^{2}$ is 1 minus the ratio of the sum of the squares of the residuals divided by <br> the sum of the squares of the differences between $Y$ fit and the mean $Y$ value). <br> This will equal 1 for a perfect fit and tend toward 0 for a bad fit. <br> In other words, $R^{2}$ is the ratio of variation that is explained by the curve-fitting <br> model to the total variation in the model. <br> In most situations, irreducible errors in measurement will prevent the model <br> from explaining all the variation. Models using a larger set of factors may <br> produce an $R^{2}$ value that is closer to 1. However, it may be that the additional <br> factors are essentially modeling noise. |
| :---: | :--- |
| $\mathbf{a R}$ | aR ${ }^{2}$ is the adjusted $R^{2}$ value. <br> aR $R^{2}$ is $R^{2}$ adjusted downward to compensate for over-fitting. The larger the <br> number of independent variables is (compared to the number of <br> observations), the lower the adjusted $R^{2}$ value will be. When using curve- <br> fitting models with a larger number of independent variables, the additional <br> variables may be simply modeling noise. |
| $\mathbf{F}$ | $F$ is the $F$-statistic. F is the ratio of the variance explained by the curve-fitting <br> model to the residual variance. |
| $\mathbf{P}$ | P is the $P$-value. $P$ is the significance of the model as a probability. It is the $P-$ <br> value of $F$ for the curve-fitting model. This compares the variance attributed to <br> the model with the variance of the residual. |
| $\mathbf{S E}$ | SE is the standard error. The standard error is the root-mean square of the <br> residuals. |

## Best Fit

The Best Fit feature will automatically find the most appropriate fit for your data. The feature processes your data with multiple curve fits and multiple weighting methods and automatically picks 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 dose-response curves.
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?

What is deemed to be the best fit can be customized. For example, you might consider the fit with the highest $\mathbf{R}^{2}$ 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 scoring method to quantify how good each fit is. The fit with the highest score is considered to be the best fit.

For convenience, the following preset scoring methods are available for selection:

- $R^{2}$
- $\mathrm{R}^{2}$ 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

Beyond these presets, you can define your own scoring methods to evaluate and compare each attempted fit.

## Scoring Method Expressions

This section describes how to define your own scoring method expressions to evaluate a fit: On completion of each fit, the fit is scored using a scoring 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.

The scoring method equation can reference the goodness measures determined from the fit:

## Goodness Measures

| Name | Description <br> $R^{2}$ is 1 minus the ratio of the sum of the squares of the residuals divided by <br> the sum of the squares of the differences between $Y$ fit and the mean $Y$ value). <br> This will equal 1 for a perfect fit and tend toward 0 for a bad fit. <br> In other words, $R^{2}$ is the ratio of variation that is explained by the curve-fitting <br> model to the total variation in the model. <br> In most situations, irreducible errors in measurement will prevent the model <br> from explaining all the variation. Models using a larger set of factors may <br> produce an $R^{2}$ value that is closer to 1. However, it may be that the additional <br> factors are essentially modeling noise. |
| :---: | :--- |
| $\mathbf{a R}$ | aR ${ }^{2}$ is the adjusted $R^{2}$ value. <br> aR $R^{2}$ is $R^{2}$ adjusted downward to compensate for over-fitting. The larger the <br> number of independent variables is (compared to the number of <br> observations), the lower the adjusted $R^{2}$ value will be. When using curve- <br> fitting models with a larger number of independent variables, the additional <br> variables may be simply modeling noise. |
| $\mathbf{F}$ | $F$ is the $F$-statistic. F is the ratio of the variance explained by the curve-fitting <br> model to the residual variance. |
| $\mathbf{P}$ | P is the P-value. $P$ is the significance of the model as a probability. It is the $P$ - <br> value of $F$ for the curve-fitting model. This compares the variance attributed to <br> the model with the variance of the residual. |
| $\mathbf{S E}$ | SE is the standard error. The standard error is the root-mean square of the <br> residuals. |

## 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 $\mathbf{x}$ of the calibrator) and its actual value calculated from the curve.

The calibration data set is the known concentration values of the standards ( $\mathbf{x}$ ) plotted against their measurements $(\mathbf{y})$. Each curve is fitted to the calibration data set.

To measure the accuracy of the curve at a particular data point, the $\mathbf{x}$ value of the known concentration (expected) is compared against the $\mathbf{x}$ value at this point computed from the curve (actual).
\% Recovery or \% Accuracy is simply:

## 100 * Actual / Expected

To simplify combining accuracy functions together and with other measures (such as $\mathbf{R}^{\mathbf{2}}$ ), the accuracy functions return a value between 0 and 1 (where 1 is perfectly accurate).


| Function Name | Description |
| :--- | :--- |
| Diff | The absolute difference between the expected value, and is the <br> 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 $x$ <br> 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 $x$ <br> value |

## Combining Measures

A scoring 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) |


| Preset | Expression |
| :--- | :--- |
| $R^{2}$ with Low-End and High-End Accuracy | $R^{2 *}$ AccuracyFactorLow(1)*AccuracyFactorHigh(1) |
| $1 /$ Standard-Error | $1 / \mathrm{SE}$ |
| $1 / \mathrm{P}-$ Value | $1 / \mathrm{P}$ |

## Standard Curve Fit Advanced Configuration

## Standard Curve Fit Custom Flag Labels

When computing concentration values from a curve, there might be samples outside certain ranges that should be flagged and reported with a custom label rather than as a result or error.

The Standard Curve Fit Custom Flag Labels feature enables rules to be defined to specify when a result should be flagged and reported using a label.

## Example Uses

A typical use of this feature is to label results for standards 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 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)

The Standard Curve Fit Custom Flag Label is an advanced option only available through XML configuration. This feature is related to the Custom Flag Label feature, in this case Standard Curve Fit Custom Flag Labels have higher precedence and override any other defined labels. You may configure custom flagging rules in the Standard Curve Fit transform based on the transform's input or output data (calculated from the curve). If any of these rules are satisfied then result is flagged with a specified label applied to it.

The rules are defined using expressions written in terms of $\mathbf{x}$ to define when a result should be flagged.

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.

## Evaluation and Results

You can define any number of Custom Flag Label rules in any order. 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). These specified rules take precedence over the default flagging settings or optionally specified CurveError. Therefore, if any of the rules with Type="Input" are evaluated as true, then these will be used in place of any curve error.

For multiple plate assays, the associated curve for the position's plate is used.
If a flag condition is satisfied and a Custom Flag Label is used, then an entry is added to the Calculation Log detailing this application. If there is any error in evaluating a Condition, the details of this is added to the error log.

## How to: Add Custom Flag Label Rules

Standard Curve Fit Custom Flag Labels are configured using XML. To add flagging rules to a Standard Curve Fit transform configuration:

1. Select the XML tab in the Assay Properties panel (If the XML tab is not immediately visible, press the << Show All Properties button to expand).
2. Locate the StandardCurveFit element.
3. Add a Flags element (as a child of the StandardCurveFit) and, optionally, a CurveError element.
4. Add a child element Flag for each required flagging rule. Set the attributes (in accordance with the following table).
5. Press Apply to save changes to the protocol.

## CurveError Optional Setting

The optional CurveError setting is used to specify a default custom flag label to use if a value cannot be computed from the curve (i.e., 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.

This is specified in the XML inside the Flags element with following syntax:
<Flags CurveError="My Custom Error Label" >

## Flag Element Attributes

The following table lists the attributes of the Flag element that must be specified to define the flag rule:

| Type | The value of $\mathbf{x}$ depends on the expression type: <br> - For Type="Input" $\mathbf{x}$ is the value of the input position. <br> - For Type="Output" $\mathbf{x}$ is the value computed for the output position. |
| :---: | :---: |
| Condition | The condition to evaluate (typically a conditional expression). <br> The flag condition expression can refer to: <br> - the value of each position using the reference $\mathbf{x}$. <br> - the computed coefficients of the curve and goodness measures. <br> - Standard Curve Named Evaluations. <br> - sample values of the input matrix. |
| Label | If a flag rule is satisfied (i.e., the Condition is evaluated to true), then the result of the transform for the position is flagged with the associated Label. If you insert $\{\mathbf{x}\}$ in the Label, it inserts the value of x (e.g., $\{\mathbf{x}\}$ is Below LLD might be reported as $\mathbf{0 . 2 5}$ is Below LLD). |

## Specifying Rules with XML

When entering conditions as 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 <br> Quote | \' |

For example, if the condition is $\mathbf{x}$ < $\mathbf{a}$ then this would be encoded in XML using $\mathbf{x}$ \< a

## Example Configuration

The following XML snippet shows a complete configuration of the StandardCurveFit element with Flag rules. With this configuration, 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">
    <Flags CurveError="Could not calculate from curve" >
    <Flag Type="Input" Condition="x &lt; min(a,d)" Label="Below Lower
Asymptote" />
<Flag Type="Input" Condition="x &gt; max(a,d)" Label="Above Lower
Asymptote" />
</Flags>
</StandardCurveFit>
```


## Example Flag Conditions

```
The following table lists further example flag conditions.
```

| XML Condition | Description |
| :---: | :---: |
| ```<Flag Type="Input" Condition="x &lt; 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 \& l ; min <br> (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 &lt; 0.125" Label= "OD &\|t; 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 \< <br> 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. |

## Standard Curve Fit Evaluations

In addition to computing concentrations, ULOQ, and LLOQ from the curve, you can evaluate expressions that:

- Calculate $\mathbf{X}$ or $\mathbf{Y}$ values on the curve (using interpolation/extrapolation)
- Reference the coefficients and goodness measures of the curve
- Can be referred to as a variable in other evaluations or Standard 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.

## How to: Add Evaluations to a Standard Curve Fit Transform Configuration

1. Select the XML tab in the Assay Properties panel (If the XML tab is not immediately visible, press the << Show All Properties button to expand).
2. Locate the StandardCurveFit element.
3. Add an Evaluations element (as a child of the StandardCurveFit).
4. Add a child element Evaluation element for each required evaluation. Set the evaluation attributes in accordance with the table below.
5. Press Apply to save changes to the protocol.

## Evaluation Attributes and Syntax

| Expression | The expression to evaluate. It can refer to: <br> - the computed coefficients of the curve, Transform Output Variables and <br> goodness measures. <br> - any defined above in the XML Standard Curve Fit Evaluation with Name <br> attribute specified. <br> - sample values of the input matrix. |
| :---: | :---: |
| Since the result is a single numerical value, the expression cannot <br> refer to $\mathbf{x}$ or $\mathbf{y}$ variables. |  |


| Type | This setting describes how the expression is treated in report: <br> - CalcX - Calculates the $\mathbf{X}$ value from the fit line using Expression as $\mathbf{Y}$ <br> value. The resulting values are reported using numerical formatting of <br> input matrix. <br> - Calc $\mathbf{Y}$ - Calculates the $\mathbf{Y}$ value from the fit line using Expression as $\mathbf{X}$ <br> value. The resulting values are reported using standard numerical <br> formatting. <br> - Parameter - Outputs the computed Expression value. |
| :--- | :--- |
| Description | Optionally added textual description of the expression. If this is not specified, <br> the Expression itself is used in report. |
| Name | Optional element that defines a name for evaluation. If it is specified, the <br> Name can be used as a variable for other XML configurations (as described <br> below). |

<Settings>
<StandardCurveFitStandardType="2" FitMethod="4PL" Concentrations="0.25,0.5, 1,2,4,8" XAxisTitle="Concentration" YAxisTitle="OD" FitToStandard="Average"
CalculateFrom="Average">
<Evaluations>
<EvaluationType="Type" Expression="Expression"
Description="Description"Name="Name" />
</Evaluations>
</StandardCurveFit>
</Settings>

## Named Evaluations

If the Name attribute is set, then the evaluation can be referred by this Name as a variable in:

- Context variables in evaluations that are defined in XML downward to it
- Standard Curve Flag Label conditions
- Transform Output Variables

The LLOQ and ULOQ are computed automatically and can be used as an evaluation and flag variables too.

## Configuring Standard Curve Evaluations

Evaluations are configured using XML and are evaluated using the plate for the associated container. This means that Blank1 always refers to the first blank sample group on the container. Further details are described in the Multiple Plate Standard Curve Fit Analysis topic.

For example, the LLD is often computed as the concentration $(\mathbf{X})$ at the average of the blank replicates +3 * standard deviation of the blank replicates. This can be computed as an expression that calculates $\mathbf{X}$ from the curve where $\mathbf{Y}=$ Blank + $\mathbf{3}$ * $\mathbf{s d}$ (Blank).

The LLOQ and ULOQ calculations are determined automatically and equal a concentration value (i.e., one of the values defined in Concentrations).

If you create named evaluation LLOQ or ULOQ, then it replaces the default LLOQ and ULOQ calculation, e.g.:
<Evaluations>
<EvaluationType="CalcY" Expression="Control1 + (10 * sd(Control1))"
Description="My LLOQ"Name="LLOQ" />
</Evaluations>

## Results and Report

The LLOQ and ULOQ are the first entries, and any further evaluations are added below them in the table.

The Evaluation data is displayed below the interactive chart and in the report as a simple two-column 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 other words, report syntax errors in a table (in same way as the Evaluation feature).

## Expressions

## Overview

Expressions are available for use throughout MyAssays Desktop to provide flexibility in dataanalysis 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 Control 1 refers to the average of the Control 1 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 Control 1 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 scoring 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)
For advanced users working with data entered directly into 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 a comma list separator).

## 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 * $\mathbf{1 0}$.

There are several situations where an expression is entered in terms of $\mathbf{x}$ (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 $\mathbf{x}$-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 $\mathbf{x}<\mathbf{1 5}$ 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., $+,{ }^{*}, /,{ }^{\wedge}$ )
- 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

(1)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 $\mathbf{x}$ minus the average of Blank1 position. |
| x > 15 | A Boolean expression that would evaluate to 1 (true) if the value of variable $\mathbf{x}$ is greater than 15 ; otherwise it evaluates to |


| Expression | Evaluated to |
| :--- | :--- |
| Ifthenelse (false). |  |
| $\mathbf{x - y} \mathbf{y} \mathbf{1 5 , \mathbf { 1 5 } , \mathbf { x } )}$ | If the value of $\mathbf{x}$ is greater than 15, then the result is $15 ;$ <br> otherwise the result is $\mathbf{x}$. |
| median(Unknown.2.All) | The difference between $\mathbf{x}$ and $\mathbf{y}$. Here $\mathbf{x}$ and $\mathbf{y}$ are the values of <br> corresponding positions from two matrices of data (as used in <br> the Expression by Matrix (Dual) transform). <br> containers. |
| Unknown1.2.3 | The average of Unknown1 sample group on the 2nd matrix of <br> 3 rd container. |
| TOV1.R2 | The R ${ }^{2}$ value of the curve fit as used in the first transform <br> (referenced using a Transform Output Variable). |

## Operators

## Unary Arithmetic Operator

| Operator | Operation | Examples |
| :--- | :--- | :--- |
| - | Minus Sign | -1.23 |
|  | $-x$ |  |

Binary Arithmetic Operators

| Operator | Operation | Example |
| :---: | :---: | :---: |
| + | Addition | 2+1 |
|  |  | $x+y$ |
|  |  | $\mathrm{x}+1$ |
| - | Subtraction | 2-1 |
|  |  | x-y |
|  |  | $\mathrm{x}-1$ |
| * | Multiplication | 2*3 |
|  |  | $x^{*} y$ |
|  |  | y*2 |
| / | Division | 2/2 |


| Operator | Operation | Example |
| :--- | :--- | :--- |
|  |  | $x / y$ |
| $x / 2$ |  |  |
|  | Raising to a power | $2^{\wedge} 3$ |
| $x^{\wedge} y$ |  |  |
| $x^{\wedge} 2$ |  |  |

## Binary Logical Operators

The numerical evaluation of 1 for true and 0 for false. Thus, $1>0=1$.

| Operator | Operation | Examples |
| :---: | :---: | :---: |
| < | Less Than | $\begin{aligned} & 1<2 \\ & x<y \\ & x<2 \end{aligned}$ |
| > | Greater Than | $\begin{aligned} & 2>1 \\ & x>y \\ & x>2 \end{aligned}$ |
| $=$ | Equal To | $\begin{aligned} & 1=1 \\ & x=y \\ & x=2 \end{aligned}$ |
| <= | Less Than Or Equal | $\begin{aligned} & 3<=9 \\ & 3<=3 \\ & x<=y \\ & x<=x \\ & x<=3 \end{aligned}$ |
| >= | Greater Than Or Equal | $\begin{aligned} & 9>=3 \\ & 3>=3 \\ & y>=x \\ & x>=x \\ & x>=9 \end{aligned}$ |
| <> | Not Equal | $2<>1$ |


| Operator | Operation | Examples |
| :--- | :--- | :--- |
|  |  | $x<>y$ <br> $x<>3$ |

## 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).

Ensure that all number values entered into the user interface are provided using the local settings of your system.

## Variables

The $\mathbf{x}$ and $\mathbf{y}$ 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 $\mathbf{x}^{*} 100$ expression, where the $\mathbf{x}$ 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 $\mathbf{x}$ and $\mathbf{y}$ variables are set to the position values of the first and second matrices. Thus, when you enter an expression $\mathbf{x + y}$, each position on the resulting matrix will be the sum of input matrices values.

| Variable | Relevant For |
| :---: | :---: |
| None | Preconfigured Protocols, Certain Endpoint: Auto Flag, Average, Matrix Difference, Median, Percentage, Percentage Coefficient of Variation, Replicate Outlier Removal, Standard Curve Fit, Standard Deviation, Variance |
| x | Certain Endpoint: Blank Correction, Dilution Curves, Dilution Factors, Expression by Matrix, Expression by Position, Factor, XY Blank Correction |
| x, y | Expression by Matrix (Dual), XY Expression (Dual) |
| y | XY Expression |

## Fit Transforms Context Parameters

XY Reduction Fit Parameter and Standard Curve Fit transforms calculate the context parameters of the fit. The former refers to the parameters in configuration settings, and the
latter uses them in flagging conditions and/or additional evaluations. These fit transform context parameters are:

- Goodness of Fit Measures calculated from the fit.

| Name | Expression Syntax |
| :---: | :--- |
| $\mathbf{R}^{\mathbf{2}}$ | r2 |
| $\mathbf{a R}^{\mathbf{2}}$ | ar2 |
| $\mathbf{F}$ | f |
| $\mathbf{P}$ | p |
| $\mathbf{S E}$ | se |

- Coefficients of the Fit - These vary depending on the selected fit method and are specified within documentation of these methods.

Standard Curve Fit also produces additional values (such as quantification limits) and any defined named evaluations. These can be optionally used for further evaluations of custom flagging within this transform.

Fit Transforms Context Parameters apply within fit transforms only and cannot be used in general configuration of the assay (e.g., validation or evaluation tables) or other transforms.

## Transform Output Variables

Any transform evaluated after the transform that produces the output variable can refer to it. This applies only where the later transform supports parameters with expression.

## 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 as being 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 read. A position on a particular matrix and plate can be specified with a period, as described in sample references in multiple container assays.

> When writing expressions, it is better 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 modified layout.

## 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: Unknown 1 refers to all non-flagged Unknown 1 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 (Unknown 1) calculates the median of all defined on the layout non-flagged Unknown 1 position values. 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 Container Assays

To simplify evaluation and avoid the need to write a different expression for each container, expressions use local group numbering. Thus, the simple Unknown1 reference always refers to the first Unknown sample group on the container being evaluated.

You can refer to a specific position, group, or type defined on specific layout plate with the syntax described below.

| Reference | Refers To |
| :--- | :--- |
| A1.2 | A1 position for 2nd container of data |
| A1.2.3 | A1 position for the 2nd matrix of 3rd container of data |
| A1..3 | A1 position for 3rd container of data |
| A1.2.All | The average of all A1 positions on matrix 2 across all containers |
| Unknown1.2 | Unknown1 sample group for 2nd container of data |
| Unknown.2.All | The average of all Unknown replicates on matrix 2 across all containers |
| Unknown1.2.All | The average of all Unknown1 replicates on matrix 2 across all containers |
| Unknown1.2.3 | Unknown1 sample group for the 2nd matrix of 3rd container of data |
| Unknown1..3 | Unknown1 sample data for 3rd container of data |

## 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 (e.g., kinetic or spectral) data is treated in analysis. To see further detains and configuration examples, please refer to 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
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 $\mathbf{X}$ 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 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 $X Y$ Reduction $X$ at $Y$ transform can be used to calculate the time $(X)$ when the halfpeak $(Y)$ 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.:

| Assay Properties |  |  |  |
| :---: | :---: | :---: | :---: |
| Transforms ${ }^{\text {a }}$ Matrices Evaluation | Validation | Report | XML |
| Input Output | Transform Configuration |  |  |
| 1. XY Reduction Peak <br> For each plot, find the maximum value. | $\begin{aligned} & \hline+ \text { Advanced } \\ & \text { - Data } \end{aligned}$ |  |  |
| $\checkmark$ Peak | X Axis | X (Time) | $\checkmark$ |
| 2. Expression by Matrix <br> For each sample group, evaluate the expression " $\mathrm{x} / 2^{\text {" }}$ where x refers to the value on the input matrix. | Y Axis | Y | $\checkmark$ |
|  | - Range |  |  |
| Peak ${ }_{\text {l }}$ ( ${ }^{\text {Half Peak }}$ | X Minimum <br> X Maximum |  |  |
| 3. $\mathbf{X Y}$ Reduction $X$ At $Y$ <br> For each plot, find the first point at which the plot equals or crosses $\mathrm{Y}=\# 3$. |  |  |  |
|  | - Settings |  |  |
|  | Cursor | \#3 | $\checkmark$ |
| $\rightarrow \square$ X At Half Peak |  | Absolute |  |
|  | Result is | Absolute | $\checkmark$ |
|  | - Units |  |  |
|  | Output Units |  |  |



## 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 Ys\}, \{list of Xs\})
- function(\{(samplereference1),(samplereference2), ..., (samplereferenceN)\}, \{operand1,operand2, ..., operandN\})


## 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 nonflagged values of that group/type.

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.

The following table lists group-enabled functions:

| Name | Description | Minimum number of parameters | Examples |
| :---: | :---: | :---: | :---: |
| average | The same as mean. | 1 | Unknown1 average ([Unknown, Blank]) |
| count | Counts the number of non-flagged values. | 1 | count <br> (Unknown) |
| mean | Calculates the mean of the non-flagged positions. | 1 | mean <br> (Unknown1) mean ([Unknown, Blank]) |
| 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 <br> (Unknown1) <br> median <br> ([Standard2, <br> Unknown4]) |
| pcv | Calculates the percentage coefficient of variance (\%CV) of a finite list of non-flagged positions. | 2 | pcv <br> (Unknown) <br> pcv <br> ([Unknown1, <br> Unknown1.2]) |
| 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). | 2 | sd <br> (Standard2) <br> sd <br> ([Unknown1, |

\(\left.$$
\begin{array}{|c|l|l|l|}\hline \text { Name } & \text { Description } & \begin{array}{l}\text { Minimum } \\
\text { number of } \\
\text { parameters }\end{array} & \text { Examples } \\
\hline \text { se } & \begin{array}{l}\text { Calculates the standard error of a finite list of non- } \\
\text { flagged positions. }\end{array} & 2 & \begin{array}{l}\text { Unknown3]) } \\
\text { (Un }\end{array} \\
\hline \text { sum } & \begin{array}{l}\text { Returns the total of all items in the finite list of non- } \\
\text { flagged positions. } \\
\text { ([Unknown, }\end{array}
$$ <br>

\hline Control])\end{array}\right]\)| 1 |
| :--- |
| var |
| Calculates the variance of a finite list of non-flagged <br> positions. Variance is a measurement of the spread <br> between positions in a data set. The variance <br> measures how far each number in the set is from <br> the mean. |
| (Unknown) |

## Example

Let's assume that we have some endpoint measurement data for a $12 \times 8$ 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.). l.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

|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ | $\mathbf{7}$ | $\mathbf{8}$ | $\mathbf{9}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ | $\mathbf{1 2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0.364 | 0.323 | 2.105 | 2.124 | 1.213 | 1.226 | 1.159 | 1.190 | 0.110 | 0.116 | 1.463 | 1.481 |
| $\mathbf{B}$ | 0.455 | 0.441 | 1.869 | 1.888 | 1.203 | 1.218 | 1.180 | 1.206 | 0.132 | 0.130 | 0.786 | 0.768 |
| $\mathbf{C}$ | 0.587 | 0.575 | 0.474 | 0.514 | 1.206 | 1.239 | 1.203 | 1.210 | 0.113 | 0.116 | 0.613 | 0.626 |
| $\mathbf{D}$ | 0.806 | 0.774 | 0.364 | 0.378 | 1.167 | 1.187 | 1.211 | 1.241 | 0.101 | 0.106 | 0.489 | 0.490 |
| $\mathbf{E}$ | 1.105 | 1.065 | 0.279 | 0.367 | 1.215 | 1.225 | 1.233 | 1.262 | 0.111 | 0.114 | 1.579 | 1.549 |
| $\mathbf{F}$ | 1.425 | 1.445 | 0.378 | 0.411 | 1.196 | 1.206 | 1.226 | 1.199 | 0.109 | 0.108 | 0.792 | 0.775 |
| $\mathbf{G}$ | 1.791 | 1.803 | 0.560 | 0.597 | 1.205 | 1.228 | 1.308 | 1.306 | 0.126 | 0.127 | 0.652 | 0.659 |
| $\mathbf{H}$ | 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

## Conditional Functions

These functions require a specified number of input parameters. Where a sample reference is used as an input parameter to a conditional function, it refers to the average of the nonflagged data points.

## Boolean Logical Functions

| Name | Description | Examples |
| :---: | :--- | :--- |
| and | Tests a number of input conditions and returns 1 if all of the con- <br> ditions evaluate to true, or 0 otherwise. | and $(\mathbf{1 , 1})$ |
| or | Tests a number of input conditions and returns 1 if any of the <br> conditions evaluate to true, or 0 otherwise. | or (1,1) <br> not $(\mathbf{x}<5, \mathbf{x}>\mathbf{1 0})$ |
| not | Returns a logical value that is the opposite of an input logical <br> value or expression (i.e., returns 0 if the supplied argument is <br> true and returns 1 if the supplied argument is false). | not $(\mathbf{x}>\mathbf{1})$ |

## Conditional Function

| Name | Description | Examples |
| :---: | :---: | :---: |
| ifthenelse | Requires 3 parameters: <br> 1. The Boolean condition to evaluate (which will evaluate to true or false). <br> 2. The result if the condition is true. <br> 3. The result if the condition is false. <br> If the value of the first condition is true, then the result is the second argument otherwise the third. | ifthenelse ( $1=1,2,3$ ) result is 2 <br> ifthenelse ( $1=0,2,3$ ) result 3 |

For example, with the reference:
IfThenElse(Unknown1 > 10, 10, Unknown1)
Unknown1 refers to the average of Unknown1 non-flagged positions. Thus, the expression evaluation result is 10, if Unknown $\mathbf{1}$ is greater than 10; otherwise the result is Unknown1.

More functions with fixed parameter length are described in Layout Analysis Functions.

## 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 results in a single numeric value.

The following table lists calculation functions.

| Name | Description | Examples |
| :---: | :---: | :---: |
| 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. | $\begin{aligned} & \operatorname{abs}(-1.23)=1.23 \\ & \mathbf{a b s}(1.23)=1.23 \end{aligned}$ |
| average | Described in group-enabled functions. | average $(1,2)=1.5$ <br> average $(-3,0.25,5)=0.75$ |
| ceiling | Returns argument ( $\{\mathbf{0} \mathbf{\}}$ ) rounded up, away from zero, to the nearest multiple of significance (\{1\}). It requires two input parameters with the following syntax ceiling(\{0\}, \{1\}), where: <br> - $\{0\}$ is the value you want to round off. <br> - $\{1\}$ is the multiple to which you want to round. <br> Regardless of the sign of a $\{\mathbf{0}\}$, a value is rounded up when adjusted away from zero. If the $\{\mathbf{0}\}$ is an exact multiple of $\{1\}$, no rounding occurs. | $\begin{aligned} & \text { ceiling }(1.23,0.05)=1.25 \\ & \text { ceiling }(-1.23,0.05)=-1.2 \end{aligned}$ |
| count | Described in group-enabled functions. | count $(1,2,3)=3$ <br> count $(-2.44,2,5,98,6)=5$ |
| exp | Returns e raised to the power of the given number. Syntax: $\exp (\{0\})$ where: <br> $\{\mathbf{0}\}$ is the exponent applied to the base $\mathbf{e}$. It accepts only a single argument. For example, the system accepts $\exp (\mathbf{A 1}+\mathbf{A} 2)$ and rejects $\exp (\mathbf{A 1}, \mathbf{A} 2)$. | $\begin{aligned} & \exp (2)=7.389056 \ldots \\ & \exp (-1)=0.367879 \ldots \end{aligned}$ |
| floor | Returns argument ( $\{\mathbf{0}\}$ ) rounded down, toward zero, to the nearest multiple of significance (\{1\}). It | floor(1.23, 0.05)=1.2 |


| Name | Description | Examples |
| :---: | :---: | :---: |
|  | requires two input parameters with the following syntax floor(\{0\}, \{1\}), where: <br> - $\{0\}$ is the value you want to round off. <br> - $\{1\}$ is the multiple to which you want to round. <br> Regardless of the sign of a $\{\mathbf{0}\}$, a value is rounded down when adjusted away from zero. If the $\{0\}$ is an exact multiple of $\{\mathbf{1}\}$, no rounding occurs. | 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 bestfit regression line plotted through the known xvalues (independent set of arguments) and known yvalues (dependent set of arguments). | $\begin{aligned} & \text { intercept }(\{1,2\},\{3,2\})=4 \\ & \text { intercept }(\{-2.44,2,5,98,6\} \text {, } \\ & \{0.1,0.2,0.3,0.4,0.5\})=- \\ & 12.152 \end{aligned}$ |
|  | 1. 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, $\{y 1, y 2, y 3\}$ and $\{x 1, x 2, x 3\} ;\{y 1, y 2, \ldots y N\}$ and $\{x 1, x 2, \ldots$ $\mathrm{xN}\}$. |  |
| In | Returns the natural logarithm of an argument. Natural logarithms are based on the constant e (2.718281828459...). The argument is supposed to be positive. | $\begin{aligned} & \ln (10)=2.302585 \ldots \\ & \ln (1.23)=0.207014 \ldots \end{aligned}$ |
|  | (1) In is the inverse of the exp function. |  |
| $\log$ | Calculates the logarithm of an argument to the base that you specify. This uses the following syntax with two input parameters: $\boldsymbol{\operatorname { l o g }}(\{\mathbf{0}\},\{\mathbf{1 \}})$ where: <br> $\{0\}$ is the positive real numerical value or expression for which you want the logarithm. | $\begin{aligned} & \log (2,4)=0.5 \\ & \log (1.23,2)=0.298658 \ldots \end{aligned}$ |


| Name | Description | Examples |
| :---: | :---: | :---: |
|  | $\{1\}$ is the base of the logarithm. If the base is omitted, it is assumed to be 10 . |  |
| $\log 10$ | Returns the base-10 logarithm of a positive argument. | $\begin{aligned} & \log 10(1.23)=0.089905 \ldots \\ & \log 10(0.1)=-1 \end{aligned}$ |
|  | Returns the largest value in a set of values. |  |
| max | 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. | $\left\lvert\, \begin{aligned} & \max (1,2,3)=3 \\ & \boldsymbol{\operatorname { m a x }}(-2.44,2,5,98,6)=98 \end{aligned}\right.$ |
| median | Described in group-enabled functions. | $\begin{aligned} & \text { median }(1,2,3,4)=2.5 \\ & \text { median }(-2.44,2,5,98,6)=5 \end{aligned}$ |
| min | Inversely to max function, returns the smallest number in a set of values. All requirements of the max apply to $\mathbf{m i n}$ too. | $\begin{aligned} & \boldsymbol{\operatorname { m i n }}(1,2,3)=1 \\ & \boldsymbol{\operatorname { m i n }}(-2.44,2,5,98,6)=-2.44 \end{aligned}$ |
| mod | Returns the remainder after the argument is divided by a divisor. The result has the same sign as the divisor. Syntax: $\bmod (\{0\},\{1\})$ where: <br> $\{0\}$ is the argument for which you want to find the remainder. <br> $\{1\}$ is the value by which you want to divide the $\{0\}$. | $\begin{aligned} & \bmod (2,0.3)=0.2 \\ & \bmod (1.23,5)=1.23 \end{aligned}$ |
| pow | Returns the result of a number raised to a power. Syntax: power(\{0\}, \{1\}) where: <br> $\{0\}$ is the base argument. <br> $\{1\}$ is the exponent to which the $\{\mathbf{0}\}$ is raised. | power(2,3)=8 <br> power(1.23,5)=2.815305... |
| slope | Returns the slope of the linear regression line through data points in Xs 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. | $\begin{aligned} & \text { slope }(\{1,2\},\{3,2\})=-1 \\ & \text { slope }(\{-2.44,2,5,98,6\} \\ & \{0.1,0.2,0.3,0.4,0.5\})=112.88 \end{aligned}$ |


| Name | Description | Examples |
| :---: | :---: | :---: |
|  | (1. 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., $\{y 1, y 2, y 3\}$ and $\{x 1, x 2, x 3\} ;\{y 1, y 2, \ldots y N\}$ and $\{x 1, x 2, \ldots x N\})$. |  |
| stdev | The same as sd in group-enabled functions. | $\begin{aligned} & \operatorname{stdev}(1,2,3)=1 \\ & \boldsymbol{\operatorname { s t d e v }}(- \\ & 2.44,2,5,98,6)=42.772359 . . . \end{aligned}$ |
| sum | Described in group-enabled functions. | $\begin{aligned} & \operatorname{sum}(1,2,3)=6 \\ & \operatorname{sum}(- \\ & 2.44,2,5,98,6)=108.56 \end{aligned}$ |
| var | Described in group-enabled functions. | ```var(1,2,6)=7 var(- 2.44,2,5,98,6)=1829.47472``` |

## Layout Analysis Functions

Layout Analysis Functions are available only if the evaluation is associated with a layout.
Otherwise an error message displays.

## Layout Evaluation Functions

Layout Evaluation functions are provided to enable sample group references to be more flexibile.

The following table lists the layout evaluation functions:

| Name | Description | Example |
| :--- | :--- | :--- |
| GroupValue() | Returns the value of the sample group with the <br> specified type and group number (The type name <br> should be specified in quotes). | GroupValue <br> ("Unknown",1) |

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 wanted to reference the Unknown group that has the same number as the current position, use: GroupValue("Unknown", PosGroup())

## Position Functions

Position Functions are only available when there is a position associated with the expression being evaluated. They take no input parameters.

The following table lists the position functions:

| Name | Description <br> PosNum() <br> PosGroup() <br> Returns the 1-based position number of each position, <br> which is assigned in accordance with position <br> numbering. | Returns the 1-based group number of the sample <br> group at the position. For example, if the position <br> contains Unknown3, then the group is 3. |
| :---: | :--- | :--- |
| PosType() | Returns the sample type number associated with the <br> position. | PosNum() |
|  | Returns the 1-based replicate number of the specified <br> in the argument position. Replicate numbers are <br> assigned in accordance with position numbering. | PosReplicate |
| PosReplicate() | () | This function is based purely on the layout <br> and does not take flagging into account. |

## Layout Functions

These functions require an associated layout.

## Layout Function Parameters

## Type

Type can be specified as a sample type number or case-insensitive sample type name in quotes, e.g.:

- LayoutNumGroups (3)
- LayoutNumGroups ("Blank")
- LayoutNumGroups ("blank")
- LayoutNumGroups ("bLaNK")
(1) "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.

The following table lists the layout functions:

| Name | Description | Example |
| :---: | :---: | :---: |
| LayoutWidth() | The number of columns in the layout (note, this is same value for all containers). | LayoutWidth() |
| LayoutHeight() | The number of rows in the layout (note, this is same value for all containers). | LayoutHeight() |
| LayoutPositions() | The total number of positions (note, this is same value for all containers). | LayoutPositions() |


| Name | Description | Example |
| :---: | :---: | :---: |
| LayoutNumContainers() | The number of containers in the layout. | LayoutNumContainers() |
| LayoutNumGroups(Type, ContainerNum) | The number of groups with the specified type. Input parameters: Type, ContainerNu m. | LayoutNumGroups(3, 1) |
| LayoutNumPositions(Type, GroupNum, ContainerNum) | The number of positions with the specified type and 1-based group number (GroupNum). Input parameters: GroupNum, Type, ContainerNu m. | LayoutNumPositions("standard", $(3,1)$ |
| LayoutNumUsedPositions (ContainerNum) | The number of positions that have a type that is not unused (i.e., Type != 1). | LayoutNumUsedPositions(2) |
| Lay- | Determines | Lay- |


| Name | Description <br> the number of <br> groups of the <br> outNumGroupsAcrossContainers <br> specified Type <br> (Type) | parameter on <br> each of the <br> containers. If <br> this is the <br> same number <br> on every <br> container <br> (including 0), <br> then this <br> value is <br> returned. <br> Otherwise -1 <br> is returned. |
| :--- | :--- | :--- |

## Integration with Readers

## 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.

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, check 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 press 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:


- Measurement height:
- Standard (approx. 8 mm .)
$\bigcirc$ User defined: $\quad \mathrm{mm}$ from bottom $\quad(3.0 .18 .0 \mathrm{~mm})$

> Temperature level checking:
> $\Gamma$ Wam if plate holder temperature differs from 25

```
Ready
```


## 3. Select the Outputs and Events tab

4. Check the File output setting
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:
$\sqrt{\checkmark}$ File output


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<br>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:
"C:\Program Files (x86)\MyAssays\MyAssays Desktop\MyAssays.Desktop.Analysis.exe" "C:\Users\Darren Cook\Documents\MyAssays\Protocols\My Endpoint 12x8 Protocol (1).assay-protocol"
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" /importraw:<OutputFileName>

This would appear in the VICTOR measurements protocol editor as follows:
-Assay end system command -
$\begin{aligned} & \text { C: } \backslash \text { Program Files } \backslash \text { MyAssays } \backslash \text { MyAssays Desktop } \backslash \text { My Assays. Deshtop. Analysis. exe } \\ & \text { Protocols } \backslash \text { My Endpoint } 12 \times 8 \text { Protocol (1).assay-protocol" /import-raw: <OutputFileName> } \\ & \text { This command will be performed when the instrument has finished measuring the assay } \\ & \text { using the edited protocol. }\end{aligned}$
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.:

Assay end system command

C:\Program Files $\backslash$ MyAssays $\backslash$ MyAssays Desktop $\backslash$ MyAssays.Desktop.Analysis.exe
jls $\backslash$ My Endpoint 12x8 Protocol (1).assay-protocol" /import-raw: <OutputFileName> /calc
This command will be performed when the instrument has finished measuring the assay using the edited protocol.

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.

## EnVision Integration

The EnVision manager software can output data in many possible export configurations. To configure the EnVision manager software 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.:


## Command Line Arguments

MAA can be launched directly from the command line with optional specific arguments.

## Syntax

## >"C:\MyAssays Installation Root path\MyAssays <br> Desktop\MyAssays.Desktop.Analysis.exe" "C:\MyAssays Folder Root path\MyAssays\Protocols\Protocol File Name.assay-protocol" /argument1 /argument2 etc.

Command line arguments are only relevant when the MAA is opened with an .assayprotocol file and can be specified in any order.

The following table lists optional command line arguments:

| Argument | Description | Example |
| :---: | :---: | :---: |
| /calc | Performs specified calculations automatically (if /import-raw is used, then calculations are performed using the imported raw data). | /calc |
| /calc-log:\{0\} | Specifies a file to save calculation progress log. | /calc-log:"Destination file path" |
| /error-log:\{0\} | Specifies a file path to save calculation errors log. | /error-log:"Destination file path" |
| /exit | Closes MAA after calculations are completed/printed. | /exit |
| /export-report:\{0\}: <br> \{1\} | Specifies the export options. $\{0\}$ is either: <br> - XLSX, PDF, XML (file export type). <br> - XSLT. Requires additional arguments to specify output filename extension and path to XSLT 1.0 file. <br> The exported file will be saved | /export-report:pdf <br> /export- <br> report:xslt1:csv:"XSLT <br> file path" |



| Argument | Description | Example |
| :---: | :---: | :---: |
|  | protocol option is selected (under File \| Save in the Analysis application), then the changes will be saved to the protocol irrespective of this option setting (e.g., when calculations are performed). |  |
| /noappwin | If this is specified, then the application window is NOT displayed. | /noappwin |
| /print | Automatically prints the report (if the calculations succeeded) with the default printer (if available). | /print |
| /tab:\{0\} | Allows you to select the tab MAA starts on. $\{0\}$ is zero-based tab <br> number: Overview $=0$; <br> Measurements $=1$; Microplate $=2$; <br> Sample IDs $=3$; Results $=4$. If this option is not specified, then the first tab will open. | /tab:1 |

The maximum command line argument is 255 characters. If the command line argument exceeds this length, then a warning message is displayed and the program is exited.

To use long command line arguments, store the command-line argument list in a text file and launch MyAssays.Desktop.Analysis.exe, passing the text file containing the command-line arguments:
MyAssays.Desktop.Analysis.exe @<CommandTxtFile>
Where <CommandTxtFile> is the name of the text file to read the command line from.

## Examples

>"C:\MyAssays Installation Root path\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe" "C:\MyAssays Folder Root path\MyAssays\Protocols\Protocol File Name.assay-protocol" /import-raw:"Raw data file path" /tab:4 /calc /export-report:xlsx:nolaunch

The selected assay protocol with specified raw data file will be computed. The MAA will start with the Results tab and the XLSX report will be saved (but not automatically launched) under \MyAssays $\backslash$ Reports $\backslash$ folder.
>"C:\MyAssays Installation Root path\MyAssays
Desktop\MyAssays.Desktop.Analysis.exe" "C:\MyAssays Folder Root path\MyAssays\Protocols\Protocol File Name.assay-protocol" /calc /print /noappwin

The selected assay protocol with specified raw data file will be computed and the results will be printed out.

These settings can be configured using the Analysis Launcher.

## Tweak Files

This section provides information about the protocol tweaks feature. The protocol tweak files are specified as optional command-line arguments.

This is an advanced feature and misuse of it could cause problems.

## Overview

You may use tweak settings to define the data analysis parameters of a protocol customization. This enables any of the assay protocol parameters to be specified by other existing 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.

## Tweak Syntax

A protocol-tweak.xml file is a 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

With your working protocol-tweak.xml file, use your instrument control or LIMS software to insert relevant protocol-tweak.xml file's data and launch the protocol from the command line when required. These tweak changes are not automatically saved to the assay file, and 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.
It is possible to launch, execute (generate reports), and exit MyAssays Desktop Pro analysis without any user intervention required.

To achieve this, we recommend developing the protocol-tweak file as follows:

1. Build or obtain an assay-protocol file that meets your data analysis requirements.
2. Identify which analysis parameters can be specified by your existing software.
3. Develop a protocol-tweak.xml file.
4. Test the protocol-tweak.xml file.

Any data analysis parameter can be modified.

## How to: Add Protocol Tweaks

1. Launch the Command Prompt.
2. Enter the file path to the protocol tweak file as a parameter of the MAA command-line arguments.

OR
Add a protocol tweaks file in the Analysis Launcher.
The system will perform certain checks on the incorporated tweaks to detect possible configuration errors in common usage scenarios.

## 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 on the Copy icon or enter it manually to your publication.

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[^0]:    MyAssays Desktop can be installed and run alongside the legacy software WorkOut. Please refer to Installing Alongside WorkOut for further details.

[^1]:    Unknown

