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MyAssays Desktop

User's Guide

www.myassays.com

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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 customise 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 detail 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 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 the whole 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 task 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 as a resource for providing further details as and when you need them.

Features

Supported Measurements

MyAssays Desktop is designed to process measurement data from any microplate or rack-based reader. In addition, it can import and analyse 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 665nm and 620nm can be imported and analysed (perhaps with a ratio calculation). Even more exotic measurements 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 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
- 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 Data Labelling
    - by name
    - by colour
    - 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 section.

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

Result Labelling

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 labelling to define your own rules accordingly.

Validation

Add automatic checking of measurements. 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, linear regression (plus legacy methods such as cubic spline, smoothed spline, cubic regression, point-to-point and many more)
- Fit data to your own user-defined curve fitting equation
- Best-Fit feature automatically compares multiple fit methods and applies the best (with customizable scoring methods)
- Goodness of fit measures reported: R^2, aR^2, SE, F-statistic, P-value (and available for further automatic scrutiny such as validation messages or best-fit scoring)
- Automatic computation of LLOQ, ULOQ, LOD based on customizable precision and accuracy thresholds
- View computed curve-fit equations in mathematical symbolic notation

Reporting

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

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

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

Excel Objects

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

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

Report Templating with Word

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

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

Export

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

- Export to XLS/XLSX/PDF/DOCX/TXT/CSV/HTML/XML
- XSLT support is provided enabling custom export definitions to be created for exacting output as required by your existing system.
- Specify the export destination folder
- Specify the naming convention of the output files, including references to imported meta data. For example, name your output files to match a barcode imported along with your measurement data).
- Configure a protocol to automatically export with these settings so no user-intervention is required.

Workflow Integration

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

For routine data analysis, your reports can be generated without any user-interaction required at all. For example, MyAssays Desktop data analysis can be performed completely automatically, with data (including any combination of measurement data, sample IDs, parameters, etc.) being imported, analysed and 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, in fact 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, utilise 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

There are three editions of MyAssays Desktop offering differing levels of functionality:

Standard: Operates only with preconfigured protocols (either those included in the installation package or through new or existing protocols available via MyAssays.com). This edition allows tweaking limited protocol parameters (such as fit method, sample concentrations, layout, etc.).

Pro: Includes all of the features of the Standard edition plus functionality for creating new custom protocols. Also, selected preconfigured protocols can be edited or extended. 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.

Enterprise: Includes all of the features of the Pro edition plus functionality for uploading and publishing protocols to MyAssays.com for online sharing.

Edition Comparison

Feature	Standard	Pro	Enterprise
Downloadable Protocols (from myassays.com)	✓	✓	✓
Preconfigured Protocols (96/384 versions):	✓	✓	✓
• ELISA	✓	✓	✓
• DNA / Protein Quantification	✓	✓	✓
• ATP lite protocol	✓	✓	✓
• Generic DELFIA	✓	✓	✓
• Generic LANCE	✓	✓	✓
• Generic Fluorescence Polarization protocol	✓	✓	✓
• Monochromator spectral	✓	✓	✓
• Kinetic for Ca2+	✓	✓	✓
• Bacterial growth	–	✓	✓
Import Script Support	✓	✓	✓
Excel Import	✓	✓	✓
Worklist Import	✓	✓	✓
Data Visualisation (3D View/Heatmap/Kinetic Overlay/Spectral Plot)	✓	✓	✓
Versioned Analysis	✓	✓	✓
Export to XLSX/DOCX/PDF	✓	✓	✓
Edit Protocols	Limited	✓	✓
Report Customisation	Limited	✓	✓
Custom Export (e.g. for LIMS)	–	✓	✓
Multiple Plate Support	–	✓	✓
Create New Protocols (New Protocol Wizard)	–	✓	✓
Matrix-Transform Data Analysis	–	✓	✓
Custom Validation Rules	–	✓	✓
Custom Evaluation Expressions	–	✓	✓
Best Fit	–	✓	✓
PLA	–	✓	✓
Publish and Share Protocols Online	–	–	✓

Getting Started

Installation

System Requirements

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

CPU:	Intel/AMD 2 GHz or faster processor (32-bit or 64-bit)
Memory:	2GB RAM
Available disk space:	300MB
Operating Systems:	Windows 10, Windows 8.x, Windows 7, Windows Vista, Windows XP SP3
Other software:	Microsoft .NET 4.0.3 or later
Display:	1024 x 768 or higher-resolution

Installation Process

Please visit the MyAssays website resource Introducing MyAssays Desktop to download the latest version.

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 are required to 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.

Activate MyAssays Desktop with your product serial code and activate your license in order to start working with the application.

Launching

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

On Windows 10:

Choose Start, 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 open MADE faster, pin it to your Start screen or the taskbar on your desktop. Right-click on application's name and choose either Pin to Start or Pin to Taskbar.

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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-myassays-desktop.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

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-multiplex-analysis.video

Folder Poll

- https://www.myassays.com/folder-poll-with-myassays-desktop.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, user ID. We refer to this data as meta-data. The software can import and repot 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 imported for supported 3rd 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 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 with colleagues.

Results

Each time an assay protocol is launched and results 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 different 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:

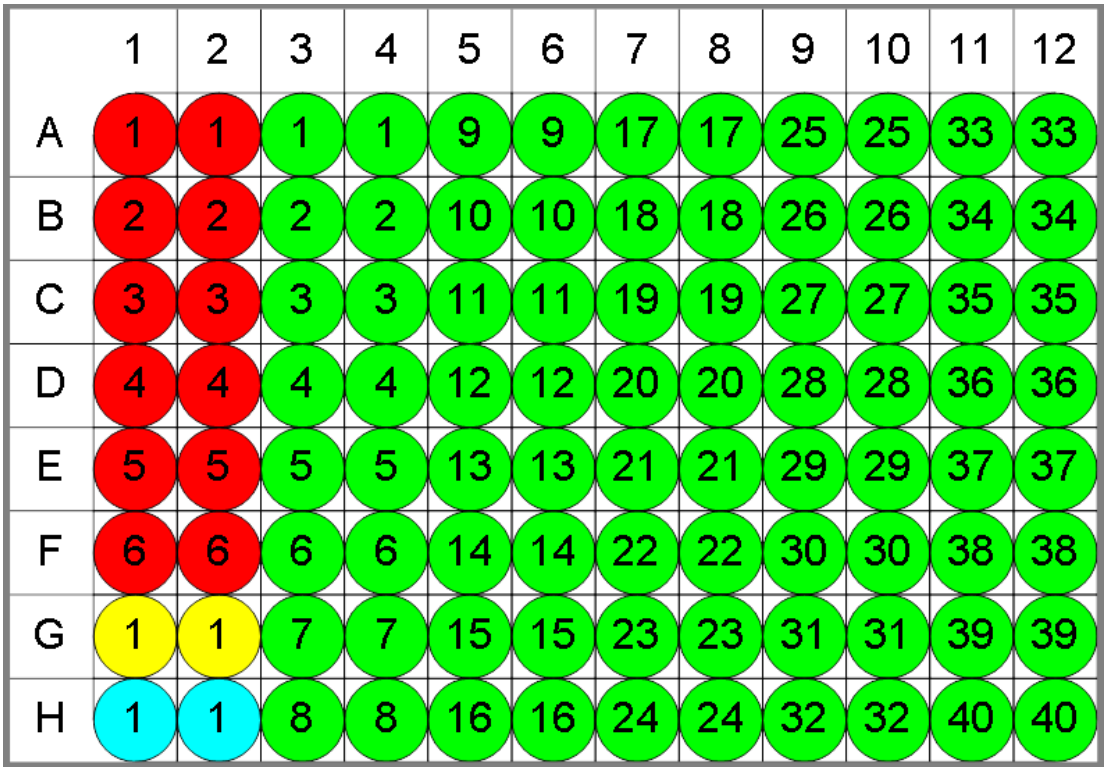
- Unknown – samples to quantify or qualify
- Standard – samples with a known quantity used for preparing a calibration or standard curve
- Control – samples used for control purposes such as inter-assay or inter-assay quality control
- Blank – a sample without any expected response used to remove background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

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

With MyAssays Desktop we use a colour to indicate sample type:

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.). I.e.



The use of a sample layout introduces a convenient layer of abstraction over the measurement data. For example, being able to refer to e.g. **Control1** 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 organise 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 amount 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 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 MyAssays database.

It also features 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** screen 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. Working with License chapter describes further details for these options.

- **View** defines whether Measurements Tab is displayed on the Folder Side Bar and Launch Assay Protocol with Options setting is displayed on preview pane in the Protocols tab.
- **Data** displays the storage path for persisting you 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 location, if its size is not fullscreen;
- **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 the **Show Quick Access Toolbar Below/Above the Ribbon** (depending on its current location), **Minimize the Ribbon** and change 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 MyAssays **Data Folder Root**. These tabs point to actual Windows folders.

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

> MyAssays Desktop arranges your data automatically in correspondent folders so that you can easily manage, share and backup your assets. You may prefer to customize how results files are named and where your data is to be 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.** *(*.TXT, *.CSV, *.XML, *.DAT, *.XLS, *.XLSX and others)*
Results	Assay results files with .assay-results extension.
Layouts	Layout files with .assay-samplelayout extension.
Reports	Report files with supported **report extension** *(*.DOC, *PPT, *.XLS, *DOCX, *XLSX, *PPTX, *.MHT, *.HTM, *.PDF)*

Selecting a tab displays its content in the main window.

File and Preview Panes

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

File Pane

List of available data files displays on the left side of 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 the 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 tabs 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 handy, when working with big data sets or with multiple versions of analyses. All sub-folders will be of the same type as their primary parent. To create a new sub-folder 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 depends on the type of file selected:

Folder Tab	Preview Pane Contents
Search Results	A summary of Assay Protocols, including the name, the instrument settings, the position used and layout and also any configured transformations.
Protocols	
Measurements	Pre-canned and custom raw data files.
Results	Comprises of two assets: • **Overview** with the assay protocol summary • **Latest Report** with the latest report of the results.
Layouts	A microplate control showing each plate layout in the layout.
Reports	Displays the preview of the PDF reports.

Welcome Screen

This is the screen that displays as you launch MADE. It contains a handful of useful options for proficient start. Get acquainted with MyAssays Desktop Explorers basic functions and begin your work on full speed.

Left pane of Welcome screen consists of:

- **Start.** Shortcuts to basic data analysis options, particularly, New Protocol..., Launch Protocol... and Open Results....
- **Recent.** Displays specified number of assay protocols and results you have worked with last. The particular title will be launched in MAA upon selection.

You can customise number of entries in **Recent** list or clear file history in Data options.

Right pane comprises of two subpanes:

- Upper subpane **Discover MyAssays Desktop** displays links to the detailed review of MyAssays tools and 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, which will help you familiarize yourself with MyAssays Desktop and its components.
  - **Support.** Contains link to **MyAssays Support** contact form and Request an Assay Protocol dialog box.

Recent Used Files Feature

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

To change the number of Recent files type it in the corresponding box or use 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 the 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 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.

To see all available assay protocols, paste "**@all**" in a search textbox.

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, which contain a keyword you have entered.

To specify the search results and ensure finding the protocol you look for, each of them 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 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 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 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 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 to online MyAssays.Com webpage of the selected assay protocol.

No Results Found

If the assay you are looking for is not yet in 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 MyAssays.com knowledge base on your PC.

Submit a Search and explore search results options of constantly evolving protocols database.

Protocols Tab

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

Only data files with .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 kit manufacturer.

In **Protocols Tab** you can:

To Create New Assay Protocol:

In MADE Welcome Screen click on **New Protocol...**.

OR

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

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

To Launch Assay Protocol File:

Navigate to 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 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 visual representation of supported command line options will appear.

How to: Launch Assay Protocol with Command Line Options:

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


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

If it is checked, corresponding option appears on preview pane of the Protocols tab upon protocol file selection.

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 a MADE Ribbon select **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 to MyAssays knowledge base.

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

You can and are welcome to attach any of 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

To View the Measurements Tab:

1. Launch MADE.
2. Select **File**tab of MADE Ribbon.
3. Select **View** screen.
4. Check the **View Measurements** checkbox.

The **View Measurements** state (checked/unchecked) persists between sessions.

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

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

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

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

Results Tab

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

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

Only assay results data files with .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 assay summary and may contain a link to Booklet Kit from manufacturer. The **Latest Report** contains the report of the selected Assay Results file.

To enlarge Preview view, clasp **Ctrl** button and push mouse scroll wheel upward.

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

Open Existing Results

How to: Launch Assay Results File:

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

- double-click on its title;
- tick the **Open** icon on the MADE Ribbons **File** group.
- tick 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.

Only data files with .assay-samplelayouts 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 files 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 Quick Access Toolbar

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

Location

You may prefer Quick Access Toolbar to be displayed above or below the Ribbon. Right-click 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 **Home**, **Tools** or **Support** tab and right-click on it. In a drop-down menu that will appear, hit on **Add to Quick Access Toolbar** command. Upon doing that, the command will be displayed in Quick Access Toolbar.

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

Advanced customizing

You may consider customizing Quick Access Toolbar to fully match your preferences. To call 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 Quick Access Toolbar and click on **More Commands** command.

Upon doing this a dialog box will appear. Select tools you prefer to be displayed 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 on arrows on the right side of the **Quick Access Toolbar** list.

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

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

Customizing 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, create custom tabs and groups with your preferred commands.

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

Minimize Ribbon

This option may be useful to expand 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 the Minimize Ribbon in a 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 **Layout Selection** pane of MAA **Microplate** tab. You can also create 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, eg. **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 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 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 position per group using the entry box.

Group numbering must start from 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 content with your changes, press the **Save + Close** button. This will save new layout to your Layouts tab and make it available to relevant assay analyses.

Multiple Plate Options

If you have selected Multiple Plate option or are editing 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 empty plate.
- **Remove Plate** - removes selected plate.
- **Duplicate plate** - copies selected plate with all defined changes.

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 each and 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 check 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 which 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.

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.

> 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 **Home** tab of the **MAA Ribbon**.
3. Select a 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.

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 {n} (pending)** label is displayed in the **Current Version selector**.

Unsaved Changes

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

This also applies to assay-protocol with no calculated changes.

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

Save Options

You can basically 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.

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 ticked.

- **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 opened 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. For example, to arrange all results into sub-folders 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 customise the naming method and target path manually, using macros or combining these approaches.

How to: Set Custom Results Naming

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

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

- Provide full path to the folder in the textbox (manually or from clipboard).
- Click **Browse...** button to provide the full path to the folder in **Browse for Folder** tree view. Press **OK** to save path or **Cancel** to close the dialog 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 **Browse...** option and use <ProtocolName><CurrentDateShort> macros from **Manage...** to specify folder name*.

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

- Type in 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 analysis type and date it was performed*.

If **Test settings when OK is clicked** checkbox is enabled, MAA will check 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 without any updates.

New Protocol Wizard

How to: Launch New Protocol Wizard:

1. Launch MADE and do one of the following:
2. Select **New Protocol...**option on MADE Welcome Screen.
3. Select **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 on the upper-right of the New Protocol Wizard window to discard all changes and exit.

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

Analysis Launcher

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

The Launcher includes:

- Controls for browsing and selecting an assay protocol, measurement data, Sample IDs and protocol tweaks files.
- Various user-friendly controls for selection of command line arguments.
- A text-box showing the full command line of the current selection.
- **Copy to clipboard** button that copies built command line with selected controls to clipboard.
- **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 **Analysis Launcher** button on the Tools tab in the **Utilities** group of the MADE Ribbon.
- Enable Launch Assay Protocol with Options feature and press the **Launch Assay Protocol with Options** button.
- Launch **MyAssays.Desktop.Analysis.Launcher** application under **MyAssays/MyAssays Desktop/** installation root folder.

If you run application from installation root, specify 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 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, which is shared with other users of the system.

How to: Set an Assay Data Folder Root:

In 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 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

Visualising Data

Heatmap Plate View

The **Heatmap View** displays a plate layout coloured in accordance with the measurement data numerical values. For example, data with smaller numerical values is depicted in dark green and data with larger numerical values is shown in red.

How to: Access the Heatmap View:

1. In MAA, select the **Measurements** or **Microplate** tab.
2. Tick the **Heatmap View** option in the lower left corner of the right pane.

Heatmap view is relevant for endpoint data only.

Structure

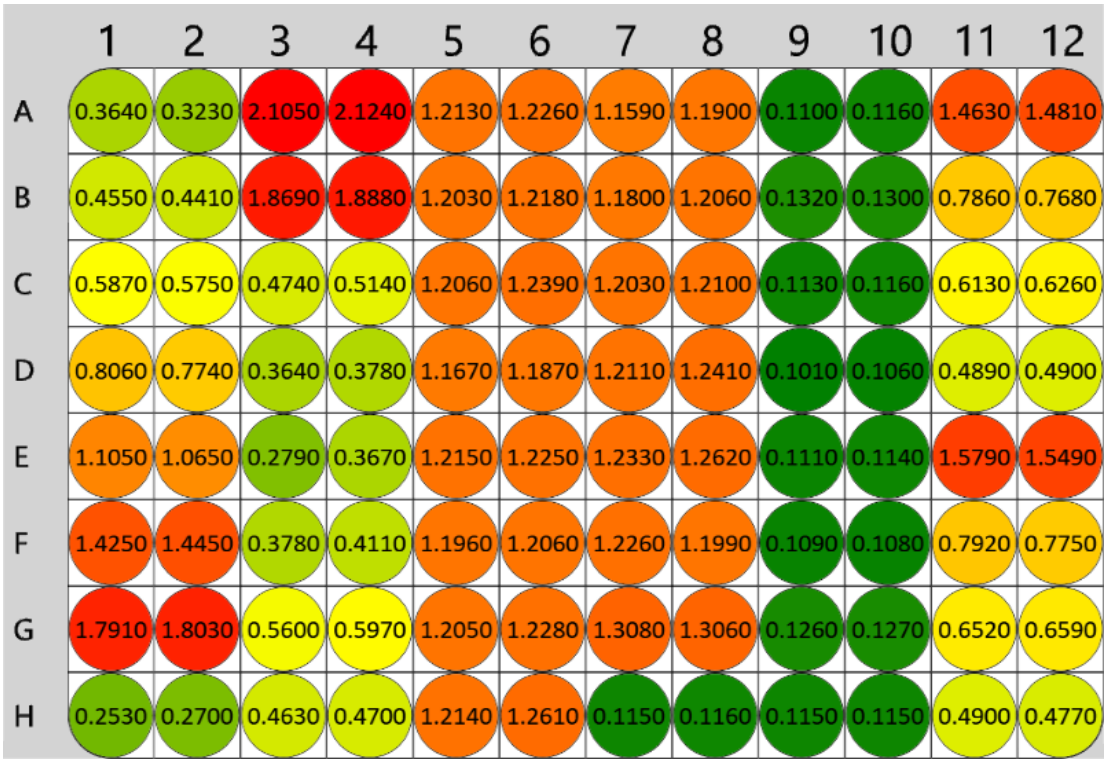
Heatmap view comprises:

- plate preview with colour of each position based on its numerical value converted to a colour within a given scale;

  Data for **Unused** positions is not displayed, the wells appear white and empty.

- heatmap scale (located under plate preview) with clickable minimum and maximum controls;
- scale function menu, which determines the heatmap scale type (linear or Log10);
- auto scale option;
- 2D/3D view buttons;



	1	2	3	4	5	6	7	8	9	10	11	12
A	0.3640	0.3230	2.1050	2.1240	1.2130	1.2260	1.1590	1.1900	0.1100	0.1160	1.4630	1.4810
B	0.4550	0.4410	1.8690	1.8880	1.2030	1.2180	1.1800	1.2060	0.1320	0.1300	0.7860	0.7680
C	0.5870	0.5750	0.4740	0.5140	1.2060	1.2390	1.2030	1.2100	0.1130	0.1160	0.6130	0.6260
D	0.8060	0.7740	0.3640	0.3780	1.1670	1.1870	1.2110	1.2410	0.1010	0.1060	0.4890	0.4900
E	1.1050	1.0650	0.2790	0.3670	1.2150	1.2250	1.2330	1.2620	0.1110	0.1140	1.5790	1.5490
F	1.4250	1.4450	0.3780	0.4110	1.1960	1.2060	1.2260	1.1990	0.1090	0.1080	0.7920	0.7750
G	1.7910	1.8030	0.5600	0.5970	1.2050	1.2280	1.3080	1.3060	0.1260	0.1270	0.6520	0.6590
H	0.2530	0.2700	0.4630	0.4700	1.2140	1.2610	0.1150	0.1160	0.1150	0.1150	0.4900	0.4770

Heatmap View Settings

Minimum and Maximum Controls

These settings allow you to set the colour scheme range displayed on the Heatmap plate preview. Each position on the layout is coloured according to its numerical value and the colour scale (using the colour range min/max values). Values outside the range are rounded to the nearest min or max colour.

How to: Change the Minimum Value:

1. Hover and click on the minimum value on the left side of the colour bar to edit the Heatmap minimum value.
2. Type in a minimum value for the Heatmap. For example, 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 the maximum value (right side of the colour bar) to edit the max value.
2. Type in a maximum value for the Heatmap. For example, 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 right hand 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 colour scale.
    - **Linear scale** – click on the **Linear scale button** (left one). The Heatmap is refreshed to display a Linear colour scale.

Auto Scale

The **Auto Scale** setting allows you to automatically scale the plate preview, if the minimum and maximum values are changed for a set of measurement data. For example, if you type a custom maximum value in the heatmap maximum control and then change the measurement data, the heatmap view will be updated with the original scale.

If you select the Auto Scale and there is a change in the measurement data, the heatmap view is updated using the new scale. In this case if the edited measurement data has a new min/max then the heatmap scale is updated accordingly.

How to: Access the Auto Scale

1. With the Heatmap View turned on click on the **Auto Scale** button (fon the right most 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 **Measurements**or **Microplate** tab.
2. Tick 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

The flagging feature is used to mark and indicate data to exclude from further analysis. This is useful for identifying outliers to ignore such as bad measurements or data for incorrectly prepared or contaminated samples.

There are two type of data that can be flagged:

- Position
- Point

For all measurements types any position can be marked as flagged (e.g. position **A1**). When the data at a position is flagged, any reference to the sample contained at that position will not include the flagged position's data.

For example, if **Standard1** comprises of 3 replicates measured at position **A1**, **A2** and **A3**, if position **A1** is flagged, **Standard1** would refer to only the not-flagged values, i.e. the average of the data at positions **A2** and **A3**.

For kinetic or spectral data any specific data point can be marked as flagged too (e.g. the data point for cycle 1 of position **A1**). Any flagged data points are not included in any further analysis. If all points of a position are flagged then the position is considered to be flagged.

For example, if the kinetic measurement data at position **A1** comprises of 10 cycles, if point 1 is flagged then a kinetic reduction operation is performed (such as computing the average of kinetic cycles in XY Reduction Average), 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 customise how flagged data is labelled in the report.

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 there result will be marked as flagged (as no further calculation is possible).

Advanced

All transforms include a setting under the **Advanced** properties group for selecting which sample types the transform should calculate results for. For those samples that are not to be calculated, the results can be set to be flagged as either:

- **Flagged with Value**
- **Flagged no Value**

Flagged Data in the Report

The report will indicate flagged data as strikethrough text (such as ~~**1.23**~~ or ~~**Flagged**~~). Where data has been flagged and there is a value associated with it, the original value appears in strikethrough.

Where there is no value associated the text Flagged appears (also in strikethrough).

For example,

Sample	Positions	Raw	Concentration
Unknown1	A3	~~1.599~~	1.53791
	A4	1.665	

Here, position **A3** has been flagged. In this case the calculation of the concentration will use only the value from position **A4**.

Here the **Raw** values in positions **A3** and **A4** have been flagged. This means that there is no result for the **Concentration**

Sample	Positions	Raw	Concentration
Unknown1	A3	~~1.599~~	~~Flagged~~
	A4	~~1.665~~	

Flagged Data in Text-Based Exports

For text base export (such as CSV, TXT) where strikethrough is not available, flagged data is identified by asterisk symbols surrounding each flagged data item, e.g.

1.23

Flagged

For example, the following export text shows three data values flagged:

```
Sample,Positions,Raw,Concentration
Unknown1,A3 A4,*1.599* *1.665*,*Flagged*
```

Custom Flag Label

If the default strikethrough text "**Flagged**" is not suitable, you can specify your own text to use instead. For example, here the text **No result** is used instead of Flagged.

Sample	Positions	Raw	Concentration
Unknown1	A3	~~1.599~~	No result
	A4	~~1.665~~	

This is an advanced setting that can only be configured through the XML editor. For more information please refer to custom flag label configuration.

Custom Flag Label Configuration

The Custom Flag Label feature enables specific labels to be defined and used to indicate flagged results instead of the default strikethrough flagged text (such as ~~**1.23**~~ or ~~**Flagged**~~).

The settings are available at different levels of the Matrix-Transform Analysis configuration; this provides a fine degree of control over how flagged results are reported. For example, you may prefer to label flagged raw data differently to flagged concentration results.

Additionally, the Standard Curve Fit transform supports conditional flagging and labelling. 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 to **Labelling** setting of Matrices Configuration 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.
2. Locate the **Transforms** element.
3. Add an **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.
2. Locate the **Transforms** element.
3. Locate **Output** element.
4. Add an **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) is 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 1 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.

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 following settings you can configure whether and how they are displayed.

General

Name	A title to be used for matrix in headers of the Sample Table and Matrix Table. If it is not specified, then the default title is used.

Numerical Formatting

Precision	A number of significant digits to be displayed for a numerical value. Precision gets a particular meaning only in combination with **Type** setting.
Type	Specifies the precision and rounding option to represent results. This can be

	expressed in terms of: • **Significant figures** – the effective figures that express a magnitude to a specified degree of accuracy that does not take decimal point into account. This accepts Precision values in range 1 through 14. • **Decimal Places** – the number of digits to the right of the decimal point. This accepts Precision values in range 0 through 14.

Report Contents

Include in Matrix Tables	It defines whether associated matrix should be included in the Matrix Tables.
Include in Sample Tables	It defines whether associated matrix should be included in the Sample Tables.
Matrix Table Ids	It defines in which Matrix Table(s) the associated matrix should be included.
Sample Table Ids	It defines in which Sample Table(s) the associated matrix should be included.
Sample Table Rep-licates	Determines how replicates of each sample group are included in the Sample table: • **Average** - the average value of all replicates is displayed. This applies to Endpoint data only. • **List** - all replicate values are included in the table. • **First** - only the first value is displayed. This simplifies view of transforms, that result in the same values for all replicates of each sample 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.

Labelling

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.

This feature is described in Labelling Samples topic.

Value Bars

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

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

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

Validation

Fundamentally, any change in measurements may affect the performance characteristics and should be validated. Thus, inherent in generating quality analytical data is to support these with a quantification of the parameters of confidence.

You can verify a set of rules that can be performed on the matrices containing endpoint data (raw or calculated). You can not add validation to the XY data notwithstanding configure validation rules for **XY Reduction** transform results.

For example, a validation condition can be created that tests that the %CV of the replicates of a control is < 15.

Each test verifies if the validation condition is satisfied or rejected and outputs **Pass** or **Fail** result, respectively. The rule for each condition is determined with an expression.

How to: Add Validation to the 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.
4. Press the **Add** button on **Tables** pane.
5. Review and edit the validation's properties as required.

Validation conditions can be performed on any endpoint matrix. Specify which matrix of data to use (you may want to use a raw or calculated matrix). Under the Validation tab you can add, edit, and remove validation conditions.

Configuration

Validation tab consists of three panes. Inside you can add to the transform 1 or more Validation Tables that display the results of 1 or more various validations.

- **Tables Pane**

Inside of this pane you can arrange the number of tables to be included in the report. These are used to store finite number of results grouped into separate tables. You may prefer to include all conditions in one single table or split them between multiple tables. Use **Add** and **Remove** action buttons to set up tables as required.

- **Conditions Pane**

For each Table you can **Add** or **Remove** Validation Conditions as required with corresponding buttons. Use **Up** and **Down** buttons to rearrange their order.

Within this pane you can specify following parameters:

Description	Optionally added textual description of the expression. If this is not specified, the default description is used in report.
Matrix	This selects which matrix (raw or calculated) to compute. If there is no available matrix (e.g. all matrices contain XY data), the **(NA)** label is displayed.

- **Conditions Configuration Pane**

Evaluations are performed with settings, provided for each Validation table's condition. Within this pane you set a validation rule to evaluate for selected matrix. This includes **Expression** to verify, validation **Type** of expression to process and **Types** of samples to include in evaluation.

General

Expression	Sets the rule for a boolean condition to be verified. Typically it is a conditional function or an expression with a logical operator.
Type	This specifies whether x variable is processed and associated with the position or group on the layout. This can be: • **Position** - the expression is evaluated for every position on the matrix of every container. • **Group** - the expression is evaluated for every group on the matrix of every container. • **Single** - the expression is evaluated once by itself and has no x variable.
Types	It allows to conveniently select which sample types the validation should apply to. The default meaning is **All**, i.e. all sample types defined on the layout. Uncheck the types you do not want to be processed.

With **Position** and **Group** evaluations, the expression may be evaluated multiple times (e.g. on every position). If the evaluation fails, then only the first failure is reported.

Validation Results

Validation rules are verified when you press **Calculate** button.

Each validation verifies the result in terms of boolean condition. Therefore, the result can be either **Pass**, **Fail** or **Inconclusive**. They are evaluated after transforms because the conditions may refer to the calculated data.

The result is:

Pass

If the validation results to **True** and does not equal 0. For **Position** and **Group** type, the result is only **Pass** if all evaluations evaluate to true.

Fail

This displays if the validation results to False and equals 0. For **Fail** the whole row appears with yellow background. For **Position** and **Group** type if any fail then **Fail** is reported.

Inconclusive

If the Expression contains syntax error (e.g. expression contains variable with **Single** type selected), the result is treated as **Inconclusive** with corresponding message shown in **Results** column.

The results of the validations are included in the calculation log and any crush appears in the error log.

Reporting Validations

All validations are evaluated (irrespective of whether they are included in the report). You may configure how and if the Validation Tables are reported.

Examples:

Here are some examples of valid rules and descriptions of their behaviour. **{0}** in these refers to any numeric value or an expression:

Rule	Validates whether
Unknown1>{0}	The average of the non-flagged **Unknown1** position values on the layout are greater than specified **{0}** value.
sd(Unknown)<{0}	The standard deviation of the non-flagged **Unknown** position type values on the layout is less than specified **{0}** value.
***x>{0}**	The value of variable **x** is greater than than specified **{0}** value.
***and(x<{0},Control<{0})**	The value of variable **x** and average of the non-flagged **Control** position type values on the layout is less than specified **{0}** value.
pcv (Unknown1)<>{0}	The percentage coefficient of variation of **Unknown1** is not equal to specified **{0}** value.
Blank1+(3*sd (Blank1))<{0}	The average of the sum of **Blank1** and tripled standard deviation of **Blank1** is less than specified **{0}** value.
median (Standard1)<1	The median of the non-flagged **Standard1** position values on the layout is less that 1.
***x-Blank1<>0**	The value of variable **x** minus the average of **Blank1** position does not equal 0.

Rules, that contain **x** variable and do not apply for **Single** type are emphasized with an asterisk (*****).

Evaluation

Evaluations can be described as calculating important information from particular analysis run (e.g. lower limit of detection (LLD), standard error, etc.). This might be useful to estimate the need for further adjustments and keep assay analysis sufficiently accurate.

Each evaluation executes an expression and results in evaluated value.

This option is relevant for endpoint data (raw or calculated) only. You can not define evaluations for XY data notwithstanding process data from **XY Reduction** transform results.

How to: Add Evaluation to the 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.
4. Press the **Add** button on **Tables** pane.
5. Review and edit the evaluation's properties as required.

Configuring Evaluation Settings

You can add to the transform 1 or more Evaluation Tables in the Evaluations tab. These tables display the results of 1 or more various evaluations typically defined by expressions.

Evaluation tab contains 3 panes in which you can configure relevant settings.

- **Tables Pane**

Inside of this pane you can arrange the number of tables to be included in the report. These are used to store finite number of results grouped into separate tables. You may prefer to include all conditions in one single table or split them between multiple tables. Use **Add** and **Remove** action buttons to set up tables as required.

- **Evaluations Pane**

For each Evaluation Table you can **Add** or **Remove** Evaluations as required with corresponding buttons. Use **Move Up** and **Move Down** buttons to rearrange their order. Within Evaluations pane you can specify following parameters:

Description	Optionally added textual description of the expression. If this is not specified, the default description is used in report.

Matrix	This selects which matrix (raw or calculated) to compute. If there is no available matrix (e.g. all matrices contain XY data), the **(NA)** label is displayed.

- **Expression Configuration Pane**

Within this pane you define the values to obtain from data of the selected matrix. This includes **Expression** to evaluate and **Numerical Formatting** to use for the result.

Settings

Expression	Determines the set of mathematical operations to be computed. The defined expression is then evaluated once by itself and may contain no **x** variable.

Numerical Formatting

Precision	A number of significant digits to be displayed for a numerical value. Precision gets a particular meaning only in combination with **Type** setting.
Type	Specifies the precision and rounding option to represent results. This can be expressed in terms of: • **Significant figures** – the effective figures that express a magnitude to a specified degree of accuracy that does not take decimal point into account. This accepts Precision values in range 1 through 14. • **Decimal Places** – the number of digits to the right of the decimal point. This accepts Precision values in range 0 through 14.

If **Numerical Formatting** is not specified, then the associated with the selected matrix settings are used.

Evaluation Results

Each evaluated expression results in a single numeric value.

The calculations are computed after transforms as the **Expression** may refer to the calculated data. If there is an error in the evaluating expression, then the error message is used as the result and is displayed in the table.

All defined Evaluations are calculated irrespective of whether they are included in the report. Evaluation results are included in the calculation log and any crush appears in the error log.

Reporting Evaluations

You may configure how and if the Evaluation Tables are reported.

Report Customisation

Accurate reporting of analysed data is important element in research. This subsection describes how to customise your reports using plenty of report elements.

Overview

Report is a summary of all of the calculation results. This option makes reporting your MyAssays output more versatile as you can select which elements to include.

The Report tab is used to configure report settings and customise any of the optional report items that are available for inclusion in the report.

How to: View Report Customisation 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.
4. Review and edit the report's elements as required.

General Report Configuration Settings

You can add to the transform various report elements that are generated from a Matrix-Transform analysis and customise the output in **Report** tab.

Report tab consists of two panes in which you can configure relevant properties.

- **Reports Pane**

This tab manages quantity and order of the report elements. Click on **Add Element** button to include an item from a drop-down list in report or **Remove** to exclude it. Select the element and press **Move Up** or **Move Down** button to change ordering of selected report item in the report.

- **Report Configuration Pane**

This pane contains general and specific options for each report element. Former, applicable to all report content, are described here while latter are covered in each relevant topic specifically.

General

Id	Optionally added custom ID for each report element. If it is not specified, the default ID is used. This ID can be used for configuring custom report templates and/or in advanced report configuration.
Include	With this checkbox you define whether element should be included in report.
Title	Optionally provided heading for a report element, which when specified, the title appears immediately before the element (with no spacing). This property can contain report macros. If it is not specified, then the element is displayed without title.

Sheet

Sheet Name	This specifies custom heading for Excel export. If **Sheet Name** is defined for one report element, then the report content is exported on 1 sheet with provided **Name**. Each report element with different **Sheet Name** is exported to a separate sheet. For each element a report macros can be specified.

Report Elements

All available report elements are listed in alphabetical order and summarised here.

The transform may output more report items than is listed here, but only those listed here can be included in the report.

How to: Add Element to the Report

1. Open the **Report** tab.
2. Select element from the **Add Element** drop-down list in the **Reports** pane.
3. Review and edit elements' settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

Evaluations Table

This element displays results of various evaluations calculated alongside transforms. It applies only to endpoint data, either raw or calculated. More...

Layout

The Layout report element is a graphical representation of the layout. It includes a layout and a sample type legend, which shows the sample types that are included in the layout. More...

Matrix Table

This is table(s) that display(s) the matrix data, either raw or calculated, in an orientation that matches the layout.

Matrix View

This report element gives a layout-based graphical representation of matrix data. Each **Matrix view** displays the data (endpoint or kinetic) of a specified matrix, using colouring as either layout or heatmap and a sample type legend.

Measurement Meta Data

This is simply a group table listing the measurements meta data in two columns.

Notes

Contains any notes you enter on a particular assay run.

Sample Table

The Sample Table lists the details of the calculations for each of the samples. A report can contain 0 or more Sample Tables. Each Sample Table can be configured to contain certain matrices of data and/or certain types and any additional report columnar content.

Transform Content

Additional report content (diagrams, charts etc.) produced by certain transforms. Depending on the configured transforms, content may be added here. For example, a Standard Curve Fit transform adds a concentration table, chart and additional evaluations.

Validations Table

It displays the results of validations defined for raw or calculated data. This option applies to endpoint matrices only. More...

Report Templating

For page-based reporting you can define a reporting template to apply to your MyAssays Desktop output. This can include headers, footers, custom images, fonts, macros, signature line, etc.

Evaluations Table

Each Evaluations Table lists the results of evaluations, which were performed alongside particular assay run. For further details on the operation itself please see Evaluations section.

Evaluations Tables Report Configuration

A report can contain one or more Evaluations Tables, which when each Evaluation is added, are included to Reports elements list automatically.

You can configure how they appear in the report using general applicable to all report content and specific for evaluations options. Former are described in the Report customisation topic while here the latter are covered.

How to: Add Evaluations Table Element to the Report

1. Open the **Report** tab.
2. Select Evaluations Table element from the **Add Element** drop-down list it the **Reports** pane.
3. Review and edit settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

By default the Evaluation data is displayed as a three-column table. The columns output **Description**, **Expression** and **Results** of each defined Evaluation.

The number of rows in the table corresponds to the number of Evaluations added. The **Results** for each of them contains the numerical value of the evaluated result.

Evaluations Table

While the **Results** are definitely included, you might prefer to hide former columns by unchecking corresponding checkboxes.

Include Description	When checked, the column contains **Description** if specified or **Expression# {index}** if it was not.
Include Expression	If included, outputs the **Expression** defined for each **Evaluation**.
Include Header	Determines whether the row with title for each column is displayed.

Layout

This element simply adds an image of the layout used in the assay to the report. This image covers a layout and a legend, which includes the sample types that are included in the layout.

How to: Add Layout Element to the Report

1. Open the **Report** tab.
2. Select Layout element from the **Add Element** drop-down list it the **Reports** pane.
3. Review and edit settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

Layout Report Configuration

As with other Report Elements, you can configure how it appears in the report using general for report content and specific to this element options. Former are described in the Report customisation topic while here the latter are covered.

In addition to general options, Layout has a similar to the Matrix View configurable setting:

Size	This allows easy configuration of sizes for generated **Layout** image in output. The options are: • **Small** – The width of an image is set to 304 px. • **Medium (Default)** – Image fits in width of A4 sheet (for **Page View**). • **Large** – The width of the image is set to 800 px.

If your protocol uses Multiple Plate Layouts, then all of them will be included in the report.

Matrix Table

Matrix Table is a simple way of outputting your data in a table. The table displays data in an orientation that matches the layout, e.g. a 12x8 matrix.

If the data is endpoint, the numeric values for each replicate will be displayed in the matrix. Tor spectral and kinetic data matrix will contain Thumb plots in each cell.

The matrix table(s) has 2 configurations:

1. One table where each position contains the data for all included matrices.
2. A separate matrix table for each included matrix.

Due to their clarity, Matrix Tables are used in the Transforms subsection of the Reference to illustrate transforms performance.

How to: Add Matrix Table Element to the Report

1. Open the **Report** tab.
2. Select Matrix Table element from the **Add Element** drop-down list it the **Reports** pane.
3. Review and edit settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

Matrix Table Report Configuration

A report can contain one or more tables that display the raw data and/or results.

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

Matrix Table

The matrix table(s) has 2 configurations that define how the results will be displayed.

Arrangement	Included matrices can be arranged as: • **Combined** – one table where each position contains the data for all included matrices (per plate). Each cell in the table lists the value of each point on the corresponding matrix. The final row of the table is a key which explains what each row of each cell refers to. • **Separate** – a separate matrix table is created for each included matrix

	data. Each table displays the name of the matrix followed by the matrix table itself.

In both cases each matrix itself is a grid corresponding to the layout.

For XY results the table will contain **Thumb Plot** in each cell. This is simply a thumbnail graphical representation of each kinetic position.

Following tables list specifications of data to create plot thumbnails.

Thumb Plot

Include Thumb Plots	With this checkbox you define whether thumb plots should be included in the report.
Thumb Plot Height	It specifies height to use for all thumbs in the report.
Thumb Plot Width	It specifies width to use for all thumbs in the report.

The plot area for each **Thumb Plot** has a minimum and maximum **X** and **Y** scales. For prototype these can be fixed values (or determined for each position). The plot lines are plotted within this scan.

Thumb Scale

Thumb Auto Scale Max X	Specifies whether the maximum **X** scale of each plot is: • **Fixed** - The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Max X** value; • **Plot** - The scale limit of each thumb plot is automatically determined by the maximum **X** data in each plot (i.e. each plot may have a different maximum **X** limit). • **Table** - The scale limit of each and every thumb plot in the table is the same. This is determined from the maximum **X** of all plots data points in the table.
Thumb Auto Scale	Specifies whether the maximum **Y** scale of each plot is:

Max Y	• **Fixed** - The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Max Y** value; • **Plot** - The scale limit of each thumb plot is automatically determined by the maximum **Y** data in each plot (i.e. each plot may have a different maximum **Y** limit). • **Table** - The scale limit of each and every thumb plot in the table is the same. This is determined from the maximum **Y** of all plots data points in the table.
Thumb Auto Scale Min X	Specifies whether the minimum **X** scale of each plot is: • **Fixed** - The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Min X** value; • **Plot** - The scale limit of each thumb plot is automatically determined by the minimum **X** data in each plot (i.e. each plot may have a different minimum **X** limit). • **Table** - The scale limit of each and every thumb plot in the table is the same. This is determined from the minimum **X** of all plots data points in the table.
Thumb Auto Scale Min Y	Specifies whether the minimum **Y** scale of each plot is: • **Fixed** - The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Min Y** value; • **Plot** - The scale limit of each thumb plot is automatically determined by the minimum **Y** data in each plot (i.e. each plot may have a different minimum **Y** limit). • **Table** - The scale limit of each and every thumb plot in the table is the same. This is determined from the minimum **Y** of all plots data points in the table.
Thumb Scale Max X	Determines custom maximum **X** scale for thumb plots if **Thumb Auto Scale Max X** is **Fixed**.
Thumb	Determines custom maximum **Y** scale for thumb plots if **Thumb Auto Scale**

Scale Max Y	**Max Y** is **Fixed**.
Thumb Scale Min X	Determines custom minimum **X** scale for thumb plots if **Thumb Auto Scale Min X** is **Fixed**.
Thumb Scale Min Y	Determines custom minimum **Y** scale for thumb plots if **Thumb Auto Scale Min Y** is **Fixed**.

Matrix Table with Multiple Plate

If the layout 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 1 matrix table for each plate.

With **Separate** there might be more than one matrix table for each plate.

Matrix View

This element displays the data (endpoint or kinetic) of a specified matrix, using colouring as either layout or heatmap. All corresponding settings of associated matrix apply to the view too.

How to: Add Matrix View Element to the Report

1. Open the **Report** tab.
2. Select Matrix View element from the **Add Element** drop-down list it the **Reports** pane.
3. Review and edit settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

Matrix View Properties

The positions appear as circles for endpoint data and as squares for XY data. Flagged positions are indicated and displayed as such for calculated data.

Matrix view can be configured with colouring of:

- **Layout.** Each position shows the numeric value in endpoint matrices and a thumb in XY data according to its sample type. Also the sample type legend is included.
- **Heatmap.** Each position displays 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.

Matrix View Report Configuration

You can add to the transform 1 or more Matrix Views. You can configure how they appear in the report using general for report content and specific to this element options. Former are described in the Report customisation topic while here the latter are covered.

Matrix View includes the following configurable settings:

General

Matrix	This defines which matrix of the data to associate with the view. Select the relevant matrix name from a drop-down list.
Size	This allows easy configuration of sizes for generated **Matrix View** image in output. The options are:

	• **Small** – The width of an image is set to 304 px. • **Medium (Default)** – Image fits in width of A4 sheet (for **Page View**). • **Large** – The width of the image is set to 800 px.

Matrix View

Colouring	If **Layout** is specified then the template shows the layout and includes layout legends. If **Heatmap** is specified then heatmap colouring and legend is displayed.

Notes

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

Entered Notes will appear under **Notes:** title.

How to: Add Notes to the Analysis

1. Launch an assay protocol or open a results file.
2. In the **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.

Notes Report Configuration

How to: Add Notes Element to the Report

1. Open the **Report** tab.
2. Select Notes element from the **Add Element** drop-down list it the **Reports** pane.
3. Review and edit settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

Notes element includes the following checkbox setting:

Notes

Exclude If Empty	This setting automatically excludes Notes from the results, if it contains no information.

Sample Table

Sample Table is a primary report element and is added to report automatically. It lists the results of the performed analysis by sample groups. Each row in the table corresponds to a sample. Flagged data is displayed as defined by associated transform and/or matrix configuration. Configuration of former is described in each transform, the latter you determine in the Matrices tab.

Optional columns can include:

- Sample groups – e.g. **Unknown1**. For unknown samples the name will be replaced by any provided Sample ID.
- Positions – e.g., **A1, B3, H12**. The positions on the layout designated as containing the sample (as provided in the Microplate tab).
- Matrices – a column for each included matrix.
- Any additional report columnar content.

Each Sample Table can be configured with:

- Which sample types to include.
- The ordering of the sample types.
- Columns to include (as configured in Matrices tab).
- Scaling for thumb plots (for XY data).

How to: Add Sample table Element to the Report

1. Open the **Report** tab.
2. Select Sample table element from the **Add Element** drop-down list it the **Reports** pane.
3. Review and edit settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

Sample Table Report Configuration

A report can contain 0 or more sample tables. Each Sample Table displays certain matrices of data (raw and/or calculated) for included sample types (**Types**). The Sample Table is configured with general report and specific to this element settings. Former are described in general report configuration settings and latter are covered below.

Sample Table

Include Positions	This checkbox defines whether the column that lists layout positions (**A1**, **A2**, etc.) is included in the report.
Replicate Orientation	It defines how positions of a sample group are listed in the report: **Vertical** - Each position is listed in a new line of the column. **Horizontal** - All positions are listed in the same line.
Types	The sample types to be included in Sample Table.

Sample Table may contain a column with thumb plots representing XY matrix data. **Thumb Plot** is simply a thumbnail graphical representation of each kinetic position.

Following tables list specifications of data to create plot thumbnails.

Thumb Plot

Include Thumb Plots	With this checkbox you define whether thumb plots should be included in the report.
Thumb Plot Height	It specifies height to use for all thumbs in the report.
Thumb Plot Width	It specifies width to use for all thumbs in the report.

The plot area for each **Thumb Plot** has a minimum and maximum **X** and **Y** scales. For prototype these can be fixed values (or determined for each position). The plot lines are plotted within this scan.

Thumb Scale

Thumb Auto Scale Max X	Specifies whether the maximum **X** scale of each plot is: • **Fixed** - The scale limit of the thumb plots used in the table is specified by the associated **Thumb Scale Max X** value; • **Plot** - The scale limit of each thumb plot is automatically determined by the maximum **X** data in each plot (i.e. each plot may have a different maximum **X** limit). • **Table** - The scale limit of each and every thumb plot in the table is the

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

Thumb Scale Max X	Determines custom maximum **X** scale for thumb plots if **Thumb Auto Scale Max X** is **Fixed**.
Thumb Scale Max Y	Determines custom maximum **Y** scale for thumb plots if **Thumb Auto Scale Max Y** is **Fixed**.
Thumb Scale Min X	Determines custom minimum **X** scale for thumb plots if **Thumb Auto Scale Min X** is **Fixed**.
Thumb Scale Min Y	Determines custom minimum **Y** scale for thumb plots if **Thumb Auto Scale Min Y** is **Fixed**.

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, such as Standard Curve Fit, comprise a number of optional content.

The different types of additional report elements are:

- **Additional Sample Table Column** – this is an optional additional column that can appear in the sample table. For example, the Dilution Factors transform outputs optional report content named Factor Column.
- **Chart** – the visual representation of a plotted curve. This optional item is included to a report by default.
- **Table** – this is a 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.

Transform Content Report Configuration

A report can contain one or more **Transform Content** elements. You can configure which optional items are actually included in report with the **Content Editor**.

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 editor comprises **Included** and **Excluded** panes. Inside of these are listed content elements which will and will not be displayed in the report, respectively.

Within editor you can add/remove items and switch their sequence in the report. To do former select the element and click on the arrow between panes to move it to different pane. Select the element and use **Up** or **Down** arrow on utmost right of the editor to do latter.

Validation Table

Similarly to Evaluations Tables, Validations Tables in the report are used to display the results of validations, which were verified for particular assay run. Further details on the validating certain conditions are provided in the Validations section.

Validations Tables Report Configuration

A table detailing whether each validation passed or failed, which when each Validation is defined, is added to a report automatically.

You can configure how they appear in the report using general applicable to all report content and specific options. Former are described in the Report customisation topic while here the latter are covered.

How to: Add Validations Table Element to the Report

1. Open the **Report** tab.
2. Select Validations Table element from the **Add Element** drop-down list it the **Reports** pane.
3. Review and edit settings as required.
4. Press **Calculate** button to perform calculations with the new settings.

By default Validation table in Report is displayed as three-column table with 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.

Validations Table

Include Description	When checked, the column contains **Description** if specified or **Condition# {index}** if it was not.
Include Expression	If included, outputs the **Condition** defined for each **Validation**.

Reference

Transforms

Transforms can be described as a set of configurable operations, which 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 priorly.

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 1 or more input matrices.
- Each transform can produce 1 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 1 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 1 or more calculated matrices to the Matrices at each step. As each transform is evaluated, each container in the results will always contain the same number of matrices (raw and calculated) as all other containers in the results.

As you add transforms, you can configure output settings and display in the report for each of them.

Expressions and Transforms

In addition to the input matrices, any transform that uses MyAssays Analysis Expressions can access data directly from the current transform (including data that is not on the input matrices). Similar to available input matrices, the data that can be accessed depends on the data that has been calculated up to this point of the evaluation (and data of the compatible type). Thus, the data accessible by an expression includes compatible raw and calculated matrices.

Transforms 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.

For each transform listed below, a transform is only relevant if the matrices collection (raw and calculated) includes the required inputs.

Relevant for Endpoint Data:

- Auto Flag
- Average
- Blank Correction
- Dilution Curves
- Dilution Factors
- Expression by Matrix
- Expression by Matrix (Dual)
- Expression by Position
- Factor
- Matrix Difference
- Median
- Percentage
- %CV (Percentage Coefficient of Variation)
- Replicate Outlier Removal
- Standard Curve Fit
- Standard Deviation
- Variance

Relevant for Kinetic/Spectral Data:

XY Transforms

- XY Blank Correction
- XY Expression
- XY Expression (Dual)
- XY Fit
- XY Join

- XY Outlier Removal
- XY Replicates Average

XY Reduction Transforms

- Average
- Fit Parameter
- Maximum Slope
- Peak
- Total
- X At Y
- Y At X

General Transform Properties

With regards to flexibility of assay setup, each transform can be configured to fully match assay requirements with a number of settings.

All transforms share the following common settings:

Advanced

Included Samples	The sample types to be computed by this transform.
Excluded Results	Sample types not selected in the **Included Samples** option will not be computed by this transform; for those cases, this setting specifies what the result will be for those excluded samples: • **Flagged With Value** – the result is flagged with the input value reported. This will appear in the report with the value with strike-through, e.g. ~~**1.23**~~. • **Flagged No Value** – the result is flagged with no value reported. This will appear in the report as ~~**Flagged**~~. • **Equal Input** – the result is set to the match the value of the input.

Units

Output	The measurement units to be included in the header of Sample Table.

Units	If the output units of the transform are the same as its input then use "ditto" units to automatically carry these units through (i.e. apply the same units to the transform's output). This short-cut means that it is not necessary to repeat settings across transforms. Ditto units are specified with two dots, i.e. ..

In addition, all **XY** and **XY Reduction** transforms can be configured with following settings.


Range settings do not apply to **XY Join** transform.

Data

X Axis	This setting determines which values to use in the **X** chart axis and for evaluations:
	• **Index** – the 1-based position number of the data point in the collection.
	• **X** – depending on the measurements data type, this option is displayed as:
	  • **X (Cycle)** – for kinetic data with no time values **X** equals the **Index**.
	  • **X (Time)** – for kinetic data, if time values are stored then this is time stamp associated with the data point.
	  • **X (Wavelength)** – for spectral data, if wavelength values are stored then this is the wavelength of the data point.
	• **Y** – each value is set to a **Y** value of the corresponding input matrix's data point.

Y Axis	This setting determines which values to consider in the **Y** chart axis and for evaluations:
	• **Index** – the 1-based position number of the data point in the collection.
	• **X**– depending on the measurements data type, this option is displayed as:
	  • **X (Cycle)** – for kinetic data with no time values **X** equals the **Index**.
	  • **X (Time)** – for kinetic data, if time values are stored then this is time stamp associated with the data point.
	  • **X (Wavelength)** – for spectral data, if wavelength values are stored

	then this is the wavelength of the data point. • **Y** – each value is set to a **Y** value of the corresponding input matrix's data point.

Range

The range settings enable the specification of a subset of the data points to consider; only data points within the specified range will be processed. When a range is set, data points outside the specified range are excluded from the calculation. Thus, only the data points inside the specified minimum and maximum range (that are also not flagged) are processed by transform.

The range can be defined by setting the **X Minimum** and **X Maximum** properties to a value or expression:

X Minimum	A numerical value or expression that defines the minimum **X** data point to include within the subset. If this is not specified, then all data points less than **X Maximum** are included.
X Maximum	A numerical value or expression that defines the maximum **X** data point to include within the subset. If this is not specified, then all data points greater than **X Minimum** are included.

In addition the range can be adjusted interactively by positioning range bars. The range bars are displayed as vertical dashed lines on the chart, which you can either:

- Drag with mouse to correct range values.
- Double-click on to reset minimum or maximum value.

Moreover, each transform has zero or more specific settings that allow customisation of the transform operations. These are covered under in each transform topic below.

Auto Flag

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform flags positions where a Boolean condition is satisfied. This is useful for automatically rejecting and ignoring data points that are outside of an expected range.

Properties:

Settings

Auto Flag	The expression to evaluate, where a single **x** variable is set to value of each position of the input matrix.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to flag all positions with a value greater than 1.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

To flag values in this matrix where the measurement is greater than 1, specify an Auto Flag expression of **x > 1**.

Calculated

The transform will generate an output matrix named **Calculated** with the value at each position matching the input data and positions that do not meet the specified condition

flagged. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	~~2.105~~	~~2.124~~	~~1.213~~	~~1.226~~	~~1.159~~	~~1.190~~	0.110	0.116	~~1.463~~	~~1.481~~
B	0.455	0.441	~~1.869~~	~~1.888~~	~~1.203~~	~~1.218~~	~~1.180~~	~~1.206~~	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	~~1.206~~	~~1.239~~	~~1.203~~	~~1.210~~	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	~~1.167~~	~~1.187~~	~~1.211~~	~~1.241~~	0.101	0.106	0.489	0.490
E	~~1.105~~	~~1.065~~	0.279	0.367	~~1.215~~	~~1.225~~	~~1.233~~	~~1.262~~	0.111	0.114	~~1.579~~	~~1.549~~
F	~~1.425~~	~~1.445~~	0.378	0.411	~~1.196~~	~~1.206~~	~~1.226~~	~~1.199~~	0.109	0.108	0.792	0.775
G	~~1.791~~	~~1.803~~	0.560	0.597	~~1.205~~	~~1.228~~	~~1.308~~	~~1.306~~	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	~~1.214~~	~~1.261~~	~~0.115~~	0.116	0.115	0.115	0.490	0.477

Average

[Input: **Endpoint** ➡ Output: **Endpoint**]

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

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to find the average position values in each sample group.

This transform averages the replicates of the sample group and stores the resulting value to each sample group replicate of the output matrix. Therefore, the result will depend on the layout configuration.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in duplicate (e.g. **Unknown1** at **A1** and **A2**, **Unknown2** at **B1** and **B2** etc.). I.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

Unknown

Average

The transform will generate an output matrix named **Average** with the value at each position being the averaged input data for each sample group. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.344	0.344	2.115	2.115	1.220	1.220	1.175	1.175	0.113	0.113	1.472	1.472
B	0.448	0.448	1.879	1.879	1.211	1.211	1.193	1.193	0.131	0.131	0.777	0.777
C	0.581	0.581	0.494	0.494	1.223	1.223	1.207	1.207	0.115	0.115	0.620	0.620
D	0.790	0.790	0.371	0.371	1.177	1.177	1.226	1.226	0.104	0.104	0.490	0.490
E	1.085	1.085	0.323	0.323	1.220	1.220	1.248	1.248	0.113	0.113	1.564	1.564
F	1.435	1.435	0.395	0.395	1.201	1.201	1.213	1.213	0.109	0.109	0.784	0.784
G	1.797	1.797	0.579	0.579	1.217	1.217	1.307	1.307	0.127	0.127	0.656	0.656
H	0.262	0.262	0.467	0.467	1.238	1.238	0.116	0.116	0.115	0.115	0.484	0.484

Blank Correction

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform subtracts the average of a specified blank group (or groups) from each sample. This is useful for subtracting background noise from measurements.

The blank value is computed from the average of the (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 - 1 blank group on each row
- by-column - 1 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 Group	The group number of the sample to use for correction. This can be defined as a number or as an expression. The expression can refer to **x** which is the group number of the sample to be corrected. For example, set this to **x** to perform a 1-to-1 correction where each group is corrected by the sample of the specified blank type with the same group number.
Blank Type	The sample type used as the blank.

Example: Single Blank

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to perform a blank correction using the average of one blank group. This blank group itself is measured in duplicate. The mean of these replicates will be subtracted from all other samples.

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

Raw

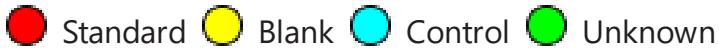
	1	2	3	4	5	6	7	8	9	10	11	12
A	0.192	0.199	0.347	0.346	0.325	0.321	0.803	0.797	1.589	1.593	0.241	0.246
B	0.293	0.300	0.586	0.584	0.800	0.793	0.402	0.401	0.839	0.837	0.562	0.564
C	0.537	0.534	0.549	0.547	0.878	0.875	0.471	0.471	0.759	0.756	1.039	1.043
D	0.858	0.855	0.320	0.325	0.531	0.530	1.552	1.551	0.429	0.427	0.424	0.424
E	1.523	1.527	0.486	0.490	1.289	1.283	1.430	1.438	1.494	1.501	1.427	1.429
F	1.622	1.621	0.621	0.626	0.667	0.663	1.350	1.347	0.631	0.634	1.695	1.694
G	0.001	0.001	0.356	0.352	0.418	0.412	1.172	1.174	1.572	1.570	0.595	0.590
H	0.297	0.297	0.796	0.801	1.517	1.515	0.960	0.965	0.534	0.527	0.585	0.584

This transform requires a layout with a minimum 1 **Blank** group.

Layout

The example uses a layout with **Standards**, **Control**, **Blank** and **Unknowns** in duplicate (e.g. **Standard1** in **A1** ans **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



To subtract the mean of the blank positions from the measurements, specify **Blank Group** to **1** and **Blank Type** to **Blank**.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the blank value from the input data. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.191	0.198	0.346	0.345	0.324	0.320	0.802	0.796	1.588	1.592	0.240	0.245
B	0.292	0.299	0.585	0.583	0.799	0.792	0.401	0.400	0.838	0.836	0.561	0.563
C	0.536	0.533	0.548	0.546	0.877	0.874	0.470	0.470	0.758	0.755	1.038	1.042
D	0.857	0.854	0.319	0.324	0.530	0.529	1.551	1.550	0.428	0.426	0.423	0.423
E	1.522	1.526	0.485	0.489	1.288	1.282	1.429	1.437	1.493	1.500	1.426	1.428
F	1.621	1.620	0.620	0.625	0.666	0.662	1.349	1.346	0.630	0.633	1.694	1.693
G	0.000	0.000	0.355	0.351	0.417	0.411	1.171	1.173	1.571	1.569	0.594	0.589
H	0.296	0.296	0.795	0.800	1.516	1.514	0.959	0.964	0.533	0.526	0.584	0.583

Example: 1-1 Blank Correction

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to perform a 1-to-1 correction, where each sample group is corrected by the blank that it is associated with. The blank numbering used in the layout defines the associations.

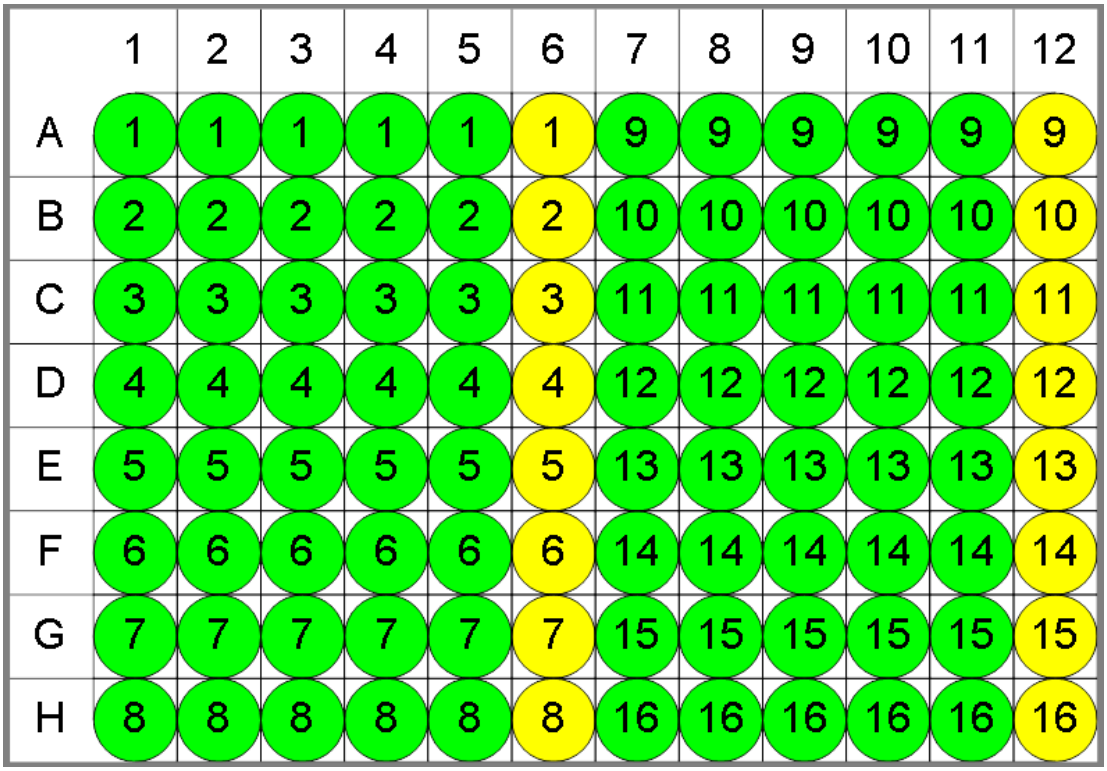
Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.962	1.999	2.038	1.922	1.995	0.002	1.628	1.670	1.624	1.554	1.701	0.000
B	0.784	0.760	0.754	0.751	0.797	0.002	1.124	1.104	1.072	1.077	1.106	0.002
C	0.586	0.575	0.582	0.590	0.576	0.001	0.724	0.737	0.690	0.711	0.717	0.002
D	0.441	0.441	0.427	0.419	0.439	0.002	0.095	0.095	0.093	0.096	0.096	0.001
E	1.956	1.970	1.875	2.043	1.959	0.001	1.449	1.479	1.428	1.395	1.385	0.001
F	1.416	1.358	1.407	1.352	1.452	0.001	0.242	0.230	0.249	0.235	0.251	0.000
G	1.438	1.429	1.488	1.401	1.372	0.002	0.943	0.952	0.956	0.912	0.969	0.002
H	0.840	0.827	0.812	0.838	0.860	0.002	1.320	1.260	1.313	1.363	1.312	0.001

Layout

The example uses a layout with 16 **Unknowns** groups (with **Unknown1** in positions from **A1** to **A5**, **Unknown2** in positions from **B1** to **B5** etc.) and 16 **Blank** singlets I.e.



To perform 1-1 correction, specify **Blank Group** to **x** and **Blank Type** to **Blank**.

With this specified, the value of each blank will be subtracted from every position of associated group, i.e. **Blank1** (stored in **A6**) value will be subtracted from **A1, A2, A3, A4, A5** (the members of **Unknown1**) and from **A6** itself. Therefore, calculated matrix will contain blank corrected **Unknown** values and all **Blanks** will be 0.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the associated blank value from the input data. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.960	1.997	2.035	1.919	1.992	0.000	1.628	1.670	1.623	1.554	1.701	0.000
B	0.783	0.758	0.752	0.750	0.796	0.000	1.122	1.102	1.070	1.075	1.104	0.000
C	0.585	0.574	0.581	0.589	0.575	0.000	0.722	0.735	0.688	0.709	0.714	0.000
D	0.439	0.439	0.425	0.417	0.437	0.000	0.094	0.094	0.093	0.095	0.095	0.000
E	1.955	1.969	1.873	2.042	1.958	0.000	1.448	1.478	1.427	1.394	1.384	0.000
F	1.415	1.358	1.406	1.352	1.451	0.000	0.241	0.229	0.249	0.235	0.251	0.000
G	1.436	1.427	1.486	1.399	1.369	0.000	0.941	0.950	0.955	0.910	0.967	0.000
H	0.839	0.825	0.810	0.837	0.858	0.000	1.319	1.260	1.312	1.362	1.311	0.000

Advanced Example: By-Row Blank Correction

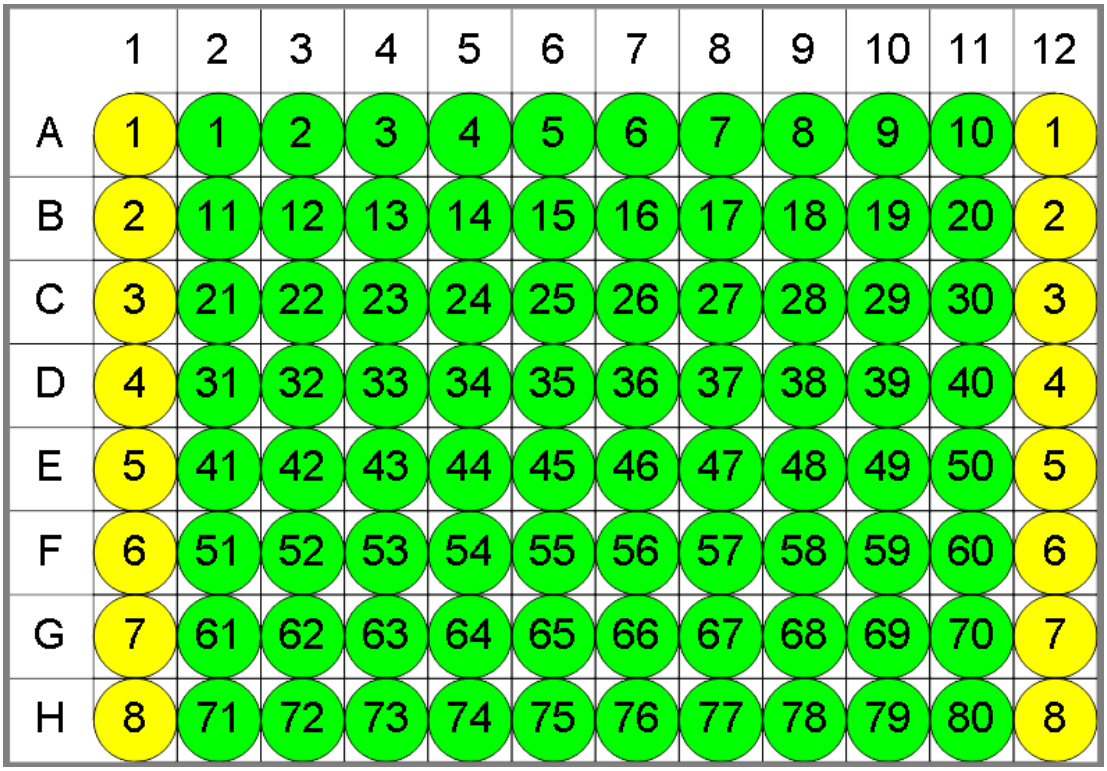
In this example we would like to configure blank correction on a row-by-row basis to blank correct each sample by the average of the two blank samples of the same row.

For better clearness of the process, this example uses simplified endpoint data for 12x8 microplate:

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	2	3	4	5	6	7	8	9	10	1
B	2	11	12	13	14	15	16	17	18	19	20	2
C	3	21	22	23	24	25	26	27	28	29	30	3
D	4	31	32	33	34	35	36	37	38	39	40	4
E	5	41	42	43	44	45	46	47	48	49	50	5
F	6	51	52	53	54	55	56	57	58	59	60	6
G	7	61	62	63	64	65	66	67	68	69	70	7
H	8	71	72	73	74	75	76	77	78	79	80	8

Layout

The example uses a layout with 80 singlet **Unknowns**and 8 **Blank** duplicates for each row (with **Blank1** in positions **A1** and **A12**, **Blank2** in positions **B1** and **B12** etc.) I.e.



Blank Unknown

With **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, i.e. for **x=1** this means **1+floor((1-1)/10),1)**, **floor=0** and the **Blank Group** is taken as 1. For the first row **x** is in range from 1 to 10 and the expression outputs 1, thus for **Unknowns** from 1 to 10 the average of **Blank1** is subtracted.

For the second x is from 11 to 20, **floor=1**, so the **Blank2** group is subtracted from **Unknowns11-20**, etc.

Blank Corrected

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

Dilution Curves

[Input: **Endpoint** ➡ 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 Type	The sample type to use for the dilution.
Dilutions	It 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 **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 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 Method	Specifies weight function for transform.
X Axis Type	A type to plot an **X** axis in a chart: • **Logarithmic** • **Linear**
X Transform	Function for **X** values transform.
Y Axis Type	A type to plot an **Y** axis in a chart:

	• **Logarithmic** • **Linear**
Y Transform	Function for **Y** values transform.

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to create a curve fit for each sample group of the **Unknown** type.

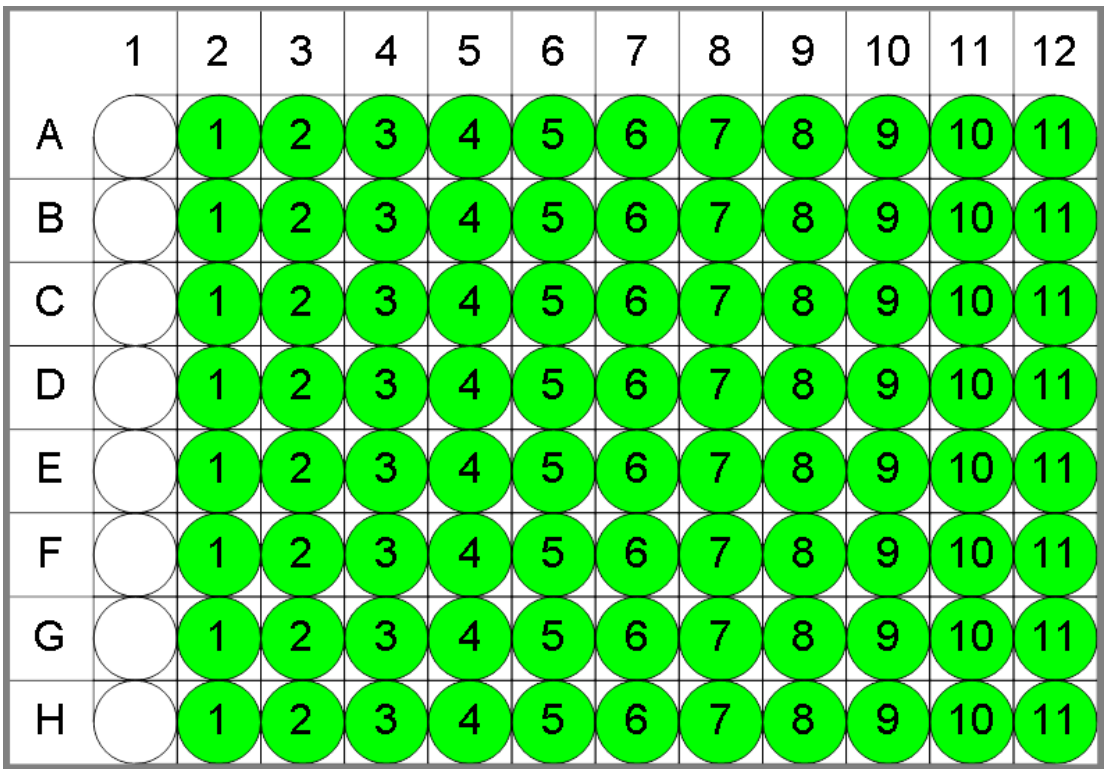
Here is some example raw data displayed here to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.000	2.682	2.345	2.612	2.732	2.675	2.664	2.574	2.580	2.361	0.871	2.839
B	0.000	2.577	1.735	2.518	2.701	2.537	2.571	2.450	2.453	2.171	0.437	2.809
C	0.000	2.537	1.290	2.497	2.683	2.447	2.490	2.273	2.344	1.695	0.222	2.783
D	0.000	2.358	0.793	2.318	2.585	2.195	2.205	1.856	2.069	1.070	0.094	2.658
E	0.000	1.958	0.369	1.799	2.224	1.636	1.661	1.192	1.485	0.550	0.037	2.322
F	0.000	1.352	0.151	1.118	1.517	0.909	0.947	0.638	0.868	0.257	0.013	1.495
G	0.000	0.745	0.053	0.540	0.872	0.425	0.485	0.282	0.417	0.094	0.002	0.862
H	0.000	0.312	0.018	0.250	0.398	0.180	0.200	0.113	0.194	0.038	0.001	0.438

Layout

The example uses a layout with one Unused column (in positions from **A1** to **H1**) and **Unknowns** in columns (e.g. **Unknown1** at positions from **A2** downward to **H2**, **Unknown2** at **A3-H3** etc.). I.e.



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

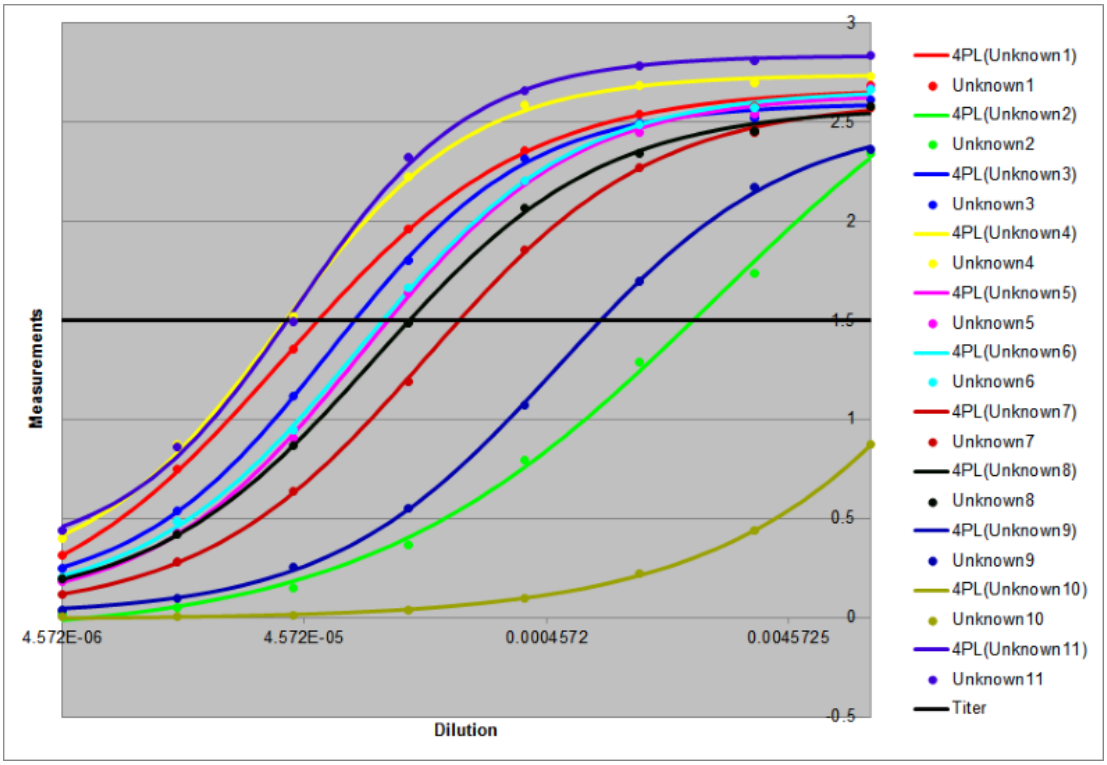
Dilutions Table

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	a	b	c	d	R^2	Result
Unknown1	-0.0584816	0.875198	0.0000376679	2.67099	0.999497	0.0000522186
Unknown2	-0.0901615	0.606878	0.00226574	3.29931	0.997736	0.00184835
Unknown3	0.103291	1.07281	0.0000588689	2.59484	0.999371	0.0000738691
Unknown4	0.176798	1.10415	0.000035979	2.73875	0.999281	0.0000381935
Unknown5	0.0355624	0.998377	0.0000794665	2.64392	0.999147	0.000101774
Unknown6	0.0581275	0.980399	0.000077654	2.66458	0.999619	0.0000965551
Unknown7	0.0190159	0.929062	0.000146444	2.60957	0.999764	0.000199822
Unknown8	0.0468791	0.936045	0.000090142	2.57555	0.999425	0.000124316
Unknown9	0.0138517	0.919968	0.000515222	2.53025	0.999769	0.000767282
Unknown10	-0.00938083	0.681115	0.135122	6.05263	0.999738	0.0267169
Unknown11	0.298789	1.20751	0.0000424681	2.83485	0.999004	0.0000389155

Chart

The chart contains 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):

	1	2	3	4	5	6	7	8	9	10	11	12
A	~~Flagged~~	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.027	0.000
B	~~Flagged~~	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.027	0.000
C	~~Flagged~~	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.027	0.000
D	~~Flagged~~	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.027	0.000
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
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** ➡ 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 Samples	The sample types to which the dilution factor should be applied.
Factors	The dilution factor to use for each selected **Factored Samples**.

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to multiply all odd **Unknown** sample groups by 2 and all even **Unknown** sample groups by 5.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank** and **Unknowns** in duplicate (e.g. **Standard1** in **A1** ans **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 Blank Control Unknown

To multiply selected sample types in this matrix by specified factors set **Factored Samples** to **Unknown** and specify **Factors** as **2** for every odd sample group and as **5** for every even sample group.

Concentration (x Dil. Factor)

The transform will generate an output matrix named **Concentration (x Dil. Factor)** with the value at each position of the selected Factored Samples multiplied by specified Factor and sample groups of other types matching the input data. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	4.210	4.248	2.426	2.452	2.318	2.380	0.220	0.232	2.926	2.962
B	0.455	0.441	9.345	9.440	6.015	6.090	5.900	6.030	0.660	0.650	3.930	3.840
C	0.587	0.575	0.948	1.028	2.412	2.478	2.406	2.420	0.226	0.232	1.226	1.252
D	0.806	0.774	1.820	1.890	5.835	5.935	6.055	6.205	0.505	0.530	2.445	2.450
E	1.105	1.065	0.558	0.734	2.430	2.450	2.466	2.524	0.222	0.228	3.158	3.098
F	1.425	1.445	1.890	2.055	5.980	6.030	6.130	5.995	0.545	0.540	3.960	3.875
G	1.791	1.803	1.120	1.194	2.410	2.456	2.616	2.612	0.252	0.254	1.304	1.318
H	0.253	0.270	2.315	2.350	6.070	6.305	0.575	0.580	0.575	0.575	2.450	2.385

Expression by Matrix (Dual)

Input: **Dual Endpoint** ➡ Output: **Endpoint**

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

Properties:

Settings

Dual Matrix Expression	The expression to evaluate, where **x** and **y** variables are set to value of each position of the input matrices.

If the expression does not contain the **x** and **y** variables, the transform will output the same evaluation result for all positions. For example, if you enter **{2^3+4}**, the resulting matrix will contain 12 in each position.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw (1)** and **Raw (2)** matrices. In this example we would like to summarise position values in these matrices.

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

Raw (1)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Raw (2)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.204	0.201	0.213	0.209	0.206	0.208	0.216	0.217	0.216	0.213	0.205	0.218
B	0.216	0.200	0.214	0.214	0.204	0.201	0.215	0.216	0.203	0.219	0.207	0.204
C	0.206	0.210	0.208	0.203	0.201	0.218	0.212	0.217	0.216	0.213	0.208	0.204
D	0.215	0.215	0.214	0.203	0.214	0.213	0.219	0.219	0.213	0.201	0.202	0.219
E	0.215	0.220	0.219	0.212	0.210	0.211	0.214	0.214	0.201	0.202	0.202	0.207
F	0.214	0.212	0.202	0.200	0.201	0.217	0.213	0.209	0.218	0.207	0.216	0.216
G	0.211	0.211	0.218	0.209	0.214	0.213	0.201	0.211	0.205	0.210	0.201	0.212
H	0.216	0.209	0.215	0.206	0.218	0.206	0.209	0.219	0.215	0.219	0.216	0.217

To add values from **Raw(2)** to corresponding values of **Raw(1)**, specify an expression of **x + y**.

Calculated

The transform will generate an output matrix named **Calculated** with the value at each position being the point by point sum of the **Raw (1)** and **Raw (2)** matrices values. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.568	0.524	2.318	2.333	1.419	1.434	1.375	1.407	0.326	0.329	1.668	1.699
B	0.671	0.641	2.083	2.102	1.407	1.419	1.395	1.422	0.335	0.349	0.993	0.972
C	0.793	0.785	0.682	0.717	1.407	1.457	1.415	1.427	0.329	0.329	0.821	0.830
D	1.021	0.989	0.578	0.581	1.381	1.400	1.430	1.460	0.314	0.307	0.691	0.709
E	1.320	1.285	0.498	0.579	1.425	1.436	1.447	1.476	0.312	0.316	1.781	1.756
F	1.639	1.657	0.580	0.611	1.397	1.423	1.439	1.408	0.327	0.315	1.008	0.991
G	2.002	2.014	0.778	0.806	1.419	1.441	1.509	1.517	0.331	0.337	0.853	0.871
H	0.469	0.479	0.678	0.676	1.432	1.467	0.324	0.335	0.330	0.334	0.706	0.694

Expression by Matrix

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform evaluates an expression defined in terms of **x** for all data points (excluding flagged samples).

Properties:

Settings

Matrix Expression	The expression to evaluate, where a single **x** variable is set to value of each position of the input matrix.

If the expression does not contain the **x** variable, the transform will output the same evaluation result for all positions. For example, if you enter **{2^3+4}**, the resulting matrix will contain 12 in each position.

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to square each measurement.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

The **Matrix Expression** setting is specified with expression of **x*x**.

Calculated

The transform will generate an output matrix named **Calc** with the value at each position being the square of the input data. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.132	0.104	4.431	4.511	1.471	1.503	1.343	1.416	0.012	0.013	2.140	2.193
B	0.207	0.194	3.493	3.565	1.447	1.484	1.392	1.454	0.017	0.017	0.618	0.590
C	0.345	0.331	0.225	0.264	1.454	1.535	1.447	1.464	0.013	0.013	0.376	0.392
D	0.650	0.599	0.132	0.143	1.362	1.409	1.467	1.540	0.010	0.011	0.239	0.240
E	1.221	1.134	0.078	0.135	1.476	1.501	1.520	1.593	0.012	0.013	2.493	2.399
F	2.031	2.088	0.143	0.169	1.430	1.454	1.503	1.438	0.012	0.012	0.627	0.601
G	3.208	3.251	0.314	0.356	1.452	1.508	1.711	1.706	0.016	0.016	0.425	0.434
H	0.064	0.073	0.214	0.221	1.474	1.590	0.013	0.013	0.013	0.013	0.240	0.228

Expression by Position

[Input: **Endpoint** ➡ Output: **Endpoint**]

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

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 coloured to match its sample type.

Position Expressions	If the protocol contains > 1 plate/analyte, select the one to specify expressions for from a drop-down list in the upper right corner of the Editor. To maximize its view click on the arrow button in the lower left corner of the Editor. Within each grid you can select and specify an expression in terms of **x** for: • a single position; • multiple positions (within a single plate) to set to a same expression. Multiple positions can be selected by: • dragging mouse (for rectangular selection). • using **Ctrl** to select random positions; • using **Shift** to select end position (rectangular selection). **Paste**, **Copy** and **Clear** commands are supported. For positions with default (simply **x**) or empty expression the output position is equal to the input position.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to multiply positions from 1 to 5 by 10, positions 10 and 96 by 100 and position 50 by 2.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Provide expressions for positions in Position Expressions Editor:

- **A1**, **A2**, **A3**, **A4**, **A5** with the expression **x*10**;
- **A10** and **H12** with the expression **x*100**;
- **E2** with the expression **x*2**.

Calculated

The transform will generate an output matrix named **Calculated** with the resulting values being the product of input data and specified expressions. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	3.640	3.230	21.050	21.240	12.130	1.226	1.159	1.190	0.110	11.600	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	2.130	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	47.700

Factor

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform multiplies data points by a common factor. The factor can be specified as a numeric value or as an expression to evaluate.

Properties:

Settings

Factor	The value to multiply all data points by. This can be specified as a number or an expression to evaluate.

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to multiply each measurement by a common factor of 2.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

The **Factor** setting for this example is specified as 2.

Factored

The transform will generate an output matrix named **Factored** with the value at each position being the product of the input data and the factor. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.728	0.646	4.210	4.248	2.426	2.452	2.318	2.380	0.220	0.232	2.926	2.962
B	0.910	0.882	3.738	3.776	2.406	2.436	2.360	2.412	0.264	0.260	1.572	1.536
C	1.174	1.150	0.948	1.028	2.412	2.478	2.406	2.420	0.226	0.232	1.226	1.252
D	1.612	1.548	0.728	0.756	2.334	2.374	2.422	2.482	0.202	0.212	0.978	0.980
E	2.210	2.130	0.558	0.734	2.430	2.450	2.466	2.524	0.222	0.228	3.158	3.098
F	2.850	2.890	0.756	0.822	2.392	2.412	2.452	2.398	0.218	0.216	1.584	1.550
G	3.582	3.606	1.120	1.194	2.410	2.456	2.616	2.612	0.252	0.254	1.304	1.318
H	0.506	0.540	0.926	0.940	2.428	2.522	0.230	0.232	0.230	0.230	0.980	0.954

Matrix Difference

Input: **Dual Endpoint** ➡ Output: **Endpoint**

This transform calculates the difference between two input matrices sample-by-sample.

If either of the matrix inputs are flagged, the result will be set to ~~Flagged~~.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw (1)** and **Raw (2)** matrices. In this example we would like to find the difference between values in these matrices.

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

Raw (1)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Raw (2)

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.204	0.201	0.213	0.209	0.206	0.208	0.216	0.217	0.216	0.213	0.205	0.218
B	0.216	0.200	0.214	0.214	0.204	0.201	0.215	0.216	0.203	0.219	0.207	0.204
C	0.206	0.210	0.208	0.203	0.201	0.218	0.212	0.217	0.216	0.213	0.208	0.204
D	0.215	0.215	0.214	0.203	0.214	0.213	0.219	0.219	0.213	0.201	0.202	0.219
E	0.215	0.220	0.219	0.212	0.210	0.211	0.214	0.214	0.201	0.202	0.202	0.207
F	0.214	0.212	0.202	0.200	0.201	0.217	0.213	0.209	0.218	0.207	0.216	0.216
G	0.211	0.211	0.218	0.209	0.214	0.213	0.201	0.211	0.205	0.210	0.201	0.212
H	0.216	0.209	0.215	0.206	0.218	0.206	0.209	0.219	0.215	0.219	0.216	0.217

If the data point values of the **Raw (2)** are greater than the values of **Raw (1)**, the resulting matrix will contain negative values.

Difference

The transform will generate an output matrix named **Difference** with the value at each position being the subtraction between values of the **Raw (1)** and **Raw (2)** matrices. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.160	0.122	1.892	1.915	1.007	1.018	0.944	0.973	-0.106	-0.097	1.258	1.263
B	0.239	0.241	1.656	1.674	0.999	1.017	0.965	0.990	-0.071	-0.089	0.579	0.564
C	0.381	0.365	0.266	0.311	1.005	1.021	0.991	0.993	-0.103	-0.097	0.405	0.422
D	0.591	0.559	0.150	0.175	0.953	0.974	0.992	1.023	-0.112	-0.095	0.287	0.271
E	0.890	0.845	0.060	0.155	1.005	1.014	1.019	1.048	-0.090	-0.088	1.377	1.342
F	1.211	1.234	0.176	0.211	0.995	0.989	1.013	0.990	-0.109	-0.099	0.576	0.559
G	1.580	1.592	0.342	0.389	0.991	1.016	1.107	1.095	-0.079	-0.083	0.451	0.447
H	0.037	0.061	0.248	0.264	0.996	1.055	-0.094	-0.103	-0.100	-0.104	0.274	0.260

Median

[Input: **Endpoint** ➡ Output: **Endpoint**]

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

The median is the middle value of the values sorted into order. If there is an even number of values, the result is the average between the two middle values.

Example

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to find median value for each measurement sample group.

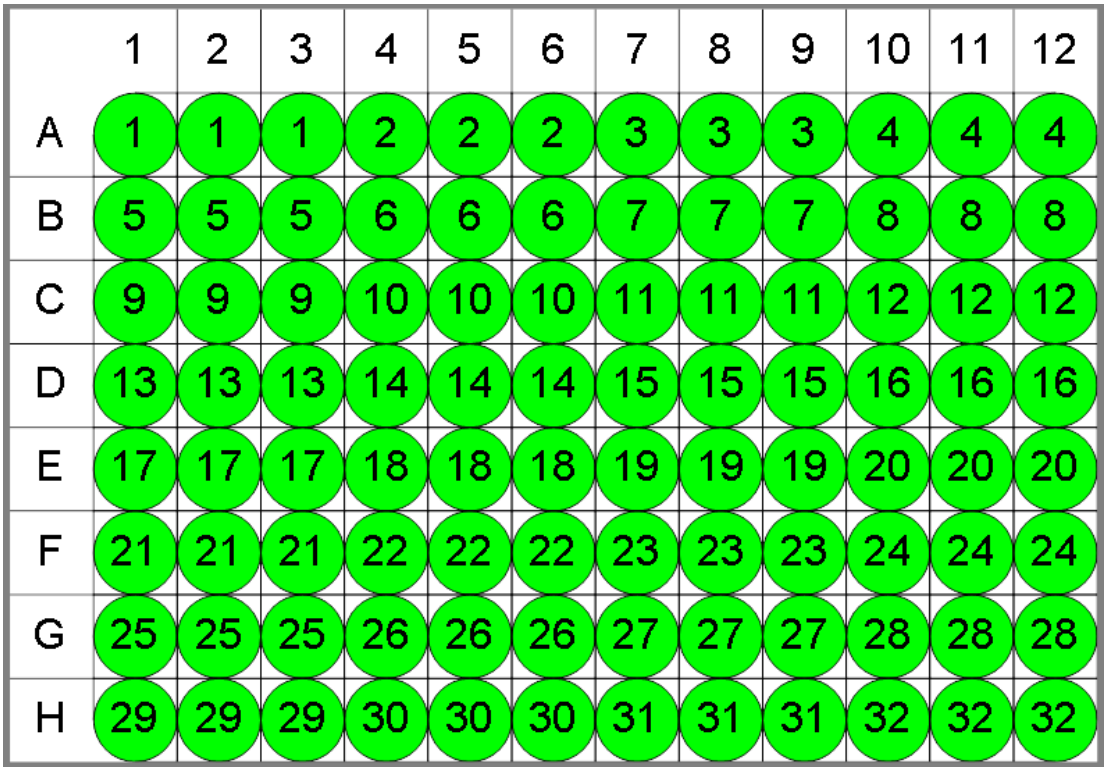
Here is some example raw data displayed here to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in triplets (e.g. **Unknown1** in positions from **A1** to **A3**, **Unknown2** in from **A4** to **A6** etc.). I.e.



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 here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.364	0.364	1.226	1.226	1.226	1.159	1.159	1.159	1.463	1.463	1.463
B	0.455	0.455	0.455	1.218	1.218	1.218	1.180	1.180	1.180	0.768	0.768	0.768
C	0.575	0.575	0.575	1.206	1.206	1.206	1.203	1.203	1.203	0.613	0.613	0.613
D	0.774	0.774	0.774	1.167	1.167	1.167	1.211	1.211	1.211	0.489	0.489	0.489
E	1.065	1.065	1.065	1.215	1.215	1.215	1.233	1.233	1.233	1.549	1.549	1.549
F	1.425	1.425	1.425	1.196	1.196	1.196	1.199	1.199	1.199	0.775	0.775	0.775
G	1.791	1.791	1.791	1.205	1.205	1.205	1.306	1.306	1.306	0.652	0.652	0.652
H	0.270	0.270	0.270	1.214	1.214	1.214	0.115	0.115	0.115	0.477	0.477	0.477

Percentage Coefficient of Variation

[Input: **Endpoint** ➡ Output: **Endpoint**]

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

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 12x8 microplate stored in the **Raw** matrix. In this example we would like to find the percentage coefficient of variation for each sample group of the input matrix.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank** and **Unknowns** in duplicate (e.g. **Standard1** in **A1** ans **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 Blank Control Unknown

%CV

The transform will generate an output matrix named **%CV** with the value at each position being the percentage coefficient of variation in each sample group. The %CV is useful for measuring the deviation between the replicates. The %CV is calculated for each sample group as the % of the standard deviation of the replicate measurements divided by their mean. Typically for replicates one might expect a %CV value to be < 15. A value greater than this might indicate a preparation or layout error. Acceptable limits depend on the application.

With the example data provided above, the results are as follows (also displayed to 3 decimal places):

- **Sample Table**

Here is a Sample Table snippet, which lists the details of the calculations. For each sample, the following details are reported:

Sample	Positions	My Raw Data	%CV
Standard1	A1	0.364	8.440
	A2	0.323	
Standard2	B1	0.455	2.210
	B2	0.441	
Standard3	C1	0.587	1.460
	C2	0.575	
Standard4	D1	0.806	2.864
	D2	0.774	
Standard5	E1	1.105	2.607
	E2	1.065	

- **Matrix Table**

Here all calculated %CV data is displayed in a Matrix Table.

	1	2	3	4	5	6	7	8	9	10	11	12
A	8.440	8.440	0.635	0.635	0.754	0.754	1.866	1.866	3.755	3.755	0.865	0.865
B	2.210	2.210	0.715	0.715	0.876	0.876	1.541	1.541	1.080	1.080	1.638	1.638
C	1.460	1.460	5.726	5.726	1.909	1.909	0.410	0.410	1.853	1.853	1.484	1.484
D	2.864	2.864	2.668	2.668	1.202	1.202	1.730	1.730	3.416	3.416	0.144	0.144
E	2.607	2.607	19.265	19.265	0.580	0.580	1.644	1.644	1.886	1.886	1.356	1.356
F	0.986	0.986	5.915	5.915	0.589	0.589	1.575	1.575	0.652	0.652	1.534	1.534
G	0.472	0.472	4.523	4.523	1.337	1.337	0.108	0.108	0.559	0.559	0.755	0.755
H	4.597	4.597	1.061	1.061	2.686	2.686	0.612	0.612	0.000	0.000	1.901	1.901

Percentage

[Input: **Endpoint** ➡ Output: **Endpoint**]

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

Properties:

Settings

P0 and **P100** can be defined as sample groups, evaluated in the context of the container. For example, if a multiple container layout contains 2 containers of data, both container 1 and container 2 include 2 **Control** groups (but in different places on each container). If **P0** is defined as **Control1** and **P100** is **Control2**, then when the analysis is performed, the %s for container 1 will be calculated using **Control1** and **Control2** on container 1, whereas the %s for container 2 will calculate %s using the **Control1** and **Control2** from container 2.

P0	The value treated as "0 %". This can be defined as a number or as an expression. All values less than **P0** will have negative value in resulting matrix.
P100	The value treated as "100 %". This can be defined as a number or as an expression. All values greater than **P100** will have values greater than 100 in resulting matrix.

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to calculate each measurement percentage value with respect to 0-3 range.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

To calculate all percentage values in this matrix specify a **P0** of 0 and **P100** of 3.

%

The transform will generate an output matrix named **%**. The value at each position will equal to its percent rank with respect to the specified 0% and 100%. With the example data provided above, the results are as follows (displayed here to 2 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	12.13	10.77	70.17	70.80	40.43	40.87	38.63	39.67	3.67	3.87	48.77	49.37
B	15.17	14.70	62.30	62.93	40.10	40.60	39.33	40.20	4.40	4.33	26.20	25.60
C	19.57	19.17	15.80	17.13	40.20	41.30	40.10	40.33	3.77	3.87	20.43	20.87
D	26.87	25.80	12.13	12.60	38.90	39.57	40.37	41.37	3.37	3.53	16.30	16.33
E	36.83	35.50	9.30	12.23	40.50	40.83	41.10	42.07	3.70	3.80	52.63	51.63
F	47.50	48.17	12.60	13.70	39.87	40.20	40.87	39.97	3.63	3.60	26.40	25.83
G	59.70	60.10	18.67	19.90	40.17	40.93	43.60	43.53	4.20	4.23	21.73	21.97
H	8.43	9.00	15.43	15.67	40.47	42.03	3.83	3.87	3.83	3.83	16.33	15.90

Replicate Outlier Removal

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform flags up to a specified number of outlier data points in each sample group. The output matrix values match the input matrix values with any outlier(s) flagged. Outliers are determined and removed as follows:

For each sample group, the transform:

1. Calculates the **%CV** of its replicates (including only the replicates not already flagged).
2. If the **%CV** is greater than the specified **%CV Threshold** then the replicate furthest from the mean is removed.

These steps are repeated until either the new **%CV** of the replicates that are not flagged is below the threshold, or until the specified number of outliers to remove has been removed.

Replicate Outlier Removal is only useful for samples measured with 3 or more replicates.

Properties:

Settings

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

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to remove 1 outlier from each sample group.

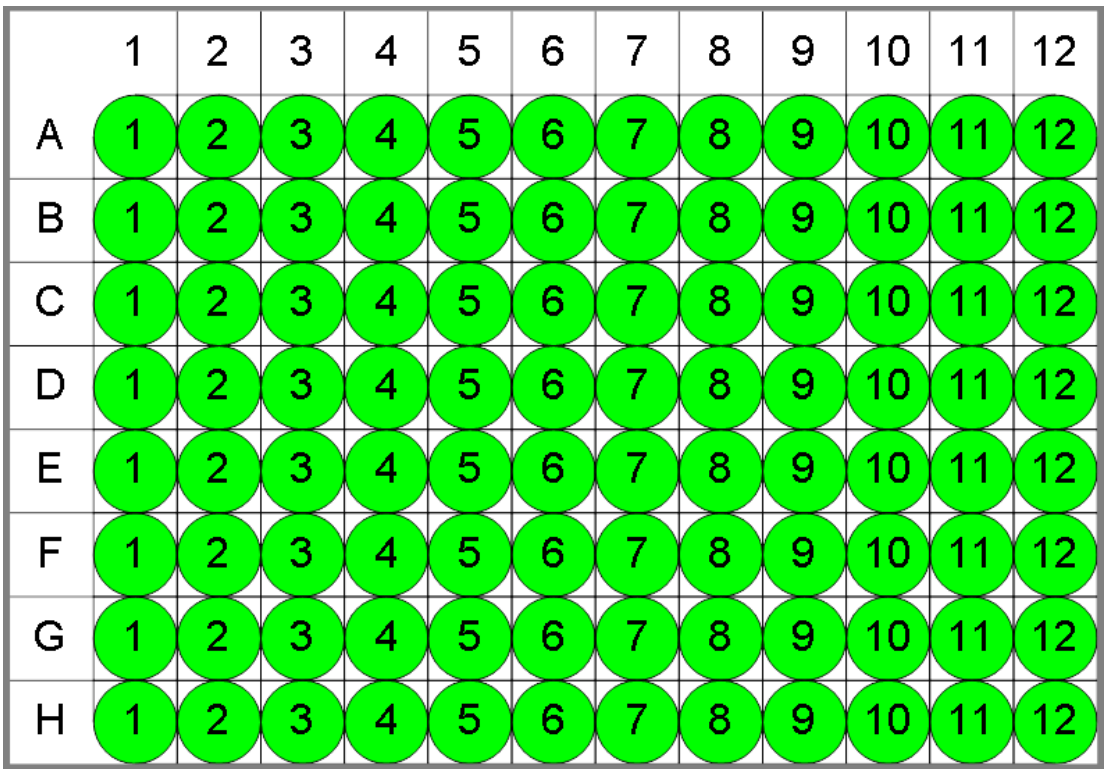
Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in columns (e.g. **Unknown1** vertically at positions from **A1**to **H1**, **Unknown2** from **B2** to **H2** etc.). I.e.



Unknown

To flag 1 outlier data point for each sample group specify a **Outliers To Remove** as 1 and **%CV Threshold** as 15%.

Calculated

The transform will generate an output matrix named **Calculated** with the value at each position matching the input data and outlier data points flagged. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	~~2.105~~	~~2.124~~	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	~~1.579~~	~~1.549~~
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	~~1.791~~	~~1.803~~	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	~~0.115~~	~~0.116~~	0.115	0.115	0.490	0.477

If there are only 2 remaining replicates (before the flag), both of them will be flagged and a message will be added to the calculation log.

Standard Curve Fit

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform:

1. Plots the specified concentration values (**X**) against the measurement data (**Y**) for each standard.
2. Fits a curve to the standard data points (optionally using weight methods).
3. Calculates concentration values from the curve.
4. Determines LLOQ and ULOQ using the specified quantification limits.
5. Optionally computes any additional values from the curve (such as LLD).

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

Properties:

For multiplex assays in this transform **Units** are not included.

Axes

X Axis Title	A name of the **X axis** on the chart.
X Axis Type	A type to plot an **X** axis in a chart: • **Logarithmic** • **Linear**
Y Axis Title	A name of the **Y axis** on the chart.
Y Axis Type	A type to plot an **Y** axis in a chart: • **Logarithmic** • **Linear**

Calibrators

Concentrations	Defines the **X** value for each point of the chart.

Standard Type	Defines a sample type to treat as a standard.

Fit

Calculate From	Defines how the output matrix results are calculated from the computed curve for each sample. I.e. is a result calculated from the curve for each replicate or for the average of the replicates? The options are: • **Replicates** – every position will contain the result of **X**, calculated from value of every replicate (**Y**). • **Average** – replicates from the same sample contain the result of **X**, calculated from averaged value of replicates (**Y**).  Any flagged positions on the input are also flagged in the output.
Fit Method	The curve fitting method to construct a curve for your data based on the specified **Standard Type**. You can also use **Best Fit** feature to plot the most appropriate fit for your data automatically.
Fit Score Method	When the **Best Fit** is selected to construct the curve, you can additionally specify the scoring method to be used in evaluating goodness of applied fit methods. It R^2 R^2 with Low-End Accuracy R^2 with High-End Accuracy R^2 with Low-End and High-End Accuracy 1/Standard-Error 1/P-Value
Fit To Standard	Defines which points are used as the calibrators to fit the curve to: • **Replicates** – all replicate points from each **Standard** sample group are used as calibrators. • **Average** – average of the replicates from each **Standard** sample group

	are used as the calibration points for the curve..
Weight Method	Specifies weight function for transform.
X Transform	This setting determines how the **X** values are interpreted in the transform: • **None** – the **X** values remain as they are. • **Log10** – each **X** point is taken as a common logarithm of **X**. • **Log2** – each **X** point is taken as a binary logarithm of **X**. • **LogN** – each **X** point is taken as a natural logarithm of **X**.
Y Transform	This setting determines how the **Y** values are interpreted in the transform: • **None** – the **Y** values remain as they are. • **Log10** – each **Y** point is taken as a common logarithm of **Y**. • **Log2** – each **Y** point is taken as a binary logarithm of **Y**. • **LogN** – each **Y** point is taken as a natural logarithm of **Y**.

Quantification Limits

Accuracy (±%)	Defines a percentage limit of accuracy for **Standard Type** sample groups. This is used to verify whether the accuracy of calibrators fits in required limits. The default value is 20%.
Precision (%CV)	Defines a %CV precision limit. This is used to verify whether %CV for each **Standard Type** sample group is lower than required limit. The default value is 20%.

The Quantification limits properties are used to determine the Lower Limit Of Quantification (LLOQ) and Upper Limit Of Quantification (ULOQ) from the fit. The LLOQ and ULOQ are computed and added to the report automatically.

The method used to calculated LLOQ and ULOQ can be overriden by setting named evaluations with corresponding **Name** settings. In this case the custom calculated values will replace the default values.

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in

the **Raw** matrix. In this example we would like to construct a curve fit and calculate concentrations for input matrix.

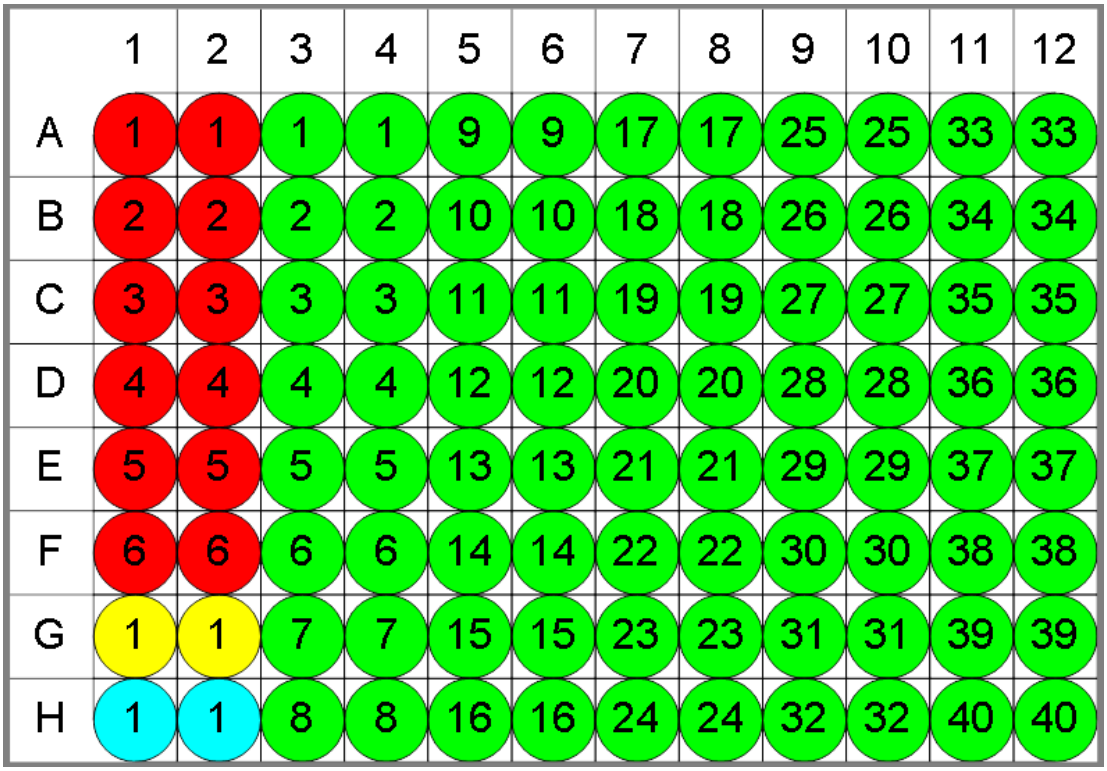
Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.192	0.199	0.347	0.346	0.325	0.321	0.803	0.797	1.589	1.593	0.241	0.246
B	0.293	0.300	0.586	0.584	0.800	0.793	0.402	0.401	0.839	0.837	0.562	0.564
C	0.537	0.534	0.549	0.547	0.878	0.875	0.471	0.471	0.759	0.756	1.039	1.043
D	0.858	0.855	0.320	0.325	0.531	0.530	1.552	1.551	0.429	0.427	0.424	0.424
E	1.523	1.527	0.486	0.490	1.289	1.283	1.430	1.438	1.494	1.501	1.427	1.429
F	1.622	1.621	0.621	0.626	0.667	0.663	1.350	1.347	0.631	0.634	1.695	1.694
G	0.001	0.001	0.356	0.352	0.418	0.412	1.172	1.174	1.572	1.570	0.595	0.590
H	0.297	0.297	0.796	0.801	1.517	1.515	0.960	0.965	0.534	0.527	0.585	0.584

Layout

The example uses a layout with **Standards**, **Control**, **Blank** and **Unknowns** in duplicate (e.g. **Standard1** in **A1** ans **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4** etc.). I.e.



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

1. Set **X Axis Title** to Concentration.
2. Set **X Axis Type** to Logarithmic.
3. Set **Y Axis Title** to Raw.
4. Set **X Axis Type** to Linear.
5. Set **Concentrations** in **Standard1** to 0.125 and a **Series** to multiply by 2.
6. Set **Standard Type** to **Standard**.
7. 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 (±%)** to 20%.
14. Set **Precision (%CV)** to 20%.

Concentration

The transform will generate an output matrix named **Concentration** with concentrations (**X**) calculation results for all samples using the curve fit. With the example data provided above, the results are as follows (also displayed here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	~~Flagged~~	~~Flagged~~	0.352	0.352	0.318	0.318	0.844	0.844	2.890	2.890	0.153	0.153
B	0.274	0.274	0.623	0.623	0.841	0.841	0.423	0.423	0.886	0.886	0.600	0.600
C	0.572	0.572	0.585	0.585	0.928	0.928	0.503	0.503	0.799	0.799	1.131	1.131
D	0.906	0.906	0.317	0.317	0.566	0.566	2.561	2.561	0.454	0.454	0.450	0.450
E	2.390	2.390	0.521	0.521	1.550	1.550	1.969	1.969	2.240	2.240	1.947	1.947
F	3.243	3.243	0.662	0.662	0.704	0.704	1.702	1.702	0.671	0.671	5.174	5.174
G	~~Flagged~~	~~Flagged~~	0.362	0.362	0.439	0.439	1.332	1.332	2.710	2.710	0.630	0.630
H	0.275	0.275	0.843	0.843	2.338	2.338	1.030	1.030	0.566	0.566	0.622	0.622

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 &lt; LLD"Label="Below LLD" />
           </Flags>
    </StandardCurveFit>
</Settings>
```

Upon calculating data with 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:

	1	2	3	4	5	6	7	8	9	10	11	12
A	Below LLD	Below LLD	0.352	0.352	0.318	0.318	0.844	0.844	2.890	2.890	0.153	0.153
B	0.274	0.274	0.623	0.623	0.841	0.841	0.423	0.423	0.886	0.886	0.600	0.600
C	0.572	0.572	0.585	0.585	0.928	0.928	0.503	0.503	0.799	0.799	1.131	1.131
D	0.906	0.906	0.317	0.317	0.566	0.566	2.561	2.561	0.454	0.454	0.450	0.450
E	2.390	2.390	0.521	0.521	1.550	1.550	1.969	1.969	2.240	2.240	1.947	1.947
F	3.243	3.243	0.662	0.662	0.704	0.704	1.702	1.702	0.671	0.671	5.174	5.174
G	Below LLD	Below LLD	0.362	0.362	0.439	0.439	1.332	1.332	2.710	2.710	0.630	0.630
H	0.275	0.275	0.843	0.843	2.338	2.338	1.030	1.030	0.566	0.566	0.622	0.622

Standard Deviation

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the standard deviation of the replicates in each sample group (flagged replicates are not included). The sample of population method is used.

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 12x8 microplate stored in the **Raw** matrix. In this example we would like to find the deviation between replicates in each sample group.

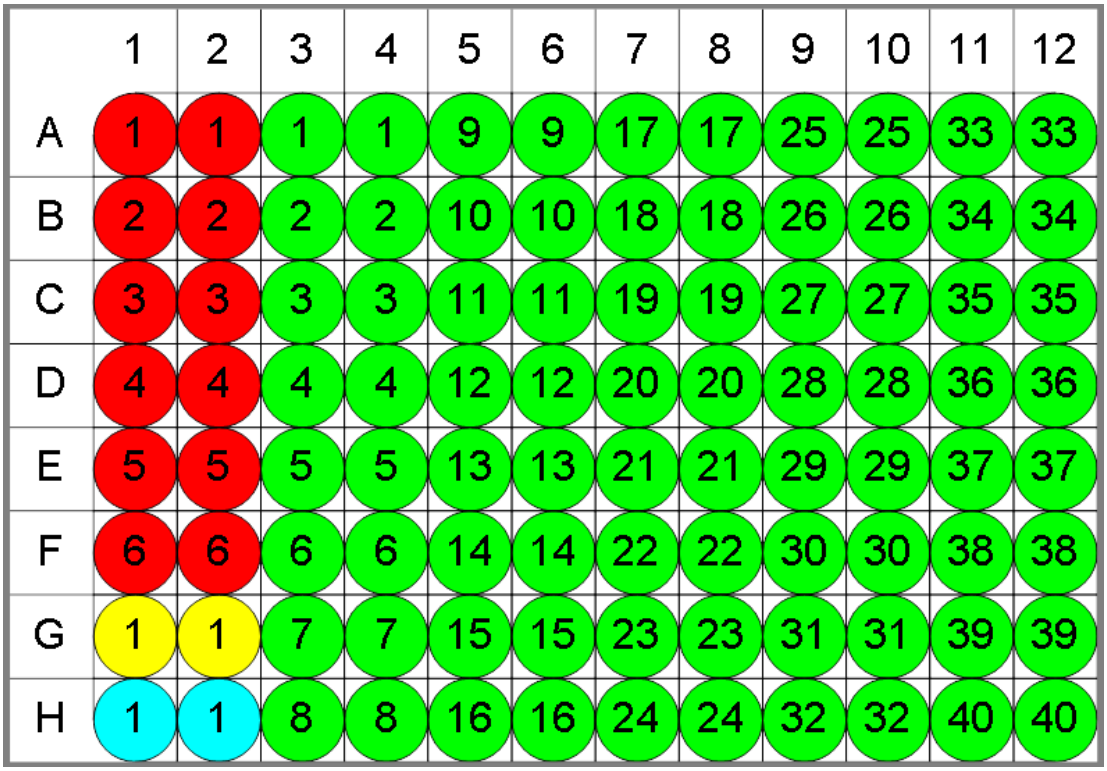
Here is some example raw data displayed here to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank** and **Unknowns** in duplicate (e.g. **Standard1** in **A1** ans **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4** etc.). I.e.



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 here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.029	0.029	0.013	0.013	0.009	0.009	0.022	0.022	0.004	0.004	0.013	0.013
B	0.010	0.010	0.013	0.013	0.011	0.011	0.018	0.018	0.001	0.001	0.013	0.013
C	0.008	0.008	0.028	0.028	0.023	0.023	0.005	0.005	0.002	0.002	0.009	0.009
D	0.023	0.023	0.010	0.010	0.014	0.014	0.021	0.021	0.004	0.004	0.001	0.001
E	0.028	0.028	0.062	0.062	0.007	0.007	0.021	0.021	0.002	0.002	0.021	0.021
F	0.014	0.014	0.023	0.023	0.007	0.007	0.019	0.019	0.001	0.001	0.012	0.012
G	0.008	0.008	0.026	0.026	0.016	0.016	0.001	0.001	0.001	0.001	0.005	0.005
H	0.012	0.012	0.005	0.005	0.033	0.033	0.001	0.001	0.000	0.000	0.009	0.009

Standard Error of Mean

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the standard error of the mean (SEM) of the replicates in each sample group (flagged replicates are not included). The sample of population method is used.

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 12x8 microplate stored in the **Raw** matrix. In this example we would like to find the SEM of each sample group.

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Unknowns** in triplets (e.g. **Unknown1** in positions from **A1** to **A3**, **Unknown2** in from **A4** to **A6** etc.). 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 here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.587	0.587	0.587	0.302	0.302	0.302	0.355	0.355	0.355	0.452	0.452	0.452
B	0.474	0.474	0.474	0.226	0.226	0.226	0.354	0.354	0.354	0.216	0.216	0.216
C	0.036	0.036	0.036	0.236	0.236	0.236	0.365	0.365	0.365	0.168	0.168	0.168
D	0.142	0.142	0.142	0.266	0.266	0.266	0.375	0.375	0.375	0.128	0.128	0.128
E	0.269	0.269	0.269	0.284	0.284	0.284	0.379	0.379	0.379	0.483	0.483	0.483
F	0.352	0.352	0.352	0.263	0.263	0.263	0.368	0.368	0.368	0.225	0.225	0.225
G	0.412	0.412	0.412	0.207	0.207	0.207	0.394	0.394	0.394	0.176	0.176	0.176
H	0.067	0.067	0.067	0.256	0.256	0.256	0.000	0.000	0.000	0.123	0.123	0.123

Variance

[Input: **Endpoint** ➡ Output: **Endpoint**]

This transform calculates the variance of the replicates in each sample group (flagged replicates are not included). The sample of population method is used.

The variance is the sum of the squares of the difference of each replicate and the mean divided by **n-1** (where **n** is the number of the replicates).

For groups with less than 2 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 12x8 microplate stored in the **Raw** matrix. In this example we would like to find the variance between measurements in each sample group.

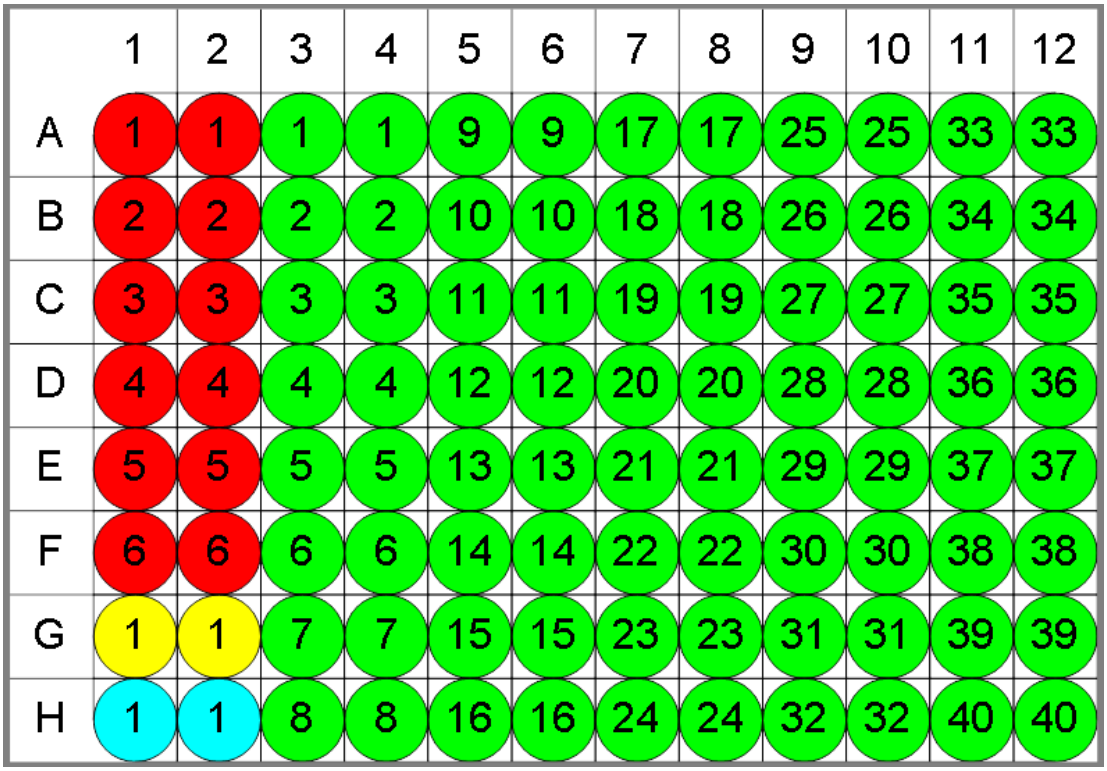
Here is some example raw data displayed to 3 decimal places:

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

Layout

The example uses a layout with **Standards**, **Control**, **Blank** and **Unknowns** in duplicate (e.g. **Standard1** in **A1** ans **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4** etc.). I.e.



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 here to 3 decimal places):

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
B	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	0.000	0.000	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000
D	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
E	0.001	0.001	0.004	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
F	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
G	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000

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.

XY Blank Correction

[Input: **XY** ➡ Output: **XY**]

This transform subtracts the average of a specified blank group (or groups) from each sample on a point-by-point basis. This is useful for subtracting background noise from measurements.

The background plot is first determined by creating an average XY plot of all replicates of the blank group. This background plot is then subtracted from each associated sample on a point-by-point basis.

Flagged positions or points are not included in the calculations.

As with other XY transforms the operation is only performed on data within specified range.

Properties:

Settings

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

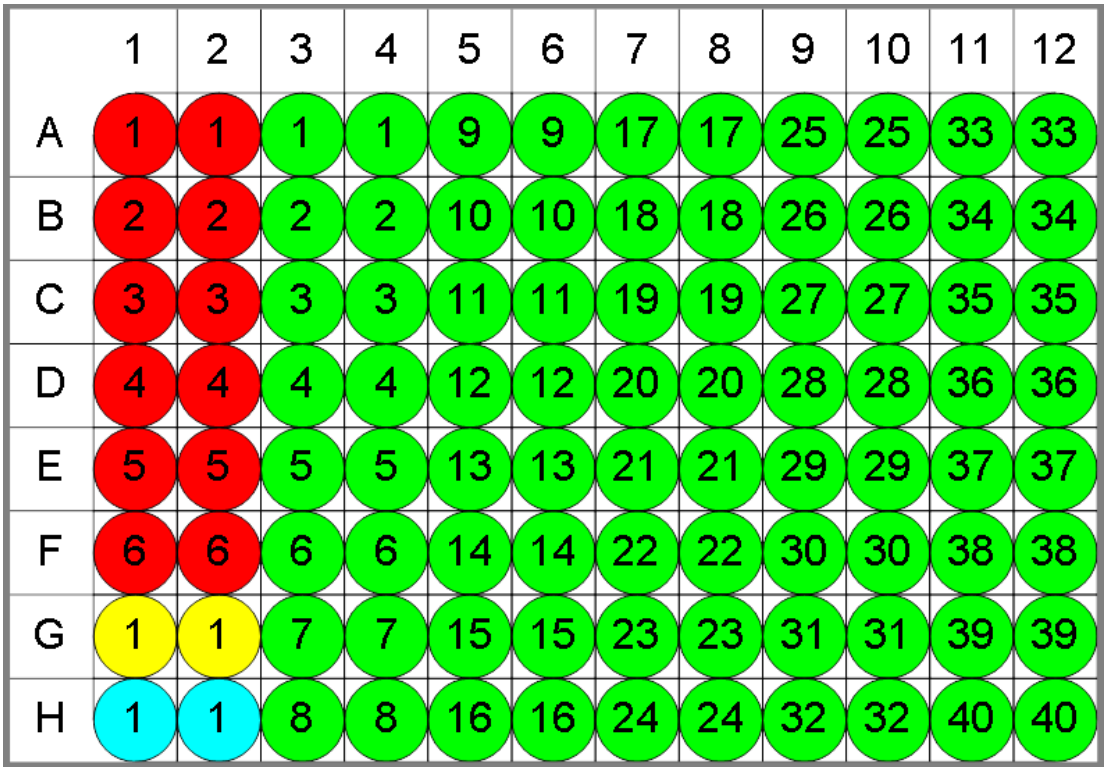
Blank Group	The group number of the sample to use for correction. This can be defined as a number or as an expression. The expression can refer to **x** which is the group number of the sample to be corrected. For example, set this to **x** to perform a 1-to-1 correction where each group is corrected by the sample of the specified blank type with the same group number.
Blank Type	The sample type used as the blank.

Example: Single Blank

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to perform a blank correction using the average of one blank group. This blank group itself is measured in duplicate. The mean of these replicates will be subtracted from all other samples.

Layout

The example uses a layout with **Standards**, **Control**, **Blank** and **Unknowns** in duplicate (e.g. **Standard1** in **A1** ans **A2**, **Unknown1** at **A3** and **A4**, **Unknown2** at **B3** and **B4** etc.). I.e.



To subtract the mean of the blank positions from the measurements, specify **Blank Group** to **1** and **Blank Type** to **Blank**.

Blank Corrected

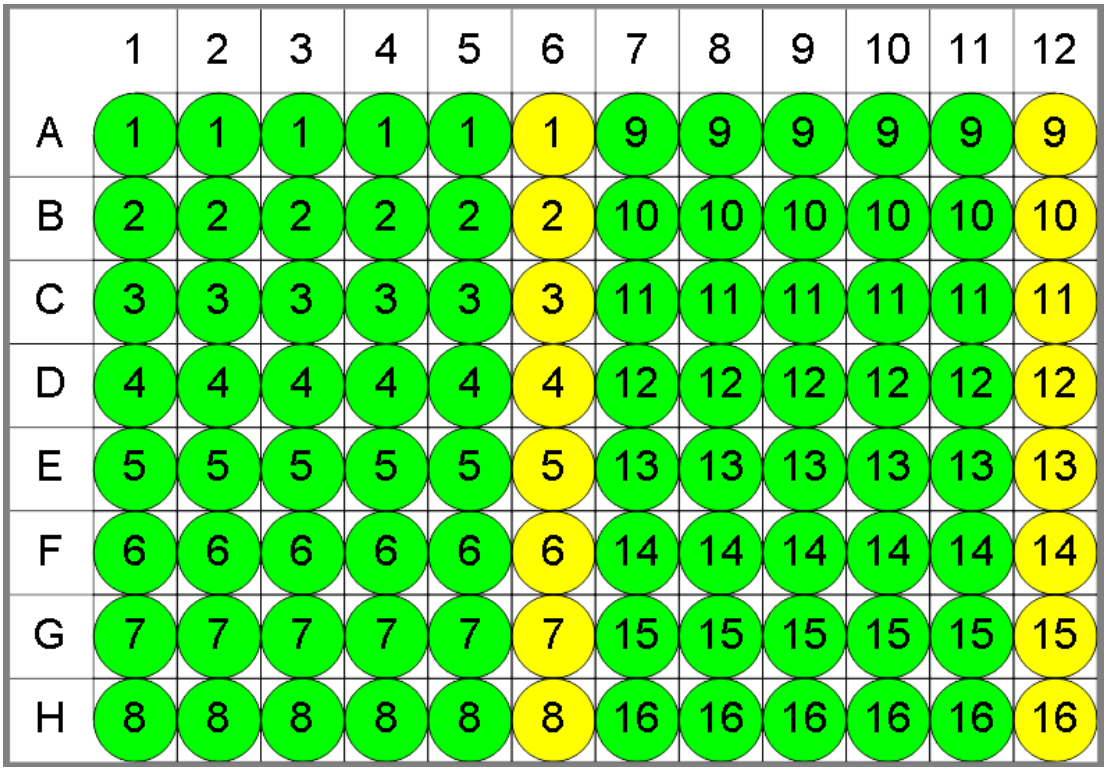
The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the average of **Blank1** sample group from the input data.

Example: 1-1 Blank Correction

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to perform a 1-to-1 correction, where each sample group is corrected by the blank that it is associated with. The blank numbering used in the layout defines the associations.

Layout

The example uses a layout with 16 **Unknowns** groups (with **Unknown1** in positions from **A1** to **A5**, **Unknown2** in positions from **B1** to **B5** etc.) and 16 **Blank** singlets I.e.



Specify **Blank Group** to **x** and **Blank Type** to **Blank** to perform 1-1 correction.

With this specified, the value of each blank will be subtracted from every replicate of associated sample group, i.e. **Blank1** (stored in **A6**) value will be subtracted from **A1, A2, A3, A4, A5** (the members of **Unknown1**) and from **A6** itself.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the associated blank value from the input data. Therefore, calculated matrix will contain blank corrected **Unknown** values and all **Blanks** will be 0.

Advanced Example: By-Row Blank Correction

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to configure blank correction on a row-by-row basis to blank correct each sample by the average of the two blank samples of the same row.

Layout

The example uses a layout with 80 singlet **Unknowns**and 8 **Blank** duplicates for each row (with **Blank1** in positions **A1** and **A12**, **Blank2** in positions **B1** and **B12** etc.) I.e.

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	1	2	3	4	5	6	7	8	9	10	1
B	2	11	12	13	14	15	16	17	18	19	20	2
C	3	21	22	23	24	25	26	27	28	29	30	3
D	4	31	32	33	34	35	36	37	38	39	40	4
E	5	41	42	43	44	45	46	47	48	49	50	5
F	6	51	52	53	54	55	56	57	58	59	60	6
G	7	61	62	63	64	65	66	67	68	69	70	7
H	8	71	72	73	74	75	76	77	78	79	80	8

Blank Unknown

With **Blank Group** setting uses the expression:

1 + floor ((x -1) / (LayoutWidth()-2),1)

This converts the group number of the sample to blank correct **(x)** to the blank number on its row, i.e. for **x=1** this means **1+floor((1-1)/10),1)**, **floor=0** and the **Blank Group** is taken as 1. For the first row **x** is in range from 1 to 10 and the expression outputs 1, thus for **Unknowns** from 1 to 10 the average of **Blank1** is subtracted.

For the second **x** is from 11 to 20, **floor=1**, so the **Blank2** group is subtracted from **Unknowns11-20**, etc.

Blank Corrected

The transform will generate an output matrix named **Blank Corrected** with the value at each position being the subtraction of the average of the associated **Blank** group from the input data.

XY Expression (Dual)

[Input: **Dual XY** ➡ Output: **XY**]

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

If the evaluation of the expression is valid then the data point is added to the output matrix (using the specified **X** and **Y** axes).

Properties:

Settings

Expression	The expression to evaluate, where variables are set to value of each position of the first (**x**) and second (**y**) input matrices. Default expression value is **x - y**.
Plot Input on Chart	When the checkbox is ticked, the chart includes both input and calculated plot. If it is unchecked, the chart shows calculated plot only.

XY Expression

[Input: **XY** ➡ Output: **XY**]

This transform evaluates specified expression for each not-flagged input XY data point within the specified range. If the evaluation of the expression is valid then the data point is added to the output matrix (using the specified **X** and **Y** axes).

Properties:

Settings

Expression	The expression to evaluate, where **y** variable is set to value of each position of the input matrix.
Plot Input on Chart	When the checkbox is ticked, the chart includes both input and calculated plot. If it is unchecked, the chart shows calculated plot only.

XY Fit

[Input: **XY** ➡ Output: **XY**]

This transform fits a specified curve to each non-flagged used XY plot within the determined range.

Properties:

Settings

Fit Method	

XY Join

[Input: **Dual XY** ➡ Output: **XY**]

This transforms accepts two XY input matrices and creates new combined XY plot for each position by appending the non-flagged data points from the second matrix to those of the first. Any flagged data points are not included in the output matrix.

This transform does not allow range specification.

Properties:

Data

If **X** is set as **Index** then the first index of the joined matrix is 1 plus the last used index.
If **X** is set as **X** then the **X** values are specified in each input matrix are used (unchanged) in the output matrix.

XY Outlier Removal

[Input: **XY** ➡ Output: **XY**]

This transform flags data points that are considered to be outliers. The values of the output matrix match those of the input matrix (the only difference being that outlier(s) might be flagged).

Properties:

Settings

Num Regression Points	The number of regression points used for each linear regression segment when determining the maximum slope. The default and minimum value is 2.
Threshold	Defines the threshold % accuracy to flag outliers. It calculates absolute % difference between back fit value and the original **y** value. The back fit is computed from slope and intercept for each **x** value in the regression set. If this % difference is **>** the specified **Threshold** then the data point is flagged on the output matrix.  Points that are flagged in one regression set are not included in calculations of following regression sets.

XY Replicates Average

[Input: **XY** ➡ Output: **XY**]

This transform calculates the XY average plot for each sample group within the specified range. Any flagged data points are not included in the analysis.

This is relevant, if there is any sample group in the layout with more than one replicate.

XY Reduction Average

[Input: **XY data** ➡ Output: **Endpoint**]

This transform reduces each XY/kinetic replicate of the input matrix to the average of its data point values within the specified range. The resulting numeric value is then stored in a corresponding position of the output endpoint matrix.

Flagged positions or points are not included in the calculations.

Example

Let's assume that we have some **XY** measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to reduce data in each position to average of its data points and store resulting value to corresponding position of an endpoint matrix.

Raw

Here is an **XY** matrix with each position containing 10 XY data points. Position data plots of the matrix are displayed in Plate Scale.

Here the reduction of data in **A1** position is shown for illustration of the transform. The raw data is displayed here to 3 decimal places:

A1 0.000;0.555 0.100;0.988 0.200;1.613 0.300;1.938 0.400;2.608 0.500;2.889 0.600;3.773 0.700;3.816 0.800;4.898 0.900;5.491

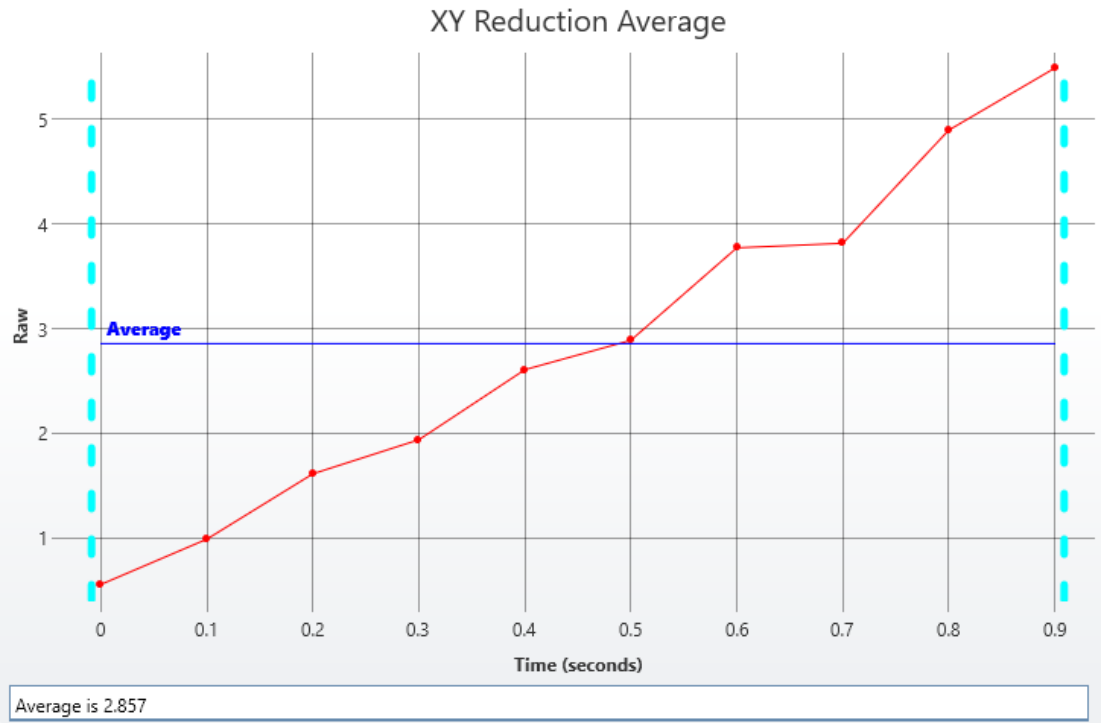
To reduce **XY** data to a average endpoint value:

1. Specify **Data**: **X Axis** as **X (Time)**, **Y Axis** as **Y**.
2. Leave **X Minimum** and **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 **Y** input data points. With the example data provided above, the resulting averaged value for **A1** plot is as follows (also displayed here to 3 decimal places):

2.857



XY Reduction Fit Parameter

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform fits a selected curve to the input XY data points within the specified range and sets the result to value of a specified fit parameter. The resulting value from each input position is stored to a corresponding position of the output endpoint matrix.

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** ➡ Output: **Endpoint**]

This reduction transform determines the maximum slope for each replicate within the specified range. The slope is determined between each pair of adjoining input XY data points using specified number of linear regressions points. The resulting maximum slope value from each input position is stored to a corresponding position of the output endpoint matrix.

Properties:

Settings

Max is	Determines the type of slope to be found by this transform. The settings are: • **Auto** – the maximum slope is determined from the general direction of each plot by using the linear regression. If the slope of the plot is positive, the **Fastest Increase** is used; if negative, the **Fastest Decrease** is used. • **Fastest Increase** – the maximum slope is the slope with the highest positive value. • **Fastest decrease** – the maximum slope is the slope with the greatest negative value.
Num Regression Points	The number of regression points used for each linear regression segment when determining the maximum slope. The default and minimum value is 2.
Result is	Specifies the result of the analysis. The settings are: • **Slope** – the result is the slope of the determined maximum slope. • **X At Centre Absolute** – the result is the **X** at the centre of the determined maximum slope. • **Y At Centre Absolute** – the result is the **Y** at the centre of the determined maximum slope. • **X At Centre Relative** – the result is the **X** at the centre of the determined maximum slope relative to the first not-flagged data point

	that is greater than **X Minimum.** • **Y At Centre Relative** – the result is the **Y** at the centre of the determined maximum slope relative to the first not-flagged data point that is greater than **X Minimum**. • **Extrapolated Y** – A value of **Y** is calculated from the determined maximum slope using the **X** value specified with **X For Extrapolation**.
X for Extrapolation	When **Extrapolated Y** option in the **Result Is** setting is chosen, then this can be used to specify an expression used to determine the **X** value to calculate **Y** for.

XY Reduction Peak

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform finds the peak **Y** value (minimum or maximum) of the input XY data points within the specified range. The resulting **X** or **Y** point value from each input position is stored to a corresponding position of the output endpoint matrix.

Properties:

Settings

Peak	This setting determines which data point is considered as the peak: • **Max** - result is the point with the maximum Y value. (This is the default value) • **Min** - result is the point with the minimum Y value.(The default value is **Max**).
Result	This setting determines which value to consider for evaluation: • **X**- X value of peak data point. • **Y**- Y value of peak data point.

XY Reduction Total

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform sums the Y values of the input XY data points within the specified range. The resulting value from each input position is stored to a corresponding position of the output endpoint matrix.

XY Reduction X At Y

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform finds the first point at which **X** value at which the **Y** value (**Cursor**) crosses or equals the **XY Data** within the specified range of the input XY matrix. The resulting point value from each input position is stored to a corresponding position of the output endpoint matrix.

X and **Y** values can be specified as a relative to the first point or as an absolute value.

Properties:

Settings

Cursor	The expression evaluated for each position that represents the target in **Y** value. The default value is 1.
Cursor Type	This defines how the **Cursor** is treated for each position. The settings are: • **Absolute** – the values specified by **Cursor** is the value to use in the calculation of **X**. • **Relative From First Measured** – the value of **Cursor** is added to the **Y** value of the first point for the position (even if the first point is ~~**Flagged**~~ or out of range). • **Relative From First In Range** – the value of **Cursor** is added to the **Y** value of the first non-flagged data point within the range.
Result is	Specifies the result of the analysis. The settings are: • **Absolute** – the computed **X** value. • **Relative From First Measured** – the computed **X** value minus the **X** value of the first point for the position (even if the first point is ~~**Flagged**~~ or out of range). • **Relative From First In Range** – the computed **X** value minus the **X** value of the first non-flagged data point within the range.

XY Reduction Y At X

[Input: **XY data** ➡ Output: **Endpoint**]

This reduction transform determines the **X** value for the specified **Y** value (**Cursor**) within the specified range of the input XY matrix. The resulting point value from each input position is stored to a corresponding position of the output endpoint matrix.

Properties:

Settings

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

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:

y = the dependent variable (i.e. what you measure as the signal)

x = the independent variable (i.e. what you control, such as, dose, concentration, etc.)

Coefficients of the Fit

The 4 parameters consist of the following:

- **a** = the minimum value that can be obtained (i.e. what happens at 0 dose)
- **d** = the maximum value that can be obtained (i.e. what happens at infinite dose)
- **c** = the point of inflection (i.e. the value of x at the point on the S shaped curve halfway between a and d)
- **b** = Hill's slope of the curve (i.e. this is related to the steepness of the curve at point c). It could either be positive or negative..

The rearranged equation to solve x is:

$$x = c\left(\frac{a-d}{y-d} - 1\right)^{\frac{1}{b}}$$

The **a** and **d** values might be flipped, however, **a** and **d** will always define the upper and lower asymptotes (horizontals) of the curve. **a** and **d** are the same units at **y**. The curve can only be used to calculate concentrations for signals within **a** and **d**. Samples outside the range of the determined **a** and **d** cannot be calculated.

4PL and IC50

A common requirement is to calculate IC50 from the fit. The IC50 is the concentration of an inhibitor where the response (or binding) is reduced by half. There are actually two ways to do this depending on what you consider IC50 to be:

- Firstly, the midpoint of the sigmoid of the 4PL is equal to the **c** coefficient of the 4PL. In this case you can simply look at the calculated **c** coefficient. Use this method if you consider the midpoint of the sigmoid to be equal to IC50. Mathematically this is the case as it is the **x** point at exactly half way between the two horizontal asymptotes.
- Alternatively, if the response is measured between 0 and 100% and you consider IC50 to be where **y** = 50 then you can calculate where **y** = 50 using the equation to solve **x** (above), substituting in the calculated coefficients.

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 (**x**). This model provides starting approximation and, although is seldom used for biological systems, is often used to visualise data relationship at a glance.

The equation for the model is:

$$y = mx + c$$

Variables

In this model we have the following:

y = the dependent variable (i.e. what you measure as the signal)

x = the independent variable (i.e. what you control, such as, dose, concentration, etc.)

Coefficients of the Fit

m = the slope of the fitted line

c = the intercept of the dependent axis

The rearranged equation to solve x is:

$$x = \frac{y-c}{m}$$

The goal is to determine values of **m** and **c** which 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 and 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

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

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 customised. For example, you might consider the fit with the highest **R^2** to be the best. You also might want to take into account the accuracy of the curve at certain regions of the fit (for example 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
- 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 defined your own scoring methods to evaluate and compare each attempted fit.

Scoring Method Expressions

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

Accuracy Functions

In addition to the Goodness Measures various accuracy functions are available to assess the accuracy of the fit at various points. These accuracy functions enable a comparison to be made between the expected value (the known **x** of the calibrator) and its actual value calculated from the curve.

The calibration data set is this is the known concentration values of the standards (**x**) plotted against their measurements (**y**).

Each curve is fitted to the calibration data set.

To measure the accuracy of the curve at a particular data point, the **x** value of the known concentration (expected) is compared against the **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 $\mathbf{R^2}$), the accuracy functions return a value between 0 and 1 (where 1 is perfectly accurate).

<table>
<tr><th>Function Name</th><th>Description</th></tr>
<tr><td>AccuracyRatio</td><td>Calculates the accuracy ratio of the expected value and its actual value. This is similar to % recovery, however, here a value between 0 and 1 where 1 is perfect accuracy (i.e. 100% recovery). A % Recovery of 120% or 80% both equal an Accuracy Ratio of 0.8. With AccuracyRatio, if the actual value differs to the expected by a factor of two or more the accuracy ratio as 0.</td></tr>
<tr><td>AccuracyFactor</td><td>Calculates an accuracy factor of the expected value and its actual value. This is computed using % Recovery and a Gaussian function such that:
<table>
<tr><th>% Recovery</th><th>Accuracy Factor</th></tr>
<tr><td>100</td><td>1</td></tr>
<tr><td>0</td><td>0.5</td></tr>
<tr><td>200</td><td>0.5</td></tr>
<tr><td><0%</td><td>Value between 0.5 and 0</td></tr>
<tr><td>> 200%</td><td>Value between 0.5 and 0</td></tr>
</table>
</td></tr>
</table>

Function Name	Description
	This function avoids reporting a value of 0 for scenarios where the % Recovery is < 0 % and > 200 %.
Diff	The absolute difference between the expected value and is actual value.

Accuracy Function Forms

Each accuracy function comes in three forms:

- At Specified X Point
- From Low end (ends with Low)
- From High end (ends with High)

The following table provides example expressions calling accuracy functions and their result.

Expression	Result
AccuracyRatio (0.125)	The accuracy ratio for calibrator where x = 0.125.
AccuracyRatioLow (1)	The accuracy ratio for the calibrator with the lowest x value.
AccuracyRatioLow (2)	The accuracy ratio for the calibrator with the second lowest x value.
AccuracyRatioHigh (1)	The accuracy ratio for the calibrator with the highest x value.
AccuracyRatioHigh (2)	The accuracy ratio for the calibrator with the second highest x value.

Combining Measures

A scroring 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 recommend 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)

Preset	Expression
R^2 with High-End Accuracy	R^2*AccuracyFactorHigh(1)
R^2 with Low-End and High-End Accuracy	R^2*AccuracyFactorLow(1)*AccuracyFactorHigh(1)
1/Standard-Error	1/SE
1/P-Value	1/P

Standard Curve Fit Advanced Configuration

Standard Curve Fit Custom Flag 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). This feature is useful in curve-fitting as there are often values outside certain ranges that should report a label rather than result or error.

The same as the general Custom Flag Label feature, Standard Curve Fit Custom Flag Label is an advanced option and is only available through XML configuration. Comparative to the former, this specific feature has higher precedence and overrides other defined labels.

It uses expressions written in terms of **x** to define when a result should be flagged and labelled as.

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.

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.
2. Locate the **StandardCurveFit** element.
3. Add an **Flags** element (as a child of the **StandardCurveFit**) and, optionally, a **CurveError** element.
4. Add a child element **Flag** t for each required flagging rule. Set the attributes (in accordance with the following table).
5. Press **Apply** to save changes to the protocol.

Custom Flag Label Attributes

Type	The value of **x** depends on the expression type: • For Type="Input"**x** is the value of the input position.

	• For Type="Output"**x** is the value computed for the output position.
Condition	The condition to evaluate (typically a conditional expression). The flag condition expression can refer to: • the value of each position using the reference **x**. • the computed coefficients of the curve and goodness measures. • Standard Curve Named Evaluations. • 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 **{x}** in the **Label** , it returns each position's value (e.g. **{x}> below LLD**).

Syntax

The valid Label syntax is displayed below. The areas for defining the Custom Flag Label attributes are highlighted in yellow.

```
<StandardCurveFit StandardType="2" FitMethod="4PL" Concentrations="0.125,0.25,0.5,1,2,4" XAxisTitle="Concentration" YAxisTitle="Raw" FitToStandard="Average" CalculateFrom="Average">
 <Flags>
        <Flag Type="Input / Output" Condition="Condition" Label="Label" />
</Flags>
</StandardCurveFit>
```

Special XML Characters

There are five characters that supposed to be defined specially in XML elements attributes. These are listed in the table below.

Operator	Description	In XML
<	Less Than	&lt;
>	Greater Than	&gt;
&	Ampersand	&amp;
"	Double Quote	&quot;

Operator	Description	In XML
'	Apostrophe/ Single Quote	&apos;

CurveError Optional Setting

The optional CurveError setting is used to specify a custom flag label to use if a value cannot be computed from the curve (i.e. is flagged on the input matrix or while calculating results). It simply replaces 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="*Label*" >

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.

Example XML Configuration

```
<StandardCurveFitStandardType="2"FitMethod="4PL"
Concentrations="0.125,0.25,0.5,1,2,4"XAxisTitle="Concentration"
YAxisTitle="Raw"FitToStandard="Average"CalculateFrom="Average">
    <FlagsCurveError="Could not calculate from curve" >
        <FlagType="Input"Condition="x &lt; Blank1+3*sd(Blank1)"Label="{x}
        Below LLD" />
        <FlagType="Input"Condition="x &lt; min(a,d)"Label="Below Lower
        Asymptote" />
        <FlagType="Output"Condition="x &lt; 0.125"Label="&lt; 0.125" />
```

```
            <FlagType="Output"Condition="x &lt; 0.125"Label="Calculated X ({x})
            &lt; 0.125" />
        </Flags>
</StandardCurveFit>
```

Standard Curve Fit Evaluations

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

- Calculate **X** or **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.

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.
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: • the computed coefficients of the curve and goodness measures. • any defined above in the XML Standard Curve Fit Evaluation with **Name** attribute specified. • sample values of the input matrix.  Since the result is a single numerical value, expression can not refer to **x** or **y** variables.
Type	This setting describes how the expression is treated in report:

	• **CalcX** - calculates the **X** value from fit line using **Expression** as **Y** value. The resulting values are reported using numerical formatting of input matrix. • **CalcY** - calculates the **Y** value from fit line using **Expression** as **X** value. The resulting values are reported using standard numerical formatting. • **Parameter** - outputs the computed **Expression** value.
Description	Optionally added textual description of the expression. If this is not specified, the **Expression** itself is used in report.
Name	Optional element, which defines a name for evaluation. If it is specified, the **Name** can be used as a variable for other XML configurations (as described 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.
- In Standard Curve Flag Label conditions.

The **LLOQ** and **ULOQ** are computed automatically and can be used as a 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 Multiple Plate Standard Curve Fit Analysis topic.

For example, the LLD is often computed as: the concentration (**X**) at the average of the blank replicates + 3 * standard deviation of the blank replicates. This can be computed as an expression that calculates **X** from the curve where **Y = Blank + 3 * sd(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. i.e. report syntax errors in table (in same way as Evaluation feature).

Expressions

You can enter an expression to evaluate for any configuration setting that accepts a numerical value as a parameter. Expressions can be used as parameters to transforms to specify custom analysis to perform.

Overview

The expressions are used to configure various analytical methods on data as required in order to achieve precise analytical results. For example, you can specify how to remove background noise from your measurements, set detection and quantification limits, etc.

The use of expressions in various levels of analysis provides:

- **great flexibility of assay design;**
- **custom analysis with familiar mathematical syntax;**
- **referencing other parts of the assay easily;**
- **taking into account flagged data;**
- **setting conditions (such as validation expressions).**

Expressions can refer to measurements or transform results from positions, sample groups, variables and other expressions. Generally, they are utilised in transforms, validation rules and custom evaluations.

Culture Settings

When providing numerical 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 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 comma list separator.

Syntax

The syntax of expressions is consistent. However, the use of the expression depends on the situation it is being used in. For example, you can enter an expression in terms of **x** in some transforms and custom flag conditions. where the expression is evaluated in every position of the layout and **x** is replaced with an endpoint value. In other situations, the expression is evaluated by itself without reference to a layout.

All expression examples given in the Help use period decimal separator(.) and comma list separator(.). Use local settings of your system when actually entering expressions.

A typical expression comprises of:

- operations, (e.g. +, *).
- operands (e.g. A1, 4, x).
- functions (e.g. pcv, floor).

The following table lists some examples of expressions you may use in your assay.

Example Expressions

Expression	Evaluated to
Unknown1	The average of the non-flagged **Unknown1** position values on the layout.
Unknown	The average of the non-flagged **Unknown** position type values on the layout.
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** and tripled standard deviation of **Blank1**. This is often used to compute LLD.

Expression	Evaluated to
pcv ([Unknown1,Unknown2])	The percentage coefficient of variation of all positions made up of **Unknown1** and **Unknown2**.
median (Standard1)	The median of the non-flagged **Standard1** position values on the layout.
x-Blank1	The value of variable **x** minus the average of **Blank1** position.
x > 15	To 1 if the value of variable **x** is greater than 15, otherwise evaluates to 0.
Ifthenelse (x>15, 15, x)	If the value of **x** is greater than 15 then the result is 15, otherwise the result is **x**.
x-y	The difference between **x** and **y**. Here **x** and **y** are the values of corresponding positions from two matrices of data.
EvalProperty(MinX)	The context-property **MinX**.
median(Unknown.2.All)	The median of all **Unknown** replicates on matrix 2 across all containers.
Unknown1.2.3	The average of **Unknown1** sample group on the 2nd matrix of 3rd container.

Operators

Unary Arithmetic Operator

Operator	Operation	Examples
-	Minus Sign	-1.23 -x

Binary Arithmetic Operators

Operator	Operation	Example
+	Addition	2+1 x+y x+1
-	Subtraction	2-1 x-y x-1
*	Multiplication	2*3

Operator	Operation	Example
		x*y y*2
/	Division	2/2 x/y x/2
^	Raising to a power	2^3 x^y x^2

Binary Logical Operators

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

Operator	Operation	Examples
<	Less Than	1<2 x<y x<2
>	Greater Than	2>1 x>y x>2
=	Equal To	1=1 x=y x=2
<=	Less Than Or Equal	3<=9 3<=3 x<=y x<=x x<=3
>=	Greater Than Or Equal	9>=3 3>=3 y>=x

Operator	Operation	Examples
		x>=x x>=9
<>	Not Equal	2<>1 x<>y x<>3

Boolean Operations

The Boolean operations (and, or, not) are implemented as Conditional Functions.

Operands

Numbers

Number operands are simply numbers, e.g. 1.23, -100, 14.

Variables

The **x** and **y** variables refer to value of each position on the associated matrix. All references to these variables in expressions are equated to the associated values.

For example, in Expression by Matrix transform you may enter **x*100** expression, where **x** variable will refer to the positions of the input matrix. In the resulting matrix all positions will be multiplied by 100. In Expression by Matrix (Dual) the **x** and **y** variables are set to position values of the first and second matrices. Thus, when you enter an expression **x+y**, each position on the resulting matrix will be the sum of input matrices values.

Variable	Relevant For
None	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 calculated context parameters of the fit. Former refers to the parameters in configuration settings and 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
R^2	r2
aR^2	ar2
F	f
P	p
SE	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 can not be used in general configuration of the assay (e.g. validation or evaluation tables) or other transforms.

Layout References

When an evaluation depends 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. upper- and lowercase letters in expressions are treated as being the same.

For example, **Unknown1** is the same as **unknown1**, **UNKNOWN1** and **UnKnOWN1**.

Position References

A position ID refers to a specific position on the layout, e.g. **A1**, **H12**. Click here to learn more about layout positions.

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**: ***Unknown1*** *refers to all non-flagged* ***Unknown1*** *sample group positions on the layout.*
- **Sample type.** If no group number is specified, then it refers to all positions of that type on the layout (e.g. all Unknowns, Blanks, Standards). **Example**: ***Unknown*** *refers to all non-flagged data points of* ***Unknown*** *type on the layout.*

The simple sample reference usually refers to the average of non-flagged positions of the type/group. Only for group-enabled functions it refers to the **list of values of each non-flagged position** that belong to the sample reference. **Example**: ***median (Unknown1)*** *calculates the median of all defined on the layout non-flagged* ***Unknown1*** *position values..*

Click here to read more about group-enabled functions.

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, simple **Unknown1** reference always refers to the first **Unknown** sample group on the container being evaluated.

Click here to view more about multiple plate analysis.

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.

Reference	Refers To
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.

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 non-flagged 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 two 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 (Unknown)**
mean	Calculates the mean of the non-flagged positions.	1	**mean (Unknown1)**

Name	Description	Minimum number of parameters	Examples
			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 (Unknown1)** **median ([Standard2, Unknown4])**
pcv	Calculates the percentage coefficient of variance (**%CV**) of a finite list of non-flagged positions.	2	**pcv (Unknown)** **pcv ([Unknown1, 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 (Standard2)** **sd ([Unknown1, Unknown3])**
se	Calculates the standard error of a finite list of non-flagged positions.	2	**se (Unknown1)** **se ([Unknown, Control])**
sum	Returns the total of all items in the finite list of non-flagged positions.	1	**sum (Unknown)** **sum ([Unknown1, Unknown1.2, Unknown1.3])**
var	Calculates the variance of a finite list of non-flagged	2	**var (Unknown4)**

Name	Description	Minimum number of parameters	Examples
	positions. Variance is a measurement of the spread between positions in a data set. The variance measures how far each number in the set is from the mean.		**var ([Unknown1, Unknown1.2])**

Example:

Let's assume that we have some endpoint measurement data for a 12x8 microplate stored in the **Raw** matrix. In this example we would like to find medium value for **Unknown1** and **Unknown2** positions.

The example uses a layout with 16 **Unknown** sample groups, where **Unknown1** at **A1**, **A2** **A3**, **A4**, **A5** and **A6**, **Unknown2** at **A7**, **A8**, **A9**, **A10**, **A11**, **A12** etc.). I.e.

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

Unknown

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

Raw

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.364	0.323	2.105	2.124	1.213	1.226	1.159	1.190	0.110	0.116	1.463	1.481
B	0.455	0.441	1.869	1.888	1.203	1.218	1.180	1.206	0.132	0.130	0.786	0.768
C	0.587	0.575	0.474	0.514	1.206	1.239	1.203	1.210	0.113	0.116	0.613	0.626
D	0.806	0.774	0.364	0.378	1.167	1.187	1.211	1.241	0.101	0.106	0.489	0.490
E	1.105	1.065	0.279	0.367	1.215	1.225	1.233	1.262	0.111	0.114	1.579	1.549
F	1.425	1.445	0.378	0.411	1.196	1.206	1.226	1.199	0.109	0.108	0.792	0.775
G	1.791	1.803	0.560	0.597	1.205	1.228	1.308	1.306	0.126	0.127	0.652	0.659
H	0.253	0.270	0.463	0.470	1.214	1.261	0.115	0.116	0.115	0.115	0.490	0.477

We use the expression:

median ([Unknown1, Unknown2])

Unknown1 and **Unknown2** refer to the lists of non-flagged data points for **Unknown1** and **Unknown2** sample groups. From this lists 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 a input parameter to conditional function, it refers to the average of the non-flagged data points.

Boolean Logical Functions

Name	Description	Examples
and	The operation tests a number of input conditions and returns 1 if all of the conditions evaluate to true, or 0 otherwise.	**and(1,1)**
or	Tests a number of input conditions and returns 1 if any of the conditions evaluate to true, or 0 otherwise.	**or (1,1)** **or (x<5, x>10)**
not	Returns a logical value that is the opposite of a input logical value or expression (i.e. returns 0 is the supplied argument is true and returns 1 if the supplied argument is false).	**not(x>1)**

Conditional Function

Name	Description	Examples
ifthenelse	Requires 3 parameters: 1. The Boolean condition to evaluate (which will evaluate to true or false). 2. The result if the condition is true. 3. The result if the condition is false. If the value of the first condition is true then the result is the second argument otherwise the third.	**ifthenelse (1=1,2,3) result is 2** **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 **Unknown1** 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 argument or list of arguments. Calculation functions use general syntax for functions and perform an operation on a list of one 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.	**abs**(-1.23)=1.23 **abs**(1.23)=1.23
average	Described in group-enabled functions.	**average**(1,2)=1.5 **average**(-3,0.25,5)=0.75
ceiling	Returns argument (**{0}**) 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:	**ceiling**(1.23, 0.05)=1.25 **ceiling**(-1.23, 0.05)=-1.2

Name	Description	Examples
	• **{0}** is the value you want to round off. • **{1}** is the multiple to which you want to round. Regardless of the sign of a **{0}**, a value is rounded up when adjusted away from zero. If the **{0}** is an exact multiple of **{1}**, no rounding occurs.	
count	Described in group-enabled functions.	**count**(1,2,3)=3 **count**(-2.44,2,5,98,6)=5
exp	Returns **e** raised to the power of the given number. Syntax: **exp({0})** where: **{0}** is the exponent applied to the base **e**. It accepts only single argument. For example, the system accepts **exp(A1+A2)** and rejects **exp(A1,A2)**.	**exp**(2)=7.389056... **exp**(-1)=0.367879...
floor	Returns argument (**{0}**) rounded down, towards zero, to the nearest multiple of significance (**{1}**). It requires two input parameters with the following syntax **floor({0}, {1})**, where: • **{0}** is the value you want to round off. • **{1}** is the multiple to which you want to round. Regardless of the sign of a **{0}**, a value is rounded down when adjusted away from zero. If the **{0}** is an exact multiple of **{1}**, no rounding occurs.	**floor**(1.23, 0.05)=1.2 **floor**(-1.23, 0.05)=-1.25
intercept	Calculates the point at which the least squares fit line will intersect the Y axis by using existing x-values and y-values. The intercept point is based on a best-fit regression line plotted through the known x-values (independent set of arguments) and known y-values (dependent set of arguments). Requires a vector of arguments as parameters.	**intercept**({1,2},{3,2})=4 **intercept**({-2.44,2,5,98,6}, {0.1,0.2,0.3,0.4,0.5})=-12.152

Name	Description	Examples
	The number of Y and X operands is required to be the same and greater than 2, i.e. {y1,y2,y3} and {x1,x2,x3}; {y1,y2, ... yN} and {x1, x2, ... xN}.	
ln	Returns the natural logarithm of an argument. Natural logarithms are based on the constant e (2.718281828459...). The argument is supposed to be positive. **ln** is the inverse of the **exp** function.	**ln**(10)=2.302585... **ln**(1.23)=0.207014...
log	Calculates the logarithm of an argument to the base that you specify. This uses the following syntax with two input parameters: **log({0}, {1})** where: **{0}** is the positive real numerical value or expression for which you want the logarithm. **{1}** is the base of the logarithm. If base is omitted, it is assumed to be 10.	**log**(2,4)=0.5 **log**(1.23,2)=0.298658...
log10	Returns the base-10 logarithm of a positive argument.	**log10**(1.23)=0.089905... **log10**(0.1)=-1
max	Returns the largest value in a set of values. To determine maximum of positions in a sample group or sample type, type in the argument it square brackets, i.e. **max ([Unknown1])**. Otherwise the reference is treated as the average of positions.	**max**(1,2,3)=3 **max**(-2.44,2,5,98,6)=98
median	Described in group-enabled functions.	**median**(1,2,3,4)=2.5 **median**(-2.44,2,5,98,6)=5
min	Inversely to **max** function, returns the smallest number in a set of values. All requirements of the **max** apply to **min** too.	**min**(1,2,3)=1 **min**(-2.44,2,5,98,6)=-2.44
mod	Returns the remainder after the argument is divided by a divisor. The result has the same sign as the	**mod**(2,0.3)=0.2 **mod**(1.23,5)=1.23

Name	Description	Examples
	divisor. Syntax: **mod({0}, {1})** where: **{0}** is the argument for which you want to find the remainder. **{1}** is the value by which you want to divide the **{0}**.	
pow	Returns the result of a number raised to a power. Syntax: **power({0}, {1})** where: **{0}** is the base argument. **{1}** is the exponent to which the **{0}** is raised.	**power**(2,3)=8 **power**(1.23,5)=2.815305...
slope	Returns the slope of the linear regression line through data points in Xs and Ys. The slope is the vertical distance divided by the horizontal distance between any two points on the line, which is the rate of change along the regression line. Requires a vector of arguments as parameters. The number of Y and X operands is required to be the same and greater than 2, i.e. {y1,y2,y3} and {x1,x2,x3}; {y1,y2, ... yN} and {x1, x2, ... xN}.	**slope**({1,2},{3,2})=-1 **slope**({-2.44,2,5,98,6}, {0.1,0.2,0.3,0.4,0.5})=112.88
stdev	The same as **sd** in group-enabled functions.	**stdev**(1,2,3)=1 **stdev**(-2.44,2,5,98,6)=42.772359...
sum	Described in group-enabled functions.	**sum**(1,2,3)=6 **sum**(-2.44,2,5,98,6)=108.56
var	Described in group-enabled functions.	**var**(1,2,6)=7 **var**(-2.44,2,5,98,6)=1829.47472

Layout Analysis Functions

Layout Analysis Functions require a list of zero or more operands.

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

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

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")

"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 con-tainers)	**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, ContainerNum.	**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, ContainerNum.	**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-outNumGroupsAcrossContainers	Determines the number of	**Lay-outNumGroupsAcrossContainers**

Name	Description	Example
(Type)	groups of the specified Type parameter on each of the containers. If this is the same number on every container (including 0) then this value is returned. Otherwise -1 is returned.	**("Unknown")**

Command Line Arguments

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

Syntax

>"C:*MyAssays Installation Root path*\MyAssays 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 .assay-protocol 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}:{1}	Specifies the export options. {0} is either: • XLSX, PDF, XML (file export type). • XSLT. Requires additional arguments to specify output filename extension and path to XSLT 1.0 file. The exported file will be saved	**/export-report:pdf** **/export-report:xslt1:csv:"XSLT file path"**

Argument	Description	Example
	under \MyAssays\Reports\ folder.	
	The optional {1} specifies whether to launch the exported file with its default associated application. If it is specified the file will not launch.	**:nolaunch** **/export-report:xml:nolaunch**
/import-containerids:{0}	Specifies a Plate IDs file to use in data analysis.  This command-line argument overrides previously configured by **Import Wizard** method.	**/import-containerids:"Data file path"**
/import-raw:{0}	Specifies the raw data file to be used for analysis.	**/import-raw:"Raw data file path"**
/import-sampleids:{0}	Specifies a Sample IDs file to use in data analysis.  This command-line argument overrides previously configured by **Import Wizard** method.	**/import-containerids:"Sample IDs file path"**
/import-tweaks:{0}:{1)	Specifies a protocol tweaks file that defines changes to the protocol configuration. • {0) - full path to the protocol tweaks file.	**/import-tweaks:"Protocol tweak file path"**
	The optional {1} specifies save setting. If it is specified, the protocol file will be saved with tweaks automatically.  If the **Save changes to**	**/import-tweaks:"Protocol tweak file path":saveprotocol**

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 to select the tab MAA starts on. {0} is zero-based **tab number**: *Overview = 0; Measurements = 1; Microplate = 2; 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 **Results tab** and the XLSX report will be saved (but not automatically launched) under \MyAssays\Reports\ 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 customisation. 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 customisations (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 Command Prompt.
2. Enter file path to protocol tweak file as a parameter of 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 Alongside WorkOut

If you install WorkOut application after MyAssays Desktop installation an error might occur:

> **ERROR - The operation failed unexpectedly. If the problem occurs again, please contact support.**
>
> **System.AccessViolationException: Attempted to read or write protected memory. This is often an indication that other memory is corrupt.**
>
> **at MIMPORTSLib.IImportScript.get_FileNameToImport()**

To resolve it, please re-install MyAssays Desktop to update shared component files to newest version.

You must activate your copy of MyAssays Desktop in order to begin your work with the application. Please consider, that your license is active on one device only, so if you want to switch your PC, you will have to deactivate it on a current one and deactivate on next one.

To add more functionality to your license you may prefer updating it. With all questions about getting a license, please contact MyAssays Support team on http://www.myassays.com/contact.aspx.

Activating License

You have to activate MyAssays Desktop with a serial code, provided by MyAssays Ltd., in order to start working with the application.

To activate **MyAssays Desktop** on your PC, please launch **MyAssays Desktop Explorer** and **Licensing Activation Wizard** will automatically appear.

In a pop-up **Licensing Activation Wizard** dialog box check '**I have a serial code to activate**' button and press **Next**.

Paste 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. Your personal information will not be shared with third parties.

Your next steps depend on availability of the internet and thus differ.

Online activation

If your PC is connected to internet, please do following:

1. Check "**Use internet connection for activation**" textbox and press **Continue** to proceed.
2. Fill in the forms in the dialog box to personalize your **MyAssays Desktop** and press **Activate**.
3. You may have to wait a few moments, while the activation is being verified. Upon that a confirmation window appears. Press **Close** to exit **Licensing Activation Wizard**.

Offline activation

If your PC is not connected to internet, please do following:

1. Uncheck "**Use internet connection for activation**" textbox and press **Continue** to proceed.
2. Then a dialog box with a link and QR-code will appear. You can either save the link and paste it in browser on an internet-connected system or scan the QR-code via network-connected device (smartphone or tablet).
3. Upon opening the link or scanning the code, you will be directed to MyAssays validation menu with a license key for activating your application.
4. Launch MyAssays Desktop Explorer. In a pop-up dialog **Licensing Activation Wizard** box check '**I have a license key obtained from activation process**' button and press **Next**.
5. Paste the license key in a textbox and press **Activate**.
6. After verifying your license key, a confirmation window appears. Press **Close** to finish activation.

Upon successful activation of the application, MyAssays Desktop Explorer will automatically launch on your PC.

Deactivating License

This option comes handy when you want to switch the PC you work on. To enable you with flexible use of your license, you can deactivate it on current device and transfer license to other without need to claim a new one.

To deactivate MyAssays Desktop on your PC, please do following:

1. Open **Information** screen of **File** tab in the MADE.
2. Click on the **Deactivate License** button.

Upon that **Deactivation Wizards Information** dialog box launches.

Your next steps depend on availability of the internet and thus differ.

Online deactivation

1. Keep the "**Use internet connection for deactivation**" textbox checked and press **Continue** to proceed with deactivation.
2. In the appearing confirmation window check the textbox and press **Deactivate**.

Offline deactivation

1. Uncheck "**Use internet connection for deactivation**" textbox and press **Continue** to proceed with deactivation.
2. In the appearing confirmation window check the textbox and press **Deactivate**.
3. After confirming deactivation, a dialog box with a link and QR-code will appear. You can either save the link and paste it in browser on an internet-connected system or scan the QR-code via network-connected device (smartphone or tablet).
4. Upon opening the link or scanning the code, you will receive confirmation e-mail at your registration e-mail address.
5. The next step is to confirm that you received the message. Check the verifying message and click on **Finish** button to complete the deactivation.

Updating License

To update your license, please do following:

1. Open **Information** screen of **File** tab in the MADE.
2. Click on the **Update Existing License** button.
3. Choose preferable updating way and press **Next**.


Your previous license deactivates, if you press **Next**.

The following steps are similar to the activation process. Upon successful update a confirmation window appears.

Licensed Features

In addition to the basic data analysis functions, MyAssays Desktop also includes some special features for performing particular types of data analysis. While the majority of the workflow could be performed with functionality, there are some complex analyses that require more complicated methods, functions and features.

Therefore, MyAssays has extended these features into optional licensable services.

To check out whether your license allows using this features, open **Information** screen of **File** tab in the MADE. The availability of licensed features is marked with the following icons:

 For active features

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