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Instructions for Use for

**magellan**

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magellan Tracker: 7.5



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## WARNING

**CAREFULLY READ AND FOLLOW THE INSTRUCTIONS PROVIDED IN THIS MANUAL BEFORE OPERATING THE INSTRUMENT.**

### **Notice**

Every effort has been made to avoid errors in text and diagrams; however, Tecan Austria GmbH assumes no responsibility for any errors which may appear in this publication.

It is the policy of Tecan Austria GmbH to improve products as new techniques and components become available. Tecan Austria GmbH therefore reserves the right to change specifications at any time with verification, validation, and appropriate approvals.

We would appreciate any comments on this publication.



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### **Declaration for EC Certificate**

Provided upon request.

### **magellan Intended Use**

See 1.2 Intended Use/Purpose of magellan.

### **About this Manual**

magellan is a universal data reduction package used to analyze data generated from microplate assays. It is designed for professional use only.

This manual instructs how to:

- Install the software
- Operate the software

### **Remark on Screenshots**

The version number displayed in screenshots may not always be the one of the currently released version. Screenshots are replaced only if content related to application has changed.

### *Change History of Instructions for Use*

Version	Changes
V 1.2	New DoC (Declaration of Conformity)

## Warnings, Cautions and Notes

The following types of notices are used in this publication; they highlight important information or warn the user of a potentially dangerous situation:



**Note**  
*Gives helpful information.*



**CAUTION**  
INDICATES A POSSIBILITY OF INSTRUMENT DAMAGE OR DATA LOSS IF INSTRUCTIONS ARE NOT FOLLOWED.














**WARNING**  
INDICATES THE POSSIBILITY OF SEVERE PERSONAL INJURY, LOSS OF LIFE OR EQUIPMENT DAMAGE IF THE INSTRUCTIONS ARE NOT FOLLOWED.



**ATTENTION**  
DIRECTIVE 2012/19/EU ON WASTE ELECTRICAL AND ELECTRONIC EQUIPMENT (WEEE)  
NEGATIVE ENVIRONMENTAL IMPACTS ASSOCIATED WITH THE TREATMENT OF WASTE.

- DO NOT TREAT ELECTRICAL AND ELECTRONIC EQUIPMENT AS UNSORTED MUNICIPAL WASTE.
- COLLECT WASTE FROM ELECTRICAL AND ELECTRONIC EQUIPMENT SEPARATELY.

## Symbols

	Manufacturer
	Date of manufacture
	CE conformity marking
	Consult the instructions for use
	<i>In vitro</i> diagnostic medical device
	United Kingdom Conformity Assessed marking shows that the labeled product is following the applicable regulation in Great Britain.
	Unique Device Identification The UDI symbol identifies the data carrier on the label.
	Catalogue number
	Serial Number
	WEEE symbol
	China RoHS symbol

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# 1. Introduction

## 1.1 Area of Application

**magellan** software is a reader control and data analysis software for analyzing data generated by measurements with a Tecan single-mode absorbance microplate reader (e.g., SUNRISE and INFINITE F50) for in vitro diagnostic use.

**Note**

***It is important to note that the proper installation of the instrument and the magellan software alone will not ensure compliance with laws and requirements. Corresponding policies concerning processes and standard operating procedures, including validation and quality control, must also be established.***

**magellan** is designed for use with the operating systems and Microsoft Office versions specified in chapter 1.4.1 System Requirements. If additional programs are installed, functionality in accordance with IVD for Europe and FDA Regulations cannot be guaranteed.

**Note**

***To prevent the misuse of user rights and falsification of data it is recommended that the User Administrator does not have magellan rights. Ideally the User Administrator should belong to the IT department.***

**Note**

***The customers' system administrator is responsible for any changes made to the computers operating system. The customer has to make sure that the appropriate user rights are set to avoid manipulation or deletion of data outside magellan software.***

**Note**

***magellan is designed to be used with one computer; it is not intended to be integrated into a network.***

**Note**

***Any serious incident that has occurred in relation to the device and software shall be reported to the manufacturer and the competent authority of the member state in which the user and/or the patient is established.***

## 1. Introduction

### 1.2 Intended Use/Purpose of magellan

**magellan** software is a reader control and data analysis software for analyzing data generated by measurements with a Tecan single-mode absorbance microplate reader (e.g. SUNRISE and INFINITE F50) for in vitro diagnostic use.

**magellan** software is intended to be used primarily for absorbance measurements and evaluation of qualitative, semi-quantitative, and quantitative IVD assays. **magellan** software is user programmable; the software needs to be configured by the user according to the assay instructions.

The product is intended for professional laboratory use by trained personnel. The product is not for home or lay person use.

**magellan** is available in two versions:

- **magellan**
- **magellan Tracker**

**magellan** Tracker offers all necessary functionality to become compliant with the FDA Regulation 21 CFR part 11 in addition to the functionality of **magellan**.



#### Note

***magellan is available in two versions: magellan and magellan Tracker.  
For ease of reference in this operating manual, the magellan version is marked as magellan Standard.***

### 1.3 User Profile

#### 1.3.1 Professional User - Administrator Level

The administrator is a person who has suitable technical training and corresponding skills and experiences. If the product is used as intended, the person can recognize and avoid dangers.

The administrator has extensive skills and can instruct the end user or the routine user in assay protocols in connection with a Tecan product within the bounds of the intended use.

Computer application skills and good English skills are required.

#### 1.3.2 End User or Routine User

The end user or routine user is a person who has suitable technical training and corresponding skills and experiences. If the product is used as intended, the person can recognize and avoid dangers.

Computer application skills and good language skills for the respective national language at the installation site and English are required.



#### Note

***Training dates, their duration and frequency are available at your customer support.  
Address and telephone number can be found in these Instructions for Use and in the web: <http://www.tecan.com/customersupport>***

## 1.4 Specifications

### 1.4.1 System Requirements

The following requirements have to be met for using **magellan**:

	Supported	Recommended
<b>PC</b>	Windows compatible PC with a Pentium compatible processor running at 1 GHz (Dual Core)	2 GHz (Dual Core)
<b>Operating System</b>	Windows 10 (32-bit)	
	Windows 10 (64-bit) Editions: Pro	
<b>Memory</b>	Windows 10 (32-bit): 1 GB RAM	2 GB RAM
	Windows 10 (64-bit): 2 GB RAM	4 GB RAM
<b>Free Hard Disk Space</b>	3 GB	5 GB
<b>Monitor</b>	Super VGA Graphics	
<b>Resolution</b>	1024 x 600 and higher	1920 x 1080
<b>Color Depth</b>	256	
<b>Mouse</b>	Microsoft mouse or compatible pointing device	
<b>Communication</b>	1 x USB 2.0	2 x USB 2.0 1 x RS232 (Serial)
<b>Devices</b>	Windows 10: DirectX 9 graphics device with WDDM 1.0 or higher driver	
<b>.NET</b>	Microsoft .NET Framework 3.5: In Windows 10 the user will be prompted to install the required .NET framework (3.5) if it is not already present.	
<b>Windows Installer</b>	3.1 If this version is not present, the install/upgrade program will install it.	
<b>Microsoft Excel</b>	2007, 2010, 2013, 2016 (32-bit), 2019 (32-bit), Microsoft Excel 365 (32-bit) <b>Only 32-bit editions supported!</b> <b>Starter editions NOT supported!</b>	2010 (32-bit) 2019 (32-bit)

## 1. Introduction

### 1.4.2 Reader Compatibility

The following Tecan readers can be used with **magellan**:

Instrument Types	Measurement Mode
SUNRISE	Absorbance
INFINITE F50	Absorbance

## 1.5 Software Installation Procedure

### 1.5.1 Automatic Software Setup Program

magellan is installed by an automatic software setup program. All necessary components are installed automatically.

Start Magellan\_Setup.exe to begin the installation procedure.

- In the first InstallShield Wizard window the components, which are required prior to installing magellan are shown. Click **Install** to continue.  
**Windows 10:** If the required .NET Framework (3.5) is not present, the user is prompted to start the installation. Select **Install this feature** (an internet connection is required). If the installation is skipped by the user, the magellan installation will not be successful.
- A **Welcome Window** appears with information about the software and the installation process. Click **Next** to continue.
- The next window displays the **License Agreement**. Read the **License Agreement** and click **I agree** to accept it and continue.
- The **Customer Information** window appears next. If you have already purchased the software, enter now your serial number, and click **Next**. If you do not yet have a serial number, click **Next** as well to continue the setup. You can register later (see chapter 2.4.3 Licensing magellan).
- The **Destination Folder** window appears next. The default installation path is displayed. Click **Browse** to change the default destination path, if desired. Click **Next** to continue.
- The **Language Selection** window appears next. Choose your preferred language.
- In the **Use For Regulated Environments** window, select magellan **Standard** or magellan **Tracker**, depending on which version you have ordered, to install the software. Click **Next** to continue.
- The setup program is now ready for installation. Click **Next** to start installation.
- Click **Finish** to end installation and to close the setup program.

The software can be started via the Windows **Start** menu by selecting magellan.

The setup program automatically detects a previous installation of **magellan**. The old version has to be de-installed before being able to install a new Magellan version. The de-installation can be performed automatically by using the installation wizard (see also chapter 1.5.5 Automatic Software Removal).



#### Note

***It is very important that the person who installs the software has administrator rights on the computer.***

**Note**

*If an older version of magellan is to be installed, the currently installed version has to be completely de-installed before the older version can be installed from scratch.*

### 1.5.2 Installation Qualification – IQ

It is recommended to use the automatic installation qualification program to check that the installation of **magellan** was successful.

Start Magellan IQ.exe from the Windows Start menu: **Start > Programs > Tecan > Magellan IQ** or directly from the file system in the default installation path specified in the setup program (typically, **C:\Program Files\Tecan\Magellan**).

The installation qualification program automatically detects the installed version of **magellan**. Click **Check** to start the installation qualification.

The IQ tool shows the state of all installed components. There are three possible states: **Successful, Warning and Failed (=Error)**. If any errors are reported, please contact your local helpdesk for support.

After the check is finished, it is possible to generate a report containing the information displayed by the IQ tool. In addition to the information of the IQ tool, the report contains a signature field, so that the report can be saved and printed for auditing purposes. Click the **Report** button in: **File > Report** to generate a report. The report can be saved as a PDF file as well as other file types.

Click **Cancel** or **Exit** to close the Installation Qualification program.

**Note**

*The installation qualification should be repeated each time magellan is installed, updated to a newer version, or the underlying system is updated or modified.*

### 1.5.3 Operation Qualification – OQ

In addition to the installation qualification check, Tecan also recommends that the calculation abilities of **magellan** are tested. For this purpose, the installation medium of **magellan** contains a workspace and report file.

Open the OQ workspace file for the installed **magellan** version and print the report. The newly printed report has to be identical to the corresponding OQ pdf report (except, of course, for the time and date information).

If the two reports differ, please contact your local dealer for support.

## 1. Introduction

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### 1.5.4 System Recovery

To repair a damaged **magellan** installation after a hardware failure, it is important to start the data backup ahead of time.

#### System Recovery with Data Backup Software

The data backup is usually performed with data backup software. This makes it possible to save the entire system, including all data, so it can be restored whenever needed.

A detailed description and precise user instructions can be found in Windows Help (for Windows backup software packages) or in the provided documentation.

The **magellan** license is tied to the computer's hardware, which means it can become invalid after a hardware change. You should therefore check to make sure your license is still valid after a system restoration. This can be done in the **About Magellan** dialog box by starting the registration wizard and checking whether the registered serial number and license number are still valid. In case of an error message, please contact Tecan's customer support to get a new license number.

#### Manual System Recovery

In those cases where a complete system restoration is not possible with the backup software (e.g. because the hardware changes are too extensive, or because a different version of the Windows operating system was installed on the new computer), **magellan** has to be re-installed and several files have to be copied from a backup archive.

In that case, the system restoration process consists of these steps:

1. Install **magellan**
2. Start **magellan** and define the **magellan** Administrator
3. Re-enter the user and user rights.
4. Copy **magellan.ini** file from the backup archive.
5. Copy **magellan** methods from the backup archive.
6. Copy sample ID lists from the backup archive.
7. Copy workspaces from the backup archive.
8. Copy exported data from the backup archive.

After the hardware changes and a relicensing of **magellan** Tracker have been completed, the user, when opening method and workspace files generated under the old license, is informed that the files originate from a different computer. To solve this problem, please follow the detailed description in chapter 10.2.4 Opening a File Created on Another PC – Add HUIDs.

#### Data Security

To make sure that the steps of the system restoration process listed above can be completed quickly, a backup archive should be set up in time. The backup archive should include **magellan** methods, workspaces, sample ID lists, exported data, audit trail files, system audit trail files, **UserManagement.xml** file, files of Pdfx Directory and the **magellan.ini** file. The contents of the backup archive should always be up to date. Tecan recommends using the **Auto Archiving** option for the backup of the methods, workspaces, and sample ID lists. You can find details about Auto Archiving in chapter 9.2.1 Archive Files / Automatic Archiving.

### magellan Paths – Windows 10

Magellan.ini	C:\Users\Public\Documents\Tecan\Magellan
Methods	Standard path: C:\Users\Public\Documents\Tecan\Magellan\mth or as set in the <b>Options</b> dialog box
Workspaces	C:\Users\Public\Documents\Tecan\Magellan\wsp or as set in the <b>Options</b> dialog box
Sample ID lists	C:\Users\Public\Documents\Tecan\Magellan\smp or as set in the <b>Options</b> dialog box
Exported data	C:\Users\Public\Documents\Tecan\Magellan\asc or as set in the <b>Options</b> dialog box
Audit Trail files	Path as shown in the Audit Trail dialogue box (under user administration)
System Audit Trail	Path as specified in 10.3 System Audit Trail
User Management	C:\ProgramData\Tecan\Tecan User Management\v1.1\UserManagement.xml
Pdfx Files	C:\Users\Public\Documents\Tecan\Pdfx

### 1.5.5 Automatic Software Removal

The **magellan** software can be removed using the standard Windows uninstall routine:

- Close **magellan**
- Select **Add/Remove Programs** from the **Settings - Control Panel** in the **Windows Start** menu.
- Select the **magellan** icon and click **Remove**.

In the removal procedure you will be asked whether or not shared components should be removed. If **Yes** is selected, **magellan** will be completely uninstalled and other Tecan programs will no longer work. Leaving these components installed will not harm your system. If you are not sure what to do, we suggest to not remove the shared components. After clicking **Yes** or **No**, the **magellan** software is uninstalled.



#### Note

**When removing all shared components, the user administration data is also removed. Some Tecan programs, for example EVOware, will not work anymore and must be re-installed.**

## 1.5.6 Cybersecurity Information

**CAUTION**

**IT IS THE USER'S RESPONSIBILITY TO TAKE THE NECESSARY PRECAUTIONS TO PROTECT THE SYSTEM FROM CYBERSECURITY THREATS.**

**WHEN INSTALLING VIRUS PROTECTION SOFTWARE OR SECURITY-RELATED UPDATES OF THE OPERATING SYSTEM PLEASE FOLLOW THE RECOMMENDATIONS OF THE LOCAL IT DEPARTMENT. BACK UP MAGELLAN FILES BEFORE STARTING UPDATES. RUN INSTALLATION QUALIFICATION (IQ), OPERATION QUALIFICATION (OQ) AND PERFORMANCE QUALIFICATION (PQ) OF MAGELLAN AFTER EVERY SYSTEM MODIFICATION.**

**Back up your data**

The importance of backing up files to be able to recover in case of a ransomware attack cannot be overstated. Be sure to create destruction-resistant backups of your critical systems and data. There are many tools and services available for file backup, restoration (of previous file versions) and recovery. Also, be sure to regularly test that the backups are working.

Use magellan archive functionality or your product of choice to backup magellan data files. For a detailed description, refer to chapter 9.2.1 Archive Files.

**Manage and control privileged access to data**

To minimize risk of credential compromise and abuse, implement unique local administrator passwords on all systems, separate and protect privileged accounts and reduce broad permissions on file repositories.

Use standard windows operators (not administrators) to operate magellan.

Use magellan Tracker functionality to control access and further secure the application.

**Operation Qualification**

In addition to the installation qualification check, Tecan also recommends that the calculation abilities of magellan are tested. For a detailed description, refer to chapter 1.5.3 Operation Qualification – OQ.



## 2. Start Working with magellan

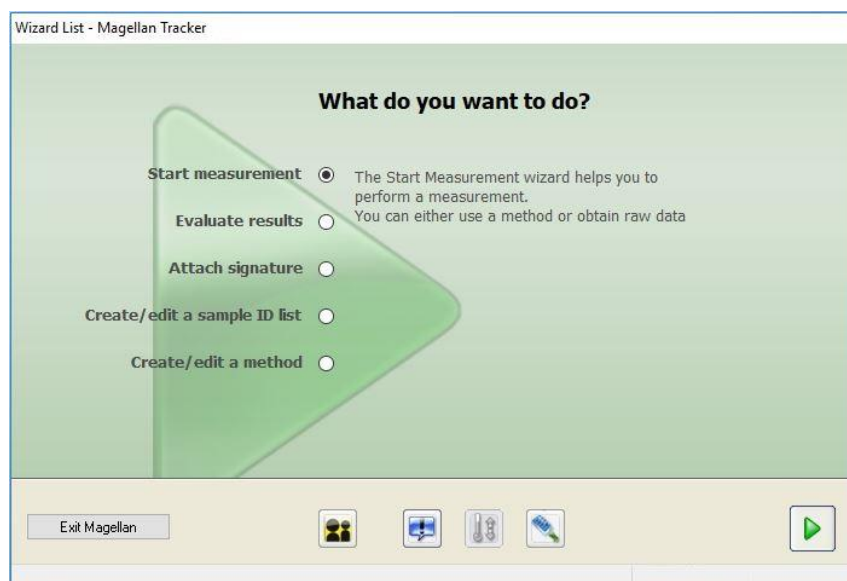
Standard **magellan** wizards represent workflow modules, which are step-by-step guides for performing complex procedures.


Occasionally, menus are available in the heading bar. The **Menu** offers a conventional way of using the software: the relevant menu item is selected from the main menus. All subsequent actions are started instantly, or a dialog box is displayed where further selections or entries can be made.

### 2.1 User Interface – Wizard List

The main type of the user interface in **magellan** is the wizard.

After launching **magellan**, the **Wizard List** appears:



Each wizard can be started either by double-clicking or by selecting it and clicking the **Next**  button.

#### Start Measurement Wizard

The **Start Measurement wizard** includes the following options:

- **Obtain Raw Data** is used to generate raw data quickly and easily by setting the required measurement parameters and starting a measurement.
- **Use Predefined Method** is used to perform measurements based on previously defined methods.
- **Start Favorite** is used to select one of the most frequently used methods from the list of numbered icons.

For a detailed description, refer to chapter 6 Start Measurement Wizard.

After the measurement is finished a workspace file is created.

#### Evaluate Results Wizard

The **Evaluate Results wizard** is used to view the raw data and to evaluate the results. The evaluation parameters can be viewed, and data can be re-evaluated.

For a detailed description, refer to chapter 7 Evaluate Results Wizard.

## 2. Start Working with magellan

### Attach Signature Wizard

The **Attach Signature wizard** is used to sign method and workspace files. This feature is only available with **magellan** Tracker.

For a detailed description, refer to chapter 8 Attach Signature Wizard.

### Create/Edit a Sample ID List Wizard

The **Create/Edit a Sample ID list wizard** is used to create new and to edit existing sample ID lists.

For a detailed description, refer to chapter 5 Create/Edit a Sample ID List Wizard.

### Create/Edit a Method Wizard

The **Create/edit a method wizard** is used to define or edit methods.

For detailed description, refer to chapter 4 Create/Edit a Method Wizard.

### Icons



#### Icon: Change Current User

If the user administration is active (refer to chapter 9.4 User Administration (magellan Tracker) and to chapter 9.5 User Administration (magellan Standard)) click this icon to log out the current user and to login a new user.

With **magellan** Standard, user administration is optional. With **magellan** Tracker user administration is obligatory.



#### Icon: Miscellaneous

Click on the **Miscellaneous** icon to select the following options:

	Instrument control		Options
	File handling		User administration
	About <b>magellan</b>		

- **Instrument control** provides quick access to several instrument functions, to service and setup options. See chapter 3 Instrument Control & Settings.
- **File handling** is used to move files to an archive location, to convert files from or to another **magellan** version and to import raw data from an ASCII-file. See chapter 9.2 File Handling.
- **Options** is used to customize certain default settings as path of generated files, clipboard and Excel copy options, the plate view and miscellaneous wizard, startup, language and password settings. See chapter 9.3 Options.
- **User administration** is used to add or disable users and to set or modify user rights. See chapter 9.4 User Administration (magellan Tracker), respectively chapter 9.5 User Administration (magellan Standard).
- **About magellan** provides license information and details on the currently installed version and components. Registration can be requested starting the **Register wizard** (see chapter 2.4.3 Licensing magellan).

**Close** the Miscellaneous window to go back to the **wizard list**.



### Icon: Temperature control

Use this icon to set the target temperature for the connected instrument.  
For a detailed description, refer to chapter 3.1.2 Temperature Control...



### Icon: Move plate

Use this icon to move the plate carrier in or out of the instrument.

## 2.2 Components & Terms – Basic Logic of magellan

### 2.2.1 File Types Used with magellan

The following file types are used with **magellan**.

**By default**, all file types associated with **magellan** are stored in subdirectories in the appropriate directory:

...\All Users\Documents\Tecan\

The subdirectories are displayed in the table below:

Type of File	File Extension	Directory
Workspace	.wsp	\magellan\wsp
Method	.mth	\magellan\mth
Sample ID List	.smp	\magellan\smp
Export Files	.asc	\magellan\asc
Standard Curve	.std	\magellan\wsp
Plate Definition	.pdf	\Reader\Pdf
	.pdfx	\Pdfx

For a detailed description on methods, sample ID lists, workspaces and standard curves, refer to the chapters 4 Create/Edit a Method Wizard, 5.2.3 Import a Sample ID List and 7 Evaluate Results Wizard.



#### Note

**INFINITE F50 instruments use the .pdfx file format, whereas SUNRISE instruments use .pdf files.**



#### Note

**The menus and toolbars available vary depending on the type of file currently opened.**






## 2. Start Working with magellan

### 2.2.2 Folder Handling

In **magellan**, it is possible to create a user-specific folder structure for saving files (methods, workspaces, standard curves and sample ID lists) in any folder of the Windows Explorer. New folders can be created by right-clicking and selecting **New folder** from the context sensitive menu. Files and folders can be moved/cut/copied in the same manner as in Windows Explorer.

#### File Type Symbols

**magellan** uses the following symbols for methods, workspaces, standard curves and sample ID lists in the file view window:

	Method
	Standard curve
	Workspace
	Password protected method
	Sample ID list

#### magellan Standard

Default paths for saving newly created files can be set via: **Wizard list** main page → **Miscellaneous** button → **Options** button → **Paths** tab.

Users can create new folders in any folder of the Windows Explorer during the saving process.

In the **Save** window, the folder, specified by the default path of the file, is opened automatically, whenever a new file is created. If an already existing file is modified, the path to the current location of the file will be opened. However, it is possible to save files in any folder of the Windows Explorer or in a newly created folder.

#### magellan Tracker

**magellan** users with administration rights can set the default paths for saving newly created files via: **Wizard list** main page → **Miscellaneous** button → **Options** button → **Paths**. These default paths are valid for all users.

Users can create new subfolders only with Windows administrator rights and only in the folder specified by the default path during the saving process.

In the **Save** window, the folder, specified by the default path of the file, is opened automatically, whenever a new file is created. If an already existing file is modified, the path to the current location of the file will be opened. However, it is only possible to save files in the default folder, or in an existing or newly created subfolder within this folder.

### 2.2.3 Standard Elements

Each wizard displays sequentially a number of windows, in which all necessary information, settings and data entry possibilities are provided.

#### Standard Elements of a magellan Wizard

For navigation from one window to another there are several buttons at the bottom of the wizard page:

<b>Back</b> button	The <b>Back</b> button is used to navigate back to the previous window within a wizard.
<b>Next</b> button	The <b>Next</b> button is used to navigate forward to the next window within a wizard.
<b>Finish</b> button	The <b>Finish</b> button is used to navigate forward to the save window of the wizard.
<b>Save</b> button	The <b>Save</b> button is only found in the last window of a wizard and replaces the <b>Next</b> button. It is used to close the wizard and save all changes or to start a process.
Cancel button	The <b>Cancel</b> button is used to close a wizard without saving any changes to settings or documents.
<b>Help</b> button	The <b>Help</b> button opens the help window.

#### Standard Elements of Microsoft Windows

<b>OK</b> button	This button confirms settings, applies and saves changes accordingly and closes the dialog box.
<b>Cancel</b> button	This button closes the dialog box without saving any changes to settings or documents.
<b>Help</b> button	Click the <b>Help</b> button to open the <b>magellan</b> online help.

#### Status Bar Information

The status bar displays the following information:

- Current command info
- User name of the currently logged in user.
- Name of connected instrument. For example: Sunrise
- Method: measurement mode and unit. For example: Absorbance [OD]
- Workspace: date and time of measurement. For example: 27.11.2002 14:13:03  
Number of selected wells. For example: 3 well(s) selected
- Keyboard status information: activity of the keyboard toggles: CAP (caps lock), NUM (Numeric block lock), SCRL (Scroll lock)
- Instrument connection state icon

### 2.2.4 The Help Button

Click the **Help** button or press 'F1' to open the **magellan** online help.

## 2. Start Working with magellan

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### 2.2.5 *The Welcome Dialog Box*

Each wizard starts with a **Welcome** dialog box, which gives a short introductory description of the procedure to be performed.

Clear the **Show welcome page** check box to suppress welcome pages when starting wizards in the future.

### 2.2.6 *Shortcuts List*

SHIFT+B	Back button
SHIFT+N	Next button
ESC	Cancel button
ENTER	Next or Finish button, if active window
F1	Help menu
CTRL+C or CTRL+INSERT	Copy
CTRL+V or SHIFT+INSERT	Paste
CTRL+X	Cut
CTRL+Y	Redo
CTRL+Z	Undo
DEL	Delete content of active well (edit sample ID, edit formula)
CTRL+SHIFT	Show formula of selected well when transformation result is viewed (Evaluate Results wizard)

## 2.3 Starting magellan

### 2.3.1 Starting Standard Version

Perform the following steps to start **magellan**:

1. Make sure that an instrument is connected or select a simulated instrument.
2. In the Windows **Start** menu, select the **Tecan** program group and click the **magellan** icon.
3. **magellan** starts.



**Note**

*magellan can be run with an instrument connected or in a demo mode, simulating an instrument. If you want to connect to an instrument (see chapter 2.4 Connecting an Instrument), switch the instrument on before starting magellan.*



**Note**

*Before starting to work with magellan, we suggest reading the Release Notes for magellan for any malfunctions in the application.*

### 2.3.2 Starting Tracker Version



**Note**

*When using magellan Tracker, the user administration system must be customized by a designated administrator, who is responsible for the setup of user accounts and for the assignment of user rights. The Administrator must always be trained by Tecan or a Tecan authorized organization.*

## Logging in for the First Time with magellan Tracker

When **magellan Tracker** is started for the first time, a dialog box appears, informing the user that a **User Administrator** must be created first. Click **OK** and the **Create Administrator** dialog box appears.

Complete the text fields and click **OK** to save the settings. At least one user administrator must be created.



**CAUTION**

**IF THE USER ADMINISTRATOR PASSWORD IS FORGOTTEN, USER ADMINISTRATION SETTINGS CANNOT BE CHANGED AND MAGELLAN MUST BE COMPLETELY REINSTALLED.**

**WE RECOMMEND CREATING AT LEAST TWO USER ADMINISTRATORS.**

For all further user definitions of the user administration (e. g. user rights), refer to chapter 9.4 User Administration (magellan Tracker) and chapter 9.5 User Administration (magellan Standard).

## 2. Start Working with magellan

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### Password

#### Initial Password (magellan Tracker only)

When a user logs in for the first time, the password assigned by the administrator has to be changed.

After entering the **User name** and **Password** and clicking **OK**, the message "Your initial password is only valid once. You have to change the password!" appears. Click **OK**; the **Change Password** window forces the user to enter a new password.

#### Password Expiration (magellan Tracker only)

When the password expires, the user will be prompted to enter a new password.

See chapter 9.4.4 User Administration Options.

### Login

Once user administration has been activated, the **Login** dialog box will appear each time **magellan** starts.

The **Login** dialog box contains the following elements:

<b>Username</b> text box	Enter your <b>UserID</b>
<b>Password</b> text box	Enter your <b>Password</b>

Click the **GO** button to enter or the **Cancel** button to terminate **magellan**.

### Application Locked

If the application has not been in use for the specified maximum of time (user defined only in **magellan** Tracker) it will be locked. The password must be entered to unlock the application.



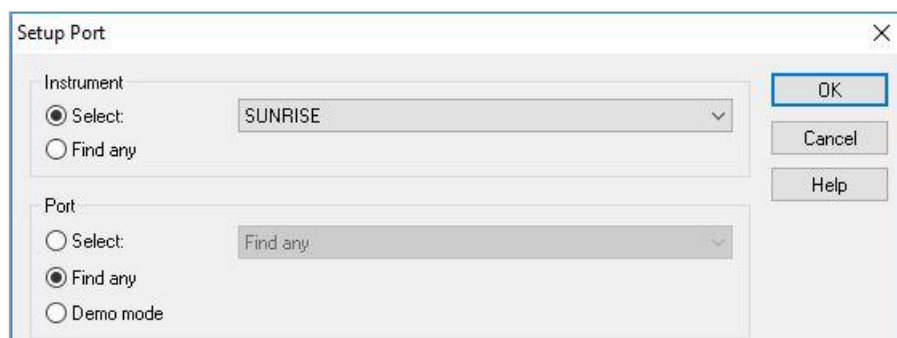
## 2.4 Connecting an Instrument

### 2.4.1 Connect to *SUNRISE* Instruments

Connect the instrument to your computer as described in the instructions for use for the instrument and switch on the instrument before starting **magellan**.

#### First Start of magellan

The first time **magellan** is started, the **Setup Port** dialog box appears:



<b>Instrument</b>	Select the connected instrument from the drop-down list or select <b>Find any</b> .
<b>Port</b>	Select the appropriate <b>COM port</b> from the drop-down list or select <b>Find any</b> and Click <b>OK</b> .

#### Change Instrument



Click the **miscellaneous** icon in the wizard list and **instrument control** in the miscellaneous list. Select **Change instrument** from **Setup & Service** to connect an instrument or to change the currently connected instrument.

#### Demo Mode

If **no instrument** is connected, select the instrument to be simulated from the drop-down list in the **Instrument** group box and select **Demo mode** in the **Port** group box. Click **OK**. **magellan** is now in demo mode.



**Demo mode allowed** (in the **Options** dialog) is selected by default.

In demo mode it is possible to perform all functions except running actual measurements.

## 2. Start Working with magellan

### 2.4.2 Connect to INFINITE F50 Instruments

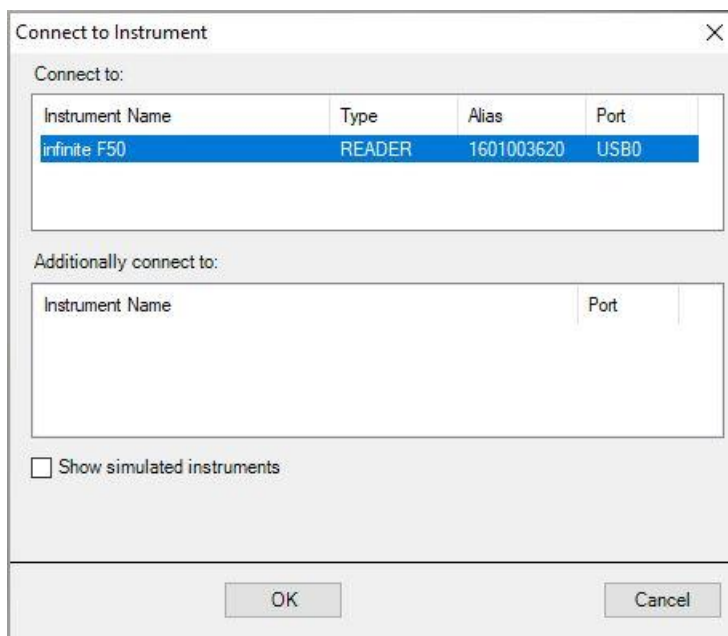
#### First Start of magellan

The first time **magellan** is started, the **Setup Port** dialog box appears:



The **Setup Port** dialog box contains two main sections: **Instrument** and **Port**. In the **Instrument** section, the **Select** radio button is chosen, and the dropdown menu shows **infinite F50**. In the **Port** section, the **Find any** radio button is selected, and the dropdown menu shows **Find any**. On the right side, there are three buttons: **OK**, **Cancel**, and **Help**.

Select **INFINITE F50** in the **Instrument** group box in the **Setup Port** dialog box. Click **OK** to display the **Connect to Instrument** dialog box.



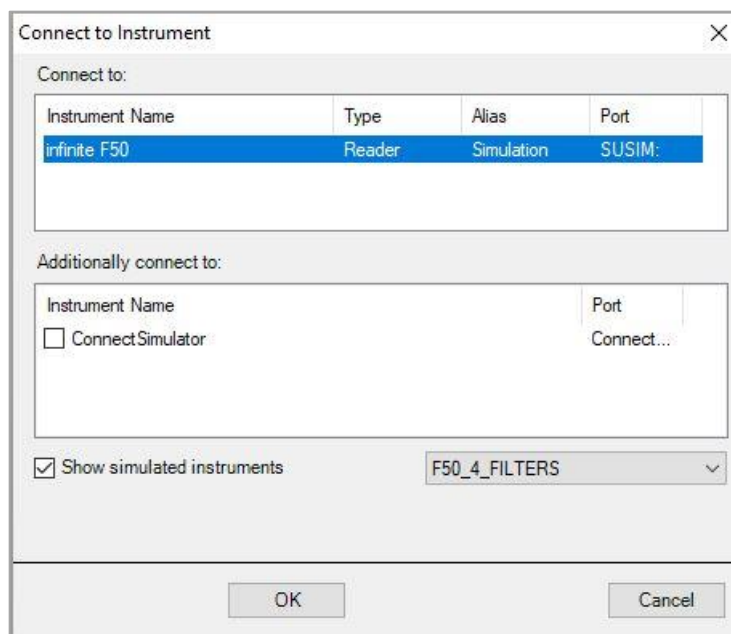
The **Connect to Instrument** dialog box features a table for selecting an instrument. The table has four columns: **Instrument Name**, **Type**, **Alias**, and **Port**. The first row is highlighted in blue and contains the values **infinite F50**, **READER**, **1601003620**, and **USB0**. Below the table, there is a section labeled **Additionally connect to:** with two empty input fields for **Instrument Name** and **Port**. At the bottom left, there is a checkbox labeled **Show simulated instruments** which is currently unchecked. At the bottom right, there are **OK** and **Cancel** buttons.

Instrument Name	Type	Alias	Port
infinite F50	READER	1601003620	USB0

Select the instrument and click **OK**.

### Demo Mode

If **no instrument** is connected, select the instrument to be simulated from the drop-down list in the **Instrument** group box of the **Setup Port** dialog.



Instrument Name	Type	Alias	Port
infinite F50	Reader	Simulation	SUSIM:

Additionally connect to:

Instrument Name	Port
<input type="checkbox"/> Connect Simulator	Connect...

☒ Show simulated instruments      F50\_4\_FILTERS

OK Cancel

For demo mode select the **Show simulated instruments** checkbox and the preferred instrument from the drop-down list, click the instrument name and click **OK**.

### 2.4.3 Licensing magellan



#### Note

*magellan can be used unregistered for 30 single days of work. If magellan is not registered after this period, the save and print options will be disabled.*

The licensing of **magellan** is performed with the **Register magellan** wizard. If **magellan** has not been registered, this wizard will automatically launch each time the program is started.

The **Register magellan** wizard can also be opened via the **miscellaneous** icon in the wizard list starting page. (**miscellaneous** → **About magellan** → **Register**).

To register **magellan**, a Magellan serial number, the hardware (PC) unit identification number (HUID) and a license number are required.

For licensing **magellan** there are two possibilities:

1. The software has been purchased. Together with the software the serial number is delivered.

After the serial number has been entered in the register **magellan** dialog box, fill out the registration form to start the license number request. The completed registration form is sent together with the individual HUID to Tecan Austria. The HUID number is generated by the software and is inserted into the registration form automatically. It is related to Windows given system drive number.

## 2. Start Working with magellan

After receiving the license number, you have to start the registration wizard again and enter it. The **Register magellan** wizard confirms the license number and summarizes the user information. Click the **Finish** button to complete the registration procedure. **magellan**'s functions will then remain fully available to the user.

2. The software was delivered as a demo version together with the instrument. A registration is possible afterwards (No serial number is delivered).

To purchase **magellan** and to receive a serial number, select the option **Order magellan to obtain a valid license** and proceed with the registration procedure as described above.



### Note

*It is very important that the person who registers the software also has administrator rights for the operating system on the computer.*

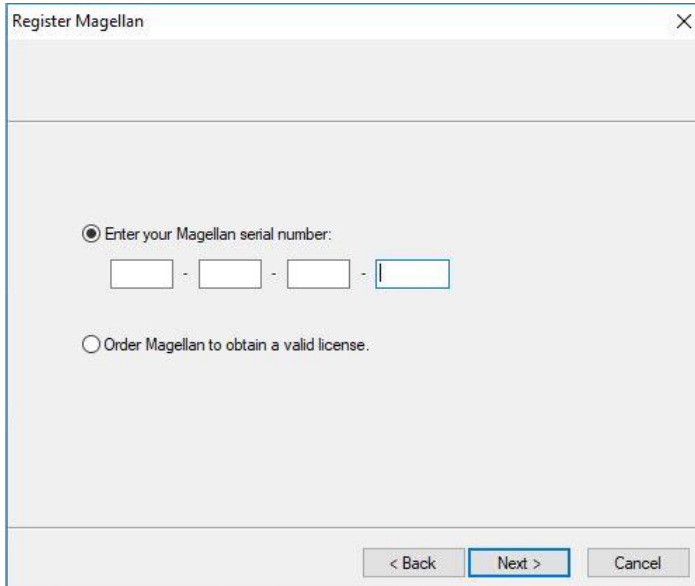
### 2.4.4 Registration Wizard

The registration wizard starts with the **Welcome** dialog box, which contains a short description of the wizard. Click **Next** and the **Serial Number** dialog box appears.

#### Serial and License Number

##### Order a Serial Number for magellan

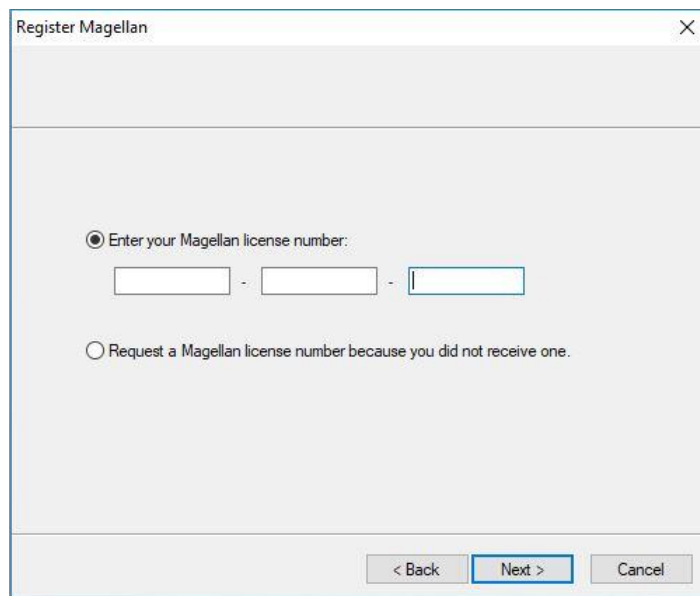
To purchase **magellan** and to receive a serial number, select the option **Order magellan to obtain a valid license**. The **Registration Form** window will then appear (see chapter Registration Form below).



##### magellan has already been purchased

Select **Enter your magellan serial number**. Enter the serial number, which is found in the **magellan** package.

After having entered the serial number, click **Next** and the **License Number** dialog box appears.

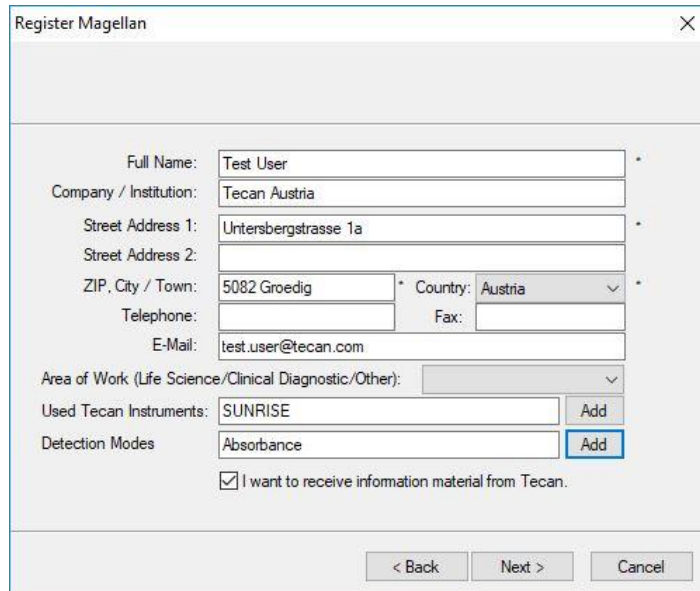


The 'Register Magellan' dialog box contains two radio button options. The first option, 'Enter your Magellan license number:', is selected and followed by three input fields separated by hyphens. The second option is 'Request a Magellan license number because you did not receive one.'. At the bottom, there are three buttons: '< Back', 'Next >', and 'Cancel'.

Users installing the software for the first time will not yet have a license number and must select **Request a magellan license number because you did not receive one**. Click **Next** and the **Registration Form** window appears.

## Registration Form

Complete the registration form. Fields marked with an asterisk are mandatory.

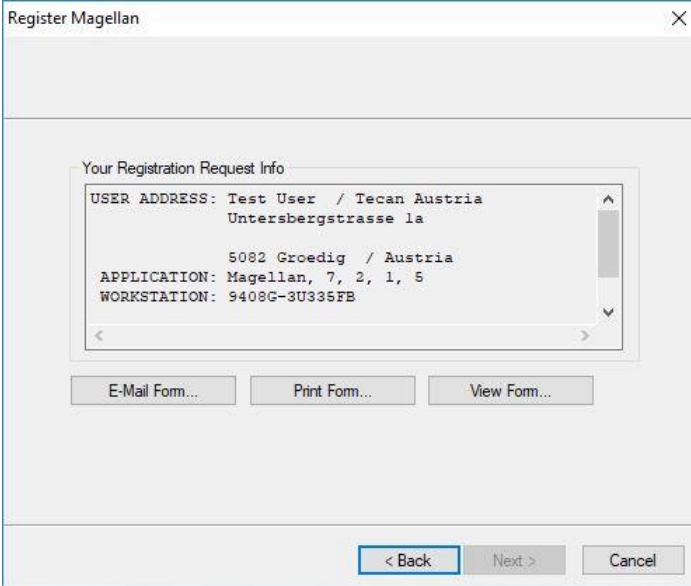


The 'Register Magellan' window displays a registration form. Fields marked with an asterisk (\*) are mandatory. The form includes: Full Name (Test User), Company / Institution (Tecan Austria), Street Address 1 (Untersbergstrasse 1a), Street Address 2, ZIP, City / Town (5082 Groedig), Country (Austria), Telephone, Fax, E-Mail (test.user@tecan.com), Area of Work (Life Science/Clinical Diagnostic/Other), Used Tecan Instruments (SUNRISE), and Detection Modes (Absorbance). There are 'Add' buttons for the last two sections. A checkbox 'I want to receive information material from Tecan.' is checked. Navigation buttons '< Back', 'Next >', and 'Cancel' are at the bottom.

Click **Next** and the license agreement window appears. Read it carefully and click the **I agree** button.

## 2. Start Working with magellan

Click **Next** and the registration information is displayed.



The image shows a Windows-style dialog box titled "Register Magellan". Inside, there is a section titled "Your Registration Request Info" which contains a text area with the following information:

```

USER ADDRESS: Test User / Tecan Austria
               Untersbergstrasse 1a
               5082 Groedig / Austria
APPLICATION:  Magellan, 7, 2, 1, 5
WORKSTATION:  9408G-3U335FB
    
```

Below the text area are three buttons: "E-Mail Form...", "Print Form...", and "View Form...". At the bottom right of the dialog box are three buttons: "< Back", "Next >", and "Cancel". The "< Back" button is highlighted with a blue border.

Click **E-Mail Form...** to send the information using the default e-mail program on your computer or click **Print Form...** to print out the registration form for faxing or mailing it to Tecan. Click **View Form...** to view the registration form using WordPad or Notepad. Within 24 hours you will receive the license number.

### Finishing Licensing magellan

After having received the license number of Tecan, repeat the steps above and insert the license number. Click **Next**. The registration wizard then confirms the license number and summarizes the user information.

Click **Finish**; the **Register magellan** wizard will close and **magellan**'s functions will remain fully available to the user.

## 3. Instrument Control & Settings

Click the **Instrument Control** button in the **Wizard List** dialog box and the **Instrument Control** dialog box appears.

Depending on the instrument connected, different instrument and setup & service options are enabled or disabled.

### 3.1 Instrument Options

#### 3.1.1 *Movements...*

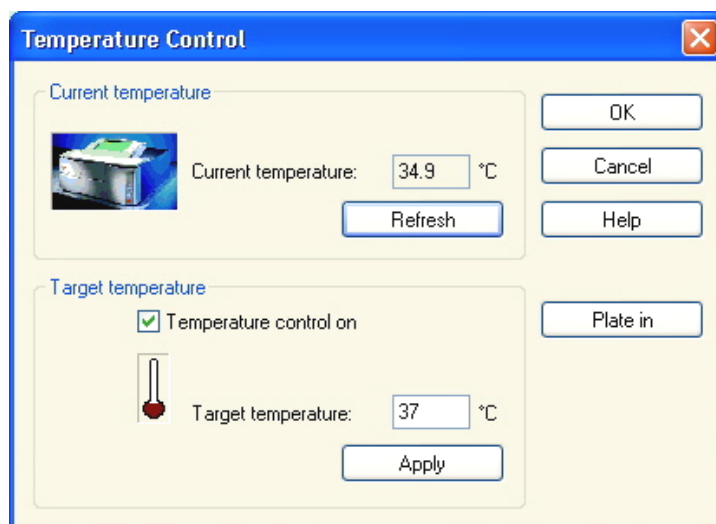
This opens the **Movements** dialog box, in which it is possible to control the movements of the plate carrier and filter slide.

#### 3.1.2 *Temperature Control...*

Only available for instruments equipped with temperature control.

This option allows the user to establish the temperature inside the reader.

This dialog is also accessible via the Start Measurement dialog box before starting a measurement. (See chapter 6.5 Start Measurement with a Predefined or Favorite Method).



#### Current temperature

The current temperature is displayed in the corresponding field. Click the **Refresh** button to update the current temperature.

#### Target temperature

To start or stop the temperature control, select or clear the check box and enter the target temperature. Click **Apply** to send the temperature to the instrument and finally **OK** to close the dialog box.

### 3. Instrument Control & Settings

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## 3.2 Setup & Service Options

### 3.2.1 Change Instrument...

In the **Setup & Service** box, click **Change instrument...** to open the **Setup Port** dialog box.

This option allows connecting **magellan** to an instrument. See chapter 2.4 Connecting an Instrument for further details.



#### Note

*If you connect another instrument to your computer or if you modify the interface parameters, you must always select this menu option. The settings will be automatically used the next time the software is launched.*

### 3.2.2 Define Filter Slides...

Standard and custom filter slides can be defined. See the corresponding chapters in the instrument Instructions for Use.

## 3.3 Log Files

During working with **magellan** log files are created. The communication between the software and the instrument and the communication between components of the software are stored in these log files.

They can be found in the following paths:

- **magellan** Log files (communication between single components of **magellan**):  
Windows 10:  
C:\Users\Public\Documents\Tecan\LogFiles\
- Collection of necessary log files  
Log files can be saved as zip archive by selecting the **Save Logfiles...** button in the **File handling** dialog (**Miscellaneous** → **File Handling**). The zip archive can now be named and saved in a defined directory. In case of any **magellan** measurement or status error(s), this archive contains all well data, status (e.g. overflow, lamp low) or calculation error(s) and can be easily sent to your local helpdesk for support request. For further information please refer to chapter 9.2 File Handling – Save Log Files.
- INFINITE F50 log files (communication between **magellan** and INFINITE F50 instrument):  
Windows 10:  
C:\Users\Public\Documents\Tecan\LogFiles\Magellan\V x.y\Instrument Serial Number
- SUNRISE Log files (RdrOle.log; communication between **magellan** and SUNRISE Instrument):  
Windows 10:  
C:\Users\CurrentUser\AppData\Local\Temp



## 4. Create/Edit a Method Wizard

### 4.1 Introduction

The **Create/Edit a Method** wizard is used to

- Create or edit methods,
- Set measurement and evaluation parameters,
- Define the plate layout,
- Select the format of the printed report and
- Set the automated data handling parameters.

### Workflow Summary

Click **Continue** on the welcome page of the **Create/Edit a Method** wizard. In the next window, select

- **Create new** if you want to define a new method or
- **Edit** if you want to modify an existing method.

In the **Define Measurement Parameters** window, measurement parameters can be set. Click **Define Evaluation** to define the plate layout, evaluation parameters, print out and automated data handling parameters. At the end of the wizard the new or modified method is saved as .mth file.



#### Note

*For a step-by-step description of how to create a method, refer to 12 Application Example.*

### File Selection Page

In the wizard list, click **Create/Edit a method** button. Click **Next** on the welcome page of the **Create/Edit a method** wizard and the **File Selection** page with the following elements appears:

<b>Create new</b> button	Select <b>Create New</b> button to create a new method.
<b>Edit</b> button	The <b>Edit</b> button must be selected to edit an existing method.
<b>Show</b> combo box	<p>In the <b>Show</b> combo box a file filter can be defined to get only those methods in the list, which fulfill the selected criteria:</p> <ul style="list-style-type: none"> <li>• All files</li> <li>• Files from this instrument</li> <li>• My files: This option is available if the user administration is enabled (always enabled in <b>magellan</b> Tracker).</li> <li>• Signed files: only available for <b>magellan</b> Tracker</li> <li>• Example files: only available if they have been installed.</li> </ul>
<b>Filename</b> list	<p>Select the method to be edited from the <b>Filename</b> list.</p> <p>A <b>Remarks</b> field next to every file name contains - if entered - a short description of the method.</p> <p>All methods available in the standard method directory will be displayed (see chapter 9.3 Options).</p>

## 4. Create/Edit a Method Wizard

**Print  
Preview...**  
button

Click the **Print Preview...** button to open the **Print Preview dialog box**, where a preview of the settings of the selected method is displayed and a printout can be started.



### Note

*If a **SUNRISE** instrument is connected, but an **INFINITE F50** method is selected, the **Instrument Mismatch** dialog appears:*

- **Connect to the proper instrument.**

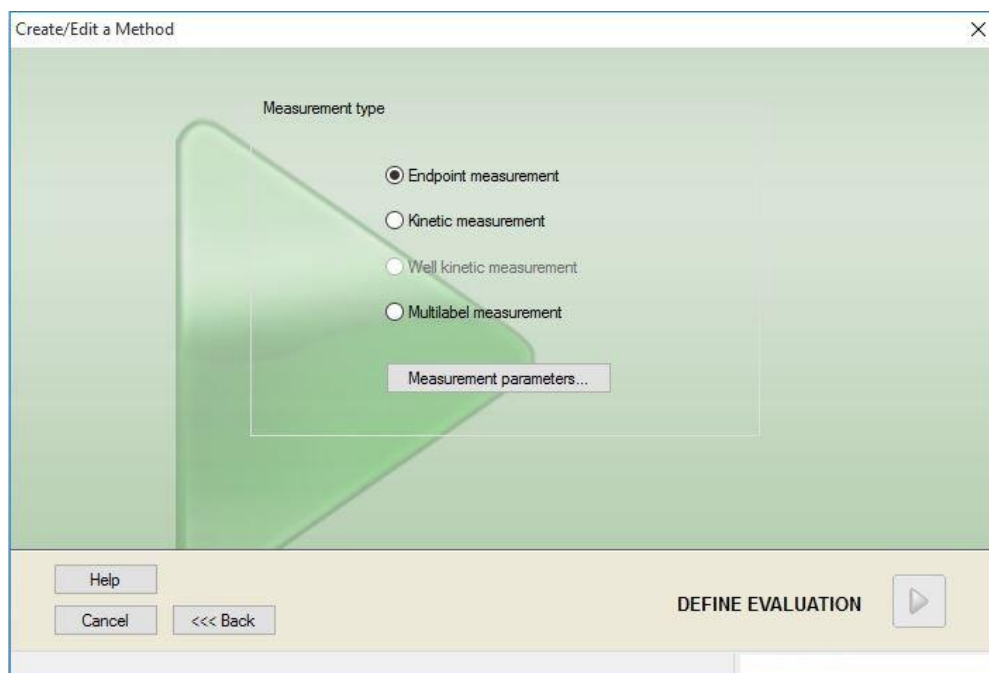
## 4.2 Define the Measurement Parameters

In the **Measurement Parameters** window it is possible to set all required parameters for the measurement, including measurement mode, wavelengths, read mode, temperature, etc. depending on the type of instrument connected.

When connected to an INFINITE F50 instrument, refer to the Instructions for Use for i-control for further details on defining measurement parameters.

### 4.2.1 Measurement Types - SUNRISE

Click **Make your selection** and the **Measurement type** dialog box appears:



The measurement type is to be selected from an option button list.

The **Measurement type** window contains the following elements (depending on the instrument connected):

**Measurement type**  
group box

- Select **Endpoint measurement** to perform a single measurement.
- Select **Kinetic measurement** to perform kinetic measurements per plate with a specified interval time.
- Select **Multilabel measurement** to perform multilabel measurements with different measurement parameters.

Click **Measurement parameters...** to open the **Measurement Parameter** dialog box.

#### 4.2.2 Measurement Parameters - SUNRISE

Select the required **Measurement type** and click **Measurement parameters...** to open the Measurement Parameter dialog box for adjustment of

- Barcode,
- Wavelengths,
- Measurement parameters (read mode),
- Kinetics
- Temperature and
- Shaking.

Click the **OK** button to save the changes and the **Cancel** button to reject them.

Depending on the instrument connected and on the measurement type selected, the **Measurement Parameters** dialog box and the respective tabs available vary.

When connected to an Infinite instrument refer to the Instructions for Use for i-control.

#### Multilabel Measurement

If the measurement type multilabel measurement was selected, the **Multilabel Measurement** dialog box is displayed.

To create a list of parameter windows the **New** button must be clicked. The **Measurement Parameters** dialog box will appear where a new set of measurement parameters can be defined. At least two sets of measurement parameters must be created in the multilabel dialog box.



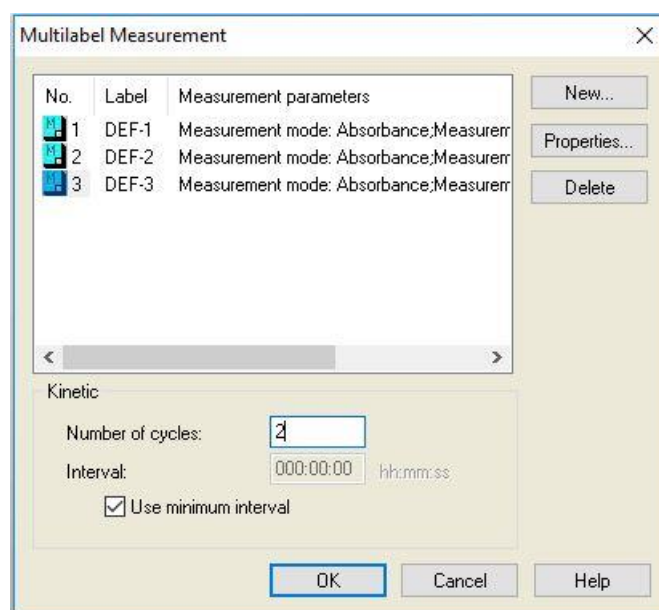
##### Note

*If Move plate out after measurement is selected when running the method, magellan displays a message box where liquids in the plate can be modified and the measurement continued. Otherwise, the measurement is performed without a break.*

The measurement parameter **Comments** can be used to label the set of measurement parameters in the list.

#### 4. Create/Edit a Method Wizard

The **Multilabel** dialog box contains the following elements:



##### Label list

In the **Multilabel** list the existing measurement parameter definitions are listed line by line. In the **No.** column a guide number counts up the existing measurement parameter definitions and a small icon is presented. The **Label** column displays a customizable name (in **Measurement Parameters – General Tab – Comment to this measurement**). The **Measurement parameters** column lists a summary of the selected measurement parameters.

##### New button

Click the **New** button and the measurement parameters of each new measurement can be defined. The **Measurement Parameters** dialog box will appear. Define names for each label. In the **Measurement Parameters** dialog box, the name written in the comment field of the **General** tab is used as label. All parameters must be entered to define a new measurement.

##### Properties... button

Click the **Properties** button and all **measurement parameters** of the highlighted label in the measurement parameters list are displayed and can be edited.

##### Delete button

Click **Delete** or press **DEL** to delete the highlighted measurement parameter(s) from the multilabel field.

##### Number of cycles

Defines the number of kinetic cycles for a multilabel kinetic measurement.

##### Interval

Defines the kinetic interval or the pause between labels (if only one cycle is defined).

### 4.2.3 Measurement Parameters - INFINITE F50

#### Defining Endpoint Measurements

The following example describes an **Absorbance Endpoint Measurement** in all wells of a 96-well microplate.

1. Select a 96-well microplate from the **Plate definition** drop-down list.
2. By default, all wells of the 96-well microplate are chosen for measurement.
3. Enter the desired measurement and reference wavelengths.

The screenshot shows the 'Part of Plate' section with a 96-well microplate grid (A-H, 1-12) where all wells are selected. Below this, the 'Absorbance' section is active, showing 'Wavelength' set to 405 nm, 'Reference' checked and set to 620 nm, and 'Label' set to 'Label1'.

#### Defining Multilabel Measurements

The following example describes an **Absorbance Multilabel Measurement** in all wells of a 96-well microplate. Three absorbance labels shall be measured.

1. Select a 96-well microplate from the **Plate definition** drop-down list.
2. By default, all wells of the 96-well microplate are chosen for measurement.
3. Enter the desired measurement wavelength.
4. Insert 2 more **Absorbance** elements and enter the measurement wavelengths.

The screenshot shows the 'Part of Plate' section with the 96-well microplate grid. Below it, three 'Absorbance' elements are defined:
 

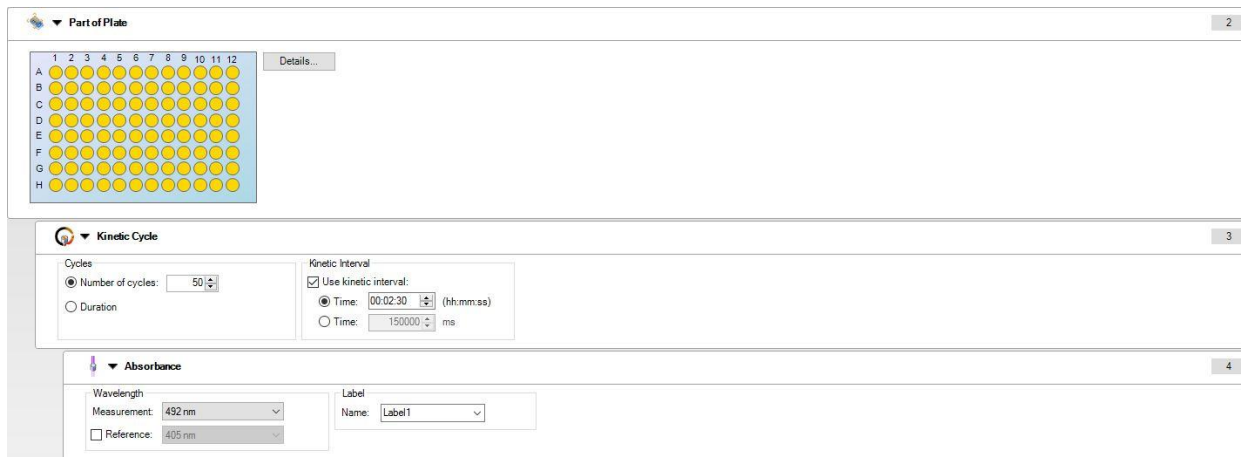
- Element 1: Wavelength 405 nm, Reference 405 nm, Label 'Label1'.
- Element 2: Wavelength 492 nm, Reference 405 nm, Label 'Label2'.
- Element 3: Wavelength 620 nm, Reference 405 nm, Label 'Label3'.

## 4. Create/Edit a Method Wizard

### Defining Kinetic Measurements

The following example describes a kinetic measurement of a 96-well microplate.

1. Select a 96-well microplate from the **Plate definition** drop-down list.
2. Insert a **Kinetic Cycle** program element between the part of plate and the absorbance element.
3. Cycles/Number of cycles: 50
4. Kinetic interval (interval between measurements): select **Use kinetic interval** and enter: 2 minutes 30 seconds.
5. Define the **Absorbance** element by entering the desired measurement wavelength.

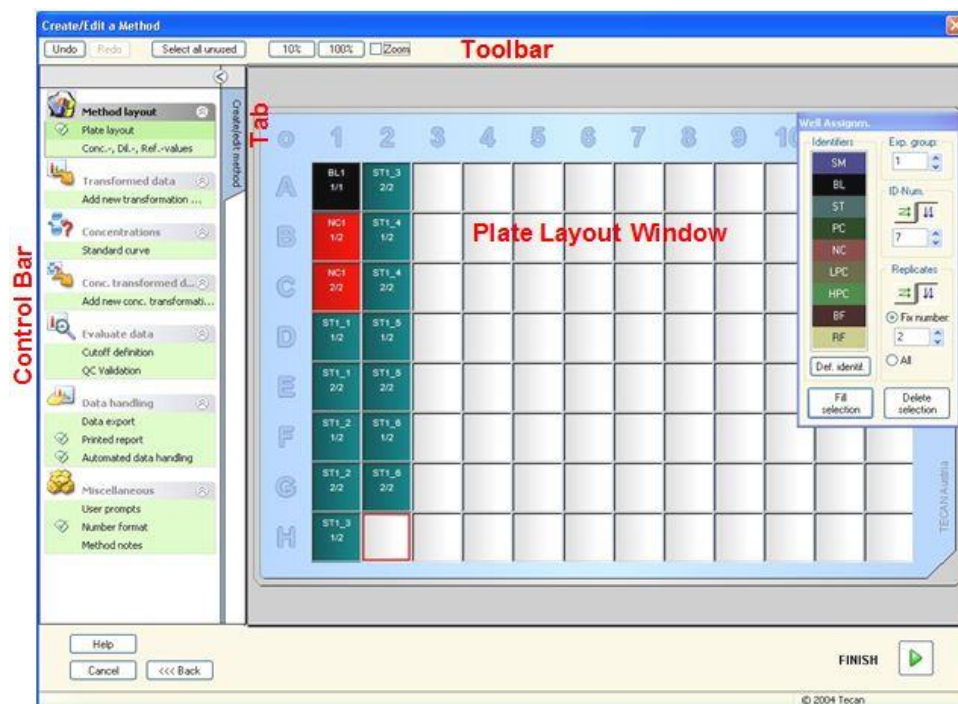


The screenshot displays the 'Part of Plate' section with a 96-well plate grid (A-H, 1-12) and a 'Details...' button. Below this, the 'Kinetic Cycle' section is active, showing 'Number of cycles' set to 50 and 'Use kinetic interval' checked with a time of 00:02:30. The 'Absorbance' section is also visible, with 'Wavelength' set to 492 nm and 'Reference' set to 405 nm.

## 4.3 Define Evaluation

### 4.3.1 The Create/Edit Method Overview Window

In the **Define Evaluation** window the user defines the plate layout, transformations and calculations, selects the format of the printed report and sets the automated date handling parameters.



#### Toolbar

On top of the window a **Toolbar** is displayed with the most common functions depending on the currently selected options:

<b>Undo</b> button	Click <b>Undo</b> to undo a previous action.
<b>Redo</b> button	Click <b>Redo</b> to redo an action that was undone.
<b>Select all unused</b> button	<b>Plate Layout mode only:</b> All unused wells of the plate are marked.
<b>Zoom to 10%</b> button	This will set the plate layout view to 10%.
<b>Zoom to 100%</b> button	This will set the plate layout view to 100%.
<b>Zoom mode</b> button	Use the <b>Zoom mode</b> button to zoom into the marked area. If activated, the user can select an area to zoom in by clicking and dragging a frame over the desired layout area. Click the right mouse button to zoom out to 100% display.

## 4. Create/Edit a Method Wizard

### Plate Layout Window

In the central area of the window the **Plate Layout Window** displays a schematically layout of a microplate.

When creating a new method select the wells for the measurement. A mouse click selects an individual well. Unselected wells will remain gray.

For the defined layout, the identifiers, transformations, and formulas selected in the **Control Bar** are displayed in the corresponding wells (see **Control Bar of Create/Edit Method** below).

#### Plate Layout: Context-Sensitive Menu

By right-clicking on a well on the plate layout, a context-sensitive menu for the marked wells is displayed. The following commands are available:

Menu	Description
<b>Summary...</b>	<b>Any plate view.</b> The <b>Summary</b> dialog box is displayed. Refer to chapter 7.4.18 Context-Sensitive Menu of a Well/ Summary Dialog for further information on the <b>Summary...</b> dialog box. This option is available if a layout has been assigned to the selected well.
<b>Fill Selection</b>	<b>Plate Layout mode only.</b> If a well or an area of the plate has been marked, it can be filled with the respective identifiers. The IDs and the color identifiers will be displayed on the plate layout.
<b>Delete Selection</b>	<b>Plate Layout mode only:</b> This command will delete the IDs and color identifiers of the selected wells and leave them blank.
<b>Select all Unused</b>	<b>Plate Layout mode only:</b> All unused wells of the plate are marked.
<b>Set / Remove Alias...</b>	<b>Plate Layout mode only:</b> Sets or removes alias designations for the well names. See chapter 4.3.2 Method Layout: How to Define a Plate Layout/ Assign Alias to the Required Well.

### Control Bar of Create/Edit Method Tab

The **Control Bar** on the left of the screen provides a number of options, which should be executed in the suggested sequence. Depending on the kind of measurement and the connected reader type, some of the options may not be available and therefore are hidden.

When selecting an item in the control bar the corresponding dialog or plate view is displayed in the **Plate Layout window** pane on the right side of the screen.

All available options will be marked with a checkmark, once they have been defined. For any kind of transformation, the transformation name is displayed.

The **Control bar - Create/edit method** tab contains the following elements:



<b>Method layout</b> group	<ul style="list-style-type: none"> <li>• Plate layout item</li> </ul> <p>The <b>Plate layout</b> window is opened, displaying the plate layout and the <b>Well assignment</b> dialog box.</p> <ul style="list-style-type: none"> <li>• Conc., Dil., and Ref.-values item</li> </ul> <p>The <b>Concentration/Dilution/Reference</b> definition dialog box is opened, displaying the dilution, concentration or reference value of each well. The standard concentrations can be established as well as the dilution factors and the reference values. An <b>Autofill</b> function provides easy assignment of concentrations in case of distinctive mathematical relations of the concentrations between the individual wells.</p>
<b>Precalculation</b>	<ul style="list-style-type: none"> <li>• Spectra data reduction for wavelength scans</li> </ul>
<b>Transformed data</b> group	<ul style="list-style-type: none"> <li>• <b>Add new transformation ...</b> item</li> </ul> <p>The <b>Plate layout</b> window is opened, displaying the plate layout and the <b>Transformations</b> dialog input field.</p>
<b>Kinetic</b> group	<ul style="list-style-type: none"> <li>• <b>Kinetic data reduction</b> item</li> </ul> <p>The <b>Kinetics Calculation Parameters</b> window is opened. The evaluation of the kinetics measurement data can be defined.</p>
<b>Kinetics transformation</b>	<ul style="list-style-type: none"> <li>• <b>Add new kinetic transformation ...</b> item</li> </ul> <p>The <b>Plate layout</b> window is opened, displaying the plate layout and the <b>Transformations</b> dialog input field (only kinetic input data can be selected).</p>
<b>Concentrations</b> group	<ul style="list-style-type: none"> <li>• <b>Standard curve</b> item</li> </ul> <p>The <b>Standard Curve</b> window is opened to set the parameters for the calculation of concentrations and the graphical display of the standard curve of the evaluated data.</p>
<b>Concentration transformation data</b> group	<ul style="list-style-type: none"> <li>• <b>Add new concentration transformation ...</b> item</li> </ul> <p>The <b>Plate layout</b> window is opened, displaying the plate layout and the <b>Concentration Transformations</b> dialog input field (only concentrations can be selected as input data).</p>
<b>Evaluate data</b> group	<ul style="list-style-type: none"> <li>• Cutoff definition item</li> <li>• <b>QC validation</b> item</li> </ul> <p>The <b>Define Cutoff</b> window is opened. In this dialog box the limits for a qualitative evaluation (screening) can be defined.</p> <p>The <b>Define QC Validation</b> window is opened. It is used to verify the validity of a test.</p>
<b>Data handling</b> group	<ul style="list-style-type: none"> <li>• Data export item</li> <li>• Printed report item</li> <li>• Automated data handling item</li> </ul>

## 4. Create/Edit a Method Wizard

### Miscellaneous group

- User prompts item
- Number format item
- Method notes item

The **Define User Prompts** window enables the assignment of data (keywords, comments or prompts) to each measurement, which can then be incorporated into a printout.

The **Number format** window allows the user to define the number format for the displayed raw data or transformed data.

In the **Method notes** it is possible to enter a description of the method.

### Control Bar – Create/Edit Method Tab: Context-Sensitive Menu

By right-clicking on any transformation, kinetic transformation and concentration transformation on the control bar, a context-sensitive menu for the marked transformation is displayed. The following commands are available:

Menu	Description
<b>Rename transformation</b>	A different name can be assigned to the selected transformation.
<b>Insert transformation</b>	Used to define a new transformation.
<b>Remove transformation</b>	Used to delete a transformation.

### 4.3.2 Method Layout: How to Define a Plate Layout

In the **Control bar** expand **Method layout** and select **Plate layout**. The **Plate view** and the **Well Assignment** dialog box are displayed.

To each well in the analysis plate an identifier can be assigned. On this basis the plate layout should be defined, (i.e. a well that is to be viewed as being a positive control, would be allocated a different identifier from that of a well that is to be viewed as being a negative control).

Standard identifiers are:

Sample	<b>SM</b> (Sample)
Blank	<b>BL</b> (Blank) <b>BF</b> (Polarization reference buffer)
Reference	<b>RF</b> (Polarization reference)
Standard	<b>ST</b> (Standard)
Control	<b>PC</b> (Positive control) <b>NC</b> (Negative control) <b>LPC</b> (Low positive control) <b>HPC</b> (High positive control) <b>CL</b> (Calibrator)

### Assign an Identifier to the Required Well

In the **Well Assignment** dialog box, well identification and layout definition can be carried out. This box also provides a number of automated ID assignment capabilities, which is an essential tool for high density plates.

The desired settings must be made in the **Well Assignment** dialog box. Generally, the wells can be selected by clicking the individual well or dragging the mouse over the required wells.

Following ways are possible to assign the selected identifier to the wells:

- Double-click when making the selection of the well
- Select the wells on the microplate and then click the **Fill selection** button (or click the right mouse button and select **Fill selection** in the context-sensitive menu) on the **Well Assignment** dialog box
- Select the wells on the microplate and then double click the identifier in the identifier list box of the well assignment dialog.
- After assigning the definitions the display in the modified wells will change.

#### Example of a labeled well:

<b>SM1_4</b>	1 <sup>st</sup> line: sample, experimental group number of 1, sample ID number of 4.
<b>1/14</b>	2 <sup>nd</sup> line: number of replicate is 1, total number of replicates is 14.
<b>x-BL1</b>	3 <sup>rd</sup> line: primary empty – filled with the transformation formula or a concentration, dilution or reference value if defined, e.g. reduce the value of this well (x) by the mean of the blanks.

#### 4. Create/Edit a Method Wizard

The **Well assignment** dialog box contains the following elements:

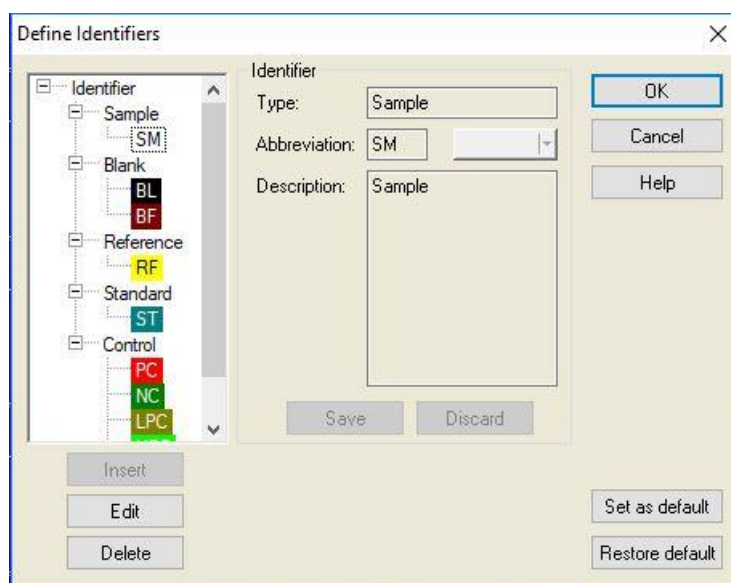
<b>Identifiers</b> group box	<p>In this group box, corresponding identifiers for the marked wells have to be selected.</p> <ul style="list-style-type: none"> <li>All available identifiers are listed in a drop-down list.</li> <li>Click the <b>Define Identif...</b> button to define additional identifiers. The <b>Define Identifiers</b> dialog box appears, see below for further details.</li> </ul>
<b>Exp. group</b> selection field	<p>If the plate is made up of more than one test, then there needs to be more than one experiment group. In the <b>Experiment group</b> selection field, define which experiment the wells belong to.</p>
<b>ID-Num.</b> group box	<p>The <b>ID Number</b> is used to assign the same ID to replicates that belong together. The ID Number is only available for samples and standards.</p> <ul style="list-style-type: none"> <li><b>ID-Num.</b> selection field The <b>ID-Num</b> option allows the user to mark those replicates that are associated with the same ID. This can be used if the replicates have been assigned to different areas of the plate.</li> <li><b>Arrow buttons</b> The ID will be calculated automatically. If a number of wells is marked, the direction in which the IDs are assigned to the wells (vertically, horizontally) can be established using the arrow buttons.</li> </ul>
<b>Replicates</b> group box	<p>Determines the number of replicates for the selected identifier type. Two option buttons allow the decision whether multiple or individual values are to be defined:</p> <ul style="list-style-type: none"> <li><b>Fix number</b> option button Only enabled for standards and samples where IDs can be used. If this option button is active a number can be entered in the corresponding text field. This number defines how many replicates are intended for this identifier. The selected wells are then filled with the entered number of replicates. Therefore, the number of selected wells must be a multiple of the entered number of replicates.</li> <li><b>All</b> option button All selected wells are defined as replicates of one identifier. If an existing ID number for the samples and standards is chosen, the selected wells are then added as replicates to the existing replicates. With all other identifier types the selected wells are added as replicates to the existing replicates.</li> </ul> <p>Two <b>Arrow buttons</b> define the direction of counting up the replicate number.</p>
<b>Fill section</b> button	<p>If an area of the plate has been marked, it can be filled with the respective identifiers. The IDs and the color of the identifiers will be displayed on the plate layout.</p>
<b>Delete section</b> button	<p>Click <b>Delete</b> or press <b>DEL</b> to delete the IDs and color identifiers of the selected wells and leave them blank.</p>
<b>Define identifier</b> button	<p>Click <b>Def. identif.</b> if a new identifier is to be defined or if an existing identifier is to be edited (see Expert's Know How, Define a New Identifier)</p>

## Assign Alias to the Required Well

To assign alias designations for defined well names, click the right mouse button in the required well, select **Set/Remove Alias...** and choose an alternative identifier name in the drop-down list. The alias is marked with an asterisk \* and has same experimental group, ID number and replicate number as the primarily defined well. This feature is used, if e.g. the 0-Standard is also used as Negative control.

## Define a New Identifier

In the **Well Assignment** dialog box, click **Def. Identif. to define** a new identifier or edit an existing one.



The identifiers are listed in groups (see table below). Highlighting an identifier, its properties are displayed in the right window.

Standard identifiers are:

Sample	<b>SM</b> (Sample)
Blank	<b>BL</b> (Blank) <b>BF</b> (Polarization reference buffer)
Reference	<b>RF</b> (Polarization reference)
Standard	<b>ST</b> (Standard)
Control	<b>PC</b> (Positive control) <b>NC</b> (Negative control) <b>LPC</b> (Low positive control) <b>HPC</b> (High positive control) <b>CL</b> (Calibrator)

The **Define Identifiers** dialog box contains the following elements:

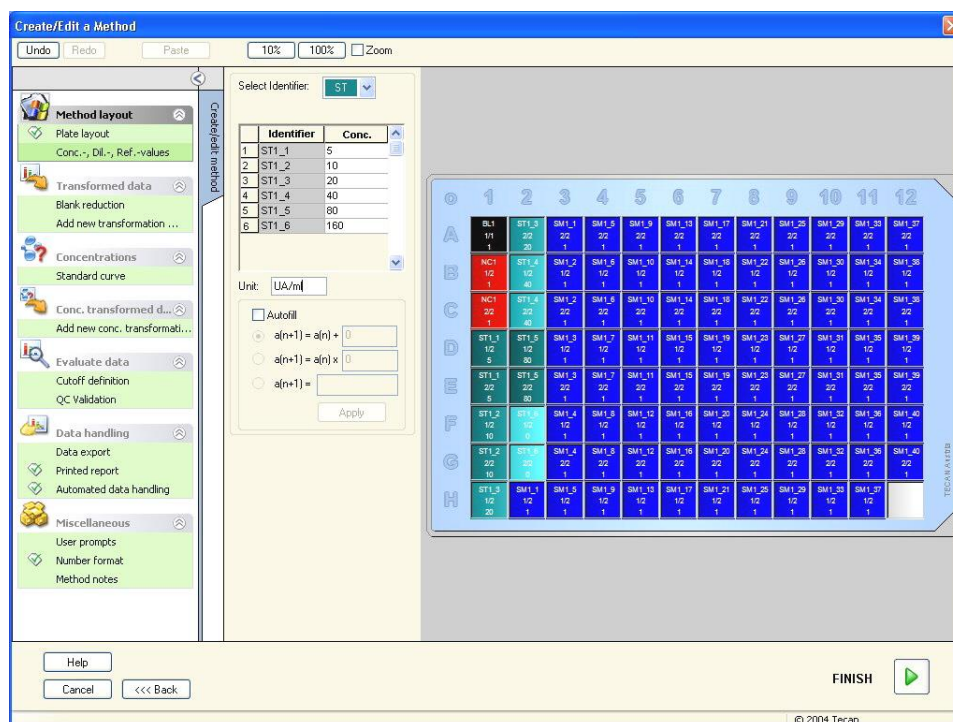
<b>Identifier</b> tree structure	A structured view of all existing identifiers, their colors and abbreviations is offered in a small window. The identifiers are listed under the groups <b>Sample</b> , <b>Blank</b> , <b>Reference</b> , <b>Standard</b> and <b>Control</b> .
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#### 4. Create/Edit a Method Wizard

<b>Identifier group box</b>	<p>The criteria held by the various identifiers used in the program will be displayed. If new identifiers are required, they can be inserted here.</p> <p>In the <b>Identifier</b> group box, the type, abbreviation, well color and description of the identifier selected in the tree structure is displayed.</p>
	<p>The <b>Identifier</b> group box is only activated for entering data, when</p> <ul style="list-style-type: none"> <li>• one of the <b>identifier groups</b> in the tree structure is selected and the <b>Insert</b> button has been clicked or</li> <li>• one of the <b>identifiers</b> in the tree structure is selected and the <b>Edit</b> button has been clicked.</li> </ul> <p>Then, in this group box, the type, abbreviation, well color and description of the new identifier need to be defined.</p>
	<p><b>Type</b> text field: The type of identifier is displayed. No changes are possible.</p>
	<p><b>Abbreviation</b> text field: The identifier's abbreviation will be used in the analysis plate display.</p>
	<p><b>Color</b> drop down list: The color of the identifier on the plate layout has to be selected here.</p>
	<p><b>Description</b> text field: A text description can be entered for each identifier.</p>
	<p>Use one of these two buttons to save changes of newly entered data or to discard any changes:</p>
	<p><b>Save</b> button: The <b>Save</b> button saves the entered color, abbreviation and description of the relevant identifier.</p>
	<p><b>Discard</b> button: The <b>Discard</b> button will cancel any changes.</p>
<b>Insert</b> button	<p>Click the <b>Insert</b> button to create a new identifier. This new identifier will be associated with the currently selected identifier group in the tree structure.</p>
<b>Edit</b> button	<p>A selected identifier can be modified.</p>
<b>Delete</b> button	<p>Click <b>Delete</b> or press <b>DEL</b> to delete any selected identifier.</p>
<b>Set as default</b> button	<p>Using this option, the settings can be defined as default for future use.</p>
<b>Restore default</b> button	<p>Using this option, the settings can be reset to the previously defined default.</p>

### 4.3.3 Method Layout: Conc., Dil. and Ref. Values

In the **Control bar** expand **Method layout** and select **Conc./Dil./Ref.-values**. The **Plate View** and the **Select Identifier** dialog box are displayed.



The **Concentration/Dilution/Reference** window contains the following elements:

**Select Identifier**  
drop-down list

The values are co-related within the individual well types; this field provides all wells currently included in the measurement. Select an identifier to edit the corresponding dilution or concentration factors. All wells, which match the selected well type identifier, are listed.

**Exp. group**  
selection field

Select the respective experimental group. If there is only one experimental group, the field cannot be edited.

Table with **Identifier**  
and **Concentration/  
Dilution** columns

This table displays all wells in the **Identifier** column, which match the selected identifier (as from the **Select Identifier** list). The corresponding dilutions, concentrations or reference values are inserted and listed in the **Dilution/Concentration/Reference** column. E.g. entering a dilution factor of 2 means that the sample has been diluted by half. The calculated concentration will therefore be multiplied by 2.

**Unit** text field

The displayed concentration unit can be determined.

**Autofill** check box

The **Autofill** function provides the calculation of the corresponding concentrations or dilution factors according to available types of series.



#### 4. Create/Edit a Method Wizard

<b>Option</b> buttons for the mathematical concentration calculation	<p>If the <b>Autofill</b> check box has been selected, the following options are available:</p> <ul style="list-style-type: none"> <li>• Arithmetic series: <math>a(n+1) = a(n) + \dots</math></li> <li>• Geometric series: <math>a(n+1) = a(n) \times \dots</math></li> <li>• User defined series <math>a(n+1) = \dots</math> Example: Each subsequent concentration should contain twice + 0.5 of the previous concentration: Formula 1: <math>a(n+1) = 2 * n + 0.5</math></li> </ul>
<b>Apply</b> button	The <b>Apply</b> button applies the selected mathematical concentration calculation to the wells as displayed in the table with <b>Identifier</b> and <b>Concentration/ Dilution</b> columns.
<b>Dilution series</b> group box	<p><b>Calculate ICx</b> check box Displays a dilution graph of the sample and automatically calculates the ICx values. This requires samples with at least 4 replicates and at least 4 different dilutions defined.</p>
	<p><b>Input Data</b> drop down list Select from the drop down list the input data.</p>
	<p><b>Calculation Condition</b> text field The intercept will be calculated with the entered percentage of the maximum value respectively maximum value minus minimum value*.</p>
	<p><b>ICx name</b> text field Data can be selected for ICx calculation. The name is filled in automatically based on the calculation condition.</p>
	<p><b>Set 0% value to</b> Intensity 0* Min. intensity of dilution series*</p>

Dilution can be edited directly in the plate layout window by right mouse clicking in one or more selected wells. In this way, it is possible to assign different dilution values to replicates.

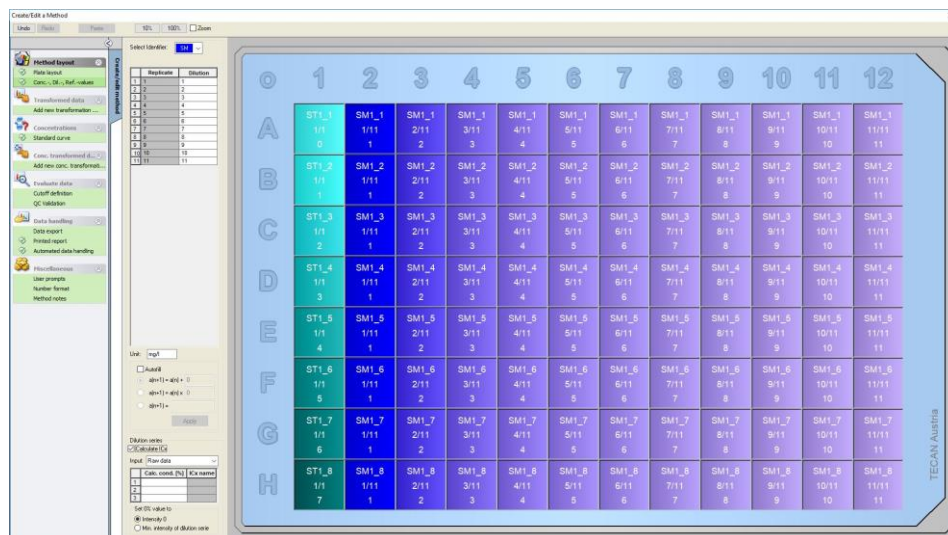


## ICx Calculation

The mathematical calculation of the fit for the dilution series is identical to the calculation of the standard curve with the Marquardt 4 parameter algorithm.

This requires at least **four replicates** with different dilutions.

In addition, the specified intercept(s), e.g. IC 50 is calculated.



It is possible to define more than one intercept for the dilution series.

It is possible to define the 0% value for the calculation by selecting:

- Intensity 0  
Using 0 OD  
The largest value of the dilution series is considered 100%, the value of 0 is considered 0%. The ICx (e.g. IC 50) is then defined as the dilution where the response reaches x% (e.g. 50%). It is only calculated if the value is within the available data (no extrapolation is used).

or

- Minimum intensity of the dilution series  
Using the minimal intensity of the dilution series



### Note

**The IC 50 is often calculated with the mean value of dilution=1:1 and dilution=1:infinity. To achieve this, the dilution series must be baseline corrected before ICx calculation.**

The largest value of the dilution series is considered 100%, the minimum intensity of the dilution series is considered 0%.

## 4. Create/Edit a Method Wizard

### 4.3.4 Precalculation: Spectra Data Reduction

This option is only available for measurements containing a two-dimensional scan (absorbance scan).

Expand **Precalculation** in the control bar and select **Spectra Data Reduction**.

Spectra data reduction allows to perform a spectra blank reduction and to extract specific data, e.g., intensities, from the scan.

The **Spectra data reduction** window contains the following elements:

#### Blank reduction check box

This option is only available if blanks are defined on the layout. The blank reduced spectra is calculated by subtracting the spectrum of the blank well from all other wells. When more blanks are defined on the plate, e.g. when multiple experimental groups are defined, an additional options button appears. This allows to define the blank to be used.

**Input data** text box: shows the input data to be processed.

**Blank reduction** option button: select, if a blank reduction should be performed on the selected experimental group.

**Reduce all by** dropdown list: select to define the identifier to be used for blank reduction.

#### Smooth check box

A spectrum containing a lot of noise can be smoothed. A smooth factor can be set in the options part. This factor defines the degree of smoothing.

**Input data** text box: shows the input data to be processed.

**Smooth factor**: to define the smooth factor.

**Wavelength pick check box**

**Wavelength pick** is used to extract intensities at specific wavelengths and calculate results like ratios. It is mandatory to set the options.

The **Wavelength pick** parameters dialog box contains the following elements:

Intensities at a specific wavelength can be extracted, ratios and areas can be calculated, and customized formulas can be entered.

	<b>Input data</b> text box: shows the input data to be processed.
	<b>Pick Wavelengths</b> option button: an intensity at a specific wavelength can be added to the list of calculated results.
	<b>Calculate Ratio</b> option button: two wavelengths can be specified. The ratio of the intensities at those wavelengths is calculated and available as result.
	<b>Area</b> : to calculate the area below the spectra curve between two defined wavelengths.
	<b>Custom</b> option button: a user defined formula can be entered. Intensities at specified wavelengths can be used in formulas.
	<b>Results</b> list box: summarizes all defined formulas
	<b>Add</b> button: the current selection is added to the list of results.
	<b>Delete</b> button: the selected result is removed from the list.
	<b>Edit</b> button: the data name of the selected result can be defined.

#### 4. Create/Edit a Method Wizard

##### Normalize check box

The **Normalize parameters** dialog box contains the following elements:

Use this option to normalize the spectrum to the intensity at a given wavelength or to the maximum intensity of the spectra graph of each well.

**Input data** text box: shows the input data to be processed.

**Normalize to:** select between maximum intensity or insert customized intensity.

##### Peak check box

A peak is defined as the position of the maximum value of the spectrum. Overflows and maxima at the left or right border of the spectrum are not treated as peaks. It is very important to sufficiently smooth the spectrum before finding a peak.

The **Peak parameters** dialog box contains the following elements:

Use this option to find the peak with the highest intensity within a defined wavelength.

The threshold (OD/RFU value) and the calculation criteria for calculation of width and area can be defined as well.

The following data will be calculated for the found path:

- peak intensity
- wavelength of the peak
- peak width
- peak area

##### Custom formulas check box

Select this check box to enter formulas to calculate the spectrum using given functions; e. g. smooth.

Refer to chapter 11.2 Spectra Data Reduction for further information.

Transformation must either return a spectrum or a single data for all wells; it is not possible to mix both. Using this option, functions can be defined which are not available in the standard selection. E.g. to find more peaks within a spectrum or to create a derivation of a spectrum.

**Available results**

Available results of all data are listed.

**S** is a spectrum

**V** is a value.

### 4.3.5 Transformed Data: Add New Transformation

In the control bar expand **Transformed data**. All defined transformations are displayed in the control bar.

To define a new transformation, select the well(s) for which the transformation is to be applied and click **Add new transformation...**

The default name should be changed immediately in the edit box. The name can be inserted or changed also later, clicking **Rename Transformation** from the context-sensitive menu.

A typical example of a transformation is the reduction of the empty value (blank) from all wells.

**Note**

*The transformation name has to be in Latin characters to make the transformation available as additional input data for further transformations with multiple input data.*

**Note**

*The name of a transformation is used to represent the result of the calculations and will also be used when the values are displayed in the specific data output menus. Calculated values of the transformations are also available as input data for further evaluations.*

**Note**

*If a blank is set in the Plate Layout, the formula to calculate the blank reduction is offered in the combo box:  $x - BL1$ .*

*The symbol  $x$  refers to the current value within a well.  $BL1$  is the average value of the blank well(s).*

**Note**

*If a multilabel measurement with two labels is defined, different formulas to reduce the multilabel data are offered in the combo box.*

*'Label1'!x/'Label2'!x ... predefined ratio calculation*

*'Label2'!x/'Label1'!x ... predefined ratio calculation*

*'Label1'!x-'Label2'!x ... predefined difference calculation*

*'Label2'!x-'Label1'!x ... predefined difference calculation*

*('Label1'!x-'Label1'!BL1)/('Label2'!x-'Label2'!BL1) ...*

*predefined ratio calculation with blank reduction*

*('Label2'!x-'Label2'!BL1)/('Label1'!x-'Label1'!BL1) ...*

*predefined ratio calculation with blank reduction*

**Note**

*If the read mode is set to absorbance, the formula to calculate the transmission is offered in the combo box:  $1/10^x$ .*

#### 4. Create/Edit a Method Wizard

A number of transformation calculations can be defined when setting up the method. A typical example of this is the deduction of the empty value (blank) from all wells. Refer to chapter 11.3 How to Write a Formula for more details.

The formula text box above the plate view is used to define these various transformation calculations, using raw data and previous transformations as input data.

On the microplate, the wells for which the transformation is to be applied must be selected.

The transformations edit field contains the following elements:

<b>Input data</b> drop down list	The list contains the measurement values, the results from precalculations and all already defined transformations, as well as the averages. If <b>Mean</b> data is selected as <b>Input</b> data for <b>Transformations</b> , then transformations will be assigned to the first replicate of an identifier only.
<b>Formula</b> text box <b>fx</b>	Formulas can be entered by typing or by selecting the needed function from the Functions&Constants list box.
<b>Formula</b> drop down list	This list contains some standard formulas (see Notes below) and all formulas which have been incorporated into the current method. A formula may therefore be selected from this list or a new formula can be added. Formulas for transformations can be entered using the appropriate variables, operators and multiple functions.
<b>Confirm</b> button	Formula edit mode only. Green hook Assigns the transformations to the selected well. Click <b>Confirm</b> button or press <b>ENTER</b> key to assign the formula definition to the well and change to <b>Select</b> mode.
<b>Cancel</b> button	Formula edit mode only. Red cross Click the <b>Cancel</b> button or press the <b>CANCEL</b> key to leave the <b>Edit</b> mode without assigning the formula definition to the well.
<b>Available data</b> drop down list	Select from this list the appropriate data, if more than one set of input data shall be used for calculations. The data set will appear in the formula text box within apostrophes followed by an exclamation sign. To complete the definition, enter the identifier's name or refer to the corresponding value within the well. E. g. 'Raw data' ! BL1  The list contains the measurement values, the results from precalculations and all, up to this moment defined transformations.
<b>Functions</b> drop down list	Lists all mathematical and Boolean functions for the definition of formulas.
<b>Options</b> button	Use this button to customize the behavior when selecting wells in the edit mode. It is possible to select between the following options: <ul style="list-style-type: none"> <li>• Identifier average name</li> <li>• Identifier replicate name</li> <li>• Plate well name</li> </ul>

<b>Constants</b> button	Click this button to open the <b>Define Constants</b> dialog box where constants for calculation can be defined.
-------------------------	--

The transformation definition has two modes:

<b>Select mode</b>	When clicking on a well, the corresponding formula is displayed in the text box. The currently active well is displayed with a red border.
<b>Edit mode</b>	When entering a formula or pressing the '=' key, the active well is displayed with a blue border. Selecting other wells adds the corresponding identifier to the current formula. When selecting the currently active well an 'x' is added to the formula. The symbol 'x' refers to the current value within a well.

Once the formula is created, it will be assigned to the selected well with pressing enter or clicking the confirm button (green hook). After assigning the formula the select mode is reached. An integrated formula checker verifies the plausibility of the formula. A warning appears in case the created formula is not executable.

Select **CANCEL** to discard the defined formula and to reach the select mode. It is also possible to use the corresponding buttons on the left of the formula text box.

When in **Select** mode click the red square in the right lower edge of the well and drag the red selection frame over those wells for which the formula should be set.

It is also possible to select the desired wells and use the functions **Set Formula** and **Remove Formula(s)** which are available from the context-sensitive menu.

These actions have to be performed for all wells, which shall contain transformations.

## Define Constants

Use the **Define Constants** dialog box to define the constant values of a method. These constants can be used wherever a formula can be entered.

Click the **OK** button to save the edited parameters.

The **Define Constants** dialog box contains the following elements:

<b>Constants</b> list	In each row, a constant can be defined. The rows are divided into 4 columns:
	<ul style="list-style-type: none"> <li>• <b>Name</b> Enter an appropriate identifier name for the constant, for example: a code or an abbreviation. Only letters can be used.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Value</b> In the <b>Value</b> text field a numerical value must be allocated to the constant.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Comment</b> Enter a short comment to the constant.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Req.</b> ("required") The <b>Req.</b> check box indicates that a measurement can only be launched on receipt or confirmation of the value for the constant.</li> </ul>



## 4. Create/Edit a Method Wizard

### 4.3.6 Kinetic: Kinetic Data Reduction

In the control bar expand **Kinetic** and select **Kinetic data reduction**.

The dialog box is structured in tabs: **Slopes**, **Onsets**, **Min./Max./Area**, **Available output data**, **Enzyme kinetics**. The unit of the values is displayed according to the selected measurement mode (for example: OD for absorbance).



**Note**  
*Unusable data (e.g., overflow values) are ignored for kinetic data calculation.*

#### Slopes Tab

This tab allows the user to establish the evaluation of the kinetic curve's slope:

<b>Input data</b> drop down list	Select the input data to be processed.
<b>Calculation</b> drop down list	Select the calculation method, linear or quadratic (refer to chapter 11 Calculations).
<b>Mean slope</b> check box	The start and end time can be typed into the provided text fields, otherwise the whole kinetic is analyzed.
	<ul style="list-style-type: none"> <li><b>Time/Points</b> option buttons: If <b>Time</b> is selected the start and end time is entered in hours, minutes and seconds. If <b>Points</b> is selected the start and end point for the analysis is given through the entered kinetic cycle number.</li> </ul>
	<ul style="list-style-type: none"> <li><b>Start</b> field: The start time (in hours, minutes, and seconds) or cycle number must be entered here.</li> </ul>
	<ul style="list-style-type: none"> <li><b>End</b> field: The end time (in hours, minutes, and seconds) or cycle number must be entered here.</li> </ul>
<b>Maximum slope</b> check box	The start and end time can be typed into the provided text fields, otherwise the whole kinetic is analyzed.
	<ul style="list-style-type: none"> <li><b>Time/Points</b> option buttons: If <b>Time</b> is selected the start and end time is entered in hours, minutes and seconds. If <b>Points</b> is selected the start and end point for the analysis is given through the entered kinetic cycle number.</li> </ul>
	<ul style="list-style-type: none"> <li><b>Start</b> field: The start time (in hours, minutes, and seconds) or cycle number has to be entered here.</li> </ul>
	<ul style="list-style-type: none"> <li><b>End</b> field: The end time (in hours, minutes, and seconds) or cycle number has to be entered here.</li> </ul>
	<ul style="list-style-type: none"> <li><b>Points</b> text field: Select for how many points the maximum slope calculation is performed.</li> </ul>

The **mean slope** option determines the mean slope (mean increase/decrease) throughout the defined interval. A start time, end time and a calculation mode (linear or quadratic) must first be entered. All measurement points that fall within



the selected interval will be determined. A regression line (linear regression or polynom 2nd degree) will be laid through the selected measurement points and the mean slope will be formed. The mean slope is defined as the arithmetical mean of the slopes that are calculated from the center points of two adjacent measurement points. The kinetics data made available through this method, includes the mean slope per second, per minute and per hour, as well as the correlation coefficient and the goodness of fit.

Using the **maximum slope** option, the maximum slope (maximum increase/decrease) achieved in the selected interval will be determined. Under the **Points** option, the number of combined points has to be entered. At the beginning the slope will be calculated from the center point of the 1<sup>st</sup> and the n<sup>th</sup> point from the first n points. Then the interval will be moved one point further and the process is repeated. This process will continue over all points within the selected interval. The result will be determined as the largest absolute value of these individual slopes. The kinetics data made available through this method includes the maximum slope per second, per minute and per hour, as well as the time span from the first measurement to the maximum slope in seconds.

## Onsets Tab

Use the **Onsets** tab to determine the time to reach a certain data point (OD value):

<b>Input data</b> drop down list	Select the input data to be processed.
<b>Time to onset</b> check box	If the <b>Time to onset</b> check box is selected, an absolute value for the onset can be entered in the following text field.
	<ul style="list-style-type: none"> <li>Text field: An <b>absolute</b> value for the onset must be entered.</li> </ul>
	<ul style="list-style-type: none"> <li><b>Basis mean of the first n points</b> option button and text field: If selected, enter the desired number of points.</li> </ul>
	<ul style="list-style-type: none"> <li><b>Basis</b> option button and text field: If selected, an absolute value for the basis must be entered in the adjacent text field.</li> </ul>
<b>Time to onset %</b> check box	If the <b>Time to onset %</b> check box is selected, a percentage value for the onset can be entered in the following text field.
	<ul style="list-style-type: none"> <li>Text field: A <b>percentage</b> value for the onset must be entered.</li> </ul>
	<ul style="list-style-type: none"> <li><b>Basis mean of the first n points</b> option button and text field: If selected, the desired number of points can be entered.</li> </ul>
	<ul style="list-style-type: none"> <li><b>Basis</b> option button and text field: If selected, an absolute value for the basis must be entered in the adjacent text field.</li> </ul>

The result data made available through this method includes the basis value, the time taken to reach the basis value, the time taken to reach the sum of basis and onset value, and the difference of these two time spans (Time Basis to Onset).

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With increasing kinetic measurement values the onset value is to be defined as a positive number, with decreasing values the onset value is to be defined as a negative number.

##### Min./Max./Area Tab

Use this tab to define the evaluation of the minimum and maximum values contained in the curve and to define the calculation of the area under the kinetic curve:

<b>Input data</b> drop down list	Select the input data to be processed.
<b>Mean minimum value</b> check box	Select to open the <b>Points</b> text field where the fixed number of points has to be entered for the minimum value. An even curve will then be generated using these points and the lowest value contained in the curve determined.
<b>Mean maximum value</b> check box	Select to open the <b>Points</b> text field where the fixed number of points must be entered for the maximum value. An even curve will then be generated using these points and the highest value contained in the curve determined.
<b>Area</b> check box	The start and end time can be typed into the provided text fields, otherwise the whole kinetic is analyzed.
	<ul style="list-style-type: none"> <li>• <b>Time/Points</b> option buttons: If <b>Time</b> is selected the start and end time is entered in hours, minutes and seconds. If <b>Points</b> is selected the start and end point for the analysis is given through the entered kinetic cycle number.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Start</b> field: The start time (in hours, minutes and seconds) or cycle number has to be entered here.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>End</b> field: The end time (in hours, minutes and seconds) or cycle number has to be entered here.</li> </ul>

Averages are taken from the number of points starting from the first kinetic measurement value and stepping through one by one until the last kinetic measurement point is included in the average calculation. The minimum/maximum value is determined from these averages.

The result data made available through this method includes minimum/maximum value and the time span from the first measurement to the minimum/maximum value in seconds.

##### Example:

With a kinetic of 5 cycles and a fixed number of 3 points, following averages are taken:

average of 1<sup>st</sup>, 2<sup>nd</sup>, and 3<sup>rd</sup> kinetic value

average of 2<sup>nd</sup>, 3<sup>rd</sup>, and 4<sup>th</sup> kinetic value

average of 3<sup>rd</sup>, 4<sup>th</sup>, and 5<sup>th</sup> kinetic value

The minimum/maximum value is determined from these 3 averages.

The area under the curve is calculated using the formula given below:

$$A = \sum_{i=1}^{n-1} y_i * (x_{i+1} - x_i) + \frac{(y_{i+1} - y_i) * (x_{i+1} - x_i)}{2}$$

### Available Data Tab

A list of the results is displayed in the Available output data tab:

<b>Data field</b>	The data field lists values as selected in the previous tabs of the Kinetic Calculation Parameters dialog box. This data field is for pure display of the listed output data only and provides no edit functions.
-------------------	--

### Enzyme Kinetics Tab

Use this tab to establish the evaluation of enzyme kinetics according to the model of Michaelis and Menten:

<b>Input data</b> drop down list	Select the input data to be processed.
<b>Calculate Km and Vmax</b> check box	Decide whether to calculate Km and Vmax selecting the corresponding check box.
<b>Calculation type</b> group box	The calculation type can be selected as:
	<ul style="list-style-type: none"> <li>Hanes (concentration versus concentration/input data)</li> <li>Eadie-Hofstee (input data/concentration versus input data)</li> <li>Lineweaver-Burk(1/input data versus 1/concentration)</li> </ul>

The result data made available through this method includes Km and Vmax for Enzyme kinetic graph of each experimental group.

Unlike the results of the other kinetic calculations, these results are displayed in the Graph: Enzyme Kinetics dialog box.

This tab is only available if standards are on the plate and either transformations or slope calculations are defined.

#### 4.3.7 Kinetics Transformations: Add New Kinetics Transformations

In the Kinetic transformations dialog box a transformation formula can be defined, which is used for transforming kinetic input data individually for every well.

In the Kinetic transformations dialog box further calculations can be performed on kinetic input data.

The window elements are similar to the Transformation input. Refer to chapter 4.3.5 Transformed Data: Add New Transformation for further information.

#### 4.3.8 Concentrations: Standard Curve

Use this option to set up standard curves for quantitative tests.

The standard curve dialog box contains various settings concerning the analysis type, the axes and the display of the standard curve. The editable fields and elements are grouped in 5 different tabs.

## 4. Create/Edit a Method Wizard

### Data Tab

This tab stipulates some basic settings like the input data source.

<b>Exp. group</b> spin control	<p>If several tests are to be performed on one plate the <b>Experiment group</b> must be selected. If the plate contains only one test, then the spin control will not be displayed.</p> <p>For each experiment group the input data can be defined individually.</p>
<b>Input data</b> drop down list	Select the <b>Input data</b> to be used for the standard curve. Select measurement data or any available transformation results.
<b>Standards from layout</b> option button	Calculate the standard curve from the standards on the layout.
<b>Standards from ext. file</b> option button	If the selected experimental group contains no standards, a standard curve can be loaded from a .std file. The <b>Select</b> button must be clicked to select the file.
<b>Standards from exp. group</b> option button	If the selected experimental group contains no standards, a standard curve from another experimental group can be used.
<b>No standard curve</b> option button	If the selected experimental group contains no standards, it can be decided to calculate no concentrations for this experimental group (in this case set per default).
<b>Additional Concentrations</b> button	Click the <b>Additional Concentrations</b> button to open the <b>Calculate Additional Concentration</b> dialog box. Select additional sets of input data, which are to be used to calculate concentrations based on the current standard curve.

The **Calculate Additional Concentrations** dialog box contains the following elements:

<b>Input data</b> drop down list	Select the input data for calculation of additional concentrations.
<b>Selected data</b> list	The list contains the input data names for calculation of additional concentrations.
<b>Add</b> button	Click the <b>Add</b> button to add the currently selected input data in the <b>Input data</b> drop down list to the <b>Selected data</b> list.
<b>Remove</b> button	Click the <b>Remove</b> button to remove the currently selected data from the <b>Selected data</b> list.

## Analysis Type Tab

Use this tab to select the analysis type. Please refer to chapter 11.4 Standard Curve Analysis Types for a detailed description of the analysis types.

**Analysis type**  
option buttons

Select which interpolation algorithm is to be employed when calculating the standard curve:

All offered analysis types are listed and can be selected:

1. Point to point
2. Linear Regression
3. Non-linear Regression
4. Cubic spline
5. Akima
6. Polynomial (including the field for selection of the polynomial order and including weight options)
7. Four Parameters (including the more button for minimum and maximum determination)
8. Four Parameters Marquardt (including the more button for definition of the weighting options)
9. Five parameters (including the more button for definition of the weighting options)
10. LogitLog (including the more button for minimum and maximum determination)

**Data scaling** drop  
down list

The analysis type is applied to scaled values. Following scaling modes can be selected:

- Lin(x)Lin(y): x and y axis are scaled linear
- Lin(x)Log(y): x axis is scaled linear, y axis is scaled logarithmically
- Log(x)Lin(y): x axis is scaled logarithmically; y axis is scaled linear
- Log(x)Log(y): x and y axis are scaled logarithmically

**Note**

***Please note, that, if one selects log-scaling for the x-axis, it is not possible to have a concentration value of 0 since it is mathematically not possible to calculate a logarithm of 0. But it is possible to use a value of for example 0.0000001.***

#### 4. Create/Edit a Method Wizard

<b>More</b> button	<p>Click the <b>More</b> button to view the following options:</p> <ul style="list-style-type: none"> <li>• <b>Standard curve</b> numeric selection field If there is more than one experimental group, for <b>LogitLog</b> and <b>Four Parameters</b> the <b>Min.</b> and <b>Max.</b> value can be selected for each curve individually.</li> <li>• <b>Weighting</b> Select <b>Use weights</b> to use one of the following weighting methods: <ul style="list-style-type: none"> <li>- Automatic using variance</li> <li>- Automatic using relative weight</li> <li>- Manual</li> </ul> </li> </ul> <p>See chapter 11.4.14 Weighting for Four / Five Parameter Fit – Marquardt / Polynomial Fit</p> <ul style="list-style-type: none"> <li>• Weighting dialog – select More button if “Automatic using variance” is selected =&gt; Error handling dialog is displayed – Define the weighting factors, which should be used if one of the two error cases (All replicates are equal or only one replicate is left) occurs, which give a variance of 0 and therefore would lead to an calculation error.</li> <li>• <b>Min/Max</b> text fields <b>Min/Max</b> allows the user to define the minimum or the maximum limit of the standard curve for <b>LogitLog</b> and <b>Four Parameters</b>.</li> </ul>
<b>Include (0,0)</b> check box	If the <b>Include</b> option is selected, (0,0) will be added as standard point. This is only available if <b>Linear</b> has been selected as the axis division for both axes.
<b>Extrapolation</b> check box	Extrapolation applies the concentration calculations to those base points which lie outside of the permitted range as well as to those which lie within the range, for example: an extrapolation factor of 3 forces a concentration calculation of values between $\text{min}-2 \cdot (\text{max}-\text{min})$ and $\text{max}+2 \cdot (\text{max}-\text{min})$ , where min and max correspond to the minimum and maximum concentration value of the standard curve.
<b>Extrapolation factor</b> numeric field	The factor data field is only active, if the <b>Extrapolation</b> check box has been selected. It defines the new limits for the concentration calculation.

#### Intercepts Tab

Use this tab to calculate concentrations for selected Y values based on the standard curve.

<b>Exp. group</b> spin control	If a number of experimental groups is available, the appropriate group can be chosen.
<b>Input data</b> drop down list	All data available for calculation is displayed in this list.
<b>Intercept name and formula</b> list field	A name for the intercept must be created first. Then, the intercept formula must be defined. A numerical value or a formula can be entered.

### Formula input operators

The selection boxes allow for the easy input of formulas by providing a variety of functions, operators and variables.

- **Variables**  
All variables accepted by the software are available using in the list box.
- **... button**  
Click this button to open the **Define constants** dialog box.
- **Operators**  
All operators accepted by the software are displayed here.
- **Functions**  
All functions accepted by the software are displayed here.

### Example

#### IC50 for standard curve:

Formula:  $(ST1\_1 + ST1\_8) / 2$

value of the smallest standard plus the value of the highest standard, divided by 2

## Axis Tab

Use this tab to define the appearance of the axes.

### X-axis group box

### Y-axis group box

Following elements are available in each group:

- **Label** text field: Enter an axis label
- **Color** button: Select a color for all elements of the axis
- **Log-scaling** check box: Select this check box to display the axes of the graph logarithmically (does not affect the calculation).
- **Auto select range** option button: The software will automatically determine minimum and maximum value of the axis
- **Range** option button: The **Min** and **Max** numeric fields are enabled. The minimum and maximum value of the axis can be specified.
- **Grid check box**: If selected, the grid will be displayed on the axis. The **Color** button and the **Line** style drop down list can be used to customize the grid.

## 4. Create/Edit a Method Wizard

### Graph Tab

Use this tab to define the appearance of the graph.

<b>Title</b> group box	<p>Following elements are available:</p> <ul style="list-style-type: none"> <li>• <b>Label</b> text field: Enter a label for the graph.</li> <li>• <b>Color</b> button: Select a color for the label of the graph.</li> </ul>
<b>Curves</b> group box	<p>Following elements are available:</p> <ul style="list-style-type: none"> <li>• <b>Experimental group</b> spin control: Select the experimental group to be customized (only available if more than one experimental group defined).</li> <li>• <b>Color</b> button: Select a color for the curve of the selected experimental group.</li> <li>• <b>Symbol</b> drop down list: Select a symbol for the base points of the selected experimental group.</li> <li>• <b>Label</b> text field: Enter a label for the curve of the selected experimental group.</li> <li>• <b>Hide curve</b> check box: If selected, the curve is not displayed.</li> <li>• <b>Line Width</b> spin control: Select the line width for the selected experimental group.</li> </ul>
<b>Font</b> group box	Select <b>Small</b> , <b>Medium</b> , or <b>Large</b> font size.
<b>Display... group box</b>	<p>Following elements can be selected to be viewed:</p> <p><b>Legend:</b> The curve color, base point style, and label are viewed together with additional information (analysis type parameters, correlation coefficient, and so on).</p> <p><b>Base points</b></p> <p><b>Intercepts:</b> If intercepts are specified, the intercepts can be displayed and labeled in the graph.</p> <p><b>Error bars:</b> If standards are defined as replicates, a bar showing the range plus/minus standard deviation is displayed for each base point.</p>

### 4.3.9 Concentrations Transformations: Add New Concentration Transformations

In the **Concentration transformations** dialog box a concentration formula can be defined, which is used for transforming concentration input data individually for every well.

In the **Concentration transformations** dialog box further calculations can be performed on concentration input data.

The window elements are similar to the **Transformation** input. Refer to chapter 4.3.5 Transformed Data: Add New Transformation for further information.

### 4.3.10 Evaluate Data: Cutoff Definition

Use this option to categorize either raw data or calculated data on threshold limits. Threshold limits can be defined as fixed numeric values or formulas.

Use the **Cutoff Definition** window to define the cutoff ranges and to assign colors and names to cutoff results.



The **Cutoff Definition** window contains the following elements:

<b>Input data</b> drop down list	Select the input data which is to be used in the evaluation.
<b>Exp. group</b> selection list	In case the plate contains more than one test, the relevant experimental group to which the cutoff should apply must be selected. If the plate contains only one test, then only one group will be available, and the field is not visible.
<p>In the <b>Cutoff</b> list, up to ten cutoff ranges can be defined. The limits for each range can be entered.</p> <p>The highest limit value must be entered on top of the list. The next lower will be placed beyond and so on. A displayed Low-High arrow shows the level. The limit values itself belong to the upper ranges (greater and equal condition).</p>	
<b>Colors</b> buttons	A color can be allocated to the individual result levels. When displaying the results these colors will be incorporated, representing the qualitative results.
<b>Labels</b> text fields	The result indicators for every value range must be named, for example: positive (pos), negative (neg), intermediate (?), ...
<b>Limits</b> text fields	The limits can be entered as a constant value or as a formula. Formulas can be entered directly into a field or via the <b>Formula input</b> fields. A maximum of up to nine limits may be defined.
<b>Formula input</b> group box	<p>Formulas to be entered into the <b>Limits</b> field can be composed by using the variables, operators and functions below. Refer to chapter 11.3 How to Write a Formula for further details.</p> <ul style="list-style-type: none"> <li>• <b>Variables</b> drop down list All available variables are displayed.</li> <li>• <b>... button</b> Click this button to open the <b>Define constants</b> dialog box.</li> <li>• <b>Operators</b> drop down list All available operators are displayed.</li> <li>• <b>Functions</b> drop down list Available functions can be selected.</li> </ul>
<b>Competitive Test</b> check box	Competitive tests allocate a positive result to low values and a negative result to high values. In the evaluation, the limits will run from top to bottom and the corresponding results symbol will be allocated when a value is found to be equal to or less than the limit. In view of this, the <b>Low-High</b> arrow will be reversed.
<b>Cutoff results selection...</b> button	Click the <b>Cutoff results selection...</b> button to open the <b>Cutoff Results Selection</b> dialog box.

## 4. Create/Edit a Method Wizard

### Cutoff Results Selection

Use this window to select whether a qualitative result for a certain identifier type is shown or not.

The **Cutoff Results Selection** contains the following elements:

<b>Cutoff display selection tree structure</b>	<p>All defined identifier names are shown in a tree structure, grouped by identifier types. Each identifier is associated with a check box.</p> <p>Selecting or clearing the check box of an identifier name indicates, whether the qualitative results of the according wells will be shown or not. After evaluation, only cutoff results for the selected identifier types are displayed.</p>
--	---

#### 4.3.11 Evaluate Data: QC Validation

Validations are used to check the validity of a test. If the defined criteria are not met, an error message will be displayed after the measurement run and no cutoff results will be displayed. (Except the user has the right to **continue evaluation when error** – see chapter 9.6 User Rights).

Upon selecting the correct input data, the desired formulas are to be entered in the **Validation Conditions** list field. A formula editor supports the user in the creation of the corresponding mathematical formulas.

##### Example:

If the validation criteria are defined as follows:

**NC1>0 and NC1<0.1**

the evaluation will check whether the negative control can be found within the given range. If this is not the case an error message will appear.

The **Define QC Validations** dialog box contains the following elements:

<b>Input data</b> drop down list	Select the relevant data, to which the validation must apply. For example: Raw data, etc.
<b>Exp group</b> selection field	If the plate contains more than one test, the relevant experimental group to which the validation should apply must be selected. If the plate contains only one test, then only one group will be available.
<b>Validation group</b> selection field	Use <b>Validation groups</b> to define validation criteria for the same experimental group with different input data.
<b>Validation Conditions</b> list field	This one-dimensional list will be filled with the formulas and logical equations, which define the <b>Validation Conditions</b> . These logical equations will generate a logical result. The program will examine the input data using this equation and, if the validation criteria are met, will return a result of TRUE. If the criteria did not meet, a result of FALSE and an error message will be displayed.

**Formula input**  
group box

Parts of the formulas to be entered into the **Validation Conditions** field can be selected from the following drop-down lists:

- **Variables** drop down list  
All available variables displayed.
- **... button**  
Click this button to open the **Define constants** dialog box.
- **Operators** drop down list  
All available operators are displayed.
- **Functions** drop down list  
Using the given palette, available functions can be chosen.
- Refer to chapter 11.3 How to Write a Formula for further details.

## Plate to Plate QC

Use this option to define a long-term QC validation (refer to chapter 7.4.2 Toolbar Menu: File/ Plate to Plate QC):

<b>Input data</b> drop down list	Select the relevant data, to which the validation must be applied, from the drop-down list.
<b>Control</b> check boxes	Select the type of control from the drop-down list, then enter the expected mean and standard deviation. A scroll bar appears next to the dialog controls to define more than 4 QC controls.
<b>Workspaces to be evaluated</b> options	Select the appropriate filter to define which workspaces should be evaluated.

### 4.3.12 Data Handling: Data Export

Data to be exported into an ASCII or Excel file can be selected using this dialog box:

<b>Available data</b> list	A list of all available data is displayed, depending on the method definition.
← and → buttons	Data for exporting can be selected simply with drag and drop or by clicking the data in the <b>Available data</b> window and then the arrow pointing towards the <b>Selected data</b> window. Data can be deselected by operating the reverse procedure.
<b>Up</b> and <b>Down</b> buttons	The order of the selected data can be changed by selecting an item and pressing the button <b>Up</b> to move it up or <b>Down</b> to move it down
<b>Selected data</b> list	This list shows all selected data, which has been transferred from the <b>Available data</b> field list.
<b>Export options...</b> button	Click this button to open the <b>Export Options</b> dialog box.

The actual exporting of data only occurs using automated data handling (see 4.3.14 Data Handling: Automated Data Handling).

#### 4. Create/Edit a Method Wizard

### Export Options

The **Export Options** dialog box contains the following elements

<b>Direction group box</b>	The user can define whether the plate data is extracted horizontally line by line or vertically column by column and written in this order to the file.
	<ul style="list-style-type: none"> <li>• <b>Horizontal</b> option button The data is collected in rows.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Vertical</b> option button The data is collected in columns.</li> </ul>
<b>Result group box</b>	Select how to export the data in the form of a matrix or of a continuous list:
	<ul style="list-style-type: none"> <li>• <b>Matrix (nested)</b> option button Data of all selected data sets is arranged in a single matrix. This matrix contains the first columns of all data sets followed by the second columns of all data sets.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Matrix (separated)</b> option button Data of each selected data set is arranged in a separate matrix.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Matrix (XFluor style)</b> option button Data of each selected data set is arranged in a separate matrix together with column and well description similar to XFluor.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Table (well data in rows)</b> option button All data of one well is arranged in horizontal direction starting with data of the well position A1.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Table (well data in columns)</b> option button All data of one well is arranged in vertical direction starting with data of the well position A1.</li> </ul>
	<p>If the <b>Add kinetic timestamps</b> check box is selected, the time stamps of the measurements are added.</p> <p>If the <b>Add Temperatures</b> check box is selected, the temperatures of the measurements are added.</p> <p>If the <b>Insert Data names</b> check box is selected, a list with the names of the exported data is displayed on top of the ASCII-file respectively the EXCEL worksheet.</p>

<b>Add data group box</b>	<p>Provides selectable data options. The selected information will be attached to the end of the data and then exported with the selected data. Select the respective check boxes:</p> <ul style="list-style-type: none"> <li>• Date/time of measurement check box</li> <li>• Method filename check box</li> <li>• Method pathname check box</li> <li>• Workspace filename check box</li> <li>• Workspace pathname check box</li> <li>• Filter wavelength value(s) check box</li> <li>• User prompts check box</li> <li>• Current user name check box</li> <li>• Measurement parameters check box</li> <li>• Multiplate plate information check box</li> <li>• Workspace audit trail check box (<b>magellan</b> Tracker only)</li> <li>• Workspace signatures check box (<b>magellan</b> Tracker only)</li> </ul>
<b>Set as default button</b>	Settings can be logged as a default for future use.
<b>Restore default button</b>	Settings can be reset to the previously defined default.

#### Example

Raw data, kinetic cycle 1, timestamp 0 s

11 12 13

21 22 23

Raw data, kinetic cycle 2, timestamp 33 s

81 82 83

91 92 93

#### 4. Create/Edit a Method Wizard

Matrix (nested), horizontal: 11 81 12 82 13 83 21 91 22 92 23 93	Matrix (separated), horizontal, with timestamps: 0 s 11 12 13 21 22 23 33 s 81 82 83 91 92 93	Matrix (XFluor style): <> 1 2 3 A 11 12 13 B 21 22 23 <> 1 2 3 A 81 82 83 B 81 82 83
Table (well data in rows), horizontal, with timestamps: 0 s 33 s 11 81 12 82 13 83 21 91 22 92 23 93	Table (well data in columns), horizontal: 11 12 13 21 22 23 81 82 83 91 92 93	Table (well data in columns), vertical: 11 21 12 22 13 23 81 91 82 92 83 93

#### Export to ASCII File

The **Export to ASCII File** dialog box contains the following elements:

<b>Decimal character</b> group box	The decimal character may be a point or a comma: <ul style="list-style-type: none"> <li>• <b>Point (x.xx)</b> option button</li> <li>• <b>Comma (x,xx)</b> option button</li> </ul>
<b>Delimiter</b> group box	This option sets a delimiter to separate the individual values within the data in the lines of an ASCII file: <ul style="list-style-type: none"> <li>• <b>Tabulator</b> option button Default option, using tabulators as delimiters.</li> <li>• <b>Other symbol</b> option button If selected, a user-defined delimiter character can be entered.</li> </ul>
<b>Path</b> group box	This option sets the path where the ASCII file will be stored: <ul style="list-style-type: none"> <li>• <b>Export default path</b> option button</li> <li>• <b>Use path</b> option button: Select any path where the ASCII file shall be stored</li> </ul>
<b>Encoding</b> group box	<ul style="list-style-type: none"> <li>• Select the export code:</li> <li>• <b>ANSI</b>: For ANSI compatible characters.</li> <li>• <b>Unicode</b>: For characters that cannot be exported with ANSI code (e.g. Chinese, Cyrillic).</li> </ul>
<b>Set as default</b> button	The settings can be logged as a default for future use.
<b>Restore default</b> button	The settings can be reset to the previously defined default.



### CAUTION

**A SUITABLE EXPORT DELIMITER MUST BE SELECTED. THE EXPORT DELIMITER AND DECIMAL CHARACTER SHOULD NOT BE THE SAME. TAB IS SET AS THE DEFAULT DELIMITER, BUT ANOTHER SYMBOL CAN BE SELECTED.**

## Export to Excel

The Export to Excel dialog box contains the following elements:

<b>Target group box</b>	<p>The option buttons define where to position the transferred data within Excel. This option is also valid for automatic Excel export.</p> <ul style="list-style-type: none"> <li>• <b>New workbook</b> option button Transferred data will be stored in the first worksheet of a new workbook. A new file will always be created, no matter if Excel is started or not.</li> <li>• <b>New worksheet</b> option button Transferred data will be put into a new worksheet within an open, active Excel workbook. If Excel is not open, when selecting this option, it will be started and a new workbook created, including the requested data into the first worksheet.</li> <li>• <b>Insert into worksheet at cell</b> option button and cell coordinates text field The first value of the transferred data will be placed into the cell indicated (default is cell A1) of an open, active Excel worksheet. If Excel is not open when selecting this option, it will be started and a new workbook will be created, inserting the requested data into the first worksheet at the defined cell.</li> <li>• <b>Append to current worksheet</b> option button This option will append the data to the current worksheet. If Excel is not open when selecting this option, it will be started and a new workbook will be created, inserting the requested data into the first worksheet.</li> <li>• Use <b>Insert into Template</b> to export data into a predefined Excel template. Path and name of the Excel template must be entered, clicking the <b>...-button</b>. The corresponding cell position must be indicated.</li> </ul>
<b>Set as default button</b>	The settings can be logged as a default for future use.
<b>Restore default button</b>	The settings can be reset to the previously defined default.

## 4. Create/Edit a Method Wizard

### 4.3.13 Data Handling: Printed Report

The Printed report dialog box provides formatting features for hardcopy printouts to customize the contents and the appearance of the printout.

The settings for the reports are grouped in four tabs, which represent certain formatting areas:

- Data Selection tab
- Page Setup tab
- Header tab
- Footer tab

#### Data Selection Tab

The **Data Selection** tab provides a list of data available for printing.

Print as group box	<p>Select whether the data is to be printed in the form of a matrix or in the form of a list:</p> <ul style="list-style-type: none"> <li>• <b>List</b> The individual list format (horizontal, vertical, sorted and alternating) must be configured in the properties dialog (see below).</li> <li>• <b>Matrix</b> The matrix selection prints the data in a 2 dimensional list (matrix).</li> </ul>
Data source and destination lists	<p>Two lists are used to define the printed data:</p> <ul style="list-style-type: none"> <li>• <b>Available data</b> list: List of all available data, which can be printed. Page breaks and dividing lines can be added to achieve the preferred layout. Elements to be printed can be selected by double-clicking; they are listed in the selected data list.</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>Selected data</b> list: List of all selected data, which will be printed. Informative notes also help to give an awareness as to how the data will be printed, for example: whether the data will be displayed in form of a matrix, a list, as data collection or as a graph. Entries that appear under a heading will be incorporated into the corresponding list or matrix format, providing possibilities to compare different sets of values, for example, measurement values and results.</li> </ul>
Append button	<p>Click this button to transfer data highlighted in the <b>Available</b> data window to the <b>Selected</b> data window. You can also use <b>drag and drop</b>.</p>
Insert button	<p>Use this option to display two pieces of similarly formatted data within the same area. First, data from the <b>Available data</b> list must be selected, then data from the <b>Selected data</b> list. When clicking the <b>Insert</b> button, the former will be included within the latter and will then occupy the same area in the print-out as its parent element. For example, if the standard deviation values are included in the measurement value element, both will be displayed within the corresponding cell of a matrix. The measurement values will, in this case, serve as the parent element and will therefore be displayed first.</p>



Remove button	Selected elements within the <b>Selected data</b> list can be deleted.
Up and Down buttons	Use these buttons to reorganize the sequence of lists, graphs, matrixes... on the printout or to reorganize items within a matrix or a list.
Properties button	Is enabled when a list is selected. Style and content of the list can be selected.
Style group box	<b>Vertical list</b> option button Prints the data in form of a vertical list (order A1, B1, and so on).
	<b>Vertical list alternating</b> option button The order of the data is alternating for each row or column (order A1, B1, ... H1, H2, G2, ... A2)
	<b>Horizontal list</b> option button Prints the data in form of a horizontal list (order A1, A2, and so on).
	<b>Horizontal list alternating</b> option button The order of the data is alternating for each row or column (order A1, A2, ...A12, B12, B11,...B1).
	<b>Sorted list</b> option button This option will sort the entries of all columns according to the entries of the first column. The alphanumerical entries in the first column are split into two parts, the first containing only letters, the second numbers. The entries are sorted first alphabetically. Entries with the same name are then sorted numerically. Example: You can use this option with sample IDs or with the layout, restricted to one experimental group. A sorting of numerical values will work only if all entries are integer values.
	<b>Sample oriented list(s)</b> button Allows the printout of individual lists per sample. The separation for the single tables is done either by the sample IDs (if available) or by the identifier names on the plate layout. Sample IDs are needed if the layout contains different experimental groups representing different parameters for the same samples. It is possible to combine the list style <b>Sample oriented list(s)</b> with other <b>parameters</b> like Identifiers, Exp. Groups and Cutoff results.

## 4. Create/Edit a Method Wizard

List options

Style

Example:

Layout			
Raw data			
Blank reduction			
Cutoff results			
1	2	3	4
A1	BL1_1	0.101~	-0.0000
A2	BL1_2	0.102~	0.0005

Layout		
Raw data		
Blank reduction		
Cutoff results		
1	2	3
A3	SM1_2_1	0.103~
A4	SM1_2_3	0.104~
B3	SM1_2_2	0.203~
B4	SM1_2_4	0.204~

Layout

Limitations

Identifiers

<input checked="" type="checkbox"/>	SM
<input checked="" type="checkbox"/>	BL
<input checked="" type="checkbox"/>	ST
<input checked="" type="checkbox"/>	PC
<input type="checkbox"/>	VS

Exp. Group(s)

☒ All experimental groups

☐ Only 1

Cutoff results

☐ All Cutoff results

☐ Only

OK

Cancel

Help

### Limitations group box

Select between the following options:

**Identifiers:** select or unselect which identifiers should be displayed in the list.

**Exp. Group:** select between all experimental groups or enter the Experimental group number you want to be displayed in the list.

**Cutoff results:** select between all cutoff results or select from the list which results should be displayed in the list.

## Page Setup Tab

In the **Page Setup** tab, general settings are defined:

### Display Header/Footer group boxes

- **Print Header** check box  
If selected, the header will be printed
- **Print Footer** check box  
If selected, the footer will be printed
- **Header** option buttons
  - **Every page** (prints the header on every page)
  - **First page only** (prints the header only on the first page)
  - **Except fist page** (prints the header on all pages except the first one)
- **Footer** option buttons
  - **Every page** (prints the footer on every page)
  - **First page only** (prints the footer only on the first page)
  - **Except fist page** (prints the footer on all pages except the first one)

**Print/Page group**

- **Color** option button  
The printout is in colors, if supported by the printer. The well specific data is printed in the color of the layout (for example: sample raw data is printed blue). The cutoff results are printed in the color of the range (for example: "pos" wells are printed red). The graph is printed as displayed.
- **Black and white** option button  
The printout is black and white.

**Margins group box**

- In the **Unit** drop down list cm or inch can be selected. There are 4 numeric fields, which define the margins:
- **Left** text field: enter the value of the left margin.
  - **Right** text field: enter the value of the right margin.
  - **Above text** field: enter the value of the top margin.
  - **Below text** field: enter the value of the bottom margin.

## Header Tab

In the **Header** tab, the content of the document header is defined:

The screenshot shows the 'Printed report' dialog box with the 'Header' tab selected. The 'Option:' column lists: Page numbers, Date, Time, File name, Program name, and Comment. The 'Adjustment:' column has radio buttons for left, centered, and right. The 'Row number:' column has numeric input fields. The 'Separators' section has checkboxes for 'Above' and 'Below'.

Option:	Adjustment:	Row number:
<input checked="" type="checkbox"/> Page numbers	<input type="radio"/> left <input type="radio"/> centered <input checked="" type="radio"/> right	3
<input checked="" type="checkbox"/> Date	<input checked="" type="radio"/> left <input type="radio"/> centered <input type="radio"/> right	2
<input checked="" type="checkbox"/> Time	<input checked="" type="radio"/> left <input type="radio"/> centered <input type="radio"/> right	3
<input checked="" type="checkbox"/> File name	<input checked="" type="radio"/> left <input type="radio"/> centered <input type="radio"/> right	1
<input type="checkbox"/> Program name	<input type="radio"/> left <input type="radio"/> centered <input type="radio"/> right	1
<input type="checkbox"/> Comment	<input type="radio"/> left <input type="radio"/> centered <input type="radio"/> right	1

Separators:  
☒ Above ☒ Below

**Option check boxes**

Use **Option** to select any of the following check boxes to be printed in the header:

- Page numbers
- Date (current)
- Time
- File name
- Program name
- Comment

The **Comment** text field is active, supposed the Comment check box has been selected.

## 4. Create/Edit a Method Wizard

<b>Adjustment</b> option buttons	Select one of the following options: <ul style="list-style-type: none"> <li>• Left</li> <li>• Centered</li> <li>• Right</li> </ul>
<b>Row number</b> list	<b>Row number</b> is a numeric field, where the row for each option can be adjusted.
<b>Separators</b> check boxes	The separators check boxes define where the bordering lines shall appear. These can be placed below, above, or both below and above the header. <ul style="list-style-type: none"> <li>• <b>Above</b> check box: Separator line appears above the header.</li> <li>• <b>Below</b> check box: Separator line appears below the header.</li> </ul>

### Footer Tab

In the **Footer** tab, the content of the document footer is defined. The **Footer** tab contains the same elements as the **Header** tab. For a description of the footer tab refer to the header tab.

The footer tab will disappear if **Print Footer** is not selected in the **Page setup** tab.

### 4.3.14 Data Handling: Automated Data Handling

After a measurement some actions can be started automatically.

Select these actions and they are executed chronologically in the following order:

- If the **load sample ID list** check box is selected, a sample ID list is automatically loaded.
- If the **save workspace** check box is selected (always selected in **magellan Tracker**), the created workspace is automatically saved.
- If the **export to ASCII file** check box is selected, the data selected for export are automatically exported to an ASCII file.
- If the **export to ASTM file** check box is selected, after running the method, the data selected for export is automatically exported in ASTM format and can be further used in compatible Laboratory Information Systems (LIS).
- If the **export to Sample Tracking** check box is selected, after running the method, the data selected for export is automatically exported to the Sample Tracking system. For more information, please refer to the corresponding manual for Sample Tracking.
- If the **export to Excel** check box is selected, the data selected for export are automatically exported to Excel.
- If the **print** check box is selected, the data selected for the printed report are automatically printed on the default printer.
- If the **view results after measurement** check box is selected, the measurement data and the calculated data are displayed for reviewing.

## More – Load Sample ID List

The **More** (Load Sample ID List) dialog box contains the following elements:

<b>Filename</b> group box	Select the filename of the sample ID list to be loaded: <ul style="list-style-type: none"> <li>• Same filename as workspace option button</li> <li>• <b>Filename</b> option button: Enter a filename in the text field.</li> </ul>
<b>Path</b> group box	Select the path where the sample ID list is stored: <ul style="list-style-type: none"> <li>• Sample ID list default path option button</li> <li>• <b>Use path</b> option button: Select any path.</li> </ul>
<b>Format</b> group box	Select the format of the sample ID list to be loaded (see chapter 5.2.3 Import a Sample ID List for details): <ul style="list-style-type: none"> <li>• Autodetect from the list of supported formats option button</li> <li>• <b>Custom file format</b> option button: Click the <b>File format...</b> button to open the <b>Custom Format</b> dialog box.</li> </ul>



### Note

*If an only partly filled sample ID list is loaded automatically, all unused samples are automatically deleted from the layout.  
If a final control (e.g. in well H12) has been defined within the layout, this control is automatically moved to the well after the last used sample well.*



### Note

*Automatically loaded sample ID lists should contain only IDs for samples and must not contain IDs for non-samples (controls, standards etc.).*

## 4. Create/Edit a Method Wizard

### More – Workspace Name

Selecting **Save workspace – More** the **Workspace Name** dialog box with the following elements appears:

<b>Format</b> group box	<p>One of the offered option buttons has to be selected for defining the default workspace name. The name can consist of the date, counter or a certain set of letters. Another possibility is to combine the date with a choice of letters. Counters used together with the date are reset daily otherwise the counter is incremented with each measurement:</p> <ul style="list-style-type: none"> <li>• Date (DDMMYYYY) + Counter option button</li> <li>• Date (YYYYMMDD) + Counter option button</li> <li>• <b>Total Counter</b> option button</li> <li>• Use available barcode option button</li> </ul>
<b>Prefix</b> text field	The entered text is added at the beginning of the workspace name as defined above.
<b>Example</b> text field	The <b>Example</b> text field shows an example of the current selection.
<b>Set as default</b> button	The settings can be logged as a default for future use.
<b>Restore default</b> button	The settings can be reset to the previously defined default.

## More – Export to LIS

The More (Export to LIS) dialog box contains the following elements:

<b>ASTM delimiter definition</b> group box	<p>Define the ASTM delimiters :</p> <ul style="list-style-type: none"> <li>• <b>Field delimiter:</b> Enter a sign for separating fields (  by default)</li> <li>• <b>Repeat delimiter:</b> Enter a sign for repeat (\ by default)</li> <li>• <b>Component delimiter:</b> Enter a sign for separating components (^ by default).</li> <li>• <b>Escape character:</b> Enter a sign for escape (&amp; by default).</li> </ul>
<b>Sender ID</b> group box	<ul style="list-style-type: none"> <li>• Define the Sender ID settings that are to be displayed in the header of an ASTM file:</li> <li>• <b>Sender ID</b> text field: Empty by default. If defined, e.g. SUNRISE, the name is displayed in the header of the ASTM file (e.g. H ^&amp;  SUNRISE^Magellan V7.2^Tracker).</li> <li>• <b>Append app. name:</b> If selected, application name, i.e. <b>magellan</b>, is exported in the header of the ASTM file (e.g. Magellan V7.2^Tracker).</li> <li>• <b>Append app. version:</b> If selected, the <b>magellan</b> version number is exported in the header of the ASTM file (e.g. <b>Standard</b> or <b>Tracker</b>).</li> </ul>
<b>LIS assay name</b> group box	<ul style="list-style-type: none"> <li>• Select the LIS assay name to be displayed in the test order record and result record of the ASTM file:</li> <li>• <b>Use method name:</b> name of the method used for the measurement.</li> <li>• <b>Use name</b> text field: define a new name to be displayed.</li> <li>• <b>Example:</b> ASTM_Test</li> <li>• Test order record: O 1 SampleID  ^^method name  Date and time of measurement</li> <li>• Result record: R 1 ^ method name^results</li> </ul>
<b>Encoding</b> group box	<ul style="list-style-type: none"> <li>• Select the export code:</li> <li>• <b>ANSI:</b> For ANSI compatible characters.</li> <li>• <b>Unicode:</b> For characters that cannot be exported with ANSI code (e.g. Chinese, Cyrillic).</li> </ul>
<b>Path</b> group box	<ul style="list-style-type: none"> <li>• Define the path for the ASTM export:</li> <li>• <b>Export default path:</b> the export is performed to the folder defined in <b>Miscellaneous</b>.</li> <li>• <b>Use path</b> text field: define a new export path.</li> </ul>
<b>Set as default</b> button	<ul style="list-style-type: none"> <li>• Using this option, the settings can be logged as a default for future use.</li> </ul>
<b>Restore default</b> button	<ul style="list-style-type: none"> <li>• Using this option, the settings can be reset to the previously defined default.</li> </ul>

#### 4. Create/Edit a Method Wizard

##### ASTM Export – Example File

Each ASTM export file (.txt) consists out of the following components:

- **Message Header Record:**  
H|\^&|||SUNRISE^Magellan V7.2^Tracker
- **Patient Information Record (P):**  
P|1||Sample ID 1 for patient 1
- **Test Order Record (O):**  
O|1|SampleID||^method name||Date and time of measurement
- **Result Record (R):**  
R|1|^method name^results
- **Message Terminator Record:**  
L|1|N

##### Example:

ASTM Export Settings:

The corresponding ASTM file:

```
H|\^&|||SUNRISE^Magellan V7.2^Tracker
P|1||sample1
O|1|sample1||^ASTM_Test||20180315091504
R|1|^ASTM_Test^Raw data^A1|0.101~|OD|
P|2||sample2
O|1|sample2||^ASTM_Test||20180315091504
R|1|^ASTM_Test^Raw data^B1|0.201~|OD|
P|3||sample3
O|1|sample3||^ASTM_Test||20180315091504
R|1|^ASTM_Test^Raw data^C1|0.301~|OD|
```



## More – View Results

The More (View Results) dialog box contains the following elements:

<b>Plate view</b> group box	<p>Select the data to be displayed in the plate view:</p> <ul style="list-style-type: none"> <li>• <b>1st line in well (fixed)</b> drop down list: Select a name from the available data names.</li> <li>• <b>2nd line in well (fixed)</b> drop down list: Select a name from the available data names.</li> <li>• <b>3rd line in well (first selection)</b> drop down list: Select a name from the available data names. In contrast to the first two lines this selection is only applied for the first time. Whenever another data to be viewed in the plate view is selected in the control bar, this data is displayed in the 3<sup>rd</sup> line. The first two lines remain unchanged.</li> </ul> <p>The 1<sup>st</sup> and 2<sup>nd</sup> line can be omitted by selecting <b>not used</b>, which makes the plate view more easily readable.</p>
<b>Text box</b> group box	<p>Select a name from the available data names. This selection is only applied for the first time. Whenever another data to be viewed in the textbox is selected in the control bar, this data is displayed in the text box.</p>

### 4.3.15 Miscellaneous: User Prompts

In the control bar expand **Miscellaneous** and select **User prompts**.

In every **Prompt** field of the list, a keyword can be entered. This keyword will then be displayed before measuring. Text can be entered, for example: lot number or the analyst's full name.

By selecting **Req.** (required), a measurement can only be launched on receipt of an input (a text information must be added in the **Prompt answer** field).

Prompts will also appear in the list of available data for printing.

### 4.3.16 Miscellaneous: Number Format

In the control bar expand **Miscellaneous** and select **Number format**.

The **Number format** dialog box is used to set up the numeric format of the display of values. Additionally, the scientific number format for values out of range can be selected.

The default setting is 5 significant digits. Selecting **User defined**, a number format of 1 - 10 integer places and 0 - 7 decimal places can be set.

If the user defined number format is selected, the two numeric data fields must be set.

Additionally, the scientific (with exponent) or the non-scientific description can be used. An example of the format of current selection is displayed.

Click **Set as default** or **Restore default** accordingly to save the entered definition.

### 4.3.17 Miscellaneous: Method Notes

In the control bar, expand **Miscellaneous** and select **Method notes**.

The **Method notes** field allows the user to add some comments to the file name, which will be displayed on the method printout.

Simple formatting like bold, italic, underlined and colored text is possible. Formatting may be omitted during printout.

## 4. Create/Edit a Method Wizard

### 4.4 Saving the Method

Click Finish save the method via the Save as window, which contains the following elements:

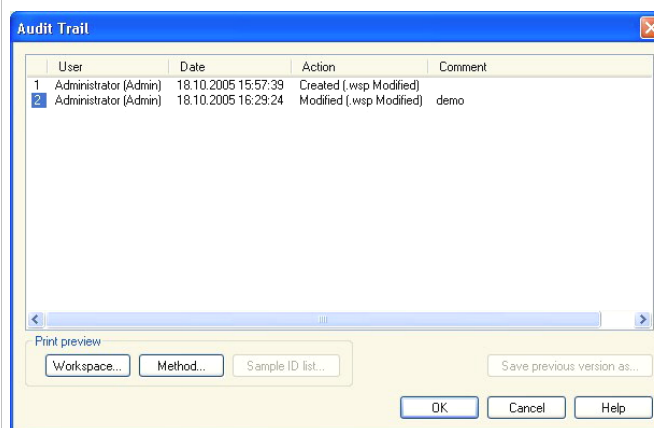
<b>Filename</b> field	Enter or modify the method's file name.
<b>File remarks</b> field	Add some comments to the file name, which will be displayed for example in the <b>Open file</b> dialog boxes.
<b>Audit trail comment</b> field	Add some comment, which will be stored in the audit trail (only available for <b>magellan</b> Tracker).
<b>Organize favorites...</b> button	Click this button to open the <b>Organize favorites</b> dialog box. See 6.4 Start Favorite for further information.
<b>Run this method now</b> check box	Select this check box to start the method immediately after finishing this wizard.

The modified document can be saved under its current file name or under a different name.

Click **Save&Finish** to save the method and close the **Create/Edit a Method** wizard.

Additional buttons in **magellan** Tracker:

<b>Audit trail...</b> button	<p>Click this button to open the <b>Audit trail</b> dialog box where the user, the date, the executed action, and a comment are displayed.</p> <p>A print preview of the workspace, the method, and the sample ID list of the current and all previous versions can be displayed clicking the appropriate buttons.</p> <p>Additionally, it is possible to save a previous version of the method under another name.</p>
------------------------------	---



<b>Signature...</b> button	<p>Click this button to open the <b>Signature</b> dialog box, where user, date, action, and comment are displayed.</p> <p>This button is only available when the file has been signed using the <b>Attach Signature</b> wizard. See chapter 8 Attach Signature Wizard for further details.</p>
<b>Method password</b> field	When entering a password for a method, this method will be password protected and cannot be modified until the correct password is entered. See detailed description below.

#### 4.4.1 Password Protection of Methods

##### Protect Method with a Password

Users who have the right to create and to edit methods can protect methods by assigning them a password.

Per default, **Administrators** and **Application Specialists** possess the required rights.

When a new method is created, the password protection can be set in the **Save as tab** of the **Create/edit a method wizard**. Enter the name of the method, type the password in the **Method password edit field** (right bottom corner of the dialog) and click **Finish**.

Confirm the password in the displayed **Method password dialog box** and click **OK**. The method is saved with the password protection.

Already saved, but not password protected methods can be protected by opening the method and setting the password in the **Save as tab** as described above.

##### Edit Password Protected Methods

For opening a password protected method enter the correct method password. The method is opened in **Edit mode**. It is possible to edit and save the method.

If **Read only** is selected, the method is opened in read only mode. It is still possible to edit the method, but it is not possible to save the changes.

##### Change the Password of a Password Protected Method

To change the password of a password protected method, open the method in **Edit mode** (password entry required) and enter a new password in the **Method password edit field** of the **Save as tab**. Click **Finish**.

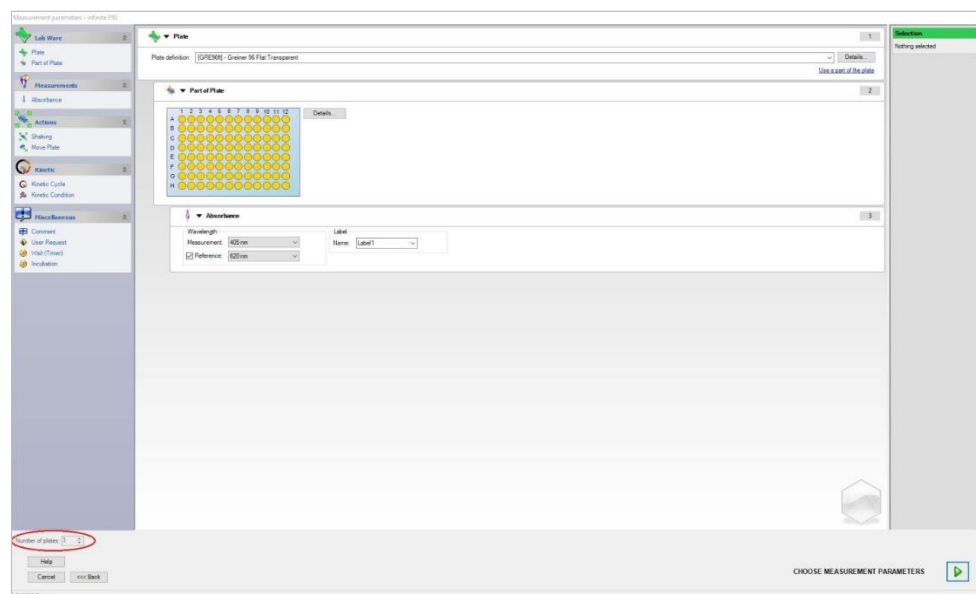
Confirm the password in the successive **Method password dialog box** and click **OK**.

## 4. Create/Edit a Method Wizard

### 4.5 Multiplate Methods

When connected to an INFINITE F50 instrument multiplate methods can be defined.

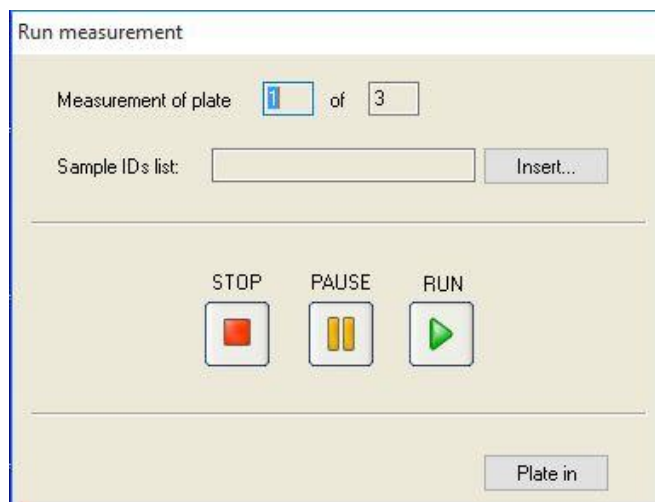
The number of plates to be measured can be set in the measurement parameters editor, during method definition.



When two or more plates are to be measured, a counter for switching between the plates is available in the **Define Evaluation** window as well.



All further parameters can be defined as is done for single plate methods. At starting a multiple plate method, the following dialog box appears:



<b>Sample IDs list</b>	For each single plate a sample ID list can be selected.
<b>STOP button</b>	Measurement is stopped. The data of the already measured plates are displayed in the created workspace and it is not possible to add measurements of additional plates.
<b>PAUSE button</b>	Measurement is paused. The data of the already measured plates are displayed in the created workspace, but it is possible to add measurements of additional plates.
<b>RUN button</b>	Measurement of the next plate is started.
<b>Plate in/ Plate out</b>	The plate is moved into or out of the instrument.

Running a multiplate method allows to pause the measurement between two plates, saving the achieved results, and continuing the measurement for the remaining plates at a later date. If **Automatic save workspace** is selected, the workspace is stored after each single measurement.



## 5. Create/Edit a Sample ID List Wizard

### 5.1 Introduction

The **Create/edit a sample ID list** wizard is used to create new sample lists or to edit existing sample lists.

#### Workflow Summary

Start the **Create/edit a sample ID list** wizard. After a welcome page, the **File selection** page appears. Select one of the options: **Create new** sample ID list or **Edit** an existing sample ID list and save the ID list using the **Save as** page.

### 5.2 Create/Edit a Sample ID List

The **File Selection** window contains the following elements:

a) <b>Create new</b> option button	A new sample ID list can be created.
b) <b>Edit</b> option button	An existing sample ID list can be modified.
<b>Show</b> combo box	The files are displayed according to the chosen selection: <ul style="list-style-type: none"> <li>• All files</li> </ul> My files: This option is available if the user administration is enabled (always enabled in <b>magellan Tracker</b> )
<b>Filename</b> list	The sample ID list to be edited must be selected. A <b>Remarks</b> field next to every file name contains - if entered - a short description of the sample ID list. All sample ID lists available in the standard sample ID list directory, which fulfill the filter criteria selected in the show combo box, will be displayed.
<b>Print Preview...</b> button	A preview of the selected sample ID list is displayed, and a printout can be started.

#### 5.2.1 Create New Sample ID List

In the **Select Plate Type** window the number of sample IDs per well and the used plate type can be selected. The **Import from external sample ID list** option allows to browse for different types of sample ID files and to import them into **magellan**.



#### Note

***Some sample ID lists may contain additional information such as concentrations and dilutions which may affect evaluation of the measurement data.***

## 5. Create/Edit a Sample ID List Wizard

The **Select plate type** dialog box contains the following elements:

Settings	
<b>Sample IDs per well</b> option buttons	Enter the number of sample IDs required per well (a maximum of three can be entered).
<b>Printout</b> option buttons	Define the layout for printing the sample ID list.
<b>Plate type</b> option buttons	<p>Four option buttons define the plate type to be selected:</p> <ul style="list-style-type: none"> <li> <b>Plate type from method</b>  Select a method to load the plate layout. Click <b>Load</b> to browse for existing method files. The Windows™ <b>Open</b> dialog box appears. Select the desired file and click <b>Open</b>. </li> <li> <b>Standard plate type</b>  Standard geometry plate types can be selected to define the plate format. When activated, a standard geometry plate type can be chosen from an associated drop-down list. </li> <li> <b>Plate type from pdf-file</b>  A predefined pdf file (SUNRISE instruments) or a pdfx file (INFINITE F50 instruments) can be used to define the plate format. </li> <li> <b>Import from external Sample ID list</b>  An external file type can be selected for import as sample ID list. See chapter 5.2.3 Import a Sample ID List. </li> </ul>

The **Enter sample IDs** button is only enabled if the required settings have been defined (method has been loaded, standard plate type or pdf-file has been selected).



### 5.2.2 Import/Edit a Sample ID List

After the selection of the plate type, the **Import/edit a sample ID list** plate window is displayed:

- Toolbar with Settings, Edit, Autofill, Delete, Undo/Redo, Print format, Print preview and Zooming buttons
- Plate view with a schematically layout of a microplate.
- Sample ID list (when **Plate type from method** has been selected)
- Dialog to insert sample IDs (when **Standard plate type** has been selected)

If a new sample ID list is to be created no sample IDs are assigned to the wells. A well can be selected by clicking in the well.

All required sample IDs have to be entered either manually or using the buttons in the tool bar or can be read by the handheld barcode scanner for sample IDs. The sample IDs can be defined and edited in the defined microplate type. Up to three sample IDs can be entered in each well. Sample IDs can be moved or copied.

When a method has been selected, on the left side a **List of all Samples from the plate layout** is displayed. Only samples without replicates are shown in the list. The sample IDs can be entered either in the list or on the plate. All changes are shown immediately.

#### Toolbar Buttons

<b>Settings... button</b>	The button opens the <b>Sample ID List Settings</b> dialog box, where the number of sample IDs per well can be selected.
<b>Edit... button</b>	The <b>Edit</b> button opens the <b>Edit Well</b> dialog box. The sample IDs of the marked well can be edited. See below for further information.
<b>Autofill... button</b>	The whole plate or a part of the plate can be selected to be automatically filled with sample IDs. After selecting the corresponding wells, click <b>Autofill</b> to open the <b>Autofill Selection</b> dialog box. See below for further information.
<b>Delete button</b>	The whole plate or part of the plate can be selected. This function deletes the sample IDs of the selected wells immediately. No dialog box asks for confirmation. Click <b>Delete</b> or press the <b>DEL</b> key to delete the sample IDs in the selected wells.
<b>Undo button</b>	Performs an undo of the last action. Click <b>Undo</b> or press <b>CTRL-Z</b> to undo a previous action.
<b>Redo button</b>	Repeats the action, which was performed before the undo step. Click <b>Redo</b> or press <b>CTRL+Y</b> to redo an action that was undone.
<b>Print format</b>	Select the layout for printing the sample ID list: <ul style="list-style-type: none"> <li>• horiz. Table</li> <li>• vert. Table</li> <li>• Matrix</li> </ul>
<b>Print preview</b>	Opens the print preview of the printed sample ID list.

## 5. Create/Edit a Sample ID List Wizard

<b>10% button</b>	This will set the plate layout view to 10%.
<b>100% button</b>	This will set the plate layout view to 100%.
<b>Zoom check box</b>	In case the well plate consists of a large number of wells, the individual well assignments cannot be displayed in the 100% zoom mode. In such a case the <b>Zoom mode</b> button allows a zoom into the marked area. If activated, the user can select an area to zoom in by clicking and dragging a frame over the desired layout area. Click the right mouse button to zoom out to 100% display.

### Context-Sensitive Menu of the Plate Layout

By right-clicking on a well on the plate layout, a context-sensitive menu for the marked wells is displayed. The following commands are available:

Menu	Description
Summary...	The <b>Summary</b> dialog box is displayed. See below for further information.
Cut	The sample IDs of the marked wells are deleted from the wells and copied to the clipboard.
Copy	The sample IDs of the marked wells are copied to the clipboard.
Paste	The sample IDs copied to the clipboard are pasted into the marked wells.
Delete	Click <b>Delete</b> or press <b>DEL</b> to delete the sample IDs of the marked wells.
Copy in ASCII-Format	The sample IDs of the marked wells are copied to the clipboard in ASCII file format. This way, they can easily be pasted into other applications (e.g. Excel, Notepad).
Paste in ASCII-Format	Sample IDs can be pasted from the clipboard in ASCII file format from other applications. See below for further information.
Edit...	The <b>Edit</b> option opens the <b>Edit Well</b> dialog box. The sample ID of the marked well can be edited. See below for further information.
Autofill Selection...	The whole plate or a part of the plate can be selected to be automatically filled with sample IDs. After selecting the corresponding wells, selecting the <b>Autofill</b> option displays the <b>Autofill Selection</b> dialog box. See below for further information.



#### Note

**When editing a Sample ID list it is possible to use Drag&Drop.  
Use the left mouse button to select and drag items.**

## Edit well...

The **Edit Well** dialog box can be accessed via the context-sensitive menu or the tool bar button.

Sample IDs for all wells on a microplate can be defined. A maximum of three sample IDs per well is possible.

The desired sample IDs for the marked well have to be entered in the **Edit Well** dialog box. This has to be repeated for every well that shall be filled with sample IDs. The navigation functions of the **Edit Well** dialog box can be used for comfortable working. Click **OK** to close the dialog box and the sample IDs for the latest marked well are saved.

The **Edit Well** dialog box contains the following elements:

<b>Left, Right, Up and Down</b> buttons	The direction buttons can be used to select another well on the plate while leaving the dialog box open and saving the changes of the current well.  The <b>Arrow keys</b> can also be used for this kind of navigation.
<b>On Enter move in vertical direction</b> check box	On clicking <b>Enter</b> or <b>Tab</b> , the entry field is moved to the next well. Use the check box to specify the direction of movement, vertically or horizontally across the plate.
<b>Edit sample IDs</b> text fields	In each well up to 3 sample IDs can be entered. Therefore, the list contains three <b>Sample ID</b> text fields and an <b>Autoincrement</b> check box associated to each of them.  A sample ID for the marked well can be entered in the text fields. The sample ID can contain letters, numbers or a combination of both. For example: Smp 1. Up to 100 alphanumeric characters can be entered. The entire plate can be filled with sample IDs.
<b>Autoincrement</b> check box	The <b>Autoincrement</b> check box can be selected, if the wells for the sample IDs are to be automatically numbered. For example: if the starter value is Smp1 then the next well is automatically named Smp2, using the <b>Enter / Tab</b> key or the arrow buttons.  Using <b>Autoincrement</b> , the sample IDs can be allocated to the wells in a numerically consecutive manner. Simply enter the initial value into the first well. The entered ID may also be alphanumeric, although it must end in a number to enable for the consecutive numbering of further wells, for example: If John1 is entered into the first well, John2 will automatically be displayed when moving to the second well.

## Autofill Selection

The Autofill Selection dialog box can be accessed via the context-sensitive menu or the tool bar button.

This dialog box allows the user to fill the selected wells with sample IDs automatically.

Select the whole plate or parts of the plate and enter the desired sample IDs and increment settings for the marked wells in the Autofill Selection dialog box. Click **OK** to close the dialog box and to fill the selected wells with the defined sample IDs. In each well up to 3 sample IDs can be entered. Therefore, the list contains three Sample ID text fields and an Autoincrement check box, a Start index text field and a Vertical check box associated to each of them.

## 5. Create/Edit a Sample ID List Wizard

The Autofill Selection dialog box contains the following elements:

<b>Use ID</b> check box	The <b>Use ID</b> check box can only be accessed, if the identical number of sample ID were selected. The checkmark determines if the autoincrement function is applied to the selected sample ID.
<b>Sample ID</b> text fields	Sample IDs for the marked well can be entered in the <b>Sample ID</b> text fields. The sample IDs can contain letters, numbers or a combination of letters and numbers.
<b>Autoincrement</b> check box	The <b>Autoincrement</b> check box must be selected, if the sample IDs for the wells are to be numbered automatically (incremented by 1).
<b>Start index</b> text field	The <b>Start index</b> text field is only editable, if the <b>Autoincrement</b> check box is selected. The starter value for the automated incrementing of the sample ID has to be entered.
<b>Vertical</b> check box	The <b>Vertical</b> check box can only be accessed, if the <b>Autoincrement</b> check box is selected. If this check box is selected, the sample IDs will be entered and numbered in vertical direction. If it is cleared, the sample IDs will be entered and numbered in horizontal direction.

### Well Summary

The **Well Summary** dialog box can be accessed via the context-sensitive menu.

This dialog box delivers an overview of all defined Sample IDs and the Sample ID list related settings of a selected well.

The **Summary** dialog box contains the following elements:

<b>Information tree</b>	The information tree gives an overview of all defined well-based parameters of the selected well. The tree is filled according to the available information. For sample ID lists the sample IDs, the pipetting status, etc. are displayed.
<b>Left, Right, Up and Down buttons</b>	The direction buttons can be used to select another well on the plate while leaving the dialog box open.
<b>Expand All / Shrink All</b>	This button displays the information tree expanded to the highest level or shrunk to the first level.

### Paste in ASCII-Format

The **Paste in ASCII-Format** function can be accessed via the context-sensitive menu.

This function pastes the contents of selected data in ASCII format from the clipboard into **magellan**.

The function allows transferring data from other software applications (for example: Excel, Notepad) into the **magellan** plate layout.

First, the relevant data must be selected in the other software application and copied to the clipboard. The rows must be separated by linefeed, the columns by tab stops. This is automatically done in Excel when selecting multiple cells.

The **Paste in ASCII-Format** function pastes the copied data in ASCII format from the clipboard into the wells. Data is always inserted starting at position A1.

### 5.2.3 Import a Sample ID List

Sample ID lists that have been created using other programs, or sample ID lists that have been defined using other forms of analytical equipment have to be imported into **magellan** before being used.



#### CAUTION

**SOME SAMPLE ID LISTS MAY CONTAIN ADDITIONAL INFORMATION SUCH AS CONCENTRATIONS AND DILUTIONS WHICH MAY AFFECT EVALUATION OF THE MEASUREMENT DATA.**

Click **Import** button in the **Sample ID list settings** dialog box to browse for existing external sample ID files. The Windows™ **Open** dialog box appears.

The window offers a list of **File names** that match the selected **File type**. The **File type** can be chosen from an associated drop-down list.

The following external file types are supported:

- Easy-Files .esy
- Tecan-files .tpl
- DD1-Files .dd1
- Hamilton-Files .pro
- APL-Files .apl
- Gemini-Files .csv
- Custom Format Files .txt

Select the requested file to be imported and click the **Open** button. The Windows™ **Open** dialog box is closed, and the file is loaded.

Confirming the **Sample ID List Setting** dialog box with **Next** will open the **Import/Edit a Sample ID List** plate window with the sample IDs displayed.

The **Import** button can also be accessed via the **Insert Sample ID List** dialog box, which is available in the **Start Measurement** window (**Insert** button) and **Evaluate Results** plate view (**Edit** toolbar menu).



#### CAUTION

**MAKE SURE THAT THE CORRECT ID LIST HAS BEEN SELECTED, OTHERWISE THE RESULTS WILL BE ASSIGNED TO ANOTHER LIST.**



#### Note

*When importing .tpl, .dd1, or custom format sample ID lists, additional information that modifies the evaluation definitions can be included.*



#### Note

*When importing sample ID lists with dilutions, the dilution must not be more than 1:1e+12 (magellan Standard and magellan Tracker).*

## 5. Create/Edit a Sample ID List Wizard

### Easy-Files .esy

These files consist of lines which contain the sample ID and the well name.

Well name:	alpha numeric, max. 3 characters
Sample-ID:	alpha numeric, max. 20 characters

The lines are separated by CR + LF.

#### Example

```
C01
B01
A01 0001
H02 0002
G02 0003
F02 0004
E02 0005
```

#### Interpretation

When **magellan** is processing an .esy-file

- Number of sample IDs is set to 1
- Sample ID is set as sample-ID in well

### Tecan-files .tpl

These files (<PLATEID>.TPL) consist of lines, which contain parameters separated by semicolons. The format is:

H;date;time

D;testno;sample-ID + control-name;position;pre-dilution;errors

L;

The file starts with an H and ends with an L. The fields are defined as follows:

date;time;testno;sample-ID	the same as in the job list (BES3)
control name	alpha numerical, max 8 characters Note! This entry contains sample-ID or the name of a control
position	alpha numerical, max. 3 characters
pre-dilution	numerical, max. 8 characters plus 1 decimal (separated by a '.')

errors	<p>alpha numerical, max. 3 characters. If an error occurred during pipetting one of the following characters is displayed here:</p> <p>First character</p> <p>&lt;Space&gt; no liquid error</p> <p>L: no or not enough liquid</p> <p>Second character</p> <p>&lt;Space&gt; no barcode error</p> <p>M: manually entered barcode</p> <p>Third character</p> <p>&lt;Space&gt; no timer overrun</p> <p>O: timer overrun</p>
--------	---

The lines are separated by CR + LF.

### Example

```
H;29-02-94;12:47:11
D;1;NEG;A1;1.0;
D;1;POS;B1;1.0;
D;1;0001;C1;1.0
L;
```

### Interpretation

When **magellan** is processing a .tpl-file

- Number of sample IDs is set to 1
- Sample ID or control name is set as sample ID in well position
- Error flags are stored for every well
- Pre-dilution is used as the dilution of the well position

## DD1-Files .dd1

These files consist of lines, which contain parameters of a fixed length.

The format is:

First line: Date (DD-MM-YY)

Second line: Time (HH:MM:SS)

Field	Pos	Length	Format / Description
TestNr	1-3	3	number (001-049)
TestName	4-23	20	Alphanumeric
SampleID	24-35	12	Alphanumeric
ControlName	36-43	8	Alphanumeric
PlateID	44-51	8	Alphanumeric
PlatePos	52-55	4	Alphanumeric
Errors	56-61	6	Alphanumeric

The lines are separated by CR + LF.

## 5. Create/Edit a Sample ID List Wizard

### Example

13-04-1999

11:01:32

953test1 KBR		KBR3	H1
953test1 KBR		KBR3	G1
953test1 KBR		KBR3	C1
953test1 KBR		KBR3	B1
953test1 KBR		KBR3	A1
953test1 KBR	0001	KBR3	H2
953test1 KBR	0001	KBR3	G2
953test1 KBR	0001	KBR3	F2
953test1 KBR	0001	KBR3	E2
953test1 KBR	0001	KBR3	D2

### Interpretation

When **magellan** is processing a .dd1-file

- Number of sample IDs is set to 1
- <Testname> specifies the **magellan** method name at the well
- <PlatePos> specifies the well
- <SampleID> or <ControlName> specifies the **magellan** sample ID
- <Errors> specifies the pipetting flag: L: Liquid error, C: Clot error, E: manually entered

When a .dd1-file is read the current layout will be modified using the layout defined in the different methods where the names are specified in the .dd1-file.



## Hamilton-Files .pro

These files consist of lines that contain the sample-ID and the well name.

A header information is available, too.

Well name: alpha numeric, max. 3 characters

Sample-ID: alpha numeric, max. 20 characters

The lines are separated by CR + LF.

### Example

14ESP-AK-Bommeli	-> Header
08403009070	-> Header
SendInfoHost=00	-> Header
SendInfoPrnt=00	-> Header
SendInfoDisk=00	-> Header

A01091111111110

A02090325228840

A03090325228930

A04090325235730

A05090336975200

### Interpretation

When **magellan** is processing a .pro-file

- Number of sample IDs is set to 1
- Sample ID is set as sample ID in well
- Header information is ignored

## APL-Files .apl

Description of .apl-files created by MiniSwift 1.3 or later or Minilyser 5.30 or later.  
The file format is defined as follows:

Field	Pos	Length	Format / Description
PlateID	1-8	8	Alphanumeric
PlatePos	9-12	4	Alphanumeric
TestNumber	13-15	3	Number
TestName	16-27	12	Alphanumeric
SampleID	28-39	12	Alphanumeric
ControlName	40-47	8	Alphanumeric
Result_1	48-55	8	Alphanumeric
Result_2	56-63	8	Alphanumeric
Errors	64-69	6	Alphanumeric
Date	70-79	10	Alphanumeric
Time	80-87	8	Alphanumeric
CutOff	88-95	8	Alphanumeric

The lines are separated by CR + LF.

## 5. Create/Edit a Sample ID List Wizard

### Example

990520S1A1	2	test1_2	BLANK		05-20-199919:12:53
990520S1B1	2	test1_2	BLANK		05-20-199919:12:53
990520S1C1	2	test1_2	NC1	LR	05-20-199919:12:53
990520S1D1	2	test1_2	PC1		05-20-199919:12:53
990520S1E1	2	test1_2	00000000010		05-20-199919:12:53
990520S1F1	2	test1_2	00000000010	V	05-20-199919:12:53

### Interpretation

When **magellan** is processing an .apl-file

- Number of sample IDs is set to 3
- <Testname> specifies the **magellan** method name at the well
- <PlatePos> specifies the well
- <SampleID> specifies the **magellan** Sample ID 1
- <ControlName> specifies the **magellan** Sample ID 2
- <Errors> specifies the **magellan** Sample ID 3
- <Errors> specifies the pipetting flag: pipetting errors L, B, N at position 1 are uncritical for samples but critical for controls, verification read and barcode errors are uncritical, too.

## Gemini-Files .csv

Description of .csv-files created by Gemini 3.40 and 3.60. The following is an example of an output file in Excel format:

Position	Tube ID	ScanError	SRCRack	SRCPos	SRCTubeID	Volume
Error	SRCRackID	GridPos	SiteOnGrid	TipNumber	DetectVol	Time
	Version 2.00	3091	Microplate	12	8	
0	9900001	18	1			3.8.1998
1		0	Tube 13*85mm	1	0001	10
0	013_000064	1	1	1		11:55:42
3		0	Tube 13*85mm	2	0002	20
0	013_000064	1	1	2		11:55:42
5		0	Tube 13*85mm	3	0003	30
0	013_000064	1	1	3		11:55:42
7		0	Tube 13*85mm	4	0004	40
0	013_000064	1	1	4		11:55:42

The file format is defined as follows:

The first line contains the column headers, which are the same for all formats, except for some which support only upper-case characters. The second line shows information about the rack / stripack, for which that file was created. Only the column Tube ID, SRCRack, SRCPos, SRCTubeID, Error, SRCRackID, GridPos, SiteOnGrid and Time are valid.

With Gemini 3.60 the SRCPos contains the number of x wells, the SRCTubeID contains the number of y wells, and the Volume contains the line to read.

The third and following lines are entries for the used wells of a rack / used tubes of a stripack.

The columns contain the following information (Column\Range\Explanation):

- Position\1 .. number of wells\Position of the well in the rack. The numbering sequence is rear to front and then left to right. (1 = A1, 2 = B1, ...) If the microplate has been pipetted in portrait mode (e.g., dimensions 8x12, iso. 12x8), the numbering sequence is left to right and then front to rear. (1 = H1, 2 = H2, ...)
- TubeID\Max. 32 characters\This column is only filled for stripacks and when the tube barcodes were scanned with a POSID command. In row 2 this column shows the version of Gemini.
- ScanError\0 .. 4294967295\This column contains possible scanning errors. Please note the table with the error codes below. In row 2 this column shows the serial number of Genesis.
- SRCRack\Max. 32 characters\Here Gemini reports for dispense commands the configuration name of the source rack. In row 2 this column shows the configuration name of the rack, for which the output file was written.
- SRCPos\1 .. number of wells\This column states for dispense commands the position in the source rack, where the liquid came from.
- SRCTubeID\Max. 32 characters\If the source for a dispense command was a stripack, Gemini reports here the barcode of the source tube.
- Volume\ -7158278 .. +7158278\This column contains the volume in µl, which was dispensed (positive value) or aspirated (negative value).
- Error\0 .. 4294967295\This column contains possible pipetting errors. Please note the table with the error codes below. In row 2 this column shows the scanning errors.
- SRCRackID\max. 32 characters\For dispense commands this is the source rack barcode. In row 2 this column shows the barcode of the rack, for which the output file was written.
- GridPos\1 .. 67 This is the grid position of the source rack for dispense commands.
- SiteOnGrid\1 .. 128\Here Gemini shows the y-position (site on the carrier) of the source rack for dispense commands.
- TipNumber\1 .. 8\Here Gemini reports the tip number, which was used for pipetting into / from this well.
- DetectVol\0 .. +7158278\If liquid detection was used, the detected volume in the well before the aspirate / dispense command is listed here.
- Time\...\This is the time (format hh:mm:ss) when the well was used.

The lines are separated by CR + LF. The columns are separated by either commas or semicolons. The columns separator is detected from the first header line.

### Interpretation

The number of lines separated by newline is counted. This number reduced by 2 is used to define the plate format, which can be 8x12, 16x24, 24x36, 32x48 (rows x columns).

## 5. Create/Edit a Sample ID List Wizard

With Gemini 3.60 the format information is extracted from the second line, SRCPos and SRCTubeID. Multiple lines per well are possible. The number in the second line, Volume, defines the line to use. If the indicated line does not exist, the sample ID list cannot be read. If any line contains an error number greater than zero, depending on the error number either a critical or an uncritical error is set.

- Position: Well position (e.g. 1 = A1, 2 = B1, ...)
- Tube ID: ignored
- Scan error: if the error number is greater than zero a critical error is set
- SRCRack: sample ID 2
- SRCPos: if SRCTubeID is empty, used as sample ID 1 (SRCRackID + "\_" + SRCPos)
- SRCTubeID: if not empty used as sample ID 1
- Volume: ignored
- Error: sample ID 3, if the error number is greater than zero a critical error is set
- SRCRackID: if SRCTubeID is empty, used as sample ID 1 (SRCRackID + "\_" + SRCPos)
- GridPos: ignored
- TipNumber: ignored
- DetectVol: ignored
- Time: ignored

### Custom Format Files \*.\*

When importing custom format files, the **Custom Format** dialog box is displayed. The **Custom Format** dialog box contains the following elements:

<b>Plate type</b> group box	In the plate type group box the plate format can be specified. If the format is already specified, the edit fields are disabled.
<b>Rows</b>	Enter the number of rows.
<b>Columns</b>	Enter the number of columns.
<b>File format</b> group box	In the File format group box the format of the specified file can be defined.
<b>File extension</b>	In the <b>File extension</b> field the file extension is displayed and the field is disabled.



#### Note

**Using this feature in the Create/Edit a method wizard, the file extension field is enabled, and the file extension has to be specified.**

<b>Column separator</b> combo box	Select the column separator used in the file. The row separator must be CR+LF.
<b>Start with line</b>	Enter a number greater than 1 if header lines shall be ignored.

### Example

Assume following settings:

Plate type

- 2 rows
- 3 columns

Format

- column separator = Tabulator
- start with line = 2
- column 1 = Plate position (A1, A2, ...)
- column 2 = Sample ID 1
- column 3 = pipetting status

### Example:

**Tecan custom file**		
A1	BLANK	0
A2	NC	0
A3	SM001	0
B1	SM002	3
B2	SM003	0
B3	SM004	0

## 5.2.4 Saving the Sample ID List

Click **Next** in the **Import/Edit a Sample ID List** window and the **Save as** window appears, in which the created or modified sample ID list can be saved:

<b>Filename</b> field	This field is intended for entering or modifying the file name of the sample ID list (.smp).
<b>File remarks</b> field	The <b>File remarks</b> field allows adding some comments to the file, which will be displayed for example in the <b>Open File</b> dialog boxes.
<b>Audit trail</b> comment field	The <b>Audit trail comment</b> field allows adding some comments, which will be stored in the audit trail (only available for <b>magellan</b> Tracker).
<b>Audit trail...</b> button	Displays the audit trail of the sample ID list (only available in <b>magellan</b> Tracker). See 4.4 Saving the Method - Audit trail for further information.


The Save&Finish button is only enabled when a document has been modified. The modified document can be saved under its current file name or under a different name.

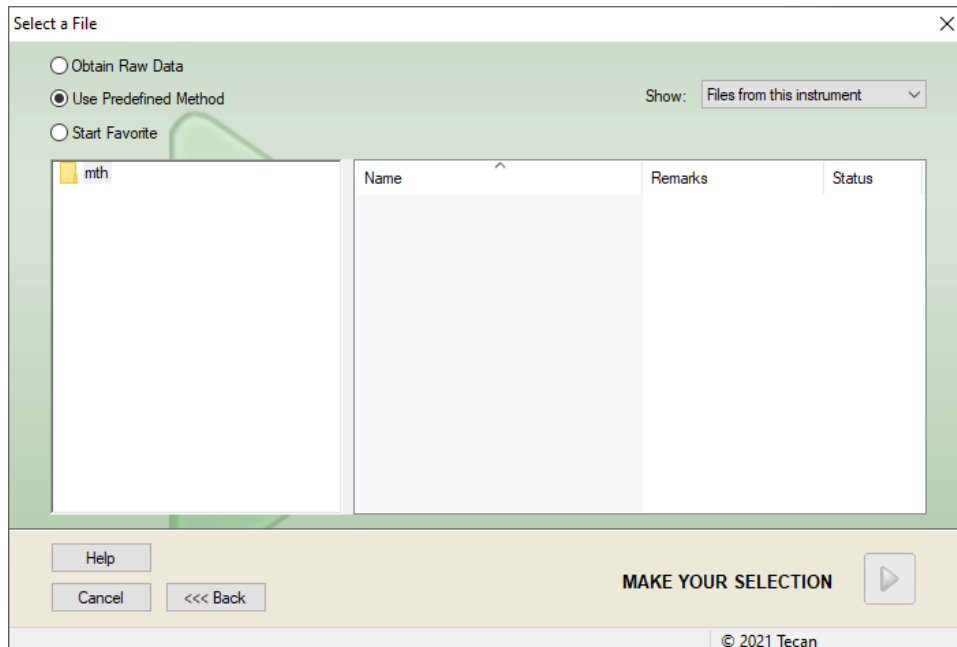
Click Save&Finish to save the sample ID list and close the Create/Edit a Sample ID List wizard.



## 6. Start Measurement Wizard

### 6.1 Introduction

In the **Wizard List** window, click **Start Measurement** to open the wizard. Click **Continue**  on the welcome page and the **Select a file** dialog box appears:



<b>Obtain Raw Data</b>	Is used to generate raw data quickly by setting the required measurement parameters.
<b>Use Predefined Method</b>	Is used to perform measurements based on already defined methods.
<b>Start Favorite</b>	Is used to select one of the most frequently used methods from the list of numbered icons.

## 6. Start Measurement Wizard

### 6.2 Obtain Raw Data

#### 6.2.1 Obtain Raw Data with the *SUNRISE* Instrument

Select **Obtain Raw Data** and click **Next** to open the **Measurement Parameter** dialog box.

In the **Measurement Parameter** dialog box, the following options are available:

<b>Endpoint measurement</b>	Use this button to perform a single measurement.
<b>Kinetic measurement</b>	For multiple measurements within a specified time interval this type of measurement is used.
<b>Measurement parameters...</b>	Click this button to define the parameters in the <b>Measurement Parameters</b> dialog box.

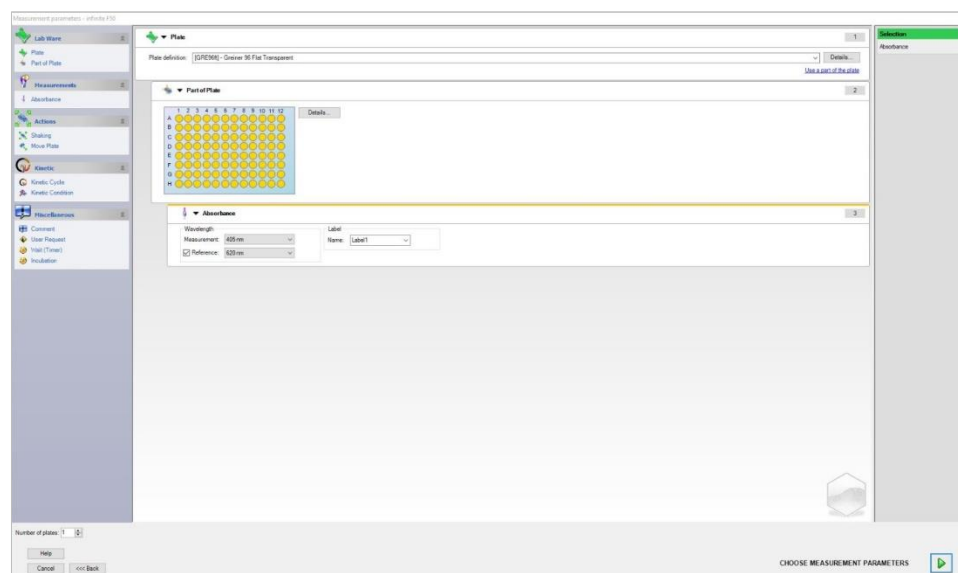


#### WARNING

**IT IS STRONGLY RECOMMENDED TO CHECK ALL OF THE MEASUREMENT PARAMETERS (EVEN PARAMETERS NOT USED IN THE CURRENT MEASUREMENT), BECAUSE PARAMETERS FROM THE PREVIOUS MEASUREMENT METHOD WILL STILL BE SET.**

#### 6.2.2 Obtain Raw Data with the *INFINITE F50* Instrument

When an INFINITE F50 instrument is connected the following window appears after selecting **Obtain Raw Data**:



Define the measurement parameters following the list on the left side.

Click **Choose Measurement Parameters**  to finish the definition. Refer to the **i-control** instructions for use for further information.



### 6.3 Use Predefined Method

Click **Use Predefined Method** and select a method from the **Filename** list.

The available methods are displayed according to the selection of the **Show** drop down list, i.e. **All files**, **Files from this instrument**, **My files**, **Signed files** or **Last selected methods**.

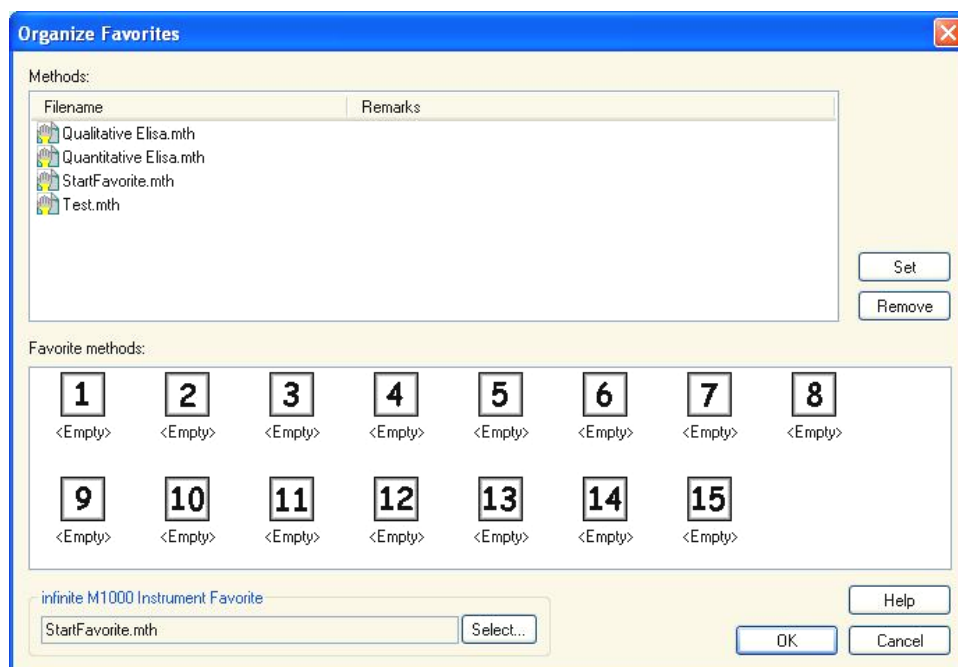
### 6.4 Start Favorite

Click **Start Favorites** to select a method, previously defined as so called favorite, frequently used method, from the list of numbered icons.

Click **Organize favorites** to add to or remove methods from the favorites list.

#### Organize Favorites

Method files can be dragged from the **Method** list onto one of the 15 icons in the **Favorite** list to save it as a favorite.



The **Organize Favorites** dialog box contains the following elements:

<b>Methods</b> list	Lists all available methods. The filename and corresponding remarks - if entered - are displayed.
<b>Set</b> button	After selecting a method from the <b>Methods Filename</b> list and selecting a method icon, click <b>Set</b> to add the selected method to the <b>Favorites</b> .
<b>Remove</b> button	Select a method icon and click <b>Remove</b> to delete a method from the <b>Favorites</b> .

## 6. Start Measurement Wizard

### 6.5 Start Measurement with a Predefined or Favorite Method

Click **Make your selection** respectively **Show Summary** in the **Select a file** dialog box to open the **Start Measurement** dialog box. Before the instrument starts to measure, the user has to (if defined) answer the report prompts and/or to confirm or change the constants.

#### Edit Prompts Dialog

If user prompts were specified in the method, the **Edit user prompts dialog box** is displayed:

<b>Prompt Answer</b> list	At each text field of this list any text prompt can be entered.
<b>Req.</b> check box	A <b>Required</b> check box next to every <b>Prompt Answer</b> text field determines that the measurement can only be started when a text has been entered.

Click **Continue** to close the user prompts dialog; the **Start Measurement** window appears. If set in the method, the **Edit Constants** dialog appears.

#### Edit Constants Dialog

The **Edit Constants** dialog box appears only, if the required flag is set for at least one constant in the selected method.

<b>Constants</b> list	At each text field of this list the value of the constant or the comment can be modified.
<b>Req.</b> check box	A <b>Required</b> check box next to every <b>Constant value</b> text field determines that this constant value needs to be confirmed. Do this by continuing to the next page.

If the method constants have been modified, the new values can be automatically transferred and saved into the corresponding method. Click **Modify constants in Method** to modify the current method with the new defined constants. Please note that this dialog is available only for **Magellan** users with the user right **Edit methods**.

Click **Continue** to close the constants dialog; the **Start Measurement** window appears.

#### Note

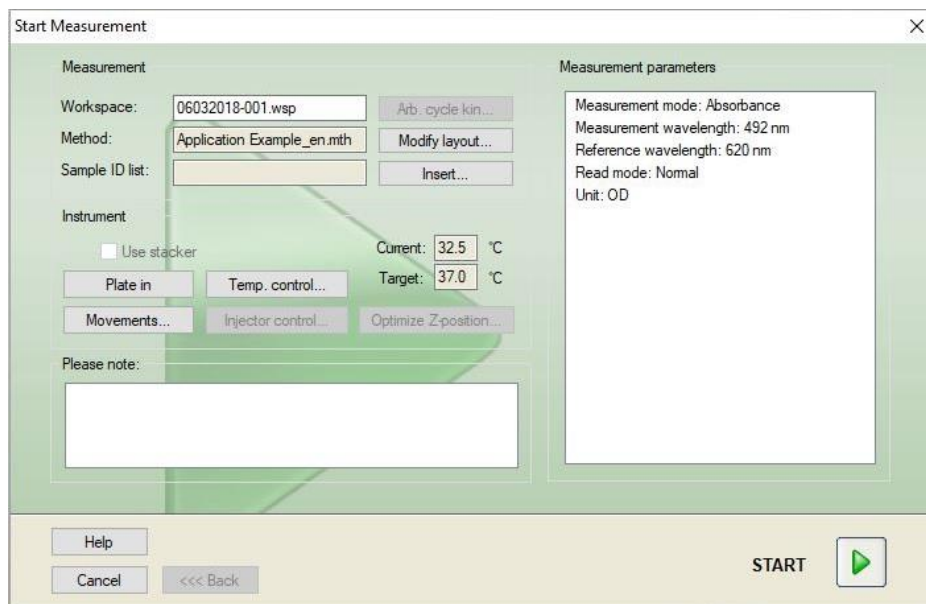
*Using magellan Tracker or magellan Standard with User administration, a default magellan Operator (refer to the chapters 9.6 User Rights and 9.5.3 Change User) can edit only the required constants. The constants without required flag set are displayed gray and cannot be edited.*

*A default magellan Administrator can also edit constants without required flag set.*

*For a default magellan Application Specialist it depends on the method he runs. Using an unsigned method, he is allowed to edit constant with and without required flag. Using a signed method, he can edit only the required constants*



After these two optional pages the **Start Measurement** dialog box is displayed:



**Measurement group box**

**Workspace** text field: The default workspace filename as defined in **Automated Data Handling** is displayed. The filename of this workspace can be renamed.

**Arb. cycle kin. ...** button: This button is available if a kinetic measurement is performed. Click this button to display the **Arbitrary Cycle Kinetic** dialog box. In this dialog box the measurement can be split up into several sub-measurements with a different number of measurement cycles and interval times. Each of these sub-measurements can be started at any time, for example: the workspace can be saved and the measurement can be continued on another day.



**Note**

***This option is not available for INFINITE F50 instruments.***

**Method** text field: The filename of the previously selected method is displayed.

**Modify layout...** button: Depending on the user rights, the plate layout can be modified. Click the **Modify layout...** button to open the **Modify Layout** dialog box. The user can move controls and remove samples, change the concentration or change the measurement parameters. **The changes are stored only in the workspace and not in the previously selected method.**  
**This button is not available when Obtain Raw Data has been selected and after inserting a sample ID list.**

**Sample ID List** text field: The filename of the currently loaded sample ID list is displayed

**Insert...** button: see also below. Click this button to open the **Insert Sample ID List** dialog box. After selection of a sample ID list file the **Sample ID List with Plate Layout Preview** dialog appears in which the user has to confirm the selection.

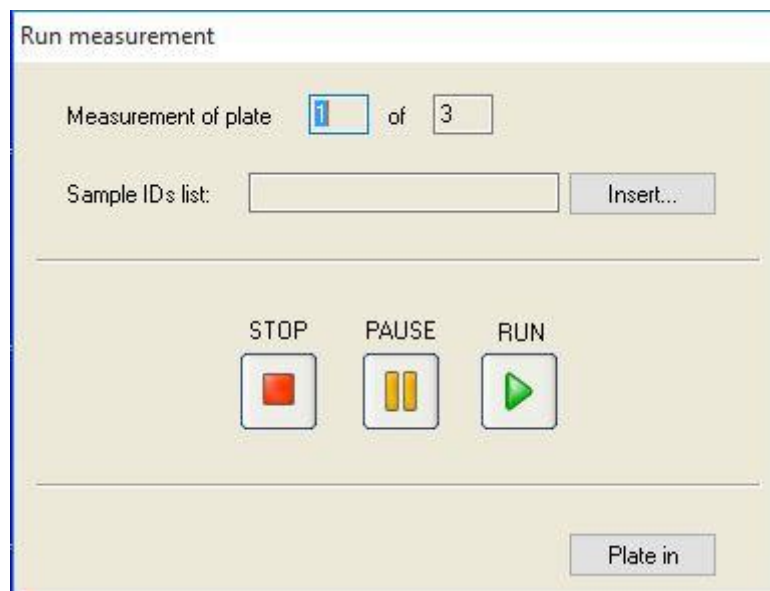
## 6. Start Measurement Wizard

<b>Instrument group box</b>	The workspaces will be stored with default workspace names. After all plates have been measured only the first workspace is open. Use <b>File Open</b> or the <b>Evaluate Results</b> wizard to open the other workspaces. <b>It is not possible to use the stacker when performing kinetic measurements.</b>
	<b>Plate In/Out</b> button: Click to move the plate carrier. This button changes its text depending on the position of the plate carrier.
	<b>Movements</b> button: Further movements of the instrument can be invoked (filter slide, mirror carriage and so on.)
	<b>Current Temperature</b> text field: The current temperature of the instrument is displayed.
	<b>Target Temperature</b> text field: The target temperature, set in the <b>Temperature Control</b> dialog box, is displayed.
	<b>Temperature Control</b> button: Click this button to open the <b>Temperature Control</b> dialog box. See chapter 3.1.2 Temperature Control... .
<b>Measurement parameters group box</b>	In a text field all configured measurement parameters are listed and can be double-checked.
<b>Please note group box</b>	Important information is displayed. Read this information and start appropriate actions before running the method.

A warning is displayed if the layout is defined for wells that will not be measured.

**Click Start to start the measurement.**

If you run a multiplate method, the **Run Measurement** dialog box appears after clicking **Start**.



It contains the following elements:

<b>Measurement of plate</b>	Displays the number of the currently processed plate.
<b>Sample ID List</b>	Insert the appropriate sample ID list for the selected plate. Sample ID lists have to be inserted plate by plate.



<b>Note</b>	
<i>Only sample ID lists created in magellan can be inserted. Import of other formats is not supported.</i>	

<b>RUN</b>	Click this button to start the measurement.
<b>PAUSE</b>	The Evaluate Results wizard is reached when clicking <b>Pause</b> ; further plates can be appended later.
<b>STOP</b>	The Evaluate Results wizard is reached when clicking <b>Stop</b> ; <b>no</b> further plates can be added.

After the measurement is completed, the **Results** dialog box appears, in which all results and calculations can be viewed. See chapter 7 Evaluate Results Wizard for more information.

## Insert Sample ID List

The **Insert Sample ID List** option is used to load a previously defined sample ID list file into a workspace:

<b>Filename</b> field	The list displays all available sample ID list files (.smp). Select a sample ID list by clicking a filename.
<b>Remarks</b> field	Available comments and remarks will be displayed.
<b>Import...</b> button	Click to open a standard Windows <b>Open</b> dialog box. External files can be imported. Refer to chapter 5.2.3 Import a Sample ID List for further information.

Select the desired sample ID list from the **Filename** field and click **OK** to view the sample ID list in the **Sample ID List with Plate Layout Preview** window. This dialog box displays the sample ID list together with the defined plate layout. If the method and the sample ID list have different plate formats, then an error message is displayed.

When the sample ID list is selected in the printed report setup then it is displayed on the printout.

The **Sample ID List with Plate Layout Preview** dialog box displays the sample ID list together with the defined plate layout. This helps the user to ensure that the correct sample ID list is selected. The dialog box contains the following elements:

<b>10%</b> button	Click to resize the displayed plate layout to show <b>10%</b> of the plate layout on the full screen.
<b>100%</b> button	Click to resize the displayed plate layout to show <b>100%</b> of the plate layout on the full screen.
<b>Zoom</b> check box	When this <b>Zoom</b> function is activated the required wells on the plate layout can be marked and the wells are automatically enlarged to fit into the full screen.
<b>Remove unused samples</b> check box	If an only partly filled sample ID list is loaded, the user can delete all unused samples from the layout by selecting this check box. If a final control (e.g., in well H12) has been defined within the layout, this control is automatically moved to the well after the last used sample well. Per default, the <b>Remove unused samples</b> option is selected.

## 6.6 Measurement Status

The **Measurement Status** dialog box is shown during the measurement performance of the instrument and contains the following elements:

<b>Status</b> text field	The text field is updated during the measurement and contains a measurement status information.
<b>Display in wells</b> group box	Select the mode of representation of data in the wells: <b>Values:</b> The measured value is displayed in the well. If more than one value is measured all values are displayed in one well.
	<b>Graph:</b> The option is enabled if a kinetic graph can be displayed. The graph is shown as soon as more than one value is available.
<b>Pause</b> button	To pause a kinetic measurement run at the next possible moment, click the <b>Pause</b> button. In the <b>Pausing Kinetic</b> dialog click the <b>Plate out / Plate in</b> button to move the plate transport out of or into the instrument. Click the <b>Continue</b> button to go on with the kinetic run.
<b>Break</b> button	Click this button to break the measurement at the next possible time point.
<b>Plate View</b> display	The <b>Plate View</b> display shows a schematic display of the microplate. According to the <b>Display in wells</b> option the contents of the wells are customized. The wells are updated as fast as the instrument delivers data. When injection or dispensing is performed, the currently used well is automatically highlighted in a different color.
<b>Cycle</b> text field	If a kinetic measurement is performed, the <b>Cycle</b> text field displays the current cycle number and the maximum number of kinetic cycles.
<b>Graph</b> display	If a kinetic or multilabel measurement is performed, the kinetic or multilabel graph of the currently selected well is displayed in a larger size at the right side of the <b>Measurement Status</b> dialog box.
<b>Previous cycle</b> group box	As long as the transmission of the data of the current cycle was not started the <b>Raw data</b> and the <b>Temperature</b> text fields contain the value and the temperature of the previous measured cycle of the currently selected well, respectively.
<b>Time</b> group box	The <b>Elapsed time</b> text field displays the time span since the start of the measurement.  The <b>Exp. run time</b> text field displays the time span expected for the whole measurement.

Scaling of the y-axis in the graph is possible by selecting either **Auto select range** or **Select range (MIN/MAX)**.



### Note

*It is possible to select multiple wells on the plate to view the selected kinetic curves in a graph. When performing kinetic measurements, the retrieved data is saved automatically every 30 min in the magellan log file directory (refer to chapter 3.3 Log Files).*

## 7. Evaluate Results Wizard

### 7.1 Introduction

The **Evaluate Results wizard** is designed to help the user analyze measurement results. Raw data, evaluation data and evaluation parameters can be viewed, and data can be re-evaluated.

#### Workflow Summary

Start the **Evaluate Results wizard** and select an existing workspace for evaluation (**Select a File** dialog box)


Click **Make your selection** to open the **Results** dialog box, in which the results can be viewed or printed (**Evaluate Results** tab) and if necessary, the used method modified (**Edit Method** tab).

Click **Finish** and use the **Save** dialog box to save a workspace file which contains method definitions, instrument data and sample ID list if configured.

Evaluated data are not stored in the workspace but recalculated every time the workspace is opened.

### 7.2 Select a File

The **Select a File** dialog box contains the following elements:

<b>Filename</b> list	The <b>Filename</b> list contains the list of all files (and their remarks) within the standard workspace directory.
<b>Show</b> combo box	<p>In the <b>Show</b> combo box, the displayed list of files can be modified according to the selection:</p> <ul style="list-style-type: none"><li>• All files</li><li>• Files from this instrument</li><li>• My files: This option is available if the user administration is enabled (always enabled in <b>magellan</b> Tracker).</li><li>• Signed files: only available for <b>magellan</b> Tracker.</li><li>• Custom definitions are possible by clicking the  button; see <b>File Selection Criteria</b> below.</li><li>• Example files: only available if they have been installed.</li></ul>



## 7. Evaluate Results Wizard

### 7.2.1 File Selection Criteria



Click the  button to open the **File Selection Criteria** dialog box.

Select one of the options under **Workspace Criteria** or enter characters in the **Containing** text field which must appear in the **Filename**. A time filter can be applied by selecting one of the options under **Workspace file created/modified** or enter a number in the **Last ... days** field. Click **OK** to save the settings.

**Select the workspace file to be evaluated from the Filename list and click Make your selection.**



#### Note

*If a **SUNRISE** instrument is connected, but an **INFINITE F50** method is selected, the **Instrument Mismatch** dialog appears:*

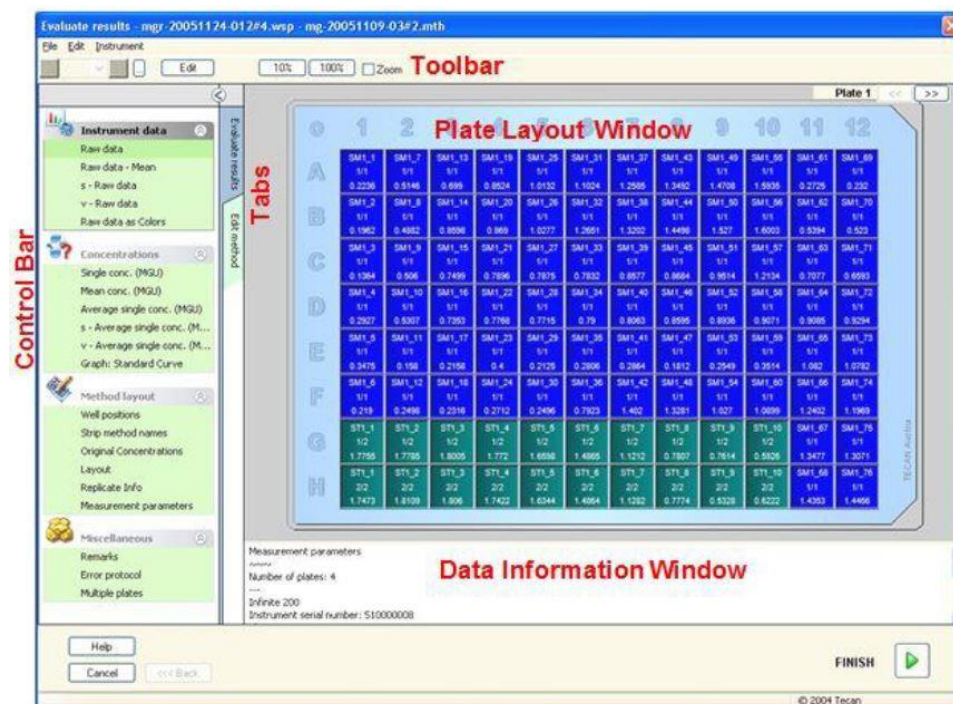
- **Connect to the proper instrument**



## 7.3 The Workspace Overview Window

The **Workspace Overview** window displays all available data of the currently selected workspace.

If the currently working user has the appropriate **magellan** rights, it is also possible to make some changes in the method by clicking on the **Edit Method** tab and perform a recalculation of the measured data.



The Workspace Overview is composed of the following elements:

- **Plate Layout** window: selected data for each well is displayed in the plate layout. If a multiplate workspace is opened, a “counter” for switching between the different plates is displayed in the right upper corner.
- **Toolbar**: for editing, zooming, switching between kinetic cycles and viewing the summary of one selected well.
- **Data Information** window: data which cannot be assigned to a single well is displayed in the text box window (for example: measurement parameters, cutoff definition, result statistic, etc.).
- **Control Bar of Evaluate Results tab**: all available data set names are displayed. Selecting a data set will either display the data in the plate layout or display the data in the **Data Information** window.
- **Control Bar of Edit Method tab**: the settings and parameters of the loaded method are displayed.

The size of the latter three windows can be changed by using the splitter bars that separate the windows.

## 7. Evaluate Results Wizard

### Plate Layout

The view displays a schematic layout of a microplate. Rows are marked alphabetically, columns numerically.

In the control bar on the left-hand side, all available data is listed. The selected data is displayed in the plate layout, in the text pane or in a separate graph window, according to the type of the selected data.

#### Context-Sensitive Menu of the Plate Layout


To display a summary of all data of one well, select the well and select **Summary** from the right mouse button menu.

### Toolbar Buttons

Available toolbar buttons are described in the following paragraphs.

Depending on the data selected, different buttons are displayed:  
when **Instrument data** is selected, the **Edit** button is available;  
when **Concentration** or **Kinetic data** is selected, the **Curve/Graph** button is available.

The following buttons are only available in the **Evaluate results** wizard.

<b>Edit</b>	Click the <b>Edit</b> button to edit or mask raw data.
 <b>button</b>	Click this button to display the <b>Summary</b> dialog box.
<b>10% button</b>	Click this button to resize the displayed plate layout to show <b>10%</b> of the plate layout on the full screen.
<b>100% button</b>	Click this button to resize the displayed plate layout to show <b>100%</b> of the plate layout on the full screen.
<b>Zoom check box</b>	When the <b>Zoom</b> check box is selected, the required wells on the plate layout can be marked and the labeled wells are automatically enlarged to fit into the full screen.
<b>Measurement cycle drop down list</b>	If the measurement is a kinetic measurement, the desired measurement cycle can be selected in the drop-down list.

### Data Information Window

Click, for example, **Miscellaneous** data in the **Evaluate Results** tab to view the corresponding information in the **Data Information** window.

## 7.4 Evaluate Results Tab

All available data set names are displayed in the **Available Data** control bar. There are several different viewing options:

- Selected data that presents a value for each well is displayed in the plate layout window. It can be viewed as values or in pseudo-colors together with a colors scale.
- Kinetic data can be viewed as a small graph in each well.
- Selected data that presents a data collection which cannot be assigned to a single well is displayed in the data information window (f.e. QC-Validation criteria).
- If a graph (standard curve, kinetics, enzyme kinetics, dilution series, multilabel, spectra) is selected, the **Graph** dialog box appears.

If a measurement sequence consisting of individual independent measurements has been executed, the results of each measurement are displayed upon selection of the relevant measurement number from a drop-down list in the toolbar (f.e. kinetic cycles in a kinetic run).

If necessary, the measurement results can be modified by clicking the **Edit** button. Manipulated data is marked with a ~ sign.



### WARNING

**THIS FUNCTION IS FOR RESEARCH USE ONLY AND MUST NEVER BE USED FOR DIAGNOSTIC TESTS.**

In each well of the plate layout, three lines of data can be displayed. Depending on which criteria selected in the control panel in the left window, different values are displayed.

### 7.4.1 Menus

<b>File</b>	ASCII File Export... ASTM File Export (LIS)... Sample Tracking Export... Excel Export... Method Export Print... Print Preview... Printer Setup... Printout Font... Plate to Plate QC...
<b>Edit</b>	Copy to Excel Copy to ASCII Format Paste from ASCII Format Insert Sample ID List... Recalculate with another Method...
<b>Instrument</b>	Movements... Temperature Control... Start Measurement...

## 7. Evaluate Results Wizard

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### 7.4.2 *Toolbar Menu: File*

#### ASCII File Export

Click **ASCII File Export** to export data as ASCII (.asc) files.

Before export procedure, the data must be selected in the **Data Export** dialog box via **Edit method tab** → **Data handling** → **Data export**.

Select the folder, where the exported data shall be stored. Enter a file name (.asc).

Upon clicking **Save** in the **Save as** dialog box, the data sets specified in the **Data Export** dialog box will be saved as an ASCII file.

#### ASTM File Export (LIS)

In the **File** menu, click **ASTM File Export** to export data to in ASTM format to compatible Laboratory Information Systems.

Select the data to be exported from the **Data Export** dialog box via **Edit method tab** → **Data handling** → **Data export**.

#### Sample Tracking Export

In the **File** menu, click **Sample Tracking Export** to export data to the Sample Tracking system

Select the data to be exported from the **Data Export** dialog box via **Edit method tab** → **Data handling** → **Data export**.

#### Excel Export

Click **Excel Export** to export data to Excel.

Select the data to be exported from the **Data Export** dialog box via **Edit method tab** → **Data handling** → **Data export**.

#### Method Export

**Click Method Export to export a method.**

Select the folder to save the method and enter the desired file name. Additionally, some comments can be added in the **Remarks** text field.

#### Print

In the **File** menu, click **Print...** or press **SHIFT-P** to print the data as defined with the **Printed Report** setup from the method. The standard Windows **Print** dialog box is opened, where the printer, page range and number of copies can be selected.

#### Print Preview

Click **Print Preview....** to see exactly how a print-out will appear without actually having to print the document.

#### Printer Setup

Click **Printer Setup....** to change the current printer or modify the printer settings.

The standard Windows **Print Setup** dialog box appears. Select printer, paper size and orientation of printout.

## Printout Font

Click **Printout Font...** to select a specific font, font style, font size, font color etc. for future printouts.

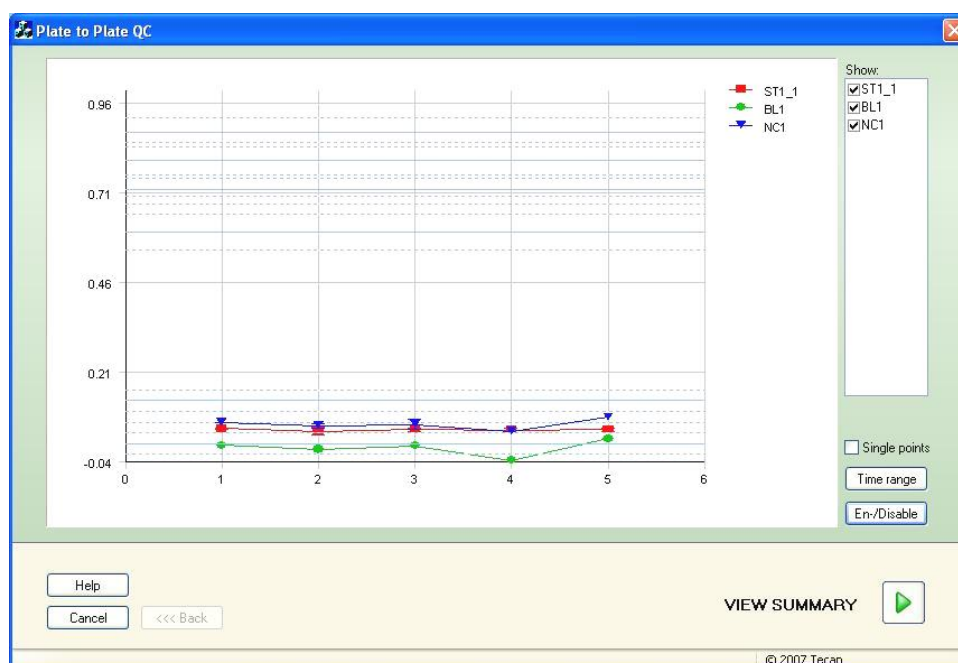
These settings will have no effect on the screen display. Large fonts should be avoided to prevent errors or misrepresentation of data.

## Plate to Plate QC

When **Plate to Plate QC** is configured in the method definition, **magellan** compares the currently observed mean value of a control against the mean and standard deviation previously defined for this method. (Refer to chapter 4 Create/Edit a Method Wizard).

### Levy-Jennings-Graph

Click **Plate to Plate QC** and the **Levy-Jennings-Graph** window appears. The Levy-Jennings-Graph displays the trend of the control values.



On the y-axes, the data values (raw data, concentrations, etc.) as set in the method definition are applied on the time scale of days (x- axes).

The control values are displayed together with the mean value and the distance lines of the standard deviations (1s, 2s, 3s).

When the cursor is placed on a measurement point, a tool-tip shows additional information (workspace name, etc.). Use the check boxes of the single elements of the **Show** list to select various controls to be displayed.

### Time Range

Click **Time range** to evaluate workspaces within a defined time range.

### Select Workspaces

Click **En-/Disable** to enable or disable certain workspaces for evaluation.

## 7. Evaluate Results Wizard



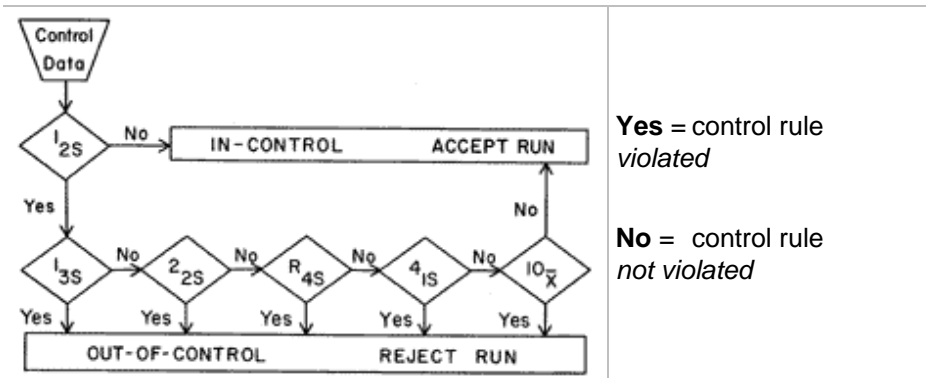
### Data Sheet

Click **View summary** to open the **Data sheet** dialog box:

<b>Workspace</b> column	A list of the evaluated workspace files. On the left-hand side of the workspace name, a green checkmark indicates fulfillment, a red cross indicates failure of the Westgard® rule evaluation (see Instructions for Use for <b>magellan</b> for further information on <b>Westgards Rules</b> ).
<b>Control</b> column	The different controls are listed.
<b>Value</b> column	The mean value of each control is displayed.
<b>Westgard® rule</b> <b>evaluation</b> columns	The individual Westgard® rules are evaluated with <b>OK</b> for a not violated control rule or <b>x</b> for a violated control rule according to the table below (see Westgard rules below).
<b>Comments</b> field	Comments to the evaluation can be entered.
<b>Print Preview</b> button	Print preview with the Levy-Jennings graph, Westgard rules check and comments.

### Westgard Rules

The Westgard® rules are a multirule QC model:



1:2s	<p>Control rule to test whether a control measurement exceeds the control limits of <b><math>\bar{x} + 2SD</math> or <math>\bar{x} - 2SD</math></b>.</p> <p>This rule is used as a warning rule to trigger careful inspection of the control data by the following control rules.</p> <p>If no control measurements exceed the mean plus 2s or the mean minus 2s control limit, then the measurement procedure is considered “<b>in-control</b>”, regardless whether any of the other rules have been violated.</p> <p>However, if one control measurement exceeds the mean plus 2s or the mean minus 2s control limit, and any of the other rules are violated, the measurement procedure is considered “<b>out-of-control</b>”.</p>
1:3s	<p>Control rule to test whether a control measurement exceeds the control limits of <b><math>\bar{x} + 3SD</math> or <math>\bar{x} - 3SD</math></b>.</p> <p>A run is rejected if a single control measurement exceeds the mean plus 3s or the mean minus 3s control limit.</p>
2:2s	<p>Control rule to test whether two consecutive control measurements exceed the same control limit of either <b><math>\bar{x} + 2SD</math> or <math>\bar{x} - 2SD</math></b>.</p> <p>A run is rejected if 2 consecutive control measurements exceed the mean plus 2s or the mean minus 2s control limit.</p>
R:4s	<p>Control rule to test whether the range, or difference, between control measurements exceeds 4SD.</p> <p>A run is rejected if 1 control measurement exceeds the mean plus 2s and another exceeds the mean minus 2s. The two control results need not be consecutive.</p>
4:1s	<p>Control rule to test whether four consecutive control measurements exceed the same control limit of either <b><math>\bar{x} + 1SD</math> or <math>\bar{x} - 1SD</math></b>.</p> <p>A run is rejected if 4 consecutive control measurements exceed the mean plus 1s or the mean minus 1s control limit.</p>
10:x	<p>A run is rejected if 10 consecutive control measurements fall on the same side of the mean. However, if one of these results falls directly on the mean, then the run is not rejected.</p>

### 7.4.3 Toolbar Menu: Edit

The **Edit** menu contains the following selections:

#### Copy to Excel

The **Copy to Excel** command allows the user to export data directly into an MS Excel worksheet.

#### Copy in ASCII-Format

Select **Copy in ASCII format** to copy the data, which is contained in the selected wells of the plate layout, to the clipboard.

This function allows transferring the well data to other software applications.

#### Paste from ASCII-Format

In the **Edit** menu, click **Paste** or press **CTRL-V**.

The contents of selected data will be pasted from the clipboard using the ASCII data format. The function allows the transferring of data from other software applications (for example: Excel) into the wells.



## 7. Evaluate Results Wizard

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First, the relevant data has to be selected with the mouse in the other software application. Then the selected data has to be copied and is transferred to the clipboard. The rows have to be separated by linefeed, the columns by tab stops. This is automatically done in Excel when selecting multiple cells.

The **Paste** function pastes the copied data in ASCII format from the clipboard into the wells. Data is always inserted starting at position A1. If the data is non numerical the value is set to 0.

In case of an unfinished kinetic with defined interval, a question is displayed asking whether the currently selected data should overwrite the original data or append the data. The time interval is taken from the measurement parameters.

### Insert Sample ID List

For detailed information see 6.5 Start Measurement - Insert Sample ID List.

### Recalculate with Another Method

A recalculation based on the settings of a newly selected method will be performed.

If an error occurs during recalculation, the procedure will be stopped.

Click this option to open the **File Open** dialog box. In an additional **Remarks** field, a text description of the file - if entered - will be displayed (available only in **magellan** Tracker). The method must be selected by either double-clicking the method file or by selecting the method file and clicking the **Open** button.

After selecting the method, the **Calculating...** dialog box is displayed. This dialog box is for display only and contains no elements for editing. It closes after the calculation is finished.

#### 7.4.4 Toolbar Menu: Instrument

For detailed information on **Movements** and **Temperature Control** see chapter 3.1 Instrument Options.

### Start Measurement

Using this option, the measurement run can be started again with the currently loaded method and current data will be overwritten if **YES** is selected in the **magellan** dialog box.

In case of an incomplete kinetic run, cycles can be added (not available for Infinite Series instruments).

For detailed information see 6.5 Start Measurement with a Predefined or Favorite Method.

#### 7.4.5 Plate Layout Window

The data, which is to be displayed within a well when opening a workspace file, can be set when defining the method (**Automated data handling → view results after measurement → More...**).

In each single well, three lines are visible; the following data is displayed as default:

1<sup>st</sup> line: layout

2<sup>nd</sup> line: replicate info

3<sup>rd</sup> line: in the third line, according to the data selected, the conventions described in the following chapter are used (cf. 7.4.6 Special Characters).



### 7.4.6 Special Characters

"None"	No data is displayed.
"~" tilde	A tilde is appended for the manipulated value of a well (simulated, edited); for example: 0.354~
"( )" parenthesis	Parenthesis are applied for the masked value of a well; for example: (0.354)
"!" exclamation mark	An exclamation mark is appended for the eliminated value of a well; for example: !0.354
"#" hash	Concentration values are marked with a '#' when the calculated concentration lies outside of the range of the standard curve that means the concentration value has been extrapolated. For example: #13.75
"*" asterisk	An asterisk marks values that have been measured using the "Use gain regulation" option, which corrects (=lowers) the gain.
Corresponding error message is displayed	The average value of a well is unusable (for example: lamp low, divide by zero, negative logarithm).
No color, third line is empty	No formula is applied to the well or Replicate well if "average s" or "v calculation" or No cutoff result.
Data of first replicate is masked or eliminated	Average value is derived without using the masked data, but the average value is displayed in the well of the first replicate
"< MIN"	The calculated concentration lies beneath the lowest standard.
"MltPt"	Multiple points; a unique concentration cannot be calculated.
"> MAX"	The calculated concentration lies above the highest standard.
"NoCalc"	Input data is not found or calculation error; calculation is not possible

### Shortcuts

When viewing transformed data, press CTRL-SHIFT to display the defined formula in the second line as long as the key is pressed.

### 7.4.7 Control Bar: Instrument Data

The user can select raw data, spectrum data, etc. and their statistics according to the performed measurement.

### 7.4.8 Control Bar: Reduced Data

The user can select reduced data, e.g. difference data according to the performed measurement.

## 7. Evaluate Results Wizard

### 7.4.9 Control Bar: Transformed Data

The user can select the required transformation to display the calculated results including their statistics, colored display, etc.

### 7.4.10 Control Bar: Kinetic Parameters

The user can view the kinetic evaluation parameters such as Mean/Max slope, Time Onset, etc. according to the measurement definition.



#### Note

**Unusable data (e.g., overflow values) are ignored for kinetic data calculation.**

### Define Kinetic Data Reduction Well Specifically

Select **Edit kinetic settings...** from the right mouse context menu when a well is selected. The Kinetic Data Reduction dialog is displayed (see chapter 4.3.6 Kinetic: Kinetic Data Reduction for further details).

For the selected well, particular parameters can be defined which can also be copied to other well(s) (select **Copy kinetic settings** from the right mouse context menu, click in the well(s) where the settings have to be copied to and select **Paste kinetic settings...**).

Changing the Kinetic Data Reduction settings in the Method tab will overwrite the well specific definitions.

### Graph: Enzyme Kinetics Dialog

The **Enzyme Kinetics Graph** dialog box enables the user to display the enzyme kinetics graph.

#### Context-Sensitive Menu of Enzyme Kinetics Graph

By right-clicking on the graph, a context-sensitive menu is displayed.

<b>Crosshair cursor</b>	A crosshair cursor is displayed to assist in placing the cursor on particular points on the graph.
<b>Copy to Clipboard</b>	Copies the graph into the clipboard as a bitmap; the bitmap can be transferred to any Windows application by using the paste function.
<b>Save as bitmap</b>	Saves the graph as a bitmap file.
<b>Print...</b>	Prints the graph.
<b>Printer setup...</b>	Displays the <b>Printer Setup</b> dialog box, in which the printer settings can be defined.
<b>Zoom to 100%</b>	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
<b>Enzyme Kinetics Data...</b>	Opens the <b>Enzyme Kinetics Data</b> dialog box. The <b>Enzyme Kinetics Data</b> dialog box displays the result of the defined enzyme kinetics analysis.
<b>Properties...</b>	Select this command to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
<b>Help...</b>	Opens the <b>magellan</b> help dialog box.

### 7.4.11 Control Bar: Concentrations

Select single concentration, mean or average single concentration to view the results, calculated according to the standard curve:

- **Single conc. (Unit)**  
Concentration of individual replicate.
- **Mean conc. (Unit)**  
The mean value of replicates is used for calculation of concentration. If replicates with different dilutions are defined, the mean concentration will not be available.
- **Average single conc. (Unit)**  
For each replicate the concentration is calculated. Then the concentrations are averaged.
- **Additional concentrations (single, mean and average concentration) if available.**
- **Graph: Standard Curve**  
Click this option to open the **Graph: Standard Curve** dialog box
- **Intercepts**
- **Values for concentration transformations if defined**
- **IC 50, r-IC 50, Graph: dilution series**

### Graph: Standard Curve Dialog

Open this dialog via the control bar or by clicking **Curve** on the toolbar to display and edit the **Standard Curve**.

This dialog box has its own menu with options to save the standard curve, change the analysis type or compare a number of curves. The graph can be exported as a bitmap, which can then be incorporated into documents of other software applications.

The **Graph: Standard Curve** dialog box contains the following elements:

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#### File menu

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The **File** menu contains the following commands:

- **New** is selected to create a new standard curve, the X and Y values can be defined in a dialog box.  
Enter measured values (Y Value) and concentration (X Value). If the **Exclude** option is selected, the corresponding point will not be incorporated into the calculation of the graph.  
On completion, click the **OK** button.
- **Open** is selected to open a previously saved standard curve.  
A standard curve, saved in the file format .std can be opened. On execution of this command, the graph will be displayed together with the already displayed standard curves.
- **Close**  
If a number of curves are open, individual curves can be closed using this option.  
The relevant curve must be selected from the available list and closed by clicking the **OK** button.
- **Save/Save as** is selected to save a standard curve for further evaluations.  
A standard curve can be saved as a .std file. The file can be included in the method by switching to the **Data** tab. If the user has selected **Save** and the curve had previously been saved, it will simply be stored without displaying any prompts. If this is not the case, the user will be invited to enter a name for the new curve.

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- **Export** is selected to export a standard curve as a bitmap file.
- **Print...** is selected to print the standard curve. This command will print the current graph.
- **Printer Setup...**  
Selecting this option displays the **Printer Setup** dialog box.
- **Exit** is selected to exit the standard curve dialog box.  
If any modifications have been made, for example a change of interpolation process, a new calculation will be performed.



### Note

**Standard curves added by New or Open are for comparison only. After closing the Standard Curve dialog box, the curves will be removed.**



## EXPERT'S KNOW HOW

A saved standard curve file can be used in methods, which do not have standards in the layout, to calculate sample concentrations. See 4.3.8 Concentrations: Standard Curve, **Standards from external file**.

### Edit menu

The **Edit** menu contains the following commands:

- Select **Copy** to copy the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the copy/paste function.
- Select **Properties** to modify the analysis type, axes, title, etc.
- Select **Standard Curve** to open the standard curve dialog box. In this dialog box, standard points may be excluded or included.  
Upon selecting the relevant curve from the available list and clicking the **OK** button, all of the base points will be displayed in the appearing window. Activate or exclude a point by clicking on the **Exclude** option. Only those points that have not been marked as excluded will be used when calculating the standard curve.  
Only base points that have been obtained from raw data, have been manually entered, or have been additionally loaded can be modified. Base points obtained from transformation, for example, can only be excluded.
- **Conc. Range:** The **Concentration Range** dialog box is displayed. Choose between **Display all** and **Display range**. If **Display range** is selected and the **Min.** and **Max.** limits are defined, only concentration values in the specified range are displayed in the plate layout window.

### View menu

The **View** menu contains the following commands:

- Select **Audit trail** to display the audit trail of an external standard curve. This option is only available for **magellan** Tracker.
- Select **Statistics** to display the statistics of the obtained values.  
To assess whether any drift or changes have occurred with the reader over a period of time, it is possible to compare a series of standard curves by means of statistics values.  
If a number of curves are loaded, the average, the standard deviation and the variation coefficient will be calculated for each of them.
- **Intercepts...** opens the **Intercepts** dialog box. The **Intercepts** dialog box displays the result of the defined intercept values.

- **Average Standard Curve** displays the standard curve averaged over the performed experimental groups.  
This option can only be activated if a number of curves are present in the window. An average curve will be generated and displayed using the collective curve data.

#### Help menu

Select **Help** to open the **magellan** help dialog box.

#### Click on points

**Clicking on points** will mask/unmask them within the standard curve. After a point is masked the line of the graph is automatically adjusted accordingly and the point is represented as a transparent symbol instead of a solid symbol.

Hint: This can be undone by pressing **CTRL+Z**.

#### X, Y cursor tool-tip

When the cursor is not moved for a short moment, a tool-tip text appears displaying the X and Y coordinates of the current cursor position.



### EXPERT'S KNOW HOW

If more than **six** standard curves are displayed in the graph, only a small legend on the right side shows the label of the graph. To view the fit functions respectively the curve fit parameters, select **Standard Curve Data** from the context-sensitive menu (see below).

#### Context-Sensitive Menu of a Standard Curve Graph

By right-clicking on the graph, a context-sensitive menu is displayed.

<b>Crosshair cursor</b>	A crosshair cursor is displayed to assist in placing the cursor on particular points on the graph.
<b>Single points</b>	View replicate values instead of mean values.
<b>Copy to Clipboard</b>	Copies the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the paste function.
<b>Save as Bitmap</b>	Saves the graph as a bitmap file.
<b>Print...</b>	Prints the graph.
<b>Printer Setup...</b>	Displays the <b>Printer Setup</b> dialog box.
<b>Undo changes</b>	Cancels recent actions.
<b>Zoom to 100%</b>	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
<b>Standard Curve Data</b>	Views the curve fit parameters of the displayed standard curve(s).
<b>Intercepts...</b>	Opens the <b>Intercepts</b> dialog box, which displays the result of the defined intercept values.
<b>Properties...</b>	Changes the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
<b>Help...</b>	Opens the standard <b>magellan</b> help dialog box.

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### Graph: Dilution Series Dialog

The **Graph: Dilution Series** dialog box displays the dilution graph with the specified intercept.

#### Context-Sensitive Menu of Dilution Series Graph

By right-clicking the graph, a context-sensitive menu is displayed.

<b>Crosshair cursor</b>	A crosshair cursor is displayed to assist in placing the cursor on special points on the graph.
<b>Copy to Clipboard</b>	Copies the complete graph into the clipboard as a bitmap; the bitmap can be transferred to any Windows application by using the paste function.
<b>Save as bitmap</b>	Saves the graph as a bitmap file.
<b>Print...</b>	Opens the <b>Print</b> dialog box from which the graph can be printed.
<b>Printer Setup...</b>	Opens the <b>Printer Setup</b> dialog box, in which the printer settings can be defined.
<b>Zoom to 100%</b>	Sets the graph display back to the 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
<b>Dilution Series Data</b>	Displays the intercept values and correlation coefficients.
<b>Properties...</b>	Select this command to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
<b>Help...</b>	Opens the standard <b>magellan</b> help dialog box.

### 7.4.12 Control Bar: Qualitative Results

The cutoff definition shows an overview of the currently used cutoff ranges and the used cutoff limits.

In the data information window on the bottom of the screen, the list of cutoff definitions is displayed (experimental groups, input data, cutoff ranges, etc.).

The user can view the cutoff results.

- Cutoff definition  
Ranges and limits of the ranges
- Cutoff results  
Cutoff result for each well
- Cutoff statistic  
Statistics of the number of hits for each range

### 7.4.13 Control Bar: Sample IDs

The user can view the sample ID list data.

### 7.4.14 Control Bar: Method Layout

The user can view the method layout, i.e. well positions, layout, replicate info, measurement parameters, etc.

### 7.4.15 Control Bar: QC Validation

The list of validations contains the experimental groups, the input data for each validation group, the validation formulas, and their results (TRUE or FALSE).

If the result is TRUE, it indicates that the validation criteria were met for this specific plate, whereas FALSE represents an invalid result for the whole plate.

### 7.4.16 Control Bar: Miscellaneous

The error protocol logs all errors that occur during the run of a method. Errors can occur during a measurement or during the calculation. Review the error protocol before using data and results.

### 7.4.17 Color Scale Box

If values contained within the analysis plate are presented in different colors, the **Color scale** dialog box is displayed. The colors allow for a fast overview of the measurement results of the individual wells. The colors, as they are used, depend on the settings defined in the color scheme.

### 7.4.18 Context-Sensitive Menu of a Well

By right-clicking on a well on the plate layout – when having selected the tab **Edit Method** –, a context-sensitive menu is displayed.

## Summary Dialog

The **Summary** dialog box provides an overview of all defined parameters of a selected well.

<b>Information tree</b>	The information tree gives an overview of all defined well-based parameters of the selected well. The tree is filled according to the available information, e.g., if sample ID list information is available the sample ID, the pipetting status, etc. are displayed. If raw data is available, additional information can be displayed depending on the measurement settings and the connected instruments, for example for kinetic measurements the time points are displayed.
<b>Left, right, up and down buttons</b>	The direction buttons can be used to select another well on the plate while leaving the dialog box open.
<b>Expand All / Shrink All</b>	Click this button to display the information tree expanded to the highest level or to shrink to the first level.
<b>OK</b>	Closes the <b>Summary</b> dialog box.



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### Details Dialog

The **Details** dialog box displays the multiple reads per well results of one well.

<b>File</b> menu	<b>Save &amp; Exit</b> is selected to save all changes and close the dialog box.
<b>Edit</b> menu	<p>The <b>Edit</b> menu contains the following commands:</p> <ul style="list-style-type: none"> <li>Click <b>Copy</b> to copy the single values into the clipboard, which then can be transferred to any Windows application by using the paste function.</li> <li>Select <b>Recalculate</b> to force the recalculation of the statistic data at the bottom of the dialog. This option is disabled if <b>Automatic Recalculation</b> is set.</li> <li>If <b>Automatic Recalculation</b> is set, the statistic data is calculated after every mask/unmask action.</li> </ul>
<b>View</b> menu	<p>The <b>View</b> menu contains the following commands:</p> <ul style="list-style-type: none"> <li><b>Values</b> can be selected to display the reads as values.</li> <li>Use this option to view multiple reads per well coarsely and quickly. <b>Graphic</b> can be selected to display the read values as colors. <b>Brightness</b> uses one color with different brightness to display the values. <b>Pseudo Colors</b> uses different colors to display the values. A color bar with a slide control is displayed to change the intensity.</li> </ul>
<b>Help</b> menu	Click <b>Help</b> to open the <b>magellan</b> help dialog box.
Click on points	Clicking <b>reads</b> will mask/unmask them. After a read is masked, the value is put in brackets. If the color display is enabled, the read is displayed in white with a black circular border.

### Edit Dialog

Use this command to edit the measured raw data of a selected well.

<b>Edit raw data</b> text field	A new value for the selected well can be entered. Data is then shown with the symbol ~ (refer to chapter 7.4.6 Special Characters).
<b>Reset</b> button	Resets the well to its original value.
<b>Mask</b> check box	Excludes the value of the well from the calculation. Data is then shown in brackets. Select the <b>Mask</b> check box again to include the value again.
<b>Left, right, up</b> and <b>down</b> buttons	The direction buttons are used to select another well on the plate while leaving the dialog box open.
<b>OK</b>	Closes the <b>Edit</b> dialog box.

### Graph: Multilabel Dialog

The **Graph: Multilabel** dialog box displays the data of the selected wells. The raw data versus well IDs is displayed.

#### Context-Sensitive Menu of Multilabel Graph

By right-clicking the graph, a context-sensitive menu is displayed.



<b>Crosshair cursor</b>	A crosshair cursor is displayed to assist in placing the cursor on particular points on the graph.
<b>Copy to Clipboard</b>	Copies the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the paste function.
<b>Save as bitmap</b>	Saves the graph as a bitmap file.
<b>Print...</b>	Opens the <b>Print...</b> dialog box from which the graph can be printed.
<b>Printer setup..</b>	Opens the <b>Printer Setup</b> dialog box in which the printer settings can be defined.
<b>Zoom to 100%</b>	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
<b>Properties...</b>	Select this command to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
<b>Help...</b>	This button opens the <b>magellan</b> help dialog box.

## Graph: Kinetics Dialog

The **Graph: Kinetics** dialog box displays the graphs of kinetic measurements of one or more selected wells. The legend contains the calculated kinetic parameters.

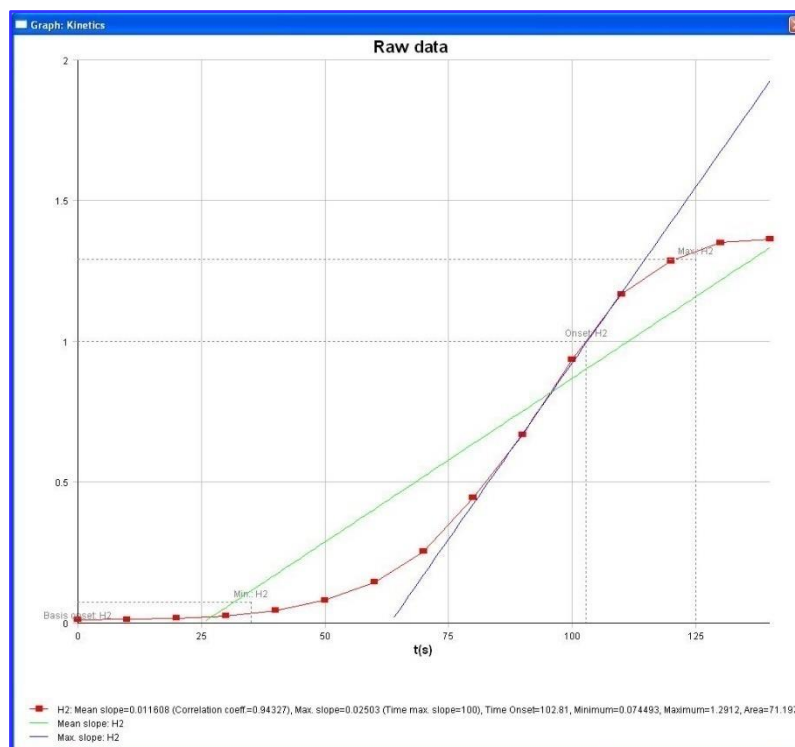
Click on points to mask/ unmask them within the kinetic graph. After a point is masked the line of the graph is automatically adjusted accordingly and the point is represented as a transparent symbol instead of a filled colored symbol.

### Context-Sensitive Menu of Kinetics Graph

By right-clicking on the graph, a context-sensitive menu is displayed.

<b>Crosshair Cursor</b>	A crosshair cursor is displayed to assist in placing the cursor on particular points on the graph.
<b>Copy to Clipboard</b>	Copies the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the paste function.
<b>Save as bitmap</b>	Saves the graph as a bitmap.
<b>Print...</b>	Opens the <b>Print...</b> dialog box from which the graph can be printed.
<b>Printer Setup...</b>	Opens the <b>Printer Setup</b> dialog box in which the printer settings can be defined.
<b>Zoom to 100%</b>	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
<b>Show Kinetic Reduced Data</b>	Calculated kinetic data (slopes, onsets, minima, maxima) can be visualized in the graph of the kinetic curve(s). Slopes are visualized as curves; onsets, minima and maxima as intercept points. The display can be enabled/disabled via the context menu item <b>Show Kinetic Reduced Data</b> in the kinetic graph dialog. The current display state is stored and will be reused for further displays.

## 7. Evaluate Results Wizard



<b>Temperature curve</b>	This option shows/hides a curve visualizing the temperature progression during kinetic measurements (if available).
<b>Kinetic parameters...</b>	Opens the <b>Kinetic parameters</b> dialog box and offers the ability to modify the kinetic settings for the selected well(s).
<b>Kinetic Data...</b>	Select this menu item to show a table of all calculated kinetic data of the selected well(s).
<b>Y-Axis scaling</b>	A range for the Y-axis can be selected.
<b>Properties...</b>	Select this button to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
<b>Help</b>	Opens the <b>magellan</b> help dialog box.



### EXPERT'S KNOW HOW

Setting different kinetic parameters for different wells is possible either by using the context sensitive menu for a well in the plate layout window or by using the context sensitive menu in the kinetic graph dialog. Editing the kinetic parameters in the Edit method tab, the kinetic parameters are set identical for all wells.

## Graph: Spectra Dialog

The **Graph: Spectra** dialog box displays the spectrum of a scan measurement.

### Context-Sensitive Menu of 2D Spectra Graph

By right-clicking on the graph, a context-sensitive menu is displayed.

<b>Crosshair cursor</b>	A crosshair cursor is displayed to assist in placing the cursor on particular points on the graph.
-------------------------	--

<b>Copy to Clipboard</b>	Copies the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the paste function.
<b>Save as Bitmap</b>	Saves the graph as a bitmap.
<b>Save as JCAMP-DX</b>	Select this command to save the graph as a JCAMP-DX 4.24 file.
<b>Save as ASCII</b>	Select this button to save the graph as a tab separated ASCII file.
<b>Print...</b>	Opens the <b>Print...</b> dialog box from which the graph can be printed.
<b>Printer Setup...</b>	Opens the <b>Printer Setup</b> dialog box in which the printer settings can be defined.
<b>Zoom to 100%</b>	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
<b>Spectra Data Reduction...</b>	Select this command to change the <b>Spectra Data Reduction</b> parameters settings.
<b>Spectra Reduced Data...</b>	Select this command to display a list of reduced spectra data. <b>Note!</b> This command is enabled only when reduced spectra data of type value is available.
<b>Data as Table</b>	Opens a dialog box showing the spectrum as table. This allows copying the data to Excel.
<b>Spectrum masked</b>	The spectrum and the reduced data are displayed as masked. This prevents further calculation of this well. Option is available only when raw spectrum is displayed.
<b>Show Prim. Spectrum</b>	The selected spectrum and the raw spectrum are displayed together. Option is available only when reduced spectrum is displayed.
<b>Properties...</b>	Select this command to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
<b>Help...</b>	Opens the <b>magellan</b> help dialog box.



**Note**

**To export scan results, go to the context-sensitive menu by right-clicking on the spectra graph. Select Data as Table in the dialog box and copy the data to Excel or save them as ASCII file.**

## 7. Evaluate Results Wizard

### 7.5 Edit Method Tab

Click this tab to change to the currently used method and its settings. Every modification of the method results in a re-calculation of all data when changing back to the Evaluate Results tab. These changes can be saved in the workspace, however, will not be applied to the originally inserted method file itself. See chapter 4 Create/Edit a Method Wizard for further information

The Edit method tab is displayed only if the currently working user has the appropriate rights (chapter 9.6 User Rights).

### 7.6 Saving the Evaluated Results

Click **Next** on the **Results** dialog box to reach the **Save in** dialog box:

<b>Save in</b> group box	<b>Filename</b> text field: a default name for the file will appear, but can be changed if desired.
	<b>File remarks</b> text field: enter remarks if necessary.
<b>Audit trail comment</b> group box	<b>Audit trail comment</b> text field: enter comments to the audit trail as necessary (only available for <b>magellan</b> Tracker).
<b>Save...</b> button:	Saves the workspace file
<b>Export...</b>	Click this button to open the Export dialog
<b>Audit Trail</b> button:	Use to view the <b>Audit Trail</b> of the file (only available for <b>magellan</b> Tracker). Refer to chapter 4.4 Saving the Method – Audit trail for further information.
<b>Signatures</b> button:	Use to view the signatures attached to this file (only available for <b>magellan</b> Tracker). Refer to chapter 4.4 Saving the Method for further information.
<b>Sign this workspace now</b>	Select <b>Sign this workspace now</b> to open the <b>Attach Signature</b> wizard (only available for <b>magellan</b> Tracker).

Click the **FINISH** button to close the **Evaluate Results** wizard. In case of unsaved changes, the user is asked to perform the saving.

Click the **Save** button for saving the data without closing the wizard.

## 8. Attach Signature Wizard

### 8.1 Introduction

Several signatures can be applied to one record and are always included in the printed report. Signed records can only be modified by users with the appropriate rights. It is possible to fully control the use of methods by allowing users to run only signed methods. Only **Method** and **Workspace** files can be signed.

**Note**

*This wizard is only available with magellan Tracker.*

Click **Attach signature** to start the **Attach signature** wizard.

After the welcome dialog box, the **Select a File** dialog box appears. Select a **Method** or **Workspace** file for signing.

**Show**  
combo box

In the **Show** combo box the displayed list of files can be modified according to the selection. Possible selections are:

- All files
- Unsigned files
- Signed files

### 8.2 Sign a File

Click **Next** and the **Sign** window appears:

## 8. Attach Signature Wizard

<b>Review</b>	Can only be signed by a user with the appropriate rights.
<b>Approval</b>	Can only be applied by a user with the appropriate rights for records with an already existing review signature. Review and approval cannot be signed by the same user. No changes may be made to the file between review and approval.
<b>Custom</b>	Enter a custom signature meaning in the text field.

The default user settings only allow administrators to attach signatures to reviews and approvals and to modify signed files.

Comments can be added in the **Comment** text box.

In the **User Name** text field, the user name of the currently logged in user must be entered. In the **Password** text field, the password of the currently logged in user must be entered.


Click **Finish** to confirm the entered information and sign the record.



**Note**

*Depending on the standard operating procedures of the company using this software, this signature may be viewed as legally binding. Therefore it is very important that the users keep their passwords secret.*

## 9. Miscellaneous Icon

Click the **miscellaneous** icon  in the wizard window and select between the following actions/ definitions:



### 9.1 Instrument Control

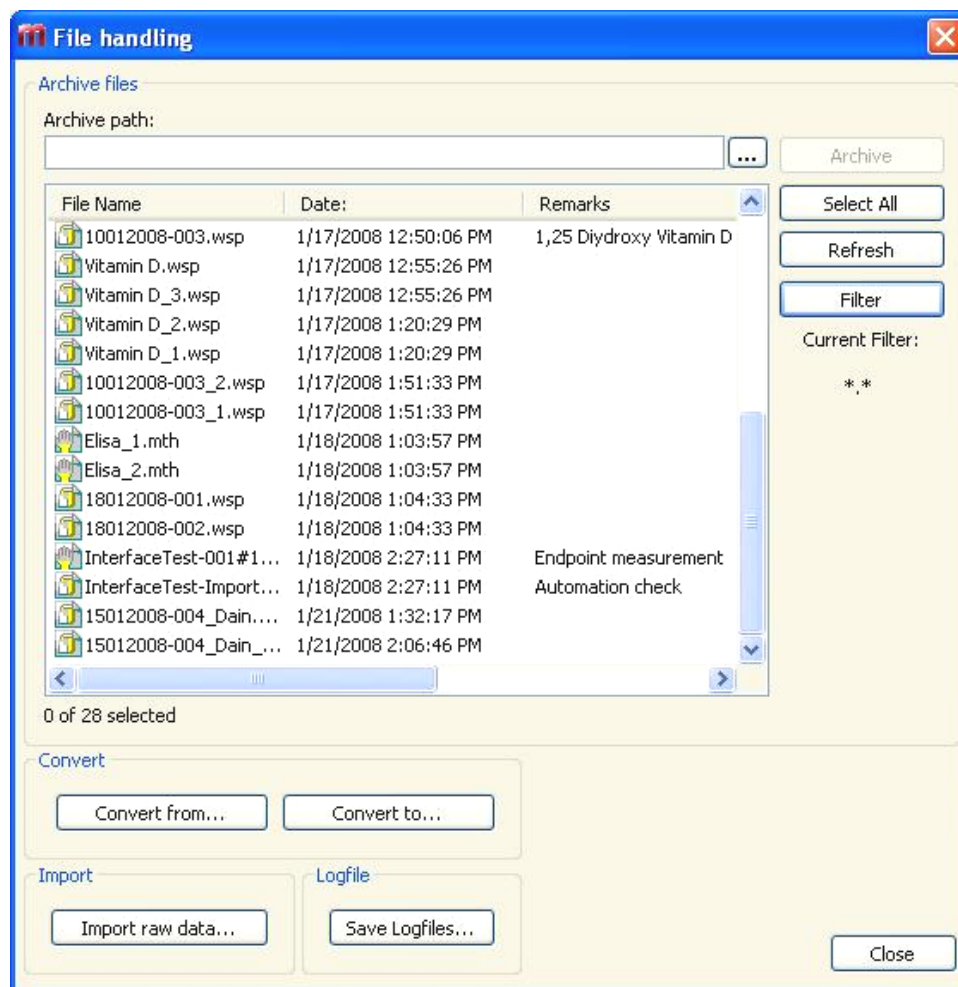
See chapter 3 Instrument Control & Settings.

### 9.2 File Handling

#### 9.2.1 Archive Files

The **Archive Files** group box gives an overview and complete control of file backup. It lists all the files (workspaces, methods, sample ID lists or temporary files) saved by **magellan**.


## 9. Miscellaneous Icon



The files for backup have to be selected from the **File Name** list. Click **Archive** to move all selected files to the specified backup directory in the appropriate subfolders.

When files have the attribute **read-only**, a warning box appears before the files are deleted.

The **Archive Files** group box contains the following elements:

<b>Archive path</b>	Define the archive path. Click the browse  button to change the path.
<b>File Name list</b>	<ul style="list-style-type: none"> <li>Lists all files saved by <b>magellan</b> filtered by the options entered via the <b>Filter</b> button.</li> </ul>
<b>Archive button</b>	Click <b>Archive</b> to move all files selected in the <b>File Name</b> list to the backup directory (cut-and-paste function).
<b>Select All button</b>	Click <b>Select All</b> to select all files displayed in the <b>File Name</b> list.
<b>Refresh button</b>	Click the <b>Refresh</b> button to cancel the current <b>Filter</b> option and to refresh the file list.
<b>Filter button</b>	<p>This button is used to display only specific files, or files with a certain string in their file names:</p> <ul style="list-style-type: none"> <li>A question mark <b>?</b> can be applied as a wildcard for one single character.</li> <li>An asterisk <b>*</b> can be applied as a wildcard for no or many characters.</li> </ul>



## Automatic Archiving

The automatic archiving function copies workspace, method, and sample files, which are either automatically or manually saved by the user, to a user-defined directory.

The **Automatic Archiving** option is only available in the **magellan Tracker** version and can only be enabled by users with **Modify general options** rights.

**Automatic archiving**  
group box

- **Enable archiving** check box: select this check box to activate automatic archiving.
- Click the file browser button (“...”) to browse for the archiving directory.



### Note

*It may happen that a selected archive directory becomes invalid, e.g., a network drive. In such a case magellan will not explicitly warn the user but will make an entry in the System Audit Trail's log file.*



### Note

*Please note that files are saved in the archiving directory only from the moment of activating the Auto Archive function. Files which have been saved before activating the Auto Archive function are not saved in the archiving directory.*

## 9. Miscellaneous Icon

### 9.2.2 Import Raw Data

By using the **ASCII File Import** function, the user can process ASCII data files in **magellan** which already contain measurement data and additional transformations. Some data format definitions must be performed in advance to guarantee correct data retrieval. For example, the individual data must be separated from the data list by specified separators.

Further options which must be specified are: Plate format, number of measurements, measurement interval, and type of data order, orientation and physical unit of the values.

Data import fails if the ASCII file does not contain as many entries as specified by the plate format.

Once the required options have been defined, select the desired file from the **files selection** field and retrieve the file data by clicking the **Open** button.

The **Open** dialog box is a standard Windows 'open file' dialog box with file navigation elements, a text field for entering a file name and a drop-down list for the selection of a file type (\*.asc).

Additionally, the **Open** dialog box contains the following elements for setting ASCII-Options:

<b>Format</b> option button	It defines the expected data format <b>Table</b> or <b>Matrix</b>
<b>Separator</b> group box	It defines which character is used for the separation of the data fields of the list or matrix: <ul style="list-style-type: none"> <li>• Tabulator if <b>Tabulator</b> is selected.</li> <li>• Any other character entered in the <b>Other</b> text-field.</li> </ul>
<b>Orientation</b> option button	It defines the orientation of the data, i.e., either <b>horizontal</b> or <b>vertical</b> .
<b>Measurement Parameters</b>	
<b>Info</b>	The box shows the following parameters: <ul style="list-style-type: none"> <li>• Plate format</li> <li>• Data unit</li> <li>• Number of measurements</li> <li>• Measurement interval</li> </ul>
<b>Measurement Parameters</b> button	Select the measurement type, the plate type, kinetic cycle number and interval.

### 9.2.3 Convert To

The **Convert Documents – Convert to** dialog box enables the user to convert **magellan** files from the current **magellan** version to files for previous **magellan** versions.



#### Note

***This option is available only when the current user has local administrator rights for the Windows system.***



**CAUTION**

**AFTER CONVERSION, METHODS MUST BE VALIDATED, BECAUSE THE CONTENT OF THE CONVERTED FILES MAY DIFFER SLIGHTLY FROM THE ORIGINAL FILE (E.G. CONTENTS OF PRINTED REPORT, ETC.)**

The **Convert Documents** dialog box contains the following elements:

<b>Document type</b> group box	Select the document type for conversion
<b>Select all</b> button	Click this button to select all displayed files in the file list
<b>Filename</b> list	All files available for conversion are displayed. Click a file to select it for conversion. By holding the Shift-key, multiple file selections are possible.
<b>Source path</b> edit field	The <b>Source path</b> edit field contains the path where the files to be converted are stored. Click the ... button on the right of the text field to change the path.
<b>Destination path</b> edit field	The <b>Destination path</b> edit field contains the path where the converted files are stored. Click the ... button on the right of the text field to change the path.
<b>Convert</b> <b>document(s)</b> button	Click this button to start conversion.
<b>Version</b> drop down menu	Select from the drop-down menu the version of <b>magellan</b> the files shall be converted to.
<b>Progress bar</b>	This bar shows the progress of the conversion.



**WARNING**

**THE FILES MAY CONTAIN FEATURES THAT ARE NOT COMPATIBLE WITH THE SELECTED FORMAT. THESE FEATURES ARE THEN UNAVAILABLE.**

## 9.2.4 Convert From

The **Convert Documents – Convert from** dialog box allows to convert **magellan** files from previous versions to the current file format. Standard **magellan** files can also be converted to **magellan** Tracker files.



**Note**

*Files for conversion are displayed only if magellan is connected with the instrument (measurement or demo mode) for which the files were generated.*



**Note**

*Files from magellan versions earlier than 4.0 must be converted to be used.*

## 9. Miscellaneous Icon



**Note**  
*Files from magellan Standard must be converted to be used with magellan Tracker.*



**CAUTION**  
**AFTER CONVERSION, METHODS MUST BE VALIDATED, BECAUSE THE CONTENT OF THE CONVERTED FILES MAY DIFFER SLIGHTLY FROM THE ORIGINAL FILE (E.G. CONTENTS OF PRINTED REPORT, ETC.)**

The **Convert Documents** dialog box contains two tabs.

The **magellan 2.x/magellan 3.x** tab contains the following elements:

<b>Document type</b> group box	Select the document type for conversion, e.g., a method.
<b>Customize new method specific options</b> group box	Several global options – in <b>magellan</b> versions lower than V4.0 – are now method specific. To set these options correctly in the method and workspace files, use one of the export buttons or the Workspace name... button.
<b>Select all</b> button	Click this button to select all displayed files in the file list
<b>File name</b> list	All files available for conversion are displayed. Click a file to select it for conversion. By holding the Shift-key, multiple file selections are possible. <b>Note!</b> Only workspaces and methods created with the currently connected instrument are displayed.
<b>Source path</b> edit field	The <b>Source path</b> edit field contains the path where the files to be converted are stored. Click the ... button on the right of the text field to change the path.
<b>Destination path</b> edit field	The <b>Destination path</b> edit field contains the path where the converted files are stored. Click the ... button on the right of the text field to change the path. <b>magellan Tracker:</b> this path cannot be modified.
<b>Convert document(s)</b> button	Click this button to start conversion.
<b>Progress bar</b>	This bar shows the progress of the conversion.



**WARNING**  
**TESTS DO NOT CONTAIN MEASUREMENT PARAMETERS. WHEN CONVERTING A TEST TO A METHOD THE MEASUREMENT PARAMETERS HAVE TO BE DEFINED. MAKE SURE THE MEASUREMENT PARAMTERS FIT TO THE SELECTED TEST.**

The **magellan 4.x / 5.x** tab—available only with **magellan Tracker**—contains the same window elements as the previously described tab, except that the following options are not necessary:

- Document type test: Tests are not available with **magellan 4.x / 5.x**.

Customize new method specific options: These options are already customized in **magellan 4.x / 5.x** files.

### 9.2.5 Save Log Files

All log files can be saved as zip archive by clicking the **Save Logfiles...** button. The zip archive can now be named and saved in a defined directory. In case of any measurement or status error during performance of **magellan**, this archive contains well data, status (e.g., overflow, lamp low) or calculation error(s) and can be easily sent to your local helpdesk for support request.

## 9.3 Options

Several selections and adjustments which are valid throughout the complete menus and wizards of **magellan** are defined in the **Options** dialog box. If **magellan** user administration is activated, several settings are user dependent. The **Options** dialog box is divided into individual tabs:

- Paths tab
- Copy tab
- Plate View tab
- Miscellaneous tab

The requested options have to be entered in the corresponding tabs. Click **OK** to save the changes and to close the dialog box.

User dependent options (every user can modify the options for his convenience) are:

- Default paths (only in **magellan** Standard)
- Copy to clipboard and Excel options
- Plate view
- Skip welcome page
- Start with wizard list or favorites page
- Move plate in after startup

The following user dependent options cannot be set in the options dialog box:

- Selected Printer
- Printout orientation.
- Printout paper size and source.
- Printout font and color.
- Default identifier types.
- Jumping direction for sample ID input.
- Import raw data settings.
- Default for Export options, Export to ASCII file, Export to Excel, and Workspace Name.
- Graph dialog box size

The following options can only be modified by a user with the appropriate right. These options are then valid for all users:

- Language
- Demo mode allowed
- Suppress 'not monotone' warning for standard curve
- Favorites
- Accepted HUIDs

## 9. Miscellaneous Icon

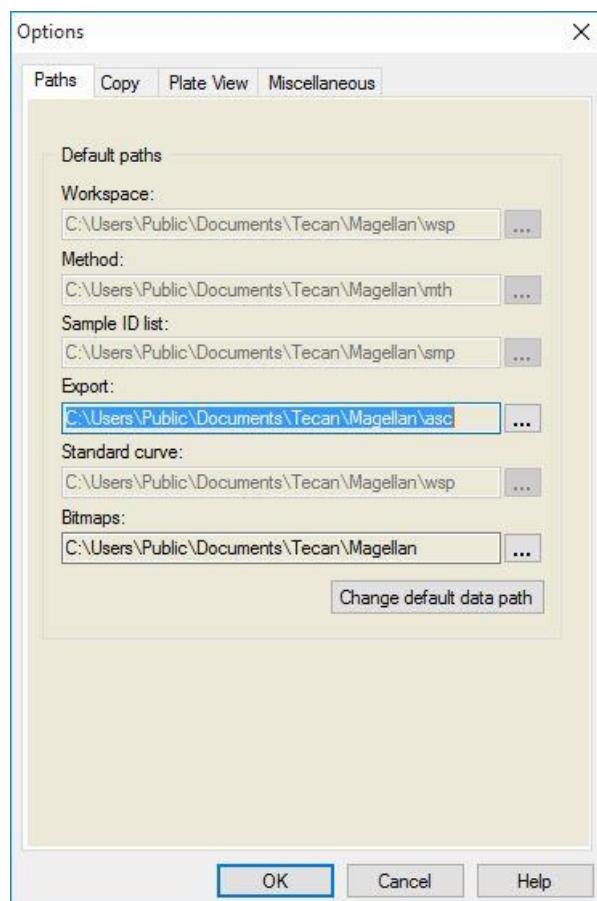


### Note

*In magellan Standard the data path can be set by the user, in magellan Tracker the data path is a general setting, valid for all users.*

### 9.3.1 Default Data Paths

This tab defines the default paths the different file types used in **magellan** are to be saved in. These predefined paths are set upon the software installation of **magellan** and can be changed in the corresponding data fields of the **Paths** tab.



The **Paths** tab contains the following elements:

#### Default paths text fields

A text field for each of the following file types is displayed, containing the corresponding default paths:

- **Workspace**
- **Method**
- **Sample ID list**
- **Export:** for measurement data exported to ASCII files.
- **Standard curve:** The path for standard curves is always the same as the path for workspaces.
- **Bitmaps:** for bitmaps created from graph dialog boxes.



#### buttons

Click the **...** buttons next to the text fields, to open a standard Window dialog box, where a different path for the generated files can be selected.

**Change default data path button**

Only available in **magellan** Tracker. Click this button to change the default data path for saving workspaces, methods, sample ID lists and standard curves files. **magellan** Administrator and System Administrator rights are necessary to modify default data paths.

**WARNING**

**THE SOFTWARE MAY NOT BE ABLE TO ASSIGN THE CORRECT FILE SYSTEM RIGHTS FOR A USER-DEFINED DEFAULT DATA PATH! THIS MUST BE DONE MANUALLY BY THE SYSTEM ADMINISTRATOR. DELETING OR MODIFYING FILES IN THE DEFAULT DIRECTORIES MUST NOT BE ALLOWED.**

**Note**

*In magellan Tracker, only the Export and the Bitmap paths can be modified.*

### 9.3.2 Copy/Export Options

In a workspace document the **Edit – Copy** and **Edit – Copy to Excel** commands allow the user to export measurement data to the clipboard or directly into an Excel worksheet. In the **Copy** tab is specified in which way the content of a plate is handled in case of a data transfer.



## 9. Miscellaneous Icon

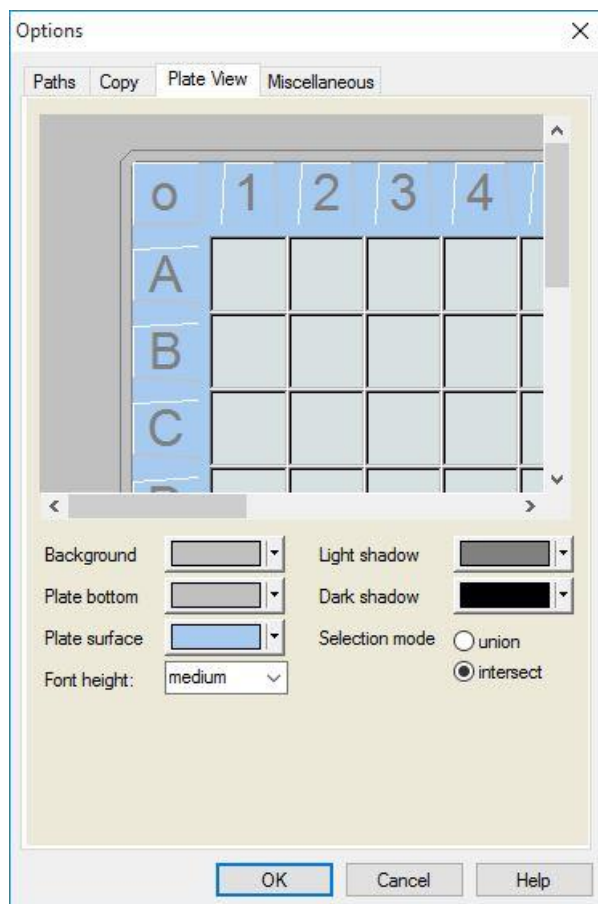
The **Copy** tab contains the following elements:

<b>Matrix format</b> group box	<p>The user also has the following opportunities to define how he would like the data to be displayed.</p> <ul style="list-style-type: none"> <li>• <b>Rows in horizontal order</b> option button Rows of data from the microplate will be copied in horizontal order.</li> <li>• <b>Rows in vertical order</b> option button Rows of data from the microplate will be copied in vertical order. This results in a transposed matrix.</li> <li>• If the <b>Add row/column labels</b> check box is selected, the row and column information like in XFluor is added when copying data.</li> </ul>
<b>Copy to clipboard options</b> group box	<p>A format for the decimal point of numbers must be selected for the transferred data:</p> <ul style="list-style-type: none"> <li>• <b>Point (x.xxx)</b> option button Example: 7.893</li> <li>• <b>Comma (x,xxx)</b> option button Example: 7,893</li> </ul>
<b>Copy to Excel options</b> group box	<p>The option buttons enable to define where to position the transferred data within Excel.</p> <ul style="list-style-type: none"> <li>• <b>New workbook</b> option button Transferred data will be stored in the first worksheet of a new workbook. A new file will always be created, no matter if Excel is started or not.</li> <li>• <b>New worksheet</b> option button Transferred data will be put into a new worksheet within an open, active Excel workbook. If Excel is not open when selecting this option, it will be opened and a new workbook will be created, the requested data is inserted into the first worksheet.</li> <li>• <b>Insert into worksheet at cell</b> option button and cell coordinates text field Transferred data will be placed into the cell indicated (default is cell <b>A1</b>) of an open, active Excel worksheet. If Excel is not open when selecting this option, it will be opened and a new workbook will be created, the requested data is inserted into the first worksheet.</li> <li>• <b>Append to current worksheet</b> option button This option will simply append the data to the current worksheet. If Excel is not open when selecting this option, it will be opened and a new workbook will be created, the requested data is inserted into the first worksheet.</li> </ul>

### 9.3.3 Plate View Settings

In the **Plate View** tab, the look of the plate view can be customized. The colors can be changed for the different regions by selecting the desired color from a drop-down list. The selection mode for marking wells can also be defined here. The font size can be adjusted as well.



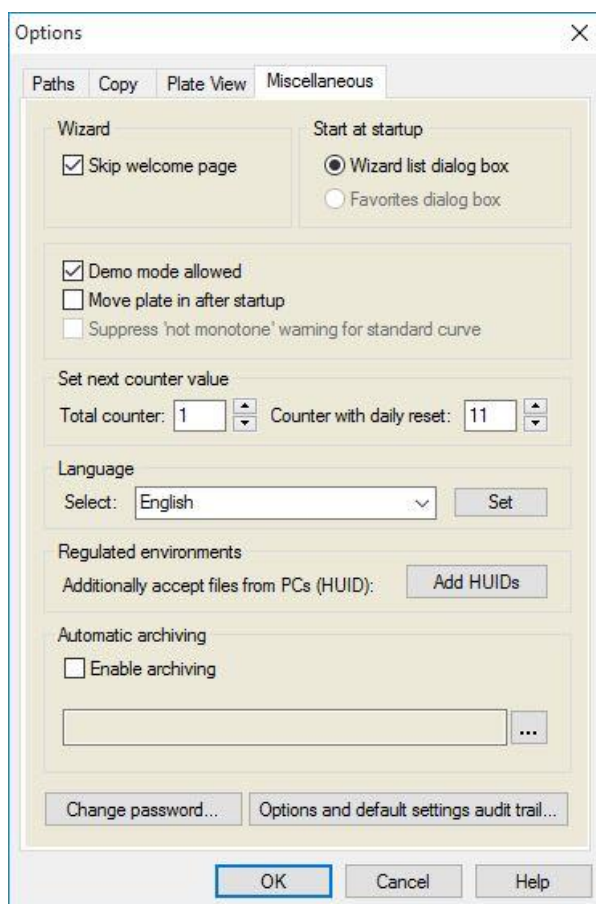


The **Plate View** tab contains the following elements:

<b>Background</b> button	The background color of the <i>Plate view</i> window can be selected.
<b>Plate bottom</b> button	The frame color of the displayed plate can be selected.
<b>Plate surface</b> button	The surface color of the displayed plate can be selected.
<b>Font height</b> drop down list	The font height for the text within the wells can be selected: <ul style="list-style-type: none"> <li>• Small</li> <li>• Medium</li> <li>• Large</li> </ul>
<b>Light shadow</b> button	The light-shadow color of the plate frame can be selected.
<b>Dark shadow</b> button	The dark-shadow color of the plate frame can be selected.
<b>Selection mode</b> option buttons	Here the selection mode for marking wells with the mouse is established: <ul style="list-style-type: none"> <li>• <b>Union</b> allows selecting wells only when the mouse has marked the complete area of the well.</li> <li>• <b>Intersect</b> allows for the selection of wells when only a part of the well has been marked with the mouse.</li> </ul>

## 9. Miscellaneous Icon

### 9.3.4 Miscellaneous



The **Miscellaneous** tab contains the following elements:

<b>Wizard</b> group box	When selecting the <b>Skip welcome page</b> check box, the welcome page of the wizard is not displayed when opening a wizard. The wizard starts at the second of its windows.
<b>Start at startup</b> group box	Selecting the <b>Favorites dialog box</b> check box defines that instead of the <i>Wizard List</i> the <i>Favorite dialog</i> will show up after the start of the <b>magellan</b> software.
Group box	<ul style="list-style-type: none"> <li>• <b>Demo mode allowed</b> check box: Select this option to allow connecting to a simulated instrument. This option is helpful if already measured data shall be evaluated. Then, no instrument is needed.</li> <li>• <b>Move plate in after startup</b> check box: If the checkbox is selected and an instrument is connected, the plate carrier is moved in automatically after startup.</li> <li>• <b>Suppress 'not monotone' warning</b> check box: Select this option to suppress the 'not monotone' warning. This option is useful if in a standard curve several points are taken in a flat area, and it is very likely that monotony is not given (i.e. the flat part of a logarithmic curve or other curve where a limit is approached). <b>Note!</b> This option is disabled in <b>magellan</b> Tracker.</li> </ul>

<b>Set next counter value</b> group box	<p>Two options are offered:</p> <ul style="list-style-type: none"> <li>• <b>Total counter</b> spin control enables to set the counter to any value. Displays the number which will appear in the name of the next workspace file created.</li> <li>• <b>Counter with daily reset</b> spin control enables to set the counter to any value. Displays the current number of workspace files that have been created during one day.</li> </ul>
<b>Language</b> group box	<p>The text field displays the applied language. A different language can be selected from the drop-down list. See <b>Set</b> below.</p>
<b>Set</b> button	<p>Select a different language and click the <b>Set</b> button to restart the program with the selected language</p>
<b>Change password</b> button	<p>Click this button to open a dialog box, where the user can change his password (only available with <b>magellan</b> User Administration activated).</p>
<b>Add HUIDs</b> button	<p>A list of additional HUIDs can be defined which allows the user to open files created on another computer (only available in <b>magellan</b> Tracker).</p>
<b>Automatic archiving</b>	<p>Select this function and specify a user-defined directory to copy all workspace, method and sample ID files which are either automatically or manually saved by the user to a user-defined archiving directory.</p>
<b>Options and default settings audit trail...</b> button	<p>Click this button to show the audit trail for options and default settings. The audit trail can be saved to an ASCII file (only available in <b>magellan</b> Tracker).</p> <p>Click <b>Save as file</b> to save this information as a .log or .txt file. The text can also be copied to a word processing program for printing.</p>

## 9. Miscellaneous Icon

### 9.4 User Administration (magellan Tracker)

There are three types of administrators mentioned in this publication:

**System Administrator** is responsible for any changes made to the computer's operating system.

The **Administrator** is responsible for user rights in the **magellan** software.

**magellan Administrator** has access to all features of the **magellan** software but cannot change user rights.

**magellan** offers password protection to prevent misuse of the software and to restrict access to parts of the software based on user rights.



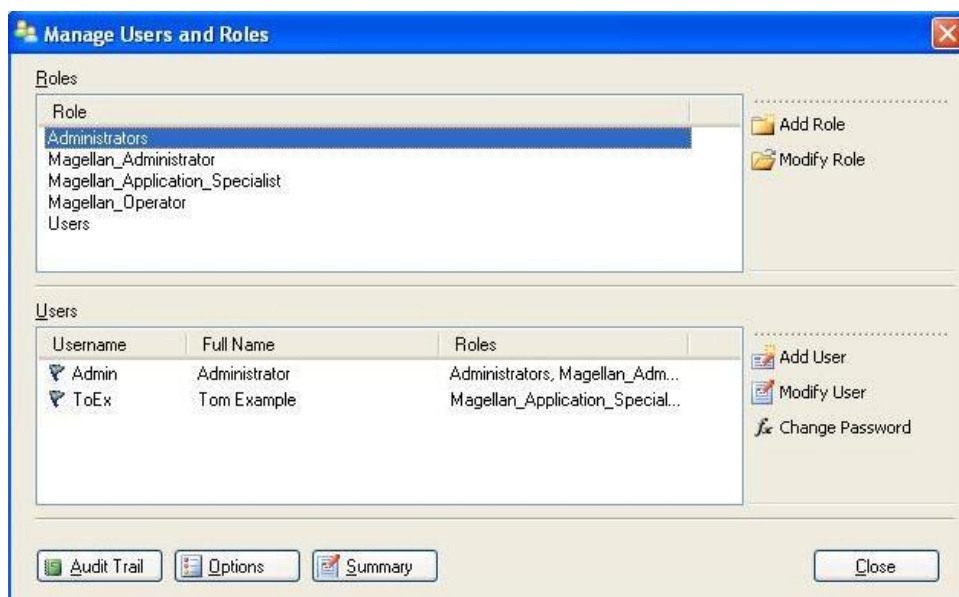
#### CAUTION

**TO PREVENT THE MISUSE OF USER RIGHTS AND FALSIFICATION OF DATA, IT IS RECOMMENDED THAT THE USER ADMINISTRATOR DOES NOT HAVE MAGELLAN RIGHTS (I.E. DOES NOT BELONG TO A MAGELLAN USER GROUP).**

**IDEALLY, THE USER ADMINISTRATOR SHOULD BELONG TO THE IT DEPARTMENT.**

Select **miscellaneous**  in the wizard window and click the **User**

**administration** icon . The **Manage Users and Roles** dialog box is displayed:



Users and roles can be added and modified; user rights can be defined. The **Manage Users and Roles** dialog box contains the following elements:

<b>Roles</b>	The <b>Roles</b> list shows all existing user groups (user levels).
<b>Add Role</b>	A new group with corresponding rights can be created.
<b>Modify Role</b>	Rights of an existing group can be modified
<b>Users</b>	The user list shows all existing users and which group they are member of.
<b>Add User</b>	A new user can be created.

<b>Modify User</b>	Full name, user level (group) or password of an existing user can be changed.
<b>Lock User</b>	A user account can be enabled / disabled. The button is visible only if a user name is selected.
<b>Audit Trail</b>	All modifications of the user administration database (e.g., creation of groups/users, change of rights, change of options, ...) are recorded in the user management audit trail written by the user management server.
<b>Options</b>	General login, password or email options can be modified
<b>Summary</b>	A detailed description of all existing users and user groups as plain text

### 9.4.1 Add/Modify User (*magellan Tracker*)

Click **Add User** in the **Manage Users and Roles** dialog box and the **Create User** dialog box appears:

The **Create User** dialog box contains the following elements:

<b>User Name</b>	A unique user name has to be entered when a new user is created. This name cannot be modified afterwards.
<b>Full Name</b>	Enter the full name of the user. This can be changed later.
<b>Password</b>	Enter the initial password. The password must be changed at the next login.

## 9. Miscellaneous Icon

Click OK and the **Modify User** dialog box appears:

The **Modify User** dialog box contains the following elements:

<b>Full Name</b>	Enter the full name of the user
<b>Roles</b>	Select from one of the existing user groups. The rights associated with that group are assigned to the user.
<b>Change picture</b>	User's picture can be added or changed.
<b>Delete picture</b>	Delete the user's picture.
<b>Change Password</b>	A new user's password can be defined. Note that the administrator needs not to provide the old password.

To modify a user, click **Modify User** in the **Manage Users and Roles** dialog box. In the **Modify User** dialog box proceed as described above.

### 9.4.2 Add/Modify Role

Click **Add Role** in the **Manage Users and Roles** dialog box and the **Create New Role** dialog box appears. Define a unique **Role Name**. Note that this name cannot be modified afterwards. Close the **Add Role** dialog box by clicking **OK**. Open the **Modify Role** dialog box:



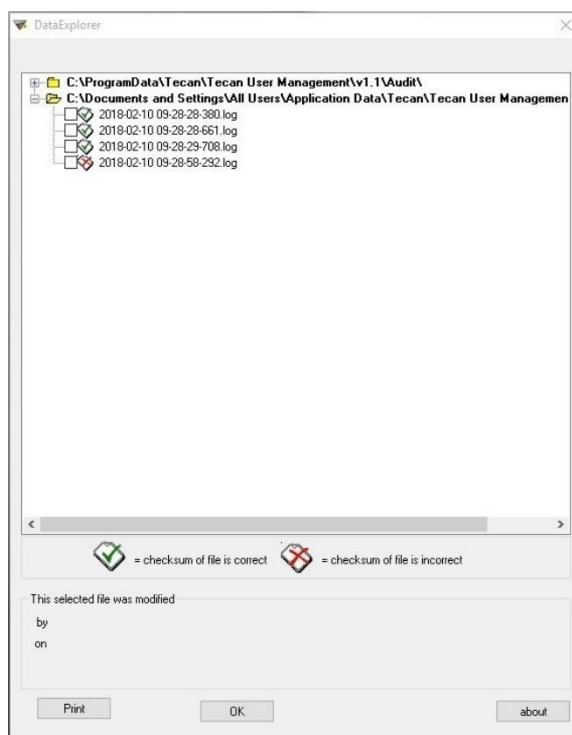
The **Modify Role** dialog box contains the following elements:

<b>Role Name</b>	The role name is defined in the <b>Add Role</b> dialog box.
<b>Application</b>	Tecan software component, i.e., Magellan.
<b>Rights</b>	The role represents a specific user level and corresponding user rights can be selected.

## 9. Miscellaneous Icon

### 9.4.3 User Administration Audit Trail

Click **Audit Trail** in the **Manage Users and Roles** dialog box and the **Audit Trail** dialog box appears:



All modifications of the user administration database are recorded in the user management audit trail written by the user management server.

To view a log file select it from the list (select checkbox) and click the **Print** button. The file is opened via pdf viewer and can then be printed. The green hook marks files with a correct checksum, the red cross marks files with an incorrect checksum.



#### Note

**Please note that the current log file always has a red cross because the file is still being altered as long as the software is open.**

## User Rights

There are three different security levels of user rights, the highest level of which is **Magellan Administrator**, who has access to all program functions. The **Application Specialist** and **Operator** levels are increasingly limited.

**magellan Standard:** The default rights are assigned as stated below.

**magellan Tracker:** Each right can be assigned or withdrawn by an Administrator and by default are assigned as stated below. The default set of rights is based on a typical laboratory environment.



#### CAUTION

**ADMINISTRATORS HAVE THE RESPONSIBILITY TO MAKE SURE THAT THE SETTINGS (AND ANY MODIFICATIONS) MATCH THE LABORATORY ENVIRONMENT DEFINED BY THE USER SOPS (STANDARD OPERATING PROCEDURES) AND COMPLY WITH APPLICABLE LAWS.**





**Note**

*For clinical diagnostic applications, the operating authority must validate all methods to ensure the safety of the results. A method is considered validated when signed by the operating authority. The operating authority is fully responsible for any results obtained.*

#### 9.4.4 User Administration Options

Click **Options** in the **Manage Users and Roles** dialog box and the **Edit Options** dialog box appears.

##### Login Options

<b>Lock application</b>	Lock of application after a specified time (1 min – 36500 h). To unlock the application the user has to reenter the password.
<b>Unsuccessful logins</b>	<p>After a number of consecutive unsuccessful logins (1 – 100), the user account is locked and optionally an alert email is sent to the system administrator.</p> <p>If the user account of a user administrator has been locked due to unsuccessful logins, this account remains locked for an idle time of 45 minutes. After this waiting time the account is unlocked and can be used again.</p>



**CAUTION**

**IF THE USER ADMINISTRATOR PASSWORD IS FORGOTTEN, USER ADMINISTRATION SETTINGS CANNOT BE CHANGED. IN THAT CASE, PLEASE UNINSTALL MAGELLAN FIRST AND PERFORM A NEW INSTALLATION AFTERWARDS (SEE CHAPTER 1.5 SOFTWARE INSTALLATION PROCEDURE).**

## 9. Miscellaneous Icon



### Note

***When uninstalling magellan, NO existing magellan files will get lost. All previous files can be found in a backup folder generated during the new installation procedure.***

## Password Options

Passwords have to contain a specific minimum number of characters. Passwords can be defined to contain non-alphanumeric characters and/or numeric digits. Password cannot be reused.

### Minimum password length:

Specify the required number of characters.

### Minimum required number of non-alphanumeric characters:

Specify the required number of non-alphanumeric characters.

### Minimum required number of numeric digits:

Specify the required number of numeric digits.

### Minimum number of password changes before re-use:

Specify the number of password changes.

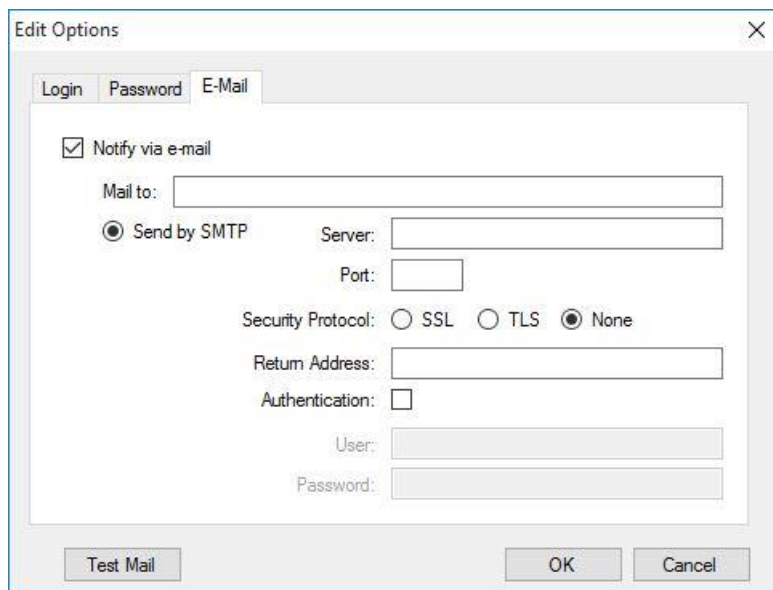
### Password expires after the specified number if of days:

User passwords expire after a configurable number of days. The user must then choose another password. Specify the required number of days (range: 1 to 36500 days).

### Allow empty password:

Select this checkbox if it is allowed to have an empty password for a user except for the administrator.

## Email Options



An administrator can be notified in case of potential security attacks (a user account has been locked because a number of unsuccessful logins).

An email can be sent to the entered email address:

- **SMTP server:** the IP address of the SMTP server has to be entered (f.e. SEUATEXCH01.eu.tecan.net)

Click **Test Mail** to send a test mail to verify that the settings are correct.



### Note

*The notification via e-mail requires an SMTP server without authentication.*

### 9.4.5 User Administration Summary

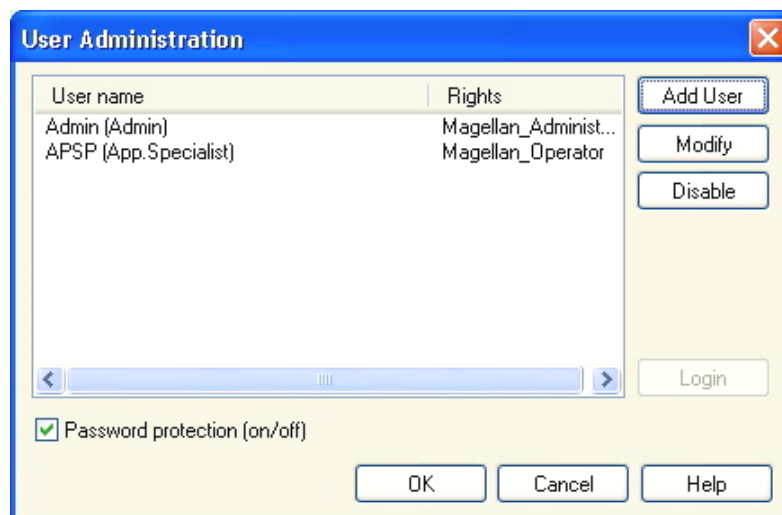
A detailed description of all existing users and user groups as plain text can be obtained by clicking **Summary** in the **Manage Users and Roles** dialog box.

The text can be copied to a word processing program for printing.

## 9. Miscellaneous Icon

### 9.5 User Administration (magellan Standard)

The **magellan** software offers protection against misuse of the software or access to the software from unauthorized users by providing a password protection facility.



User profiles can be defined at three different security levels. The highest level of security within the software is that of the **magellan Administrator**. This level gives access to all the program's functions and data editing facilities. For **Application Specialist** and **Operator** level, options are increasingly restricted.

Only the **User Administrator** can enable or disable the software's password protection, define new users or delete old users. If the users are logged in under their user name, the system will only give access to options according to their user rights definition.

The **User administration** dialog box contains the following elements:

<b>Login</b> button	The <b>Login</b> dialog box is displayed. A user can log in with his user name.
<b>User list</b>	<ul style="list-style-type: none"> <li>All currently setup users with their <b>User name</b> and <b>Rights</b> are displayed within this list.</li> </ul> Any user to be edited or deleted can be selected here.
<b>Add User</b> button	The <b>Add User</b> button opens the <b>User Rights</b> dialog box, in which a password, name, and user ID can be entered to define a new user.
<b>Modify</b> button	The <b>Modify</b> button opens the <b>User Rights</b> dialog box for modifying the selected user in the user list.
<b>Disable</b> button	The <b>Disable</b> button will disable the selected user in the current user list.
<b>Password protection (on/off)</b> check box	This check box enables to switch on/off the software's password protection facility. If enabled, the <b>Login</b> dialog box will be displayed upon starting <b>magellan</b> .

### 9.5.1 Add/Modify User (magellan Standard)

This dialog allows adding or editing of users and assigning them to a User group. For the rights of different user groups see chapter 9.6 User Rights .

The **User Rights** dialog box contains the following elements:

<b>User name</b> text field	Enter the full name of the user – as it shall be displayed
<b>UserID</b> text field	Define the user ID that the user has to enter for login
<b>User rights</b> option buttons	Define the level of access to the software's facilities available for the user: <ul style="list-style-type: none"> <li>• Operator</li> <li>• Application Specialist</li> <li>• Administrator</li> </ul>
<b>Password</b> text field	Define the user password (at least 5 characters)
<b>Confirm password</b> text field	Re-enter the password. For security concerns, in this field, the password characters are displayed as symbol.

Click the **OK** button to save and close the dialog box.

Click the **Cancel** button to close the dialog box without saving the entered settings.



#### Note

*If no users have been defined at all and the user administration shall be used, an administrator has to be defined first. Therefore, upon clicking the Login button, a short message is displayed. After that, the User Rights dialog box is displayed for entering the user information of the administrator (see chapter 2.3 Starting magellan/ Login).*

### 9.5.2 Login

This button is only enabled if user administration is activated but **Password protection** was not selected. Therefore, at startup the **Login** dialog was not displayed. To activate the password protected user administration, click the **Login** button.

### 9.5.3 Change User

To change the active user, click the **Change user** icon  in the wizard window. The **Login** dialog box is displayed.

## 9. Miscellaneous Icon

### 9.6 User Rights

There are three different security levels of user rights, the highest level of which is **Administrator**, who has access to all program functions. The **Application Specialist** and **Operator** levels are increasingly limited.

**magellan Standard:** The default rights are assigned as stated below.

**magellan Tracker:** Each right can be assigned or withdrawn by a User Administrator and by default are assigned as stated below. The default set of rights is based on a typical laboratory environment.



#### CAUTION

**USER ADMINISTRATORS HAVE THE RESPONSIBILITY TO MAKE SURE THAT THE SETTINGS (AND ANY MODIFICATIONS) MATCH THE LABORATORY ENVIRONMENT DEFINED BY THE USER SOPS (STANDARD OPERATING PROCEDURES) AND COMPLY WITH APPLICABLE LAWS.**



#### Note

*For clinical diagnostic applications, the operating authority must validate all methods to ensure the safety of the results. A method is considered validated when signed by the operating authority. The operating authority is fully responsible for any results obtained.*

The user rights are summarized in the table below and valid for both **magellan** versions, i.e., **magellan Tracker** and **magellan Standard**, unless otherwise stated:

User Rights	magellan Administrator	magellan Application Specialist	magellan Operator
Sample ID List			
<b>Create sample ID lists</b> Create a new sample ID list or save an existing one with a new name.	Yes	Yes	Yes
<b>Edit sample ID lists</b> Edit an existing sample ID list and save it with the same name.	Yes	Yes	No
<b>Sign sample ID lists*</b> Sign an existing sample ID list for review/approval.	Reserved for future use.		
<b>Modify signed sample ID lists*</b> Edit or change sample IDs in a signed sample ID list.	Reserved for future use.		
<b>Method</b>			
<b>Create methods</b> Create a new method or save an existing one with a new name.	Yes	Yes	No

User Rights	magellan Administrator	magellan Application Specialist	magellan Operator
<b>Edit methods</b> Edit an existing method and save it with the same name.	Yes	Yes	No
<b>Sign methods*</b> Sign an existing method for review/approval. Note: The right <b>Sign methods</b> alone is not enough to sign method files. You also need the right <b>Edit methods</b> . Additionally, the <b>Modify signed methods</b> right is also needed to add the <b>Approval signature</b> to files that already have a <b>Review</b> signature.	Yes	No	No
<b>Modify signed methods*</b> Edit a signed method and save it with the same name.	Yes	No	No
<b>Run unsigned methods*</b> With this right alone only approved methods can be used. Note: This right can be used in combination with the right <b>Run not approved methods</b> to allow the user to run all methods.	Yes	Yes	No
<b>Setup favorites</b> Add/Remove methods from the favorite list.	Yes	No	No
<b>Define multilabel measurement</b> Define methods using multilabel measurements.	Yes	Yes	No
<b>Define kinetic transformations</b> Define methods using kinetic transformations.	Yes	Yes	No
<b>Define concentration transformations</b> Define methods using concentration transformations.	Yes	Yes	No
<b>Define alias</b> Define methods using aliases for identifiers.	Yes	Yes	No
<b>Workspace</b>			
<b>Create workspaces</b> Perform a measurement and save the workspace with a new name – or – save an existing workspace with a new name.	Yes	Yes	Yes
<b>Edit workspaces</b> Edit an existing workspace and save it with the same name.	Yes	Yes	No

## 9. Miscellaneous Icon

User Rights	magellan Administrator	magellan Application Specialist	magellan Operator
<b>Sign workspaces*</b> Sign an existing workspace for review/approval. Note: The right <b>Sign workspaces</b> alone is not enough to sign workspace files. You also need the right <b>Edit workspaces</b> . Additionally, the <b>Edit signed workspaces</b> right is also needed to add the <b>Approval signature</b> to files that already have a <b>Review</b> signature.	Yes	No	No
<b>Edit signed workspaces*</b> Edit a signed workspace and save it with the same name.	Yes	No	No
<b>Continue evaluation when error</b> Continue calculation after errors have occurred	Yes	Yes	No <sup>1</sup> /Yes <sup>2</sup>
<b>Modify raw data (samples)</b> Edit or mask measurement data of samples.	Yes	No	No
<b>Modify raw data (standards)</b> Edit or mask measurement data of standards, controls, blanks.	Yes	No	No
<b>Import raw data</b> Import raw data from ASCII file in an existing workspace.	Yes	No	No
<b>Modify evaluation</b> Change evaluation (method) settings in an existing workspace.	Yes	Yes	No
<b>Reevaluate with another method</b> Reevaluate an existing workspace with another method.	Yes	Yes	No
<b>Modify layout</b> Change measurement parameters, concentration, and layout before starting a measurement.	Yes	Yes	No
<b>Standard curve</b>			
<b>Create standard curve files</b> Create a new standard curve and save it with a new name.	Yes	Yes	No
<b>Edit standard curve files</b> Edit an existing standard curve and save it with the same name	Yes	Yes	No
<b>Sign standard curve files*</b> Sign an existing standard curve for review/approval.	Reserved for future use.		



User Rights	magellan Administrator	magellan Application Specialist	magellan Operator
<b>Modify signed standard curve files*</b> Edit and change settings in a signed standard curve file.	Reserved for future use.		
<b>General</b>			
<b>Archive files</b> Move files to an archive location	Yes	No	No
<b>Set default paths**</b> Set individual paths for saving workspace, method, sample ID list, export and bitmap files.	Yes	Yes	Yes
<b>Define filter slides</b> Change the filter definition of the instrument	Yes	No	No
<b>Modify general options</b> Select language, suppress not monotone warning, allow demo mode.	Yes	No	No
<b>Print unsigned workspaces*</b> The results of an unsigned workspace can be printed.	Yes	Yes	Yes
<b>Run not approved methods*</b> This right alone allows the user to run already reviewed, but still not approved methods and approved methods. Note: This right can be used in combination with the right <b>Run unsigned methods</b> to allow the user to run all methods.	Yes	Yes	No
<b>Edit reviewed method*</b> Reviewed (but not approved) methods can be edited.	Yes	No	No
<b>Edit reviewed workspace*</b> Reviewed (but not approved) workspaces can be edited.	Yes	No	No
<b>Reader Server</b>			
<b>Save plate definition files</b> Create or edit plate definition files.	Yes	No <sup>1</sup> /Yes <sup>2</sup>	No
<b>Save spin profile</b> Create or edit spin profile files.	Yes	No	No

\* user rights available in magellan Tracker only

\*\* user rights available in magellan Standard only


<sup>1</sup> magellan Tracker

<sup>2</sup> magellan Standard

## 9. Miscellaneous Icon

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### 9.7 About magellan

Select **About magellan**  to display the copyright information and software disclaimer:

In the **About magellan** dialog box, information about the currently installed version of the **magellan** software, the version numbers of the components (tab **components**), UDI information and the program license of the user are displayed (tab **license**).

### Register Wizard

For further details on the **Register magellan Wizard** see chapter 2.4.4 Registration Wizard.

## 10. Additional Features for magellan Tracker

### 10.1 User Administration

In **magellan** Tracker a user administration is obligatory. Refer to chapter 9.4 User Administration (magellan Tracker) for further details.

#### 10.1.1 Audit Trail

To become compliant with the **FDA Regulation 21 CFR part 11** every step done in **magellan** Tracker is documented. In the **Audit Trail** all modifications concerning the following data are listed:

- a method file
- a workspace file
- a Sample ID list
- a standard curve file
- the user administration database or
- options and default settings.

Each entry consists of the user (name and full name), date and time of change, whether the file was created or modified, and any audit trail comments.

#### Audit Trail of Methods, Workspaces, Sample ID lists

You can view the Audit trail using the **Audit trail** button at the save page of the wizards.

#### Audit Trail of a Standard Curve

Standard curves can be saved and afterwards be used for evaluation of data from another workspace. For the feature to load a standard curve from external file refer to chapter 4.3.8 Concentrations: Standard Curve of the Create/Edit a Method Wizard. For opening a previously saved standard curve in the standard curve graph refer to chapter 7.4.11 Control Bar: Concentrations.

To view the audit trail of the loaded standard curve, select **Audit trail** from the **View** menu in Standard Curve Graph dialog box.

#### Audit Trail of the User Administration Database

To view the Audit trail of the User Administration Database, select **Miscellaneous** icon in the **Wizard List** starting page and click **User Administration**.

#### Audit Trail of Options and Default Settings

To view the Audit trail of all options and default settings select **miscellaneous** icon in the **Wizard List** starting page and click **Options**. In the **Miscellaneous** tab the **Audit trail** button can then be selected.

## 10. Additional Features for magellan Tracker

### 10.2 File Handling

The measured data is always saved directly after the measurement.



**Note for magellan Tracker only:**  
*To guarantee that no manipulation (deleting) of data is possible  
 magellan users should not be Windows administrators.*

#### 10.2.1 Saving a File

A file, created and saved in **magellan** Tracker, is indicated with a “#” sign in its file name. The added “#” sign can only be seen in the appropriate subdirectory of **magellan**.

Example

method#1.mth

workspace#1.wsp

sampleIDlist#1.smp

#### 10.2.2 Changing a Method or Workspace File

Every time a method or workspace file is modified and saved, the number behind the “#” in the file name is automatically increased (e.g.: first version of a workspace: name#1.wsp; edit and save the new version to get name#2.wsp; After the next change name#3.wsp is created...). All versions of a file are listed in the appropriated subdirectories of **magellan**.



**Note**  
*When transferring Tracker files, it is necessary to transfer all versions of the file.*

#### 10.2.3 Opening a File

Only the last saved version of a file is available in the wizards of create/edit a method, create/edit a sample ID list, evaluate results and start measurement.

To view a previous version of a file, open the **Audit trail** in the saving page of the file, select the preferred version of the file by clicking once on the number and click **Save previous version as...** button. Rename the file and add some file remarks or Audit trail comments and open the file with the **Create/Edit a Method** wizard.



**Note**  
*If you want to compare a method with its previous versions a printout must be made, because two print preview windows cannot be opened simultaneously.*

### 10.2.4 Opening a File Created on Another PC – Add HUIDs

In the licensing process of **magellan**, three numbers are involved:

- Serial number of the software
- HUID (**H**ardware **U**nit **I**dentification Number) and
- License number (refer to chapter 2.4.3 Licensing magellan).

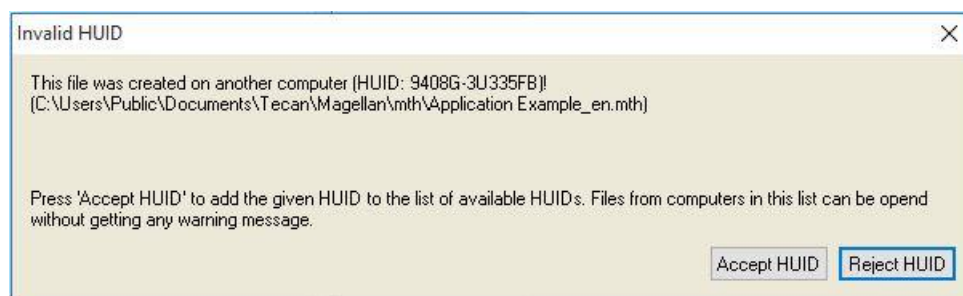
The HUID of a Personal Computer is configured during **magellan** registration and all files created and saved on this PC are linked to this special HUID.

If there is the need to work with **magellan** Tracker files, which were created on another PC, the HUID of this other PC must be accepted.

When a user with the right to **Modify general options** tries to open a document (sample ID list, method, workspace) from another PC, i.e. with a different HUID number, the user is automatically asked to add that number to the list of known HUID numbers. If the button **Accept HUID** is clicked, the HUID number will be added to the list and the document will be opened without further interactions.

**Hence this HUID number is always accepted.**

To view the list of accepted HUID numbers of other PCs click **Miscellaneous** icon in the wizard list starting page → **Options** → **Miscellaneous** tab. Click the **Add HUID** button and the dialog box with the other PCs HUID numbers is displayed.



## 10.3 System Audit Trail

The system audit trail is only available in the **magellan Tracker** version. The system audit trail function writes several **magellan** events into a log file (see table below). A new log file is created once per week and is stored under

**Windows 10:** C:\Users\Public\Documents\Tecan\LogFiles\SystemAuditTrail

A checksum, computed over the entire log file, is used to guarantee log file consistency and to protect the files against intentional and accidental changes. Log file consistency is always checked at start up. Invalid files will be immediately closed, marked as invalid by appending ".invalid" to the log file's name, and a new one will be created in its place.

Old or invalid logfiles are moved to the Archive folder, where they are protected against deletion.

## 10. Additional Features for magellan Tracker

### Magellan Events to be Tracked

Event	Event Type	Description
Magellan Start	StartUp	Magellan was started.
Magellan Exit	Exit	Magellan was closed.
Successful User LogOn	Login	A user logged in successfully.
Failed User LogOn	FailedLogin	Login failed, due to wrong username or password.
User LogOff	Logout	A user logged out.
New Workspace	New	A new workspace was created.
Load Workspace	Load	An existing workspace file was loaded into Magellan.
Save Workspace	Save	A workspace was saved.
New Method	New	A new method was created.
Load Method	Load	An existing method file was loaded into Magellan.
Save Method	Save	A method was saved.
New Sample ID List	New	A new sample ID list was created.
Load Sample ID List	Load	An existing sample ID list was loaded.
Save Sample ID List	Save	A sample ID list was saved.
Start Measurement	Measure	A new measurement was started.
Attach Signature	Signature	A workspace or method file was signed.
Export Results	ExportASCII ExportExcel ExportASTM ExportSampleTracking	Results were exported.
Prints Results	Print	Results were printed.
Automatic Archive	ArchiveFailed	The archiving of a workspace, method or sample ID list file failed.
CRC Failure	CRCFailed	Checksum of the previous log file was invalid.

# 11. Calculations

## 11.1 Evaluate Results – Calculation Procedure

Depending on the settings the calculation follows the procedure below:

1. Precalculation
  - 1.1 Spectra calculation
2. Check if data and evaluation settings fit together
3. Raw data statistic calculation
4. Transformation calculation
5. Kinetic parameter calculation
6. Kinetic transformation calculation
7. Concentration calculation
8. Concentration transformation calculation
9. Cutoff range determination
10. QC Validation
11. Statistic calculation

The procedure is repeated if

- QC Validation eliminated values using the eliminate functions.
- Interpolation parameters in the transformations are required.

Equal values for transformations in kinetic and multilabel measurements will be suppressed.

For calculations with different dilutions the Mean concentrations will be discarded.

In case the evaluation procedure is aborted through errors, results calculated until that point can be displayed.

In case some values are found to be FALSE, the following **Occurred Errors** dialog box will appear:

<b>Message</b> text field	The error message and a short explanation is displayed in a text field.
<b>Save as</b> file button	Click the <b>Save as file</b> button and the error protocol can be stored in an ASCII file.

In case the curve fit failed, depending on the user right, a question is displayed, where the user can decide to change the Analysis Type settings. After changes the evaluation procedure will be started from beginning.

In case the validation failed, depending on the user right, an error message box is displayed, or a question message box is displayed, where the user can decide to continue the calculation anyway. If the calculation is aborted, cutoff results cannot be accessed. However, on a printout a validation failed message will be included.

In case values or settings have been changed, a **message box** will appear.

<b>Message</b>	The instrument values have been changed. Do you want to re-start the result calculation?
<b>Yes</b> button	Click the <b>Yes</b> button to re-calculate the evaluation values.
<b>No</b> button	Click the <b>No</b> button to close the message. No re-calculation will be performed.

## 11. Calculations

### 11.1.1 Statistics

If a statistical value is calculated over e.g., the  $n$  replicates with values  $x_1 \dots x_n$  of a sample following formulas are used:

Name	Formula
Mean value, average value	$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$
Standard deviation	$s = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2}$ and $s=0$ for $n=1$
Variation coefficient in percent	$v = 100 \frac{s}{\bar{x}}$

For more information refer to chapter 11.3.5 Statistical Functions.

## 11.2 Spectra Data Reduction

Spectra data contains much more information than single wavelength measurements. Typical information extracted from spectra are intensities at specified wavelengths or at found peaks. During calculation it is also possible to calculate spectral blank reduction and ratio calculation.

### 11.2.1 Mathematical Description

**Blank reduction** is performed by subtracting the blank spectrum from the sample spectrum.

**Smoothing** is done with the Savitzky-Golay algorithm. The filter coefficients are calculated by a polynomial with degree 2. The smooth factor is treated as number of points:

$$g_i = \sum_{n=-n_L}^{n_R} c_n f_{i+n} \quad \text{where } n_R - n_L + 1 = \text{number of points}$$

The smoothing window is symmetrical, e.g., for a smooth factor of 5,  $n_L = -2$ ,  $n_R = 2$ .

For the lower and upper border of the spectrum, the window is asymmetrical, thus  $n_L = 0$ ,  $n_R = 4$  or  $n_L = -4$ ,  $n_R = 0$  respectively.

Before smoothing, all overflow values are removed from the spectrum.

#### Wavelength pick

- **Pick wavelength** – Retrieves the intensity of the selected wavelength
- **Calculate ratio** – Calculates the ratio by dividing the intensities at the selected wavelengths
- **Area** – Calculates the area under the spectrum within the selected wavelength range
- **Custom** – Reduces the spectrum using a user defined formula

#### Normalize

Reduces the spectrum into a range from 0 to 1.



### Peak find

The spectrum is differentiated, and all null points of the result are treated as potential peaks. The corresponding peaks are sorted by value and all invalid peaks are removed (e.g., overflows, local minima, values below the defined threshold). The highest value of the remaining items is selected as peak.

In practice this is often the maximum value of the spectrum.

### Custom formulas

Ability to define various data reductions for the spectra (refer to chapter 11.3.8 Spectra Functions).



#### WARNING

**SINGLE OUTLIERS CAUSED BY NOISE WILL ALSO BE DETECTED AS PEAK! THEREFORE, IT IS HIGHLY RECOMMENDED TO SMOOTH THE SPECTRUM BEFORE USING PEAK FIND!**

## 11.3 How to Write a Formula

### 11.3.1 Introduction

A variety of formulas are necessary for the calculations, the cutoff requirements and the validation. These formulas resemble the syntax of BASIC commands.

**All values are calculated in double precision although they are displayed depending on the desired number format.**

### 11.3.2 Formula Variables

All of the previously defined abbreviations for the identifiers contained within the analysis plate can be employed as variables in calculations.

For example:

PC1, SM1\_1, BL1...Average values

PC1\_1, SM1\_1\_1, BL1\_1...Individual values, individual replicates



#### Note

***The program differentiates between lower- and upper-case letters when dealing with these labels.***

It is also possible to work with the well coordinates.

**For example: A2, B3, H12**



#### Note

***Well coordinates must always be written using upper case letters.***



#### Note

***The symbol x refers to the current value within a well. For example: x-BL1...subtracts the empty value (blank) from the current value.***

## 11. Calculations



### Note

*The different cycles for kinetic measurements can be accessed by indices [ ], where "0" indicates the first cycle.*

For example:

*SM1\_1[0]... Average value of sample 1 of the first cycle*

*x[1]... value of current well of the second cycle*

*x[i] ... value of the current well and the current cycle*

### Serial Kinetic Subtraction – Calculation of Difference between Kinetic Cycles

Calculations over kinetic data can be defined by using the iteration variable 'i' in formulas. For instance, a numerical derivative of a kinetic curve can be performed using the formula  $x[i]-x[i-1]$ , which subtracts each kinetic cycle by the previous. But use of that formula would automatically lead to an error for cycle number 1. Therefore, set the formula  $\text{if}(i>0) \text{ then}(x[i]-x[i-1]) \text{ else ignore}()$  in the transformation edit field to prevent the subtraction of the first cycle.

The use of constants in formulas is identical to all other variables, the only difference being that a constant can contain characters (f.e. alpha, dilution).

There are two predefined accessors.

**concX ...**

**returns the concentration of the standard of the current well**

**dilX ...**

**returns the dilution of the sample or control of the current well**



### Note

*If more than one set of input data shall be used for calculations, select the appropriate data from the available data drop down list, activated in transformation edit fields of the Create/edit a method tab (refer to chapter 4.3.5 Transformed Data: Add New Transformation and chapter 7.4.9 Control Bar: Transformed Data).*



### Note

*Using one of the mathematical functions described in the following chapters, an "intellisense" help is activated to support correct writing of special formulas.*

### Formula Operators

Operator	Description
+	Plus
-	Minus
*	Multiplication
/	Division

Operator	Description
^	To the power of the exponent The symbol used to represent the expression “to the power of” is ‘^’. This character can be obtained by pressing the SHIFT key together with the number 6 key (but not on the numerical keypad.) Example: $x^3$ The value of the well will be increased to the power of three.
<	Less than
<=	Less than or equal to
>	Greater than
>=	Greater than or equal to
==	Equals
!=	Is not equal to
=	Assigned to



**Note**

**The difference between equals (==) and assign to (=).**  
**For example: If ( $x = 0.000$ ), then  $x = 1.000$  (If the current value of  $x$  is equal to 0 then set the value of  $x$  to 1)**

### 11.3.3 Formula Functions

The expressions “and” and “or” can be incorporated into the same equation using logic functions. The result from a logical equation will be either TRUE or FALSE and is therefore a Boolean value. The individual equations must be enclosed in brackets.

#### Logical Expressions

##### and

In equations of this nature, the result will be TRUE if both expressions are found to apply, otherwise a result of FALSE will be given. Example:

Where the value held by the well is 0.3

$(x > 0.0)$  and  $(x < 1)$  = TRUE

$(x > 0.0)$  and  $(x < 0.1)$  = FALSE

##### or

In equations of this nature, at least one of the expressions involved must be found to apply in order that a result of TRUE can be given.

**Example:** where the value held by the well is 0.3

$(x > 0.0)$  or  $(x < 0.1)$  = TRUE

$(x > 0.4)$  or  $(x < 0.1)$  = FALSE

## 11. Calculations

### if(...) then(...) else(...)

The following expressions are used in the program and, as an example, can be written in the following manner:

if (statement) then Term A else Term B

The statement:

The statement must be either true or false and written in brackets. If the statement is arrived at by means of logical operators (and/or), then the whole expression must be written here and enclosed in brackets.

Terms A and B:

If the statement is true, Term A will apply and if the statement is false Term B will apply.

It is not always necessary to include the else expression. If it is not present in the equation, no response will be given in the event of a false result.

The "if(...) then(...) else(...)" expression can also be used with Boolean terms for QC Validation.

#### **Example:**

*Check whether the value of a well lies within a defined range. If the result is yes, the well will be represented by the value 0.0, if the result is no, the value 1 will be used.*

*if (( x>-0.005) and (x<0.0)) then(0.0) else(1.0)*

### 11.3.4 Basic Functions

#### abs(argument)

This function gives the absolute sum of the argument.

Therefore  $(-1 \cdot x)$  where  $x < 0$  and  $(x)$  where  $x \geq 0$ .

#### **Example:**

*abs(-1) = 1*

*abs(1) = 1*

#### exp(argument)

This function raises the Euler (e) value to the power of the argument.

**Example:** *exp(1) =  $e^1 = 2.718$*

#### frac(argument)

This function separates out the fraction section of argument.

frac(): delivers the fraction section of a decimal value.

**Example:** *frac(1.7) = 0.7*

#### int(argument)

This function separates out the integer sections of argument.

int(): delivers the integer section of a decimal value.

**Example:** *int (1.7) = 1*

### Log(argument)

$\log(\text{arg1};\text{arg2})$

This function takes the logarithm of arg2 to the base of arg1.

**Example:**

The well holds a value of 100.

$\log(x;10)$

**The result here will be 0.5.**

### ln(argument)

This function takes the natural logarithm of argument.

**Example:**  $\ln(10) = 2,303$

### lg(argument)

This function takes the logarithm to base 10 of argument.

**Example:**  $\lg(10) = 1$

### round(argument)

This function rounds argument to an integer value.

**Example:**

To round 12.579 to two decimal places use the following formula:

$\text{round}(12.579*100)/100$

The result is 12.58.

### sqr(argument)

This function raises argument to the power of 2

**Example:**  $\text{sqr}(3) = 9$

### sqrt(argument)

This function takes the square root of argument

**Example:**  $\text{sqrt}(9) = 3$

## 11.3.5 Statistical Functions



**Note**

**Use single and not average or mean data as input data for transformations with statistical functions.**

### avg(argument) and mean(argument)

This function calculates the average value of argument. The argument must be an identifier.

**Example:**

$\text{avg}(\text{SM1})$

The average of all the samples in the first experimental group will be formed. Furthermore, the replicates of a value can be averaged:

$\text{avg}(\text{ST1\_1})$

**Averages all replicates of the first standard.**

## 11. Calculations

---

### **median(argument)**

This function determines the median of argument. The argument must be an identifier. The individual replicates are ordered in terms of size and the median determined by taking the middle value in the order. If the number of values is an even number, the average of the two middle values will be determined.

**Example:**

*Median (NC1)*

*Assume NC1\_1=0.1, NC1\_2=0.05, NC1\_3=0.04*

*The median value of these negative controls will be determined as follows.*

*The order of the values gives:*

*0.04 0.05 0.1*

*The median is therefore 0.05.*

### **medianPlate()**

The median of the whole plate can be determined using this function. The individual values are ordered in terms of size and the median determined by taking the middle value in the order. If the number of values is an even number, the average of the two middle values will be determined.

**Example:**

*medianPlate()*

Assume BL1=1, NC1=2, PC1=3, SM1\_1=4, SM1\_2=5 and no other wells defined.

The median of the whole plate is 3.

### **max(argument) and min(argument)**

This function calculates the minimum/maximum of argument. The argument must be an identifier.

**Example:**

*max(SM1)*

The maximum of all the samples in the first experimental group will be formed.

*min(ST1\_1)*

Determines the minimum of the individual replicates of the first standard.

### **maxAvg(argument) and minAvg(argument)**

This function gives the maximum/minimum average value of argument. The argument must be an identifier.

**Example:**

*minAvg(SM1)*

If a number of results are found for SM1, only the minimum average will be given.

### PointwiseCV(argument)

The average point wise coefficient of variation (CV) is determined. The result can be used to validate the standard curve. The argument must be an identifier.

#### Example:

*PointwiseCV(ST1)*

Assume

ST1\_1\_1=0.54 ST1\_1\_2=0.52 cv=2.668

ST1\_2\_1=0.72 ST1\_2\_2=0.77 cv=4.746

ST1\_3\_1=1.08 ST1\_3\_2=0.99 cv=6.148

The result of *pointwiseCV* is the average of the CV of ST1\_1, ST1\_2 and ST1\_3 and is 4.5209.

### Sum(argument)

This function calculates the sum of argument.

#### Example:

*sum(SM1)*

The sum of all the samples in the first experimental group will be formed.

*sum(ST1\_1)*

Determines the sum of the replicates of the first standard.

### stddev(argument)

This function calculates the standard deviation of argument. The argument must be an identifier.

#### Example:

*stddev(NC1)*

The standard deviation of the negative control in the first experimental group will be formed.

## 11.3.6 Elimination Functions

The elimination functions will be employed in the validation. In this way the user can make sure that the measurement values lie within a valid interval and delete any rogue values.

Three differing elimination functions can be employed when defining the validity intervals. The identifier that is to be influenced by the function is always the first parameter required when defining the elimination criteria.

All three elimination functions produce a logical result. TRUE is given when there are enough valid measurement values available and FALSE is given when less than the requirement is valid.

Invalid measurement values will be labeled with an exclamation mark.

## 11. Calculations

### eliminate (arg1; arg2; arg3; arg4)

The validation interval will be defined using a defined value.

This function eliminates values that lie outside of the validation range defined in arg2.

*arg1: Identifier name (NC1,PC1).*

*arg2: Value used to represent the range, dependent upon arg4.*

*arg3: Number of valid, individual values that must be available in order that an average can be generated. If too few values are available following the elimination, a result of FALSE will be given.*



#### Note

**For arg3:**

**a value of "2" or higher has to be defined. "1" is not accepted.**

*arg4: Represents the selection of whether testing will use the range average-arg2 to average+arg2 (argument of 1) or it will be checked whether the individual values lie below average+arg2 (argument of 0). In this case (argument of 0) there is no lower limit.*

The elimination function here determines the average of arg1. The value with the highest absolute deviation to the average value is then checked to ensure that it lies within the range according to arg4. Is the value lying outside of this range it will be viewed as being invalid. In this case the average calculation will begin again, excluding the previously discovered invalid value, and continue in this manner until no more rogue values can be found.

A result of TRUE will be delivered when enough valid individual values are available.

#### Example:

*eliminate(NC1;0.15;2;0)*

The average value will be generated for the negative controls. It will then be seen whether the individual negative controls lie above NC1+0.15. (There is no lower limit). If this is the case, the rogue value(s) will be eliminated as described above. If on completion, at least 2 individual values are valid, a result of TRUE will be returned; otherwise, a result of FALSE will be given.

### eliminatePerc (arg1; arg2; arg3; arg4)

The validation interval will be defined using a percentage of the average value.

This function eliminates values as described for function eliminate. The validation range is defined using a percentage (arg2) of the identifier.

#### Example:

*eliminatePerc(NC1;10;2;1)*

Individual values will be invalid if they deviate to an extent of more than 10% below or above the average. On completion, a minimum of 2 individual values must be valid in order that the negative controls are declared as being valid.



### eliminateRange (arg1; arg2; arg3; arg4)

This function eliminates values that lie outside of the validation range defined by arguments 2 and 3.

*arg1: Identifier name (NC1,PC1)*

*arg2: Lower limit of the selected range*

*arg3: Upper limit of the selected range*

*arg4: The number of valid, individual values that must be to proceed. If too few values are available following the elimination, a result of FALSE will be given.*

A result of TRUE will be delivered when enough valid individual values are available.

**Example:**

*eliminateRange(NC1; 0.0 ; 0.1 ; 2)*

The individual values for the negative controls must fall within the range of 0.0 and 0.1 to be valid. To achieve a result of TRUE, at least 2 of the values must be viewed as being valid.

### eliminateCV (arg1; arg2; arg3)

This function eliminates replicates until the CV of the remaining replicates is lower than the given CV (arg2). The replicates are eliminated step by step, beginning with the value with the highest difference to the mean value.

*arg1: Identifier name*

*arg2: Limit of accepted CV value*

*arg3: The number of valid, individual values that have to be left to deliver a positive result. If too few values are available following the elimination, a result of FALSE will be given.*

A result of TRUE will be delivered when enough valid individual values are available.

**Example:**

*eliminateCV(NC1; 15; 3)*

The calculated CV of the individual values of the negative control shall be below 15%. After the elimination, at least 3 replicates must be left to get TRUE as result.

### countDeleted(arg1; arg2)

This function checks if there are enough valid values available and returns TRUE or FALSE.

*arg1: The identifier, whose quantity is to be checked.*

*arg2: The lowest number of replicates that must be available.*

**Example:**

*countDeleted(NC1; 2)*

This function works in conjunction with the Eliminate functions in equations:

The Validation contains the following line:

if (NC1>0.5) then eliminateRange(NC1; 0; 0.5; 2)

If the average of the negative control lies above 0.5, then all replicates that lie outside of the range should be omitted.

This elimination will be processed once. If values for elimination are found, a new calculation will follow making sure that the average lies under 0.5 and a result of TRUE will be given.

## 11. Calculations

At this point it is not yet certain that the necessary number of replicates is available. This is then determined using the countDeleted function within an else statement:

if (NC1>0.5) then eliminateRange(NC1; 0; 0.5; 2) else countDeleted(NC1; 2)

The equation process (of the second run following the elimination) uses the else statement. The countDeleted function then checks, whether the given identifier in arg1 is available in the quantity specified in arg2. If this is the case a result of TRUE will be given, if not FALSE.

### Step by step example eliminate respectively eliminatePerc

The only difference between eliminate and eliminatePerc is the way for calculating the limits for the valid range (see above). The calculation sequence is the same for both functions. For the step-by-step description, eliminate is used.

**eliminate(NC1;0.15;2;0)**

<b>Individual values:</b>	<b>NC1_1 = 0.217</b>	$\overline{NC1} = 0.288$
	<b>NC1_2 = 0.439</b>	
	<b>NC1_3 = 0.208</b>	

Step 1: The individual values are sorted by their distance to the average.

$ NC1\_1 - \overline{NC1} $	<b> 0.217-0.288 </b>	<b>0.071</b>	<b>→</b>	<b>NC1_2 (0.439)</b>
$ NC1\_2 - \overline{NC1} $	<b> 0.439-0.288 </b>	<b>0.151</b>		<b>NC1_3 (0.208)</b>
$ NC1\_3 - \overline{NC1} $	<b> 0.208-0.288 </b>	<b>0.08</b>		<b>NC1_1 (0.217)</b>

Step 2: Calculation of upper limit:  $0.288+0.15 = 0.438$

Step 3: first comparison:

$0.439 > 0.438$  and therefore out of the valid range → Step 4: value of NC1\_2 is eliminated, and the average and the limit are recalculated.

Step 4: New avg =  $(0.217+0.208)/2 = 0.2125$

New limit =  $0.2125+0.15 = 0.3625$

Step 5: second comparison:

$0.208 \leq 0.3625 \rightarrow$  valid

$0.217 \leq 0.3625 \rightarrow$  valid

#### Result:

The replicate NC1\_2 doesn't fit into the given range and therefore has been eliminated.

Function returns TRUE because there are still two replicates left.

Note: In each calculation cycle (Step 1 to Step 4), only one replicate is deleted (the replicate with the highest distance to the average). The cycle is repeated until no replicate is deleted during the comparison step within the cycle.

### 11.3.7 Other Functions

#### ignore()

This function omits the values of chosen wells so they will not be incorporated into the calculations. Ignored values are displayed with a leading '!' and handled like eliminated values.

**Example:**

*if(x<0.9\*SM1\_1) then ignore()*

#### isInvalid()

This function gives a Boolean value, whether values within the well are valid or not. Invalid values for example can be caused by overflow values of the reader.

**Example:**

*if(isInvalid()) then x=3.0*

If the well contains an invalid value, the value 3.0 will be assigned. In this way, further calculations are possible, in spite of such values.

#### calcAlways(argument)

This function enables to calculate formulas on wells independent of the state of the value. argument can be any valid formula. The formula will be calculated even if the value is masked or invalid. This function can be used to calculate results that do not depend on the value of the used well.

**Example:**

*calcAlways(A)*

The value of parameter A of the standard curve formula is returned.

#### concX

This function can be used in concentration transformations. The result of **concX** is the original concentration of the well and can therefore only be used in wells with standards as identifier.

**Example:**

$x - \text{concX}$  gives the difference between the calculated and the original concentration of the well.

### 11.3.8 Spectra Functions

#### smooth(numPts)

Smooths with the given number of points.

#### minimum()

Delivers the minimum as data pair (wavelength, intensity).

#### maximum()

Delivers the maximum as data pair (wavelength, intensity).

#### normalize(wl)

Normalizes by using the intensity at the given wavelength.

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### **peak(threshold;wlStart;wlEnd;peakIndex:percLimit)**

Delivers the peak as data set (intensity, wavelength, width, area). Peaks lower than the threshold will not be found.

Peak search is done in the given wavelength range.

peakIndex = -1 → returns max. peak

peakIndex = -2 → returns min. peak

peakIndex = 0, 1, 2, ... → returns peak at the given index

percLimit is a percentage used for calculating width and area.

### **numPeaks(threshold;wlStart;wlEnd)**

Delivers the number of peaks found in the given wavelength range. Peaks lower than the threshold will not be found.

### **derive(degree)**

Calculates the derivate of the given degree. Valid degrees are 1 and 2; e.g. derive(2).

### **intensity(function)**

Delivers the intensity of either a data pair or a peak; e.g. intensity(minimum()).

### **wavelength(function)**

Delivers the wavelength of either a data pair or a peak; e.g. wavelength(maximum())

### **width(function)**

Delivers the width of a peak; e.g. width(peak0.5;450;650;-1;50)).

### **area(function)**

Delivers the area of a peak, e.g. area(peak0.5;450;650;-1;50)).

## 11.3.9 Examples

### Transformations

Transformations modify the current value of the well. The result must always be a numerical value.

#### **Blank reduction:**

$$x - BL1$$

The empty value (blank) will be deducted from the current value of the well.

#### **Blanking of a kinetic run:**

$$x - x[0]$$

The value of first point of the kinetic is used as blank and will be deducted from the values of all kinetic cycles.



#### **Note**

**The index "0" represents the first measurement of a kinetic run.**

**Ratio:**

$$x/PC1 * 100$$

Calculates the ratio between a sample and a control in percentages.

**DNA/Protein ratio:**

$$'Label1'!x/'Label2'!x$$

To calculate the DNA/protein ratio, a multilabel measurement must be defined. The first measurement uses a wavelength of 260 nm, the second measurement uses a wavelength of 280 nm.

**Conditional result:**

$$\text{If } (x < 0.0) \text{ then } 0 \text{ else } x$$

If the value of the well is less than 0, it will be represented by 0, otherwise it remains unchanged.

**Cutoff**

The cutoff dictates the limits to be applied when evaluating. The result must always be a numerical value.

**Label: POS**

Limit:  $NC1 * 1.15$

**Label: ??**

Limit:  $NC1 * 0.85$

**Label: -**

The result is positive (POS) when the absorbance is more than 15% above the average of the negative controls and negative (-) when it is more than 15% below the average. A result is declared as open (??) if it lies between these two values.

**QC Validation**

The validation serves to examine the validity of the test. The result must always be a logical statement, TRUE or FALSE.

$$(BL1 > -0.005) \text{ and } (BL1 < 0.120)$$

If the average value of the empty value falls within the range of -0.005 to 0.12, a result of TRUE will be declared.

$$\text{eliminateRange}(NC1; -0.005; 0.12; 2)$$

If a minimum of two negative controls fall within the range of -0.005 to 0.12, a result of TRUE will be declared.

$$\text{abs}(PC1 - NC1) > 0.25$$

The distance between the averages of positive controls and the negative controls must be greater than 0.25. If this is the case, a result of TRUE will be declared.

## 11. Calculations

### 11.4 Standard Curve Analysis Types

#### 11.4.1 Definitions

Given n base points  $(x_1, y_1), \dots, (x_n, y_n)$ ,  $x_1 < \dots < x_n$

Name	Formula
Correlation coefficient	$r = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2}}$
Average square deviation	$d = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2}$
Goodness of fit	$goodness = 1 - d$

#### 11.4.2 Analysis Type Parameters

The analysis type parameter (e.g., the slope A and the intercept B for linear regression) can be used in calculation. The available parameters are described below. **If there is more than one experimental group**, the analysis type parameters have a postfix of "B" for the second experimental group, "C" for the third experimental group and so on. Example: The slope of a linear regression in experimental group 3 can be accessed as "AC".

#### 11.4.3 Error Messages

If any of the values in the calculated concentrations lie outside of the range stipulated by the standards, the entry **>Max** or **<Min** will be displayed within the plate's wells respectively. If the user would nevertheless like to incorporate these values into the calculation, the Extrapolation option must be selected.

If the curve is not strictly monotone, an error message is generated.

If there are multiple solutions for a concentration calculation for a measured value, the entry MultPt will be displayed within the plate's wells.

#### 11.4.4 Point to Point

Using this process, the adjacent base points will be joined by means of a straight line.

A minimum of 2 base points is required for this calculation.

Extrapolation is not possible. There are no parameters for use as variables in the transformations.

If no concentration can be calculated the entry NoCalc will be displayed within the plate's wells.

##### Mathematical Description

Interpolation function:

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i} \cdot (x - x_i) \quad \text{if } x \in [x_i, x_{i+1}]$$

### 11.4.5 Linear Regression

A straight line will be formed, where the sum of the squared deviations of all base points is a minimum.

A minimum of 2 base points is required for this calculation.

If necessary, extrapolation can also be implemented in this process. In an evaluation with one experimental group, the slope and ordinate intercept serve as the variables A and B in the transformations. Furthermore, the correlation coefficient r may also be implemented.

In the Standard Curve dialog box following additional information is displayed:

Formula with coefficient values A (slope) and B (intercept)

Average square deviation d

Absolute value of the correlation coefficient r

#### Mathematical Description

Approximation function:

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto A \cdot x + B$$

where A and B are determined by minimizing the error function

$$err(A, B) = \sum_{i=1}^n (f(x_i) - y_i)^2$$

The solution is unique if

$$rank \begin{pmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{pmatrix} = n, \text{ which is true if } x_i \neq x_j \forall i, j = 1, \dots, n \text{ (see general condition)}$$

### 11.4.6 Non-Linear Regression

This approximation is designed especially for hyperbolical data. Ideally the measured values for low concentrations are high and the measured values for high concentrations are low and the region of interest is in the high concentration range.

The parameter calculation supported by the linear regression x/y is used for y.

A linear regression is carried out using the transformed data.

The result is expressed as the slope k and the intercept d.

From this result  $A = 1/k$  and  $B = d/k$  can be determined.

A minimum of 2 base points is required for this calculation.

If necessary, extrapolation can also be implemented in this process. In an evaluation with one experimental group, the coefficients A and B serve as variables in the transformations. Furthermore, the correlation coefficient r may also be implemented. The approximation is always applied to the unscaled base point values.

In the Standard Curve dialog box following additional information is displayed:

Formula with coefficient values A and B

Average square deviation d

Absolute value of the correlation coefficient r



**WARNING**

**THIS APPROXIMATION IS NOT CONTINUOUS AND THEREFORE IMPROPER DATA CAN CAUSE HUGE DEVIATIONS BETWEEN THE GIVEN BASE POINTS AND CALCULATED POINTS!**

**Mathematical Description**

Approximation function:

$$f : [x_1, x_n] - \{-b\} \rightarrow R$$

$$x \mapsto \frac{A \cdot x}{B + x}$$

where A and B are determined by solving the linear regression problem for the transformed base points

$$(x_1, \frac{x_1}{y_1}), \dots, (x_n, \frac{x_n}{y_n})$$

Linear regression:

$$g : [x_1, x_n] \rightarrow R$$

$$x \mapsto k \cdot x + d, \text{ minimizing}$$

$$err(k, d) = \sum_{i=1}^n (g(x_i) - \frac{x_i}{y_i})^2$$

The parameters A and B are calculated from k and d by

$$A = \frac{1}{k} \text{ and } B = \frac{d}{k}$$

This function f is not continuous at -B.

### 11.4.7 Polynomial

2<sup>nd</sup> order: parabolic or quadratic

3<sup>rd</sup> order: cubic

The user can select between a polynomial of order 2 calculation or a polynomial of order 3 calculation.

A minimum of 3 base points is required for a polynomial of order 2 calculation, whereas a minimum of 4 is required for the polynomial of order 3 calculation.

If necessary, extrapolation can also be implemented in this process. The parameters  $A = a_0$ ,  $B = a_1$  and  $C = a_2$  can be used in transformations with polynomial of order 2. For polynomial of order 3, the variables  $A = a_0$ ,  $B = a_1$ ,  $C = a_2$  and  $D = a_3$  can be implemented.

In the Standard Curve dialog box following additional information is displayed:

Formula with coefficient values A, B and C for polynomial of order 2 or formula with coefficient values A, B, C and D for polynomial of order 2

Average square deviation



### Mathematical Description

Approximation function:

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto \sum_{i=0}^{order} a_i \cdot x^i, \text{ order} = 2 \text{ or } 3$$

(n>order)

where  $a_{order}, \dots, a_0$  are determined by minimizing the error function

$$err(a_{order}, \dots, a_0) = \sum_{i=1}^n (f(x_i) - y_i)^2$$

The solution is unique if

$$rank \begin{pmatrix} x_1^{order} & \dots & x_1 & 1 \\ \vdots & & \vdots & \vdots \\ x_n^{order} & \dots & x_n & 1 \end{pmatrix} = order + 1$$

, which is true if  $x_i \neq x_j \forall i, j = 1, \dots, n$

## 11.4.8 Cubic Spline

The adjacent base points will be joined through the polynomial of order 3 calculation. The determination of the parameters is performed using the not-a-knot condition.

A minimum of 3 base points is required for this calculation.

Extrapolation is not possible. There are no parameters for use as variables in the transformations.

### Mathematical Description

Interpolation function features:

Piecewise polynomial of order 3.

Continuous second derivation at all base points.

$$\int_{x_1}^{x_n} \left( \frac{d^2 f}{dx^2} \right)^2 dx$$

Minimizes the integral, which is a simplified term for the deformation energy of a spline.

Not-a-knot condition: at  $x_2$  and  $x_{n-1}$  also the third derivation is continuous.

## 11.4.9 Akima

The Akima interpolation creates in some cases a smoother curve as the spline interpolation.

A minimum of 3 base points is required for this calculation.

Extrapolation is not possible. There are no parameters for use as variables in the transformations.

### Mathematical Description

This interpolation method uses piecewise polynomials of order 3.

The piecewise interpolation polynomial itself and its first derivation are continuous.

## 11. Calculations

### Method

The slopes  $m_i$  at all base points are estimated from the neighbor points by a special function:

$q_i = \frac{y_i - y_{i-1}}{x_i - x_{i-1}}$  are the slopes of the linear interpolator between point  $i$  and point  $i-1$ ,  $i=2, \dots, n$

$$m_i = \frac{q_i |q_{i+2} - q_{i+1}| + q_{i+1} |q_i - q_{i-1}|}{|q_{i+2} - q_{i+1}| + |q_i - q_{i-1}|}, i=3, \dots, n-2$$

Special cases:

Is  $q_i = q_{i+1}$ , set  $p'(x_i) = q_i = q_{i+1}$ .

Is  $q_{i-1} = q_i$  and  $q_{i+1} \neq q_{i+2}$ , so is  $y'_i = q_i$  (analog for  $q_{i+1} = q_{i+2}$ ).

$$m_i = \frac{q_i + q_{i+1}}{2}.$$

Is  $q_{i-1} = q_i$  and  $q_{i+1} = q_{i+2}$ , set

For the indexes 1, 2,  $n-1$ ,  $n$  the slopes cannot be estimated by this algorithm.

Now we have the following conditions for the 3<sup>rd</sup> order interpolation polynomial  $p_i$ ,  $i=1, \dots, n-1$

$$p_i(x_i) = y_i$$

$$p_i(x_{i+1}) = y_{i+1}$$

$$p'_i(x_i) = m_i$$

$$p'_i(x_{i+1}) = m_{i+1}$$

which are four conditions for each 3<sup>rd</sup> order interpolation polynomial  $p_i$ .

### 11.4.10 LogitLog

LogitLog is designed for sigmoid standard curves. LogitLog will always produce an S-shaped curve. The curve will asymptotically reach an upper and a lower limit, which can be independently established as the minimum and maximum limits. If the user has not established any limits here, the minimum and maximum base point value will be used. The approximation is always applied to the unscaled base point values.

A minimum of 4 base points is required for this calculation.

If necessary, extrapolation can also be implemented in this process. The parameters A, B, C and D can be employed as parameters in the transformations.

In the Standard Curve dialog box following additional information is displayed:

Coefficient values A, B, C and D

Average square deviation  $d$

Absolute value of the correlation coefficient  $r$  (correlation of data and fit)

#### Restrictions for the Process Application

LogitLog and Four Parameter approximation may only be employed when working with standard curves that meet following requirements:

- Sigmoid process applied to the standard data in relation to the concentrations
- Symmetrically generated curve in relation to the IC-50 value

- To calculate the curve correctly it is necessary to have a concentration value of zero and a value of infinite standard concentration (saturated value), so that the asymptotes can be determined. If these two values are not present within the standard curve, they can be defined manually using the **More standard curve parameters** option (Min, Max). If no Min and Max values are defined, **magellan** will base the process on the smallest and largest values present respectively.



### WARNING

**IF THESE REQUIREMENTS ARE NOT MET, APPROXIMATION OF THIS NATURE CANNOT BE CORRECTLY EMPLOYED.**

### Mathematical Description

The LogitLog regression is a function

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto D + \frac{A - D}{1 + \left(\frac{x}{C}\right)^B}$$

for the description of sigmoid correlation of data.

The parameter can be interpreted as:

$$A = \lim_{x \rightarrow 0} f(x)$$

$$D = \lim_{x \rightarrow \infty} f(x)$$

$$f(C) = \frac{A + D}{2}$$

A, D are determined as the minimum respectively maximum (or vice versa if the function is decreasing).

Then the linear regression problem is solved for transformed base points.

$$X = \log_{10} x$$

$$Y = \ln \left( \frac{\frac{D - y}{D - A}}{1 - \frac{D - y}{D - A}} \right)$$

$$g : [X_i, Y_i] \rightarrow R$$

$$x \mapsto k \cdot x + d, \text{ minimizing the error function}$$

$$err(k, d) = \sum_{i=1}^n (g(x_i) - Y_i)^2$$

The parameters B, C are determined from k, d:

$$B = -m \cdot \log_{10}(e)$$

$$C = e^{\frac{b}{B}}$$

## 11. Calculations

The parameters A,B,C,D, have appealing geometric interpretations.

A = response at a dose (x-value) of zero (keep in mind that x=0 does not appear on logarithmic plots)

D = response at an infinitely high dose

C = is the point of symmetry on the curve (IC50); and below this point the curve is a mirror image

B = is a measure of the steepness of the curve at the inflection point; in fact, it is (within a possible change of sign) the slope of the curve written in its Logit form

Notice that the curve is always decreasing (if A>D) or increasing (if A<D).

### 11.4.11 *Four Parameters*

Four parameter approximation needs to fulfill the same base point requirements as LogitLog.

The resulting curve will be produced using the Nelder and Mead Downhill-Simplex method. This method produces an increasingly more accurate approximation of the result throughout the interval. The four-parameter method requires considerably more time to be processed. As with LogitLog, an S-shaped curve is produced.

A minimum of four base points is required for this calculation.

If necessary, extrapolation can also be implemented in this process. The parameters A, B, C, and D can be employed as parameters in the transformations. The approximation is always applied to the unscaled base point values.

In the Standard Curve dialog box following additional information is displayed:

Coefficient values A, B, C and D

Average square deviation d

Absolute value of the correlation coefficient r (correlation of data and fit)

#### **Restrictions for the Process Application**

Refer to chapter 11.4 Standard Curve Analysis Types – LogitLog for further information.

#### **Mathematical Description**

Approximation function:

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto D + \frac{A - D}{1 + \left(\frac{x}{C}\right)^B}$$

### Method

First a LogitLog approximation is calculated.

The parameters A, B, C, D are optimized by the Downhill-Simplex algorithm, a minimization algorithm that needs only function evaluations but no function derivation.

The algorithm stops if an accuracy of 0.001 is reached (success) or the maximum number of 10,000 iterations is exceeded (failure) before the given accuracy is reached.

### Bibliography

Nelder, J.A., and Mead, R. 1965, Computer Journal, vol. 7, pp 308-313

## 11.4.12 Four Parameters – Marquardt

The four-parameter approximation needs to fulfill the same base point requirements as LogitLog.

The resulting curve will be produced using the Levenberg-Marquardt method. This method produces an increasingly more accurate approximation of the result throughout the interval. The four-parameter method requires considerably more time to be processed. As with LogitLog, an S-shaped curve is produced.

A minimum of four base points is required for this calculation.

If necessary, extrapolation can also be implemented in this process. The parameters A, B, C and D can be employed as parameters in the transformations. The approximation is always applied to the unscaled base point values.

In the Standard Curve dialog box following additional information is displayed:

- Coefficient values A, B, C and D
- Average square deviation d
- Absolute value of the correlation coefficient r (correlation of data and fit)

### Restrictions for the Process Application

Refer to chapter 11.4 Standard Curve Analysis Types – LogitLog for further information.

### Mathematical Description

Approximation function:

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto D + \frac{A - D}{1 + \left(\frac{x}{C}\right)^B}$$

### Method

First a LogitLog approximation is calculated.

The parameters A, B, C, D are optimized by the Levenberg-Marquardt algorithm, an iterative technique that finds a local minimum of a function that is expressed as the sum of squares of nonlinear functions.

The algorithm stops if an accuracy of 1E-7 (FLT\_EPSILON) is reached (success) or the maximum number of 30,000 iterations is exceeded (failure) before the given accuracy is reached.

## 11. Calculations

### 11.4.13 Five Parameters – Marquardt

The five-parameter approximation basically needs to fulfill the same base point requirements as LogitLog. The sigmoid curve may however be non-symmetric.

The resulting curve will be produced using the Levenberg-Marquardt method. This method produces an increasingly more accurate approximation of the result throughout the interval. The five-parameter method requires considerably more time to be processed. As with LogitLog, an S-shaped curve is produced.

A minimum of five base points is required for this calculation.

If necessary, extrapolation can also be implemented in this process. The parameters A, B, C, D, and E can be employed as parameters in the transformations. The approximation is always applied to the unscaled base point values.

In the Standard Curve dialog box following additional information is displayed:

- Coefficient values A, B, C, D, and E
- Average square deviation d
- Absolute value of the correlation coefficient r (correlation of data and fit)

#### Restrictions for the Process Application

Refer to chapter 11.4 Standard Curve Analysis Types – LogitLog for further information.

#### Mathematical Description

Approximation function:

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto D + \frac{A - D}{\left(1 + \left(\frac{x}{C}\right)^B\right)^E}$$

#### Method

The parameters A, B, C, D, E are optimized by the Levenberg-Marquardt algorithm, an iterative technique that finds a local minimum of a function that is expressed as the sum of squares of nonlinear functions.

The algorithm stops if an accuracy of 1E-7 (FLT\_EPSILON) is reached (success) or the maximum number of 30000 iterations is exceeded (failure) before the given accuracy is reached.

### 11.4.14 Weighting for Four / Five Parameter Fit – Marquardt / Polynomial Fit

Weighting influences the standard optimization algorithm.

The algorithm tries to optimize the weighted sum of least squares.

A weighting factor of one means no weighting.

Weighting factors greater than one mean that the specified point has higher priority for the resulting fit.

Weighting factors smaller than one indicate that the point is taken less into account.



#### WARNING

**WEIGHTS SHOULD ONLY BE USED IF THERE IS SEVERE STATISTICAL EVIDENCE, THAT GATHERED DATA AND ALGORITHM ARE APPROPRIATE.**

#### Mathematical Description

Average weighted square deviation

$$d = \sqrt{\frac{1}{\sum_{i=1}^n k_i} \sum_{i=1}^n k_i (y_i - f(x_i))^2}$$

#### Automatic calculation of weights using variance:

The weights are automatically calculated with  $1/SD^2$  where SD is the standard deviation of the replicates of the actual base point.

This means that data with high standard deviation is less weighted than data with low standard deviation.



#### WARNING

**WEIGHTING USING VARIANCE IS DANGEROUS WHEN TOO FEW REPLICATES ARE USED, BECAUSE THE STANDARD DEVIATION CAN THEN HAVE A HIGH RANDOM PORTION WHICH CONSIDERABLY INFLUENCES THE OPTIMIZATION ALGORITHM.**

#### Automatic calculation of weights using relative weights:

The weights are automatically calculated with  $1/Y^2$  where Y is the mean value of the actual base point. This means that the algorithm minimizes the relative distances of the data to the curve.

## 11. Calculations

### 11.5 Calculation of Dilution Series

#### 11.5.1 Detection of Dilution Series

The following criteria must be fulfilled to force **magellan** to detect a dilution series on the layout:

- Sample(s) with a minimum of four replicates
- Usage of at least four different dilution factors for the single replicates of a sample

**magellan** checks the whole layout and picks all found dilution series.

#### 11.5.2 Curve Parameter Calculation

Curve parameters are calculated for every found dilution series using the **Four Parameters – Marquardt** algorithm. In case of a failure the calculation is redone using the **Four Parameters** algorithm. Please refer to chapter 11.4 Standard Curve Analysis Types for more detailed information about the algorithms mentioned above.

#### 11.5.3 Calculation of IC Values

First the maximum intensity ( $I_{\max}$ ) and the minimum intensity ( $I_{\min}$ ) of every dilution series is picked.

##### Calculation of IC-intensity

If the 0% value is set to intensity 'Intensity 0'

$$I_{IC} = \frac{ICx}{100.0} * I_{\max}$$

If the 0% value is set to 'Min. intensity of dilution series'

$$I_{IC} = I_{\min} + \frac{(I_{\max} - I_{\min}) * ICx}{100.0}$$

##### Calculation of dilution at ICx

Using the curve parameters calculated in step 12.6.2 and the calculated IC-intensity the resulting dilution is calculated.

$$dilution = C * \left( \frac{A - I_{IC}}{I_{IC} - D} \right)^{\frac{1}{B}}$$



## 12. Application Example

### 12.1 Step-by-Step Example: Quantitative ELISA

A step-by-step example (quantitative test) of how to create a method in **magellan** is provided in this chapter. By following the instructions, you will learn how to define evaluations from a test kit description in **magellan**.

The method was created using a Sunrise in demo mode, but it is also possible to define the methods with another Tecan instrument connected, if it can measure absorbance.

#### 12.1.1 Test Kit Description

In the manufacturer's test kit description of a quantitative IgM – Antibody detections – ELISA the following instructions are found: Plate Layout

	1	2	3	4	5	6	7	8	9	10	11	12
A	BLK	C3	S1									
B	NC	C4	S2									
C	NC	C4	S2									
D	C1	C5	S3									
E	C1	C5	S3									
F	C2	C6	...									
G	C2	C6	...									
H	C3	S1										

BLK = Blank, NC = Negative control, C1 – C6 = Calibrators (Standards),  
S1 – S... = Samples

#### Measurement and Evaluation

Read plate at a wavelength of 492nm, reference at 620nm.

Blank reader/plate on well A1.

Concentrations of the Calibrators (Standards):

Calibrator 1	5 UA/mL
Calibrator 2	10 UA/mL
Calibrator 3	20 UA/mL
Calibrator 4	40 UA/mL
Calibrator 5	80 UA/mL
Calibrator 6	160 UA/mL

After the blank correction the optical densities (OD<sub>492</sub>–OD<sub>620</sub>) are plotted versus the concentration. The regression line that goes through these points is the standard curve.

## 12. Application Example

Interpretation of the test results:

IgM < 18 UA/mL	Negative
18 UA/mL ≤ IgM < 22 UA/mL	Intermediate
IgM ≥ 22 UA/mL	Positive

The calculated IgM concentration of both negative controls must be under 8 UA/mL.

### Data Handling

After the measurement, the data file (workspace) is stored automatically and a report containing the measurement parameters, plate layout, blanked values, standard curve, IgM-concentrations, cutoff definition, qualitative results of the samples and validations is created.

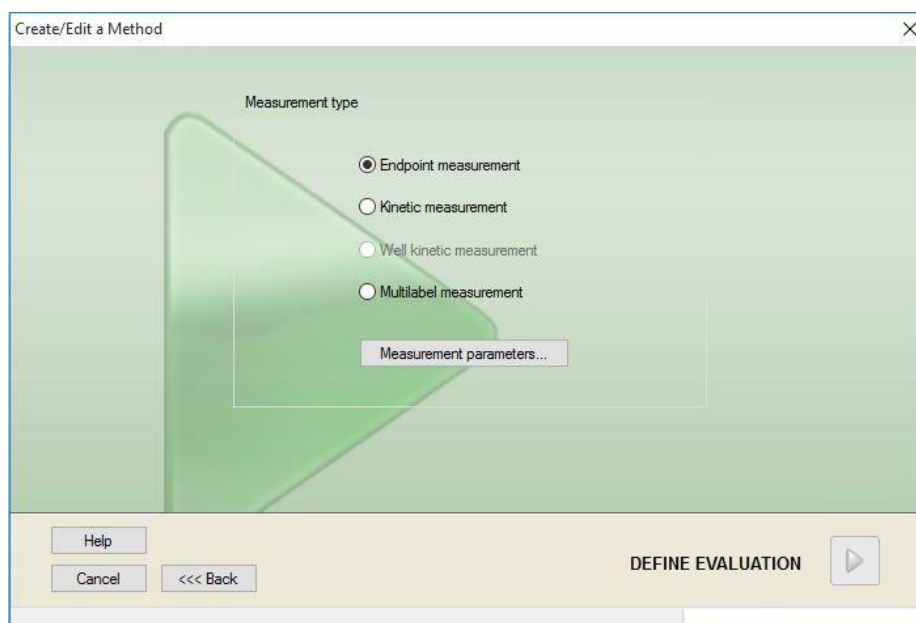
Additionally, the layout and the qualitative results are be stored as ASCII file.

#### 12.1.2 Create a Method

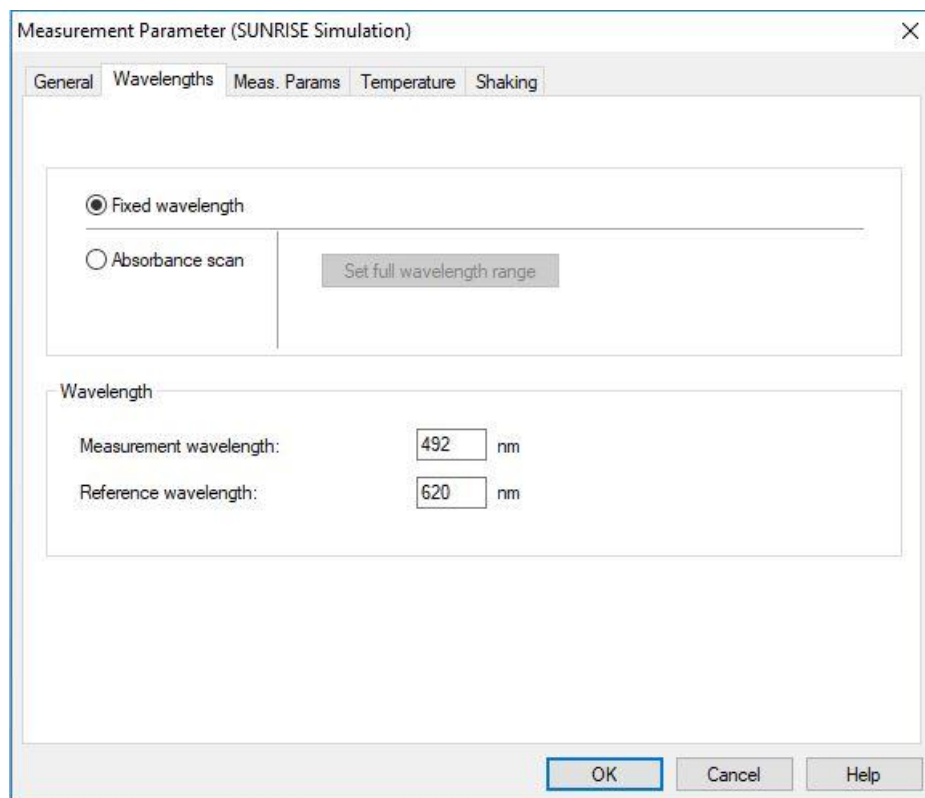
In the **Wizard List** dialog box, select **Create/edit a method** and click **OK**. Click next on the **Welcome** page of the **Create/edit a method wizard** and the **Select a file** dialog box appears. Select **Create new**.

### Measurement Parameters

Click **Next** and the **Measurement parameter** dialog box appears.



Select **Endpoint measurement** and click the **Measurement parameters** button. The following dialog box appears:

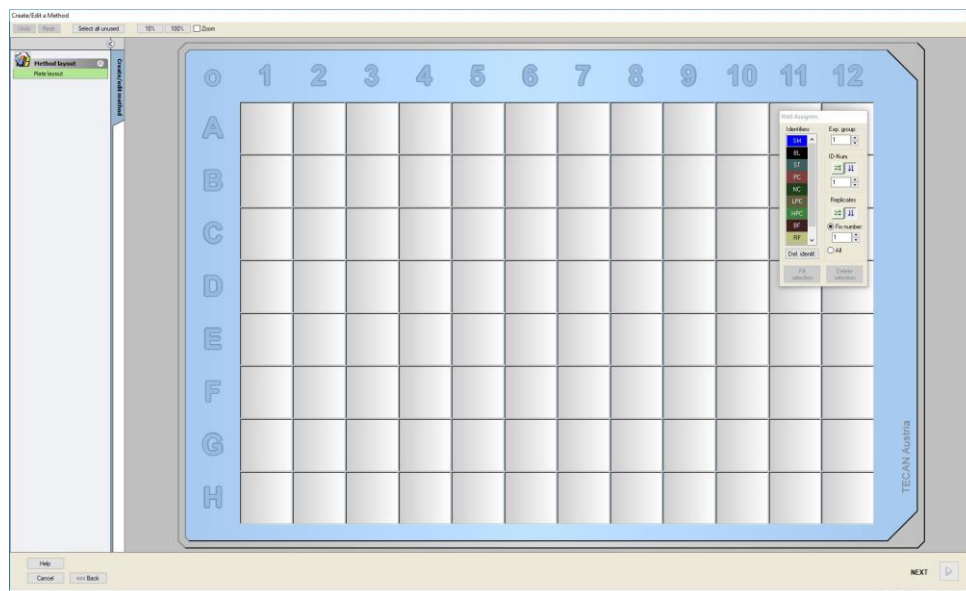


On the **General** tab select **Absorbance**.

On the Wavelengths tab select 492nm as Measurement wavelength and 620nm as Reference wavelength.

Click **OK** to return to the **Measurement parameter** dialog box.

Click **Define evaluation** and the **Plate layout** window is displayed.



## 12. Application Example

### Design Layout

Define the plate layout using the **Well Assignment** dialog box on the right side of the screen.

In the **Identifiers** group box, select **BL (Blank)**.

In the **Experimental** group box, the number **1** remains.

In the **Replicates** group box, select **All**.

Click well **A1**, which is then marked with a red border.

Click **Fill selection** and the well is labeled with the selected identifier type.



#### Note

***A single well can also be filled by double-clicking it.***

Now choose the following settings in the **Well Assignment** dialog box:

In the **Identifiers** group box, select **NC (Negative Control)**.

In the **Experimental** group box, the number **1** remains.

**All** is selected in the **Replicates** group box.

Starting at well **B1** click and drag the mouse to **C1**. The wells **B1** to **C1** are then marked with a red border.

Click **Fill selection** and the wells are labeled with the selected identifier type.

Next, calibrators (standards) must be assigned to wells **D1** to **G2**. Select the following settings in the **Well Assignment** dialog box:

In the **Identifiers** group box, select **ST (Standard)**.

In the **Experimental** group box, the number **1** remains.

In the **Replicates** group box, choose between **Fix number** and **All**:

#### Fix number

Only enabled for standards and samples where IDs can be used.

If this **Fix number** button is active a number can be entered in the corresponding text field. This number defines how many replicates are intended for this method. In the selected wells, the entered number of replicates for every ID is created.

Therefore, the number of selected wells must be a multiple of the entered number of replicates.

### All

All selected wells are defined as replicates. If an existing ID number for the samples and standards is chosen, the selected wells are then added as replicates to the existing replicates. With all other identifier types the selected wells are added as replicates to the existing replicates.



Two arrow buttons define the direction of the replicate and ID number sequence (horizontal or vertical).

In this example select **Fix Number** and **2**.

In the **ID-Number** box and in the **Replicates** group box select the **vertical arrows**.

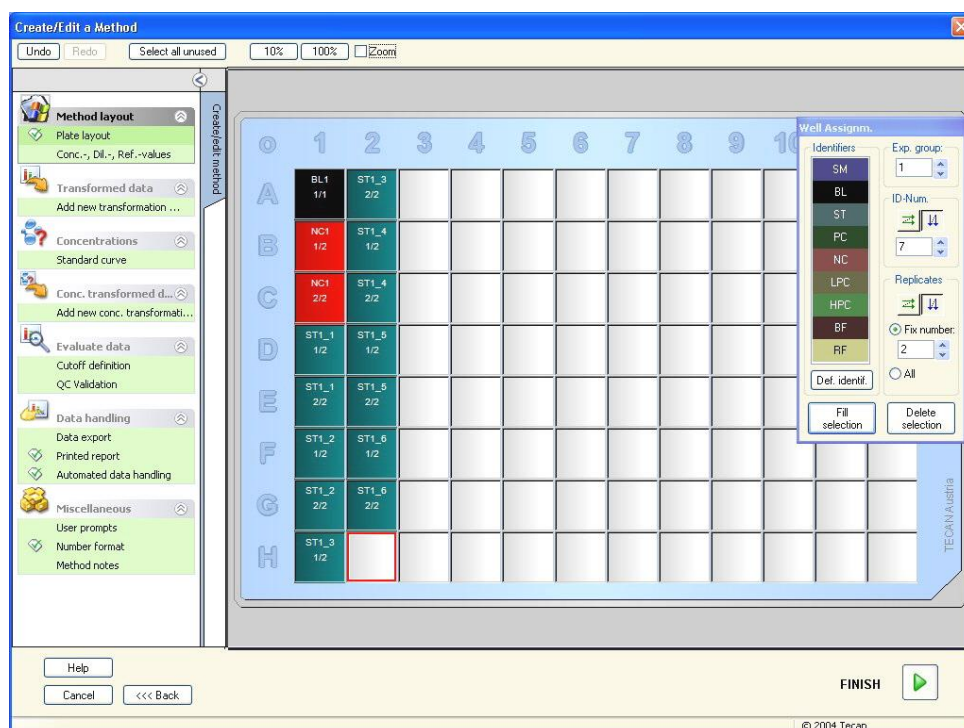
Then select the wells D1 to G2 and click **Fill selection**.



### Note

**Select the wells as follows: Starting at well D1 click and drag the mouse over the required wells to H1. Then hold down the control (Ctrl) key and drag the mouse over the required wells from A2 to G2.**

The **Plate Layout** appears as follows:



Click **Select all unused** from the toolbar to select all empty wells on the plate. Then hold down the control (Ctrl) key and click the well **H12**, so that it remains blank and unmarked.

In the **Well Assignment** dialog box select **SM (Sample)** under **Identifiers**.

In the **Experimental** group box, the number **1** remains.

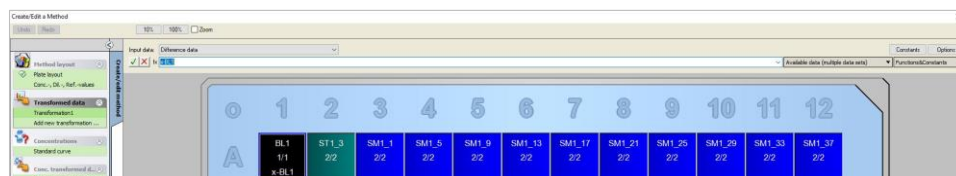
In the **Replicates** group box choose **Fix number** and **2**.

In the **ID-Number** box leave 1 and in the **Replicates** group box select the **vertical arrows**. Click then **Fill selection**. The layout definition procedure is complete.

## 12. Application Example

### Transformations


In the control bar on the left of the window select the next option, **Add new transformation...** from the **Transformed data** item, to define blank reduction.

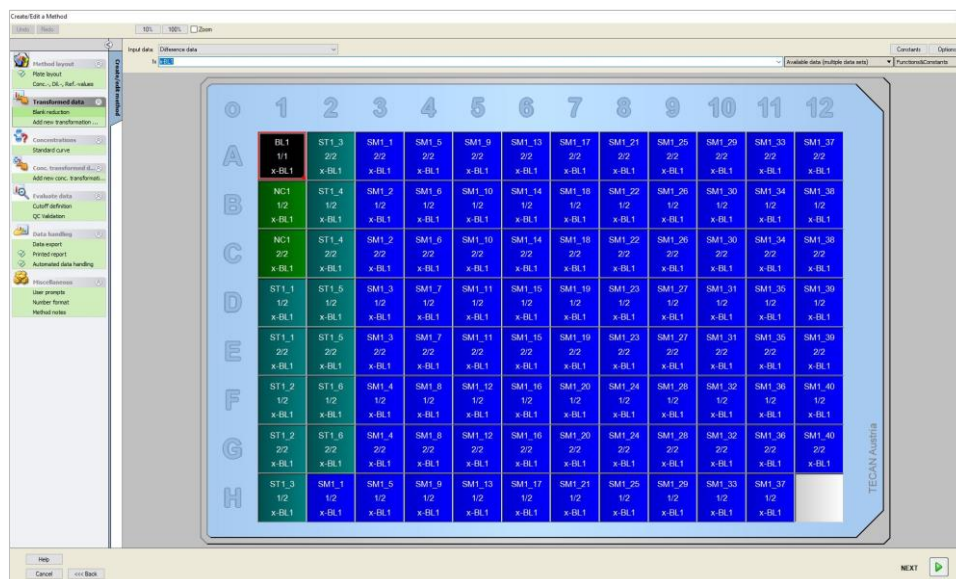


A dialog box appears asking you if you want to define a blank reduction. Click **Yes**.

Select **Difference Data** in the **Input data** box. By default, the transformation is named Transformation1 (see control bar). If you have confirmed the definition of a blank reduction before, the software automatically names it **Blank reduction**.

In the **Formula** box automatically appears **x-BL1** for this blank reduction, where **x** refers to the current input data value in a well and **BL1** is the mean value of the blank wells of experimental group 1.

Now select the whole plate by clicking the  sign in the upper left corner of the microplate and click the green hook next to the formula window to assign the transformations to the wells. For further details and explanations concerning the definition and assignment of transformations, refer to chapter 4.3.5 Transformed Data: Add New Transformation. The following window appears:



In each well the following information appears (example well A5):

<b>SM1_9</b>	Sample, experimental group number 1, sample ID number 4.
<b>2/2</b>	Number of replicate is 2, total number of replicates is 2.
<b>x-BL1 or 1.000</b>	Assigned transformation x-BL1 (when Transformation is selected) or Dilution Factor value of 1 (when Conc., Dil., Ref.-values is selected).



## Concentration / Dilution / Reference Value Definition

In the control bar select **Conc.**, **Dil.**, **Ref.-values** from the **Method layout** item to define the respective values as described in the test kit.

Calibrator 1	5 UA/mL
Calibrator 2	10 UA/mL
Calibrator 3	20 UA/mL
Calibrator 4	40 UA/mL
Calibrator 5	80 UA/mL
Calibrator 6	160 UA/mL

Make sure **ST** is selected in the **Select Identifier** list .

In the **Identifier** list, a list of the standards from the Exp. Group 1 appears. In the corresponding **Concentration** box of **ST1\_1** type the number **5** and in the **Unit** box, type UA/mL. In the corresponding **Concentration** box of **ST1\_2** type the number **10**. The unit only needs to be defined once and is valid for all standards. Type the values for the ST1\_3 to ST1\_6 in the same way.

The screen showing the plate layout and the concentration is displayed:

The screenshot displays the Tecan software interface for defining plate layout and concentrations. The main area shows a grid with columns numbered 1 to 12 and rows lettered A to H. Each cell in the grid contains a sample identifier and its corresponding concentration and unit. For example, in row A, column 1, the identifier is BL1 with a concentration of 1/1. In row A, column 2, the identifier is ST1\_3 with a concentration of 2/2. The grid continues with various SM1 identifiers and their concentrations. The left sidebar shows the 'Method layout' section with options like 'Conc.', 'Dil.', and 'Ref.-values'. The 'Select Identifier' dropdown is set to 'ST1'. The bottom of the interface has a 'NEXT' button and a 'Back' button.

## 12. Application Example

### Standard Curve

In the control bar click **Standard curve** from the **Concentrations** item to define the appropriate standard curve.

The following is in the test kit description:

After the blank correction, the optical densities (OD 492 – OD 620) are plotted versus the concentration. The regression line that goes through these points is the standard curve.

On the **Data tab**, select **Blank reduction** as input data.

The screenshot shows the 'Standard curve' dialog box with the 'Data' tab selected. The 'Input data' dropdown is set to 'Blank reduction'. Under the 'Standards' section, 'Standards from Layout' is selected. There is a 'Select...' button next to the 'Standards from ext. file' option. An 'Additional concentrations...' button is at the bottom.

On the **Analysis type** tab, select **Linear regression**.

The screenshot shows the 'Standard curve' dialog box with the 'Analysis type' tab selected. Under 'Analysis Type', 'Linear regression' is selected. The 'Data scaling' dropdown is set to 'Lin(x)Lin(y)'. Other options include 'Point to point', 'Non-linear regression', 'Cubic spline', 'Akima', 'Polynomial', 'Four parameters', 'Four parameters Marquardt', 'Five parameters', and 'LogitLog'. There is a 'More...' button. At the bottom, there are checkboxes for 'Include (0,0)' and 'Extrapolation factor' with a value of 1.



On the **Axis** tab, define the labeling and the scaling of the axis as shown below:

Standard curve

Data Analysis type Intercepts **Axis** Graph

X-axis

Label:

Color:

☐ Log. Scaling

☒ Auto select range

☐ Range Min.:  Max.:

☒ Grid Color:  Style:

Y-axis

Label:

Color:

☐ Log. Scaling

☒ Auto select range

☐ Range Min.:  Max.:

☒ Grid Color:  Style:

On the **Graph** tab, define the graph title, curves, font and graph display.

Standard curve

Data Analysis type Intercepts Axis **Graph**

Title

Label:

Color:

Curves

Label:

Color:

Symbol:

Size:

☐ Hide curve

Line width:

Font

☒ Small

☐ Medium

☐ Large

Display...

☒ Legend

☒ Intercepts

☒ Base points

☒ Error bars

## 12. Application Example

### Define Cutoffs

In the control bar select **Cutoff definition** from the **Evaluate data** item to define the limits for the qualitative evaluation.

The test kit description contains the following instructions:

Interpretation of the test results:

IgM < 18 UA/mL	Negative
18 UA/mL <= IgM < 22 UA/mL	Intermediate
IgM >= 22 UA/mL	Positive

Use the following procedure to define the appropriate cutoffs:

In the Input data box, select Mean conc. (UA/mL).

The **Cutoffs** table represents a scale indicating the high and the low end for the **Limits** and **Labels**. In **Limits**, type 22 as the first (higher) limit and 18 as the second (lower) limit.

In **Labels**, enter the test interpretation (**Positive**, **Intermediate** and **Negative**) into the individual boxes. Use the drop-down color palette to assign a color:

Positive – Red

Intermediate – Blue

Negative – Green

The screen contains the following:

Click **Cutoff results selection** to select the identifier types for which the cutoff results must be shown.

## Define QC Validations

In the control bar, click **QC Validations** from the **Evaluate data** item. Validation criteria for the test must be defined, so that the validity of the test results is guaranteed.

In this example the following requirement must be fulfilled:

The calculated IgM-concentration of both negative controls must be under 8 UA/mL.

In the **Input** box, select **Single conc. (UA/mL)**.

In the first row, type **NC1\_1<8**, or enter the formula using the available **variables**, **operators** and **functions**.



### Note

**NC1\_1 means Negative control of experimental group 1, replicate 1.**

In the second row, type **NC1\_2<8**.

The **QC Validations** dialog box is now displayed as follows:

Validation Conditions	
1	NC1_1<8
2	NC1_2<8
3	
4	
5	
6	
7	
8	

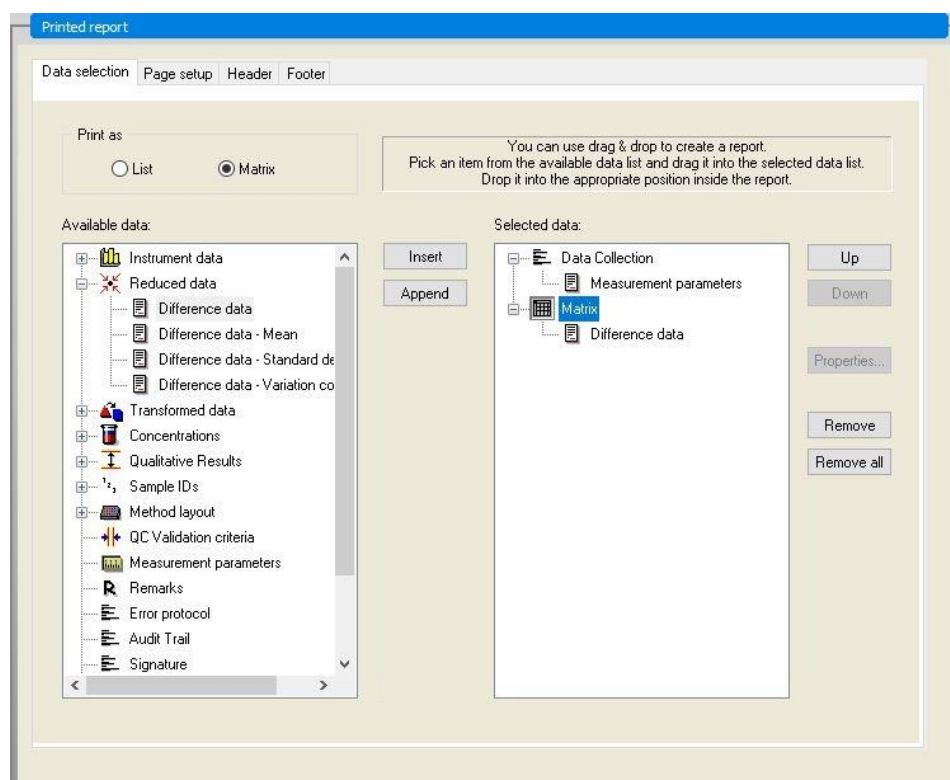
Formula input

Variable: BL1    Operators: +    Functions: and

## 12. Application Example

### Organize Printed Report

In the control bar, click **Printed report** from the **Data handling** item. The following screen is displayed:



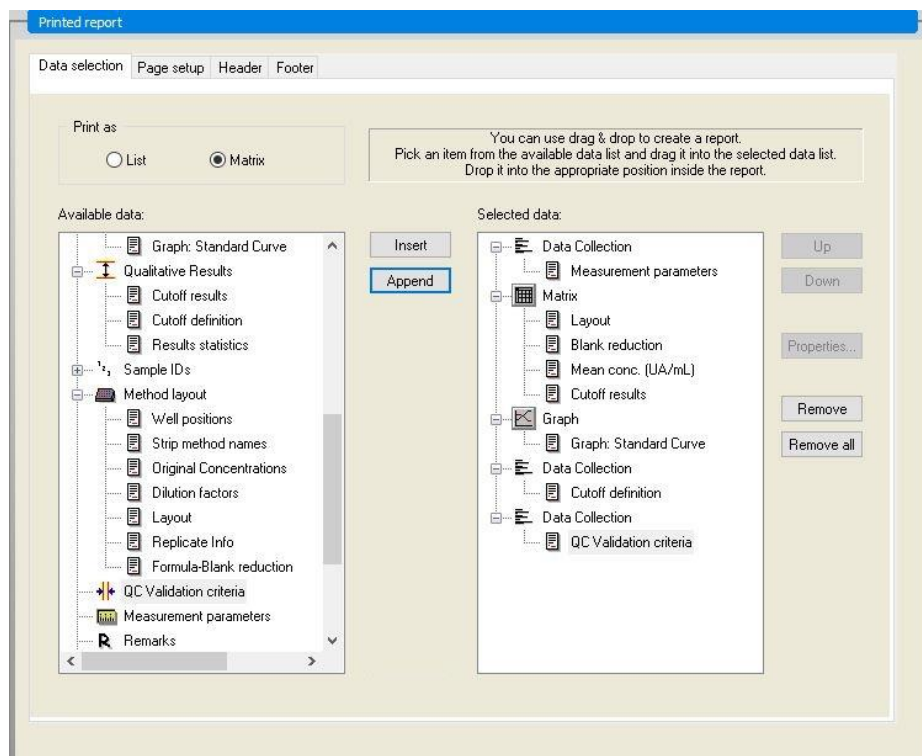
On the **Data selection** tab, all available report data is contained in the **Available data** box. Using the **Insert** and **Append** buttons, data can be transferred into the **Selected data** box. Data can also be transferred using drag-and-drop. In the **Print as** box, choose between printing the data as a matrix or as a list with a special orientation.

In this example a report containing the measurement parameters, plate layout, blanked values, standard curve, IgM-concentrations, cutoff definition, qualitative results of the samples and validations should be created.

Before creating the report, the default **Matrix Difference data** must be removed from the **Selected data** box. So only **Measurement parameters** remain in the **Selected data** box.

Select **Method layout/Layout** in the **Available data** box and attach it as a matrix to the report by clicking **Append**. Then insert **Blank reduction**, **Mean conc. (UA/mL)** and **Cutoff results** into the matrix by selecting the corresponding items and clicking **Insert**.

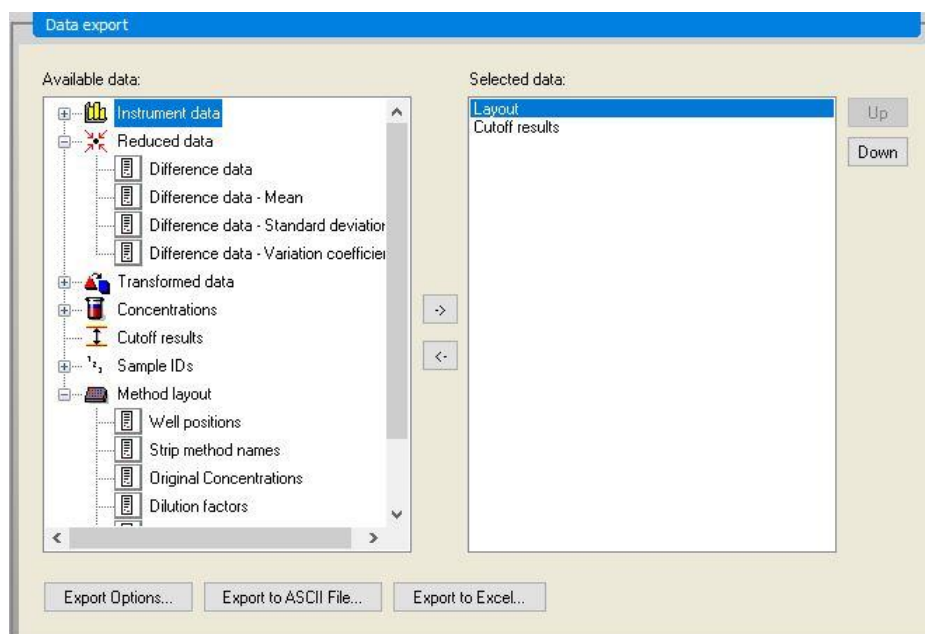
**Append Graph: Standard curve, Cutoff definition, and QC Validation criteria** to the selected data. The data setup part of the report definition procedure is complete; the **Printed Report** dialog box looks like this:



On the **Header** and **Footer** tabs, define the layout of the header and the footer of the report (see chapter 4.3.13 Data Handling: Printed Report for further details).

## Data Export

In the control bar, select **Data export** from the **Data handling** item. In this example, the layout and cutoff results should be stored as ASCII file. Select **Layout** and **Cutoff** results from the **Available data** window; click the → arrow to insert them into the **Selected data** window. The screen displays the following information:



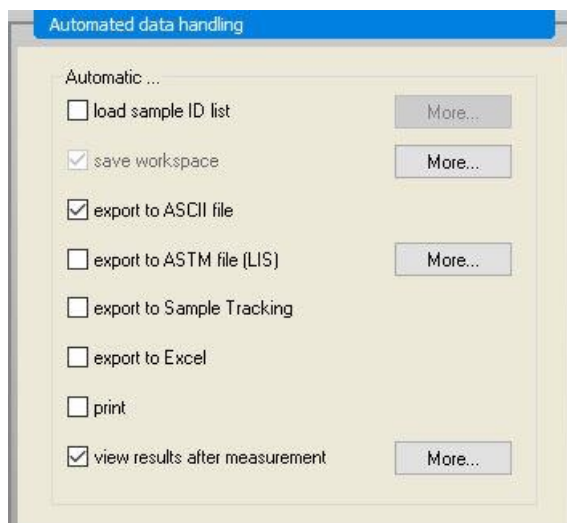
### Note

**Exported data should always contain the Layout or Sample ID List.**

## 12. Application Example

### Automated Data Handling

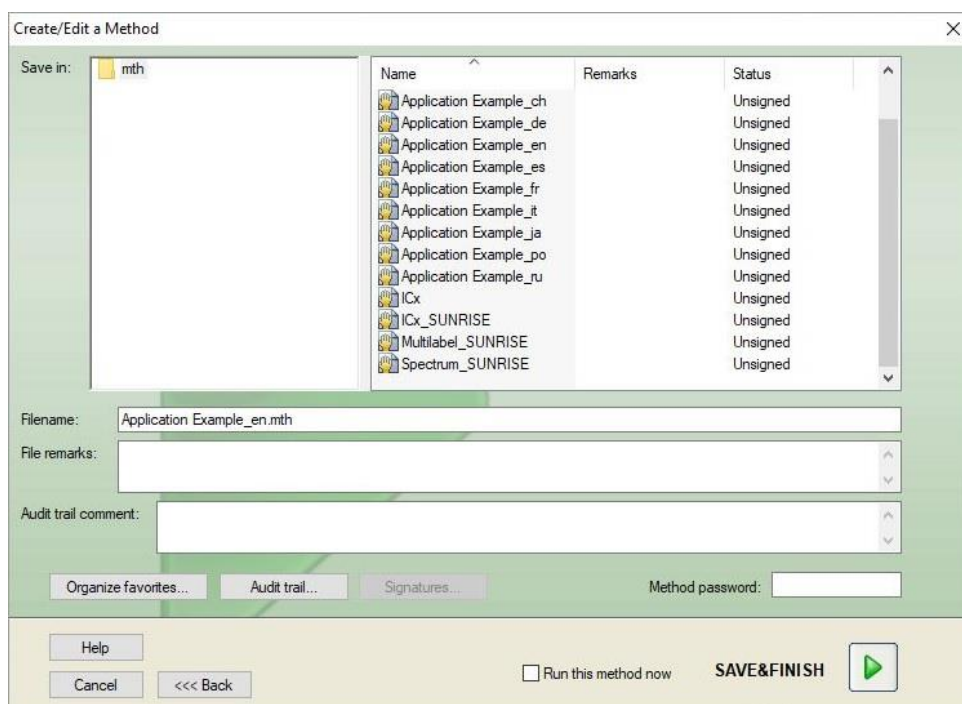
In the control bar, select **Automated data handling** from the **Data handling** item.



Select **export to ASCII file**, and **view results after measurements**. In **magellan Tracker**, **save workspace** is selected by default and cannot be modified.

### Save the Method

Click **FINISH** to open the **Save as** window. Enter the method filename and complete any other field if appropriate.

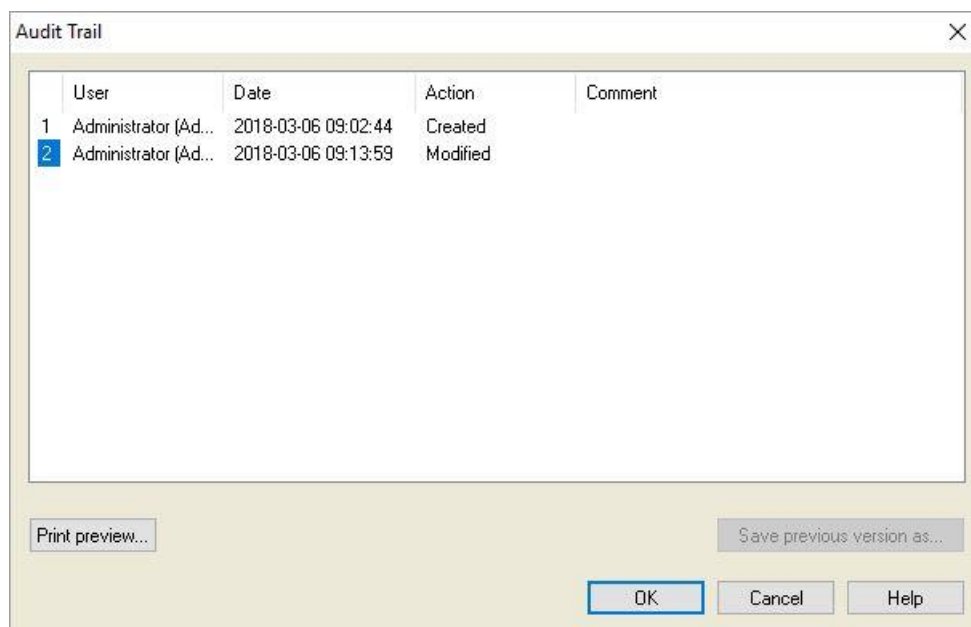


<b>Filename</b> text field	A filename must be entered. A default filename is suggested automatically but can be changed.
<b>File remarks</b> text field	Comments entered here will be saved and displayed with the filename.
<b>Audit trail comment</b> text field	Comments entered here will be stored in the audit trail. <i>This option is only available with <b>magellan Tracker</b>.</i>

<b>Audit trail...</b> button	The <b>Audit Trail</b> dialog box appears. <i>This option is only available with magellan Tracker.</i>
<b>Organize Favorites...</b> button	The <b>Organize Favorites</b> dialog box appears. (See chapter 6.4 Start Favorite – Organize Favorites).
<b>Signatures...</b> button	The <b>Signature</b> dialog box appears. <i>This option is only available with magellan Tracker.</i>
<b>Method password</b>	Enter a method password if you want to protect the method to be saved (see chapter 4.4.1 Password Protection of Methods).
<b>Run this method now</b> check box	The method will be run immediately after having finished the wizard.

## Audit Trail

Click **Audit Trail** to view the **Audit Trail** dialog box:



The audit trail shows a list of all modifications made to the method. Each entry consists of the user (name and full name), date and time of change, whether the file was created or modified, and any audit trail comments.

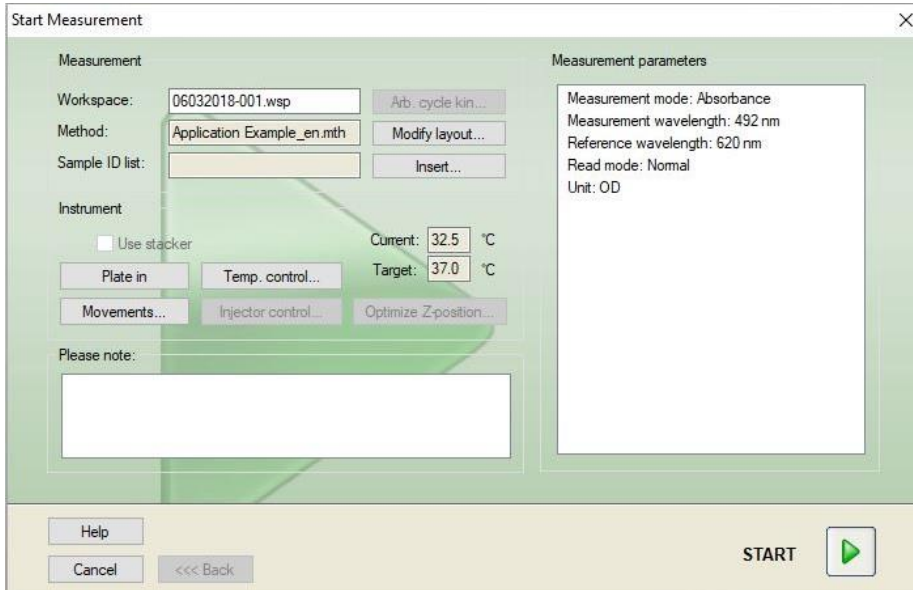
Click **Print preview...** to get a preview of the file. To compare a method with its previous versions a printout must be made, because two print preview windows cannot be opened simultaneously.



## 12. Application Example

### 12.1.3 Run the Method

If **Run this method now** is selected in the **Save as** dialog box of the **Create/edit a method wizard**, the **Start Measurement Wizard/ Start Measurement** dialog box will appear after **Save** is clicked:



The **Start Measurement** dialog box is divided into two main sections: **Measurement** and **Measurement parameters**.

**Measurement section:**

- Workspace:** 06032018-001.wsp
- Method:** Application Example\_en.mth
- Sample ID list:** (empty field)
- Instrument:**
  - ☐ Use stacker
  - Current:** 32.5 °C
  - Target:** 37.0 °C
- Buttons:** Plate in, Temp. control..., Movements..., Injector control..., Optimize Z-position..., Arb. cycle kin..., Modify layout..., Insert...
- Please note:** (empty text area)

**Measurement parameters section:**

- Measurement mode: Absorbance
- Measurement wavelength: 492 nm
- Reference wavelength: 620 nm
- Read mode: Normal
- Unit: OD

**Bottom section:**

- Buttons:** Help, Cancel, <<< Back, START (with a green play button icon)

Click **Start** to start the measurement. A workspace will be created automatically, which contains all previously entered information and will collect all measurement values. While the measurement is being executed, a measurement status dialog box appears indicating the progress of the measurement.

After the measurement is completed, the **Results** dialog box appears, in which all the results and calculations can be viewed.

### 12.1.4 Evaluate the Result

**Evaluate results** enables you to view and evaluate raw data. The evaluation parameters can be viewed, and data can be re-evaluated.

This section guides you through the **Evaluate Results wizard** using the example workspace file created by running the quantitative ELISA method.



#### Note

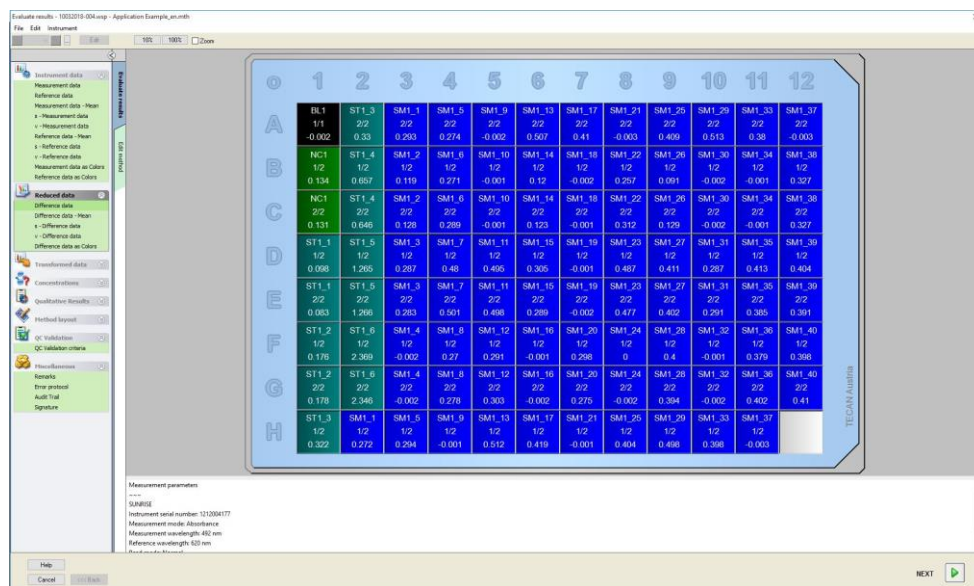
**Example files automatically appear in the Method List in magellan Standard. For magellan Tracker, these files are available in the default data path and must be converted.**

In the Wizard List dialog box, click Evaluate results.

Click **Next** on the **Welcome** page of the **Evaluate Results wizard** and the **Select a file** dialog box appears.

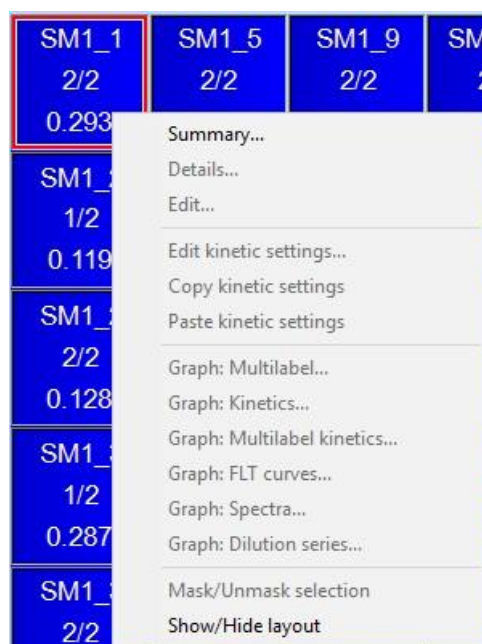
Select the workspace **Quantitative Elisa example\_Sunrise.wsp** from the file list and click **Make your selection**. Calculations are executed and the following plate layout window is displayed:





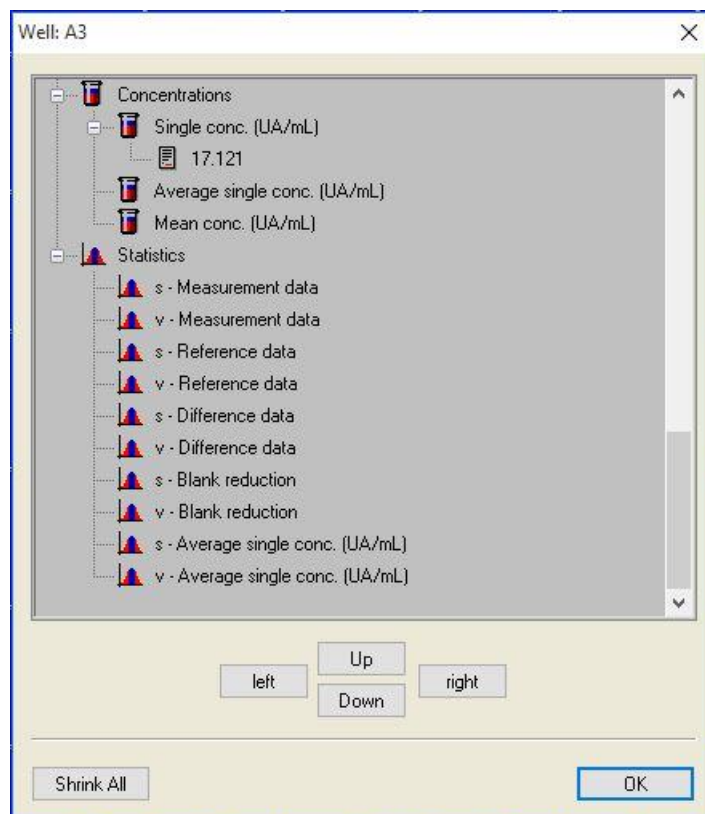
In each single well the calculated value is displayed. Depending on the selected item in the control bar, the plate layout window changes correspondingly. Parameters and settings can be changed using the items in the control bar. If the method is to be modified, click on the **Edit method** tab.

Click in the well with the right mouse key and the context-sensitive menu appears:



Selecting **Summary**, the following window is displayed providing detailed information of the definition and the settings of the chosen well:

## 12. Application Example



Click **Finish** in the plate layout window and the **Save as** dialog box appears, where you can enter a file name and remarks. Click the small **Save** button on the left of the window to save the file; you can continue working on the method or workspace. Click the **Save** button on the right side at the bottom of the screen to save the file and to close the wizard. The program goes back to the wizard list.

## 12.1.5 Summary of Definition of Quantitative ELISA in magellan

### 1. Subtract Blank value

#### Definitions in magellan

Click on **Add new transformation** in the control bar and a window appears, asking if you want to define a **Blank reduction**. Click **Yes** and the **Blank reduction** formula is assigned automatically to all wells.

### 2. Define Concentrations

#### Definitions in magellan (Control bar – Method layout/ Conc.-, Dil.-, Ref.- values)

Selected identifier: ST

Unit: UA/ml

ST1_1	5	(ST1_1.....Standard 1 first experimental group)
ST1_2	10	(ST1_2.....Standard 2 first experimental group)
ST1_3	20	(ST1_3.....Standard 3 first experimental group)
ST1_4	40	(ST1_4.....Standard 4 first experimental group)
ST1_5	80	(ST1_5.....Standard 5 first experimental group)
ST1_6	160	(ST1_6.....Standard 6 first experimental group)

### 3. Define Standard Curve

#### Definitions in magellan (Control bar – Concentrations/ Standard curve)

Input data	blank reduction
Analysis type	linear regression
X-axis	linear
Y-axis	linear

### 4. Define Cutoffs

#### Definitions in magellan (Control bar – Evaluate data/ Cutoff definition)

- Input data: Mean conc. (UA/mL)

Limits      22  
                 18

Positive>=22>intermediate>=18>negative

Non competitive test#

### 5. QC Validation

#### Definitions in magellan (Control bar – Evaluate data/ QC validation):

- Input data: Single conc. (UA/mL)

Validation condition 1      NC1\_1<8

Validation condition 2      NC1\_2<8

NC1\_1.....Negative Control first replicate first experimental group

NC1\_2.....Negative Control second replicate first experimental group



## 13. Glossary of Terms

Term	Definition
<b>Average single conc. (???)</b>	Concentration calculated by averaging the single concentrations
<b>Basis OD</b>	Kinetic Parameter: Basis OD value of the onset calculation
<b>Basis OD %</b>	Kinetic Parameter: Basis value of the onset calculation in %
<b>Clipboard</b>	The clipboard is the medium by which programs under Windows exchange data with each other. Data can be selected in one Windows application by cutting or copying it to the clipboard and then added into another application by pasting it from the clipboard.
<b>Correlation coeff.</b>	Correlation coefficient, indicates the strength and direction of a linear relationship between two random variables.
<b>Cutoff limit</b>	The cutoff limit enables the user to define the limits between two conditions (for example: positive or intermediate). These criteria are used in the evaluation of the results.
<b>Cutoff results</b>	Name of the cutoff range the value lies in as defined under cutoff definition
<b>Cutoff definition</b>	Definition of all cutoff ranges and calculated limits
<b>Dilution factors</b>	Defined dilution factors of the samples and controls. A dilution factor of 2 represents a 1:2 dilution.
<b>Dilution series</b>	A sample with replicates in different dilutions.
<b>Goodness of fit</b>	1 minus average relative square deviations of the base points from the curve
<b>Graph</b>	Graphs can be displayed for kinetic measurements, enzyme kinetics, multilabel measurements, dilution series or standard curves.
<b>Hidden</b>	Displayed if well data is hidden when printing
<b>HUID</b>	<b>H</b> ardware <b>U</b> nit <b>I</b> dentification Number
<b>IC 50</b>	The dilution/concentration which results in 50% of the maximum response
<b>Invalid</b>	Value is invalid, no calculation possible
<b>Graph: Kinetic</b>	Graph of kinetic measurements
<b>Lamp low</b>	No values from measurement because of absorbance instrument error.
<b>Layout, Plate Layout</b>	Defines where samples or controls are placed on the microplate
<b>Max. slope OD/hr</b>	Kinetic Parameter: Maximum slopes of the kinetic curves per hour
<b>Max. slope OD /min</b>	Kinetic Parameter: Maximum slopes of the kinetic curves per minute
<b>Max. slope OD /sec</b>	Kinetic Parameter: Maximum slopes of the kinetic curves per second
<b>Maximum OD</b>	Kinetic Parameter: Maximum value of the kinetic curves
<b>Mean slope OD /hr</b>	Kinetic Parameter: Average slopes of the kinetics curves per hour
<b>Mean slope OD /min</b>	Kinetic Parameter: Average slopes of the kinetics curves per minute
<b>Mean slope OD /sec</b>	Kinetic Parameter: Average slopes of the kinetics curves per second
<b>Mean. conc (???)</b>	Concentration calculated from the mean of the replicates of the input data

### 13. Glossary of Terms

Term	Definition
<b>Measurement data</b>	Dual wavelength absorbance measurement: Data measured using the measurement filter
<b>Measurement parameters</b>	Defines measurement mode, wavelength, plate size, shaking, etc.
<b>Measurement type</b>	The measurement type can be endpoint measurement, kinetic measurement, multilabel measurement or well-kinetic measurement.
<b>Method</b>	Methods contain of the measurement parameters and the evaluation definition. Running a method leads to a workspace that contains the measured and calculated data.
<b>Minimum OD</b>	Kinetic Parameter: Minimum value of the kinetic curves
<b>MultPt</b>	The standard curve is not monotone and delivers more than one concentration at the given input data.
<b>NoCalc</b>	No value returned from the calculation.
<b>Original Concentrations</b>	Concentrations of the standard curve defined in the method.
<b>Pipetting status</b>	If a sample ID list is imported from a pipetting software, the pipetting status can be displayed.
<b>QC Validation</b>	The QC validation criteria are defined in the method and stipulate whether a measurement is valid or invalid. The criteria can, for example, indicate if the measurement values lie too far apart from each other, or if they deviate too far from an expected value. The program automatically warns the user if the criteria are not met.
<b>Raw data</b>	Data measured by the instrument.
<b>Reference data</b>	Dual wavelength absorbance measurement: Data measured using the reference filter
<b>Results statistics</b>	Summary of the number of values in the different cutoff ranges
<b>Sample ID List</b>	Sample IDs are assigned to each well on the basis that the associated probe can be identified. The IDs are usually barcodes imported from sample ID lists stored by a pipetting software.
<b>Sample IDs</b>	IDs of the samples
<b>Single. conc (???)</b>	Concentration calculated from the input data of each replicate
<b>Test</b>	In previous versions a test contained the evaluation settings but not the measurement parameters. Tests are no longer supported in <b>magellan</b> and are replaced by the more powerful methods.
<b>Time Basis OD</b>	Kinetic Parameter: Time until the basis value is reached
<b>Time Basis OD %</b>	Kinetic Parameter: Time until the basis value % is reached
<b>Time Basis to Onset OD</b>	Kinetic Parameter: Time between basis value and onset value
<b>Time Basis to Onset OD %</b>	Kinetic Parameter: Time between the basis and the onset value %
<b>Time max. slope sec</b>	Kinetic Parameter: Kinetic Parameter: Time point of the maximum slope
<b>Time maximum OD</b>	Kinetic Parameter: Time until the maximum is reached
<b>Time minimum OD</b>	Kinetic Parameter: Time until the minimum is reached
<b>Time Onset OD</b>	Kinetic Parameter: Time until the defined onset value is reached
<b>Time Onset OD %</b>	Kinetic Parameter: Time until the defined onset in % is reached
<b>Time points</b>	Time stamps of the single measurements of a kinetic measurement

Term	Definition
<b>Unavailable</b>	Requested data is not available
<b>Unused</b>	No data measured; no layout defined in this well
<b>User Prompts</b>	User Prompts are references that are setup in the method. They are displayed before the measurement and the user has to add text to them. This text will then be incorporated in a printout.
<b>Validation criteria</b>	Summary of validation condition results
<b>Well position</b>	Name of the well, for example: A1, A2, ...
<b>Workspace</b>	All available data within the program can be found in the Workspace, for example the measurement data, the print definition and the method definition. The Workspace is used for loading methods and running measurements.
<b>!</b>	Precedes values that have been eliminated during calculation
<b>#</b>	Precedes concentration values that have been calculated using extrapolation and lie outside the range of the standard curve
<b>( )</b>	Parenthesis surround values that have been masked
<b>*</b>	An asterisk marks values that have been measured using the "Use gain regulation" option, which corrects (=lowers) the gain.
<b>??? – Mean</b>	Calculated averages (for example: Raw data – Mean)
<b>??? – Standard deviation s - ???</b>	Calculated standard deviations (for example: Raw data – Standard deviation or s – Raw data)
<b>??? – Variation coefficient v - ???</b>	Calculated variation coefficients (for example: Raw data – Variation coefficient or v – Raw data)
<b>~</b>	Added to values that have been edited or simulated
<b>&lt;Min</b>	Calculated concentration is lower than minimum
<b>&gt;Max</b>	Calculated concentration exceeds maximum
<b>&lt;Blank&gt;</b>	Printed report: Insert empty matrix or table printout
<b>&lt;Page break&gt;</b>	Printed report: Print next item on the next page
<b>&lt;Separator&gt;</b>	Printed report: Print line between two items
<b>x</b>	Symbol <b>x</b> refers to the current value within a well
<b>concX</b>	Symbol <b>concX</b> refers to the concentration of the standard in the current well.
<b>dilX</b>	Symbol <b>dilX</b> refers to the dilution of the sample or control in the current well.
<b>'???'</b>	Available data set if more than one set of input data shall be used for calculations
<b>[ ]</b>	Indices access the different cycles of a kinetic measurement whereas [0] indicates the first cycle
<b>*</b>	The asterisk marks identifiers that have been set as aliases.





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