



Instructions for Use for

magellan

Document Part No.: 30143531
2021-11

Document Revision No.: 1.4

Software Revisions:



magellan: 7.5

magellan Tracker: 7.5



30143531 04



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.



Manufacturer

Tecan Austria GmbH
Untersbergstr. 1A
A-5082 Grödig, Austria
T: +43 6246 89330
F: +43 6246 72 770
www.tecan.com
E-mail: office.austria@tecan.com

Copyright Information

The contents of this manual are the property of Tecan Austria GmbH and are not to be copied, reproduced or transferred to another person or persons without our prior written permission.

Copyright © Tecan Austria GmbH
All rights reserved.
Printed in Austria.

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.

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

Table of Contents

1. Introduction	9
1.1 Area of Application.....	9
1.2 Intended Use/Purpose of magellan	10
1.3 User Profile	10
1.3.1 Professional User - Administrator Level	10
1.3.2 End User or Routine User	10
1.4 Specifications.....	11
1.4.1 System Requirements	11
1.4.2 Reader Compatibility	12
1.5 Software Installation Procedure.....	12
1.5.1 Automatic Software Setup Program	12
1.5.2 Installation Qualification – IQ.....	13
1.5.3 Operation Qualification – OQ.....	13
1.5.4 System Recovery	14
1.5.5 Automatic Software Removal	15
1.5.6 Cybersecurity Information.....	16
2. Start Working with magellan.....	17
2.1 User Interface – Wizard List.....	17
2.2 Components & Terms – Basic Logic of magellan.....	19
2.2.1 File Types Used with magellan.....	19
2.2.2 Folder Handling	20
2.2.3 Standard Elements	21
2.2.4 The Help Button.....	21
2.2.5 The Welcome Dialog Box	22
2.2.6 Shortcuts List.....	22
2.3 Starting magellan	23
2.3.1 Starting Standard Version	23
2.3.2 Starting Tracker Version.....	23
2.4 Connecting an Instrument.....	24
2.4.1 Connect to SUNRISE Instruments.....	24
2.4.2 Connect to INFINITE F50 Instruments	25
2.4.3 Licensing magellan.....	27
2.4.4 Registration Wizard	27
3. Instrument Control & Settings.....	31
3.1 Instrument Options.....	31
3.1.1 Movements.....	31
3.1.2 Temperature Control.....	31
3.2 Setup & Service Options.....	32
3.2.1 Change Instrument.....	32
3.2.2 Define Filter Slides.....	32
3.3 Log Files.....	32
4. Create/Edit a Method Wizard.....	33
4.1 Introduction	33
4.2 Define the Measurement Parameters.....	34
4.2.1 Measurement Types - SUNRISE.....	34
4.2.2 Measurement Parameters - SUNRISE	35
4.2.3 Measurement Parameters - INFINITE F50.....	36
4.3 Define Evaluation.....	38

4.3.1	The Create/Edit Method Overview Window.....	38
4.3.2	Method Layout: How to Define a Plate Layout	41
4.3.3	Method Layout: Conc., Dil. and Ref. Values.....	46
4.3.4	Precalculation: Spectra Data Reduction.....	49
4.3.5	Transformed Data: Add New Transformation.....	52
4.3.6	Kinetic: Kinetic Data Reduction	55
4.3.7	Kinetics Transformations: Add New Kinetics Transformations	58
4.3.8	Concentrations: Standard Curve	58
4.3.9	Concentrations Transformations: Add New Concentration Transformations.....	63
4.3.10	Evaluate Data: Cutoff Definition	63
4.3.11	Evaluate Data: QC Validation.....	64
4.3.12	Data Handling: Data Export.....	65
4.3.13	Data Handling: Printed Report	70
4.3.14	Data Handling: Automated Data Handling	74
4.3.15	Miscellaneous: User Prompts.....	78
4.3.16	Miscellaneous: Number Format	78
4.3.17	Miscellaneous: Method Notes	78
4.4	Saving the Method	79
4.4.1	Password Protection of Methods.....	80
4.5	Multiplate Methods	81
5.	Create/Edit a Sample ID List Wizard	83
5.1	Introduction	83
5.2	Create/Edit a Sample ID List.....	83
5.2.1	Create New Sample ID List.....	83
5.2.2	Import/Edit a Sample ID List.....	85
5.2.3	Import a Sample ID List.....	89
5.2.4	Saving the Sample ID List.....	96
6.	Start Measurement Wizard.....	97
6.1	Introduction	97
6.2	Obtain Raw Data.....	98
6.2.1	Obtain Raw Data with the SUNRISE Instrument.....	98
6.2.2	Obtain Raw Data with the INFINITE F50 Instrument.....	98
6.3	Use Predefined Method	99
6.4	Start Favorite.....	99
6.5	Start Measurement with a Predefined or Favorite Method	100
6.6	Measurement Status	104
7.	Evaluate Results Wizard	107
7.1	Introduction	107
7.2	Select a File	107
7.2.1	File Selection Criteria	108
7.3	The Workspace Overview Window	109
7.4	Evaluate Results Tab.....	111
7.4.1	Menus	111
7.4.2	Toolbar Menu: File	112
7.4.3	Toolbar Menu: Edit.....	115
7.4.4	Toolbar Menu: Instrument	116
7.4.5	Plate Layout Window	116
7.4.6	Special Characters.....	117
7.4.7	Control Bar: Instrument Data.....	117
7.4.8	Control Bar: Reduced Data	117
7.4.9	Control Bar: Transformed Data	117
7.4.10	Control Bar: Kinetic Parameters.....	118

7.4.11	Control Bar: Concentrations	118
7.4.12	Control Bar: Qualitative Results.....	122
7.4.13	Control Bar: Sample IDs.....	122
7.4.14	Control Bar: Method Layout.....	122
7.4.15	Control Bar: QC Validation	122
7.4.16	Control Bar: Miscellaneous.....	122
7.4.17	Color Scale Box.....	123
7.4.18	Context-Sensitive Menu of a Well.....	123
7.5	Edit Method Tab.....	128
7.6	Saving the Evaluated Results	128
8.	Attach Signature Wizard.....	129
8.1	Introduction	129
8.2	Sign a File	129
9.	Miscellaneous Icon	131
9.1	Instrument Control	131
9.2	File Handling	131
9.2.1	Archive Files.....	131
9.2.2	Import Raw Data.....	134
9.2.3	Convert To.....	134
9.2.4	Convert From.....	135
9.2.5	Save Log Files.....	137
9.3	Options.....	137
9.3.1	Default Data Paths	138
9.3.2	Copy/Export Options	139
9.3.3	Plate View Settings.....	140
9.3.4	Miscellaneous.....	142
9.4	User Administration (magellan Tracker)	144
9.4.1	Add/Modify User (magellan Tracker)	145
9.4.2	Add/Modify Role	147
9.4.3	User Administration Audit Trail	148
9.4.4	User Administration Options.....	149
9.4.5	User Administration Summary	151
9.5	User Administration (magellan Standard).....	152
9.5.1	Add/Modify User (magellan Standard).....	153
9.5.2	Login.....	153
9.5.3	Change User	153
9.6	User Rights	154
9.7	About magellan	158
10.	Additional Features for magellan Tracker	159
10.1	User Administration.....	159
10.1.1	Audit Trail	159
10.2	File Handling	160
10.2.1	Saving a File.....	160
10.2.2	Changing a Method or Workspace File	160
10.2.3	Opening a File	160
10.2.4	Opening a File Created on Another PC – Add HUIDs	160
10.3	System Audit Trail.....	161
11.	Calculations.....	163
11.1	Evaluate Results – Calculation Procedure	163
11.1.1	Statistics	164
11.2	Spectra Data Reduction.....	164

11.2.1	Mathematical Description	164
11.3	How to Write a Formula	165
11.3.1	Introduction	165
11.3.2	Formula Variables	165
11.3.3	Formula Functions	167
11.3.4	Basic Functions.....	168
11.3.5	Statistical Functions	169
11.3.6	Elimination Functions	171
11.3.7	Other Functions.....	174
11.3.8	Spectra Functions	174
11.3.9	Examples	175
11.4	Standard Curve Analysis Types.....	176
11.4.1	Definitions	176
11.4.2	Analysis Type Parameters	177
11.4.3	Error Messages.....	177
11.4.4	Point to Point.....	177
11.4.5	Linear Regression	177
11.4.6	Non-Linear Regression	178
11.4.7	Polynomial.....	179
11.4.8	Cubic Spline	179
11.4.9	Akima	180
11.4.10	LogitLog	180
11.4.11	Four Parameters	182
11.4.12	Four Parameters – Marquardt.....	183
11.4.13	Five Parameters – Marquardt.....	183
11.4.14	Weighting for Four / Five Parameter Fit – Marquardt / Polynomial Fit.....	184
11.5	Calculation of Dilution Series	185
11.5.1	Detection of Dilution Series	185
11.5.2	Curve Parameter Calculation	185
11.5.3	Calculation of IC Values.....	185
12.	Application Example	187
12.1	Step-by-Step Example: Quantitative ELISA.....	187
12.1.1	Test Kit Description	187
12.1.2	Create a Method	188
12.1.3	Run the Method.....	201
12.1.4	Evaluate the Result	202
12.1.5	Summary of Definition of Quantitative ELISA in magellan	204
13.	Glossary of Terms	205
	Index.....	209
	Trademarks.....	212
	Tecan Customer Support	213

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.

1.2 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/customer-support>

1.4 Specifications

1.4.1 System Requirements

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

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

1.5.4 System Recovery

In order 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 Options dialog box
Workspaces	C:\Users\Public\Documents\Tecan\Magellan\wsp or as set in the Options dialog box
Sample ID lists	C:\Users\Public\Documents\Tecan\Magellan\smp or as set in the Options dialog box
Exported data	C:\Users\Public\Documents\Tecan\Magellan\asc or as set in the Options 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

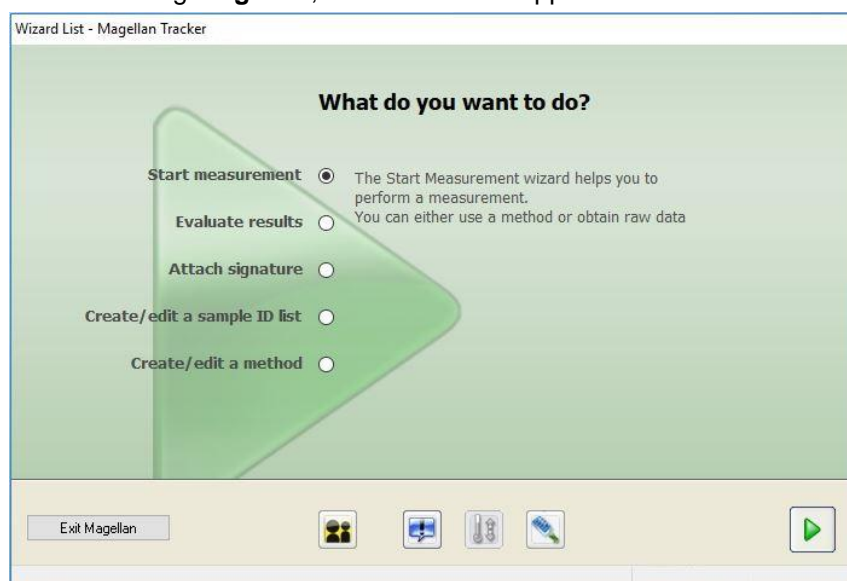
Standard **magellan** wizards represent workflow modules, which are step-by-step guides for performing complex procedures.


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 magellan		

- **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 .pdfx	\Reader\Pdf \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:

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

Standard Elements of Microsoft Windows

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

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 TO CREATE 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

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:

Username text box	Enter your UserID
Password text box	Enter your Password

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.

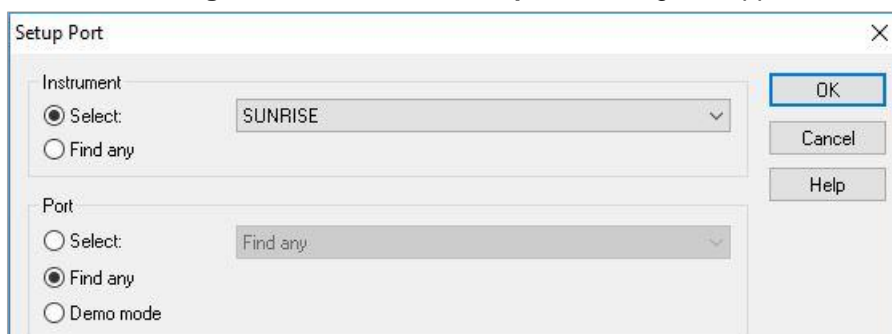
2.4 Connecting an Instrument

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:



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

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.

2.4.2 Connect to INFINITE F50 Instruments

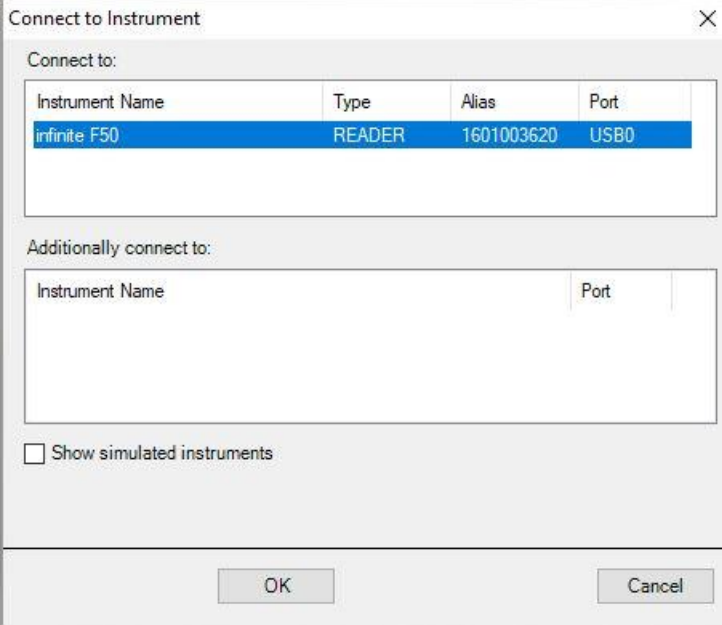
First Start of magellan

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



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

2. Start Working with magellan

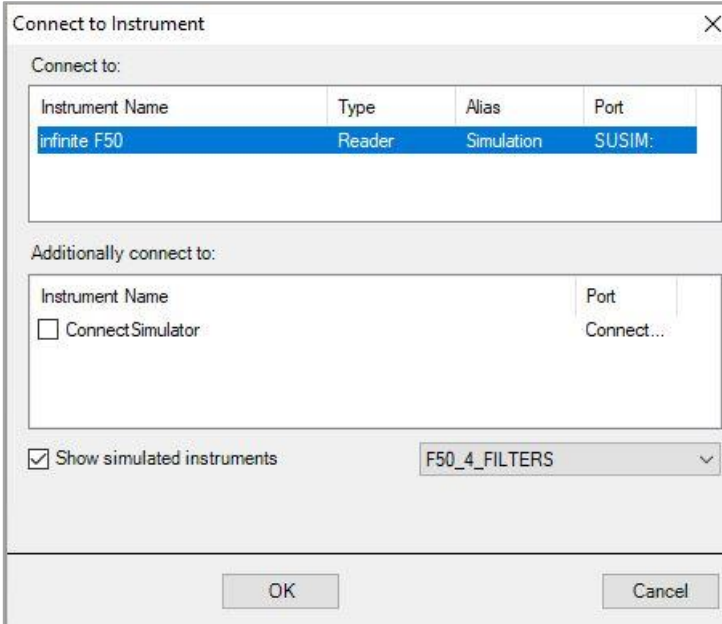


Instrument Name	Type	Alias	Port
infinite F50	READER	1601003620	USB0

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:

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 launch automatically 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**).

In order 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.

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

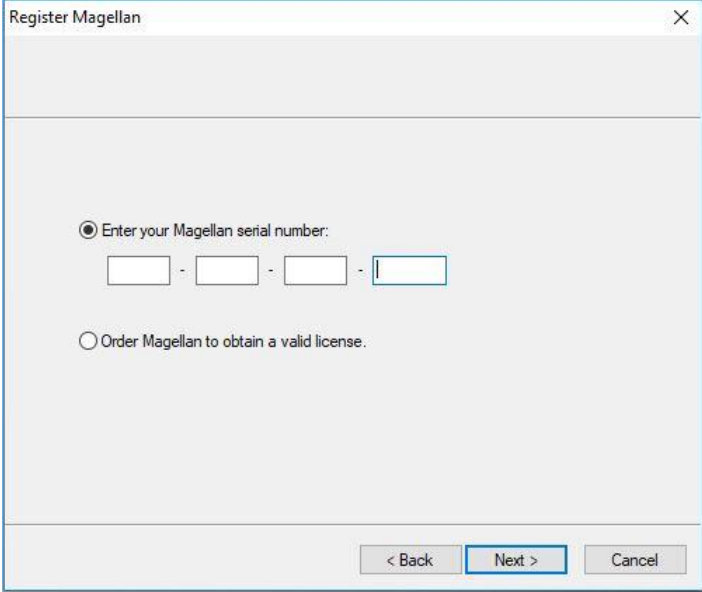
The registration wizard starts with the **Welcome** dialog box, which contains a short description of the wizard. Click **Next** and the **Serial Number** dialog box appears.

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).

2. Start Working with magellan



Register Magellan

Enter your Magellan serial number:

- - -

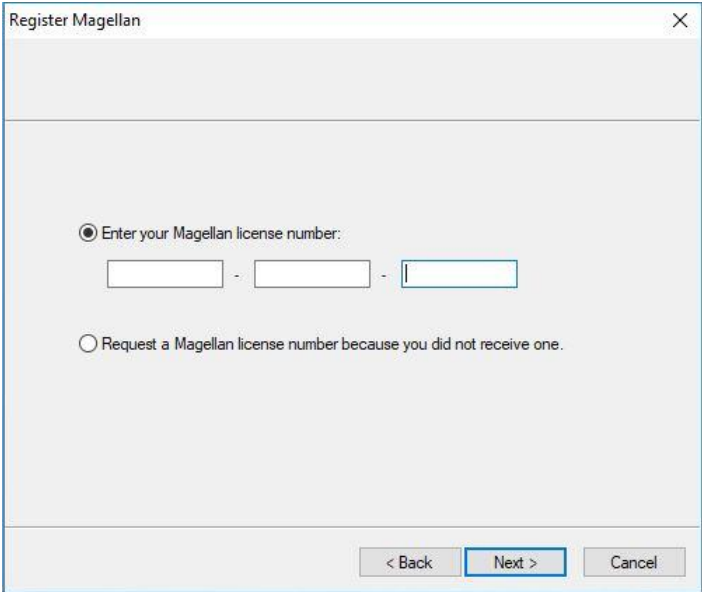
Order Magellan to obtain a valid license.

< Back Next > Cancel

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.



Register Magellan

Enter your Magellan license number:

- -

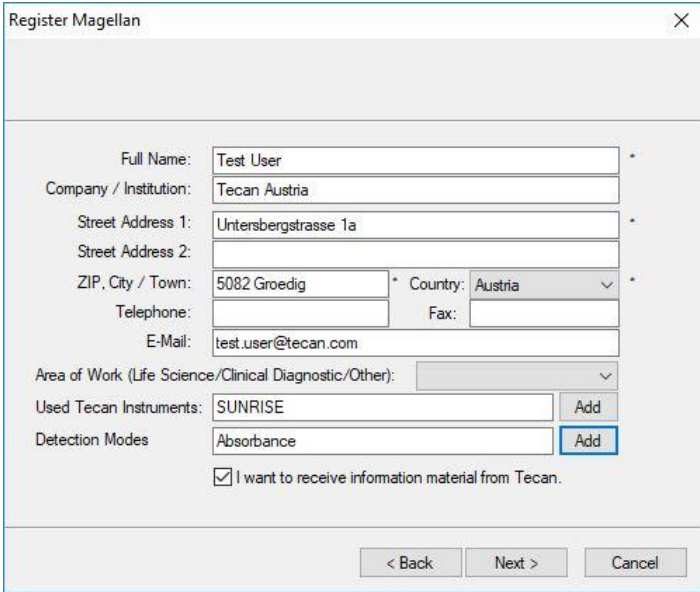
Request a Magellan license number because you did not receive one.

< Back Next > 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.

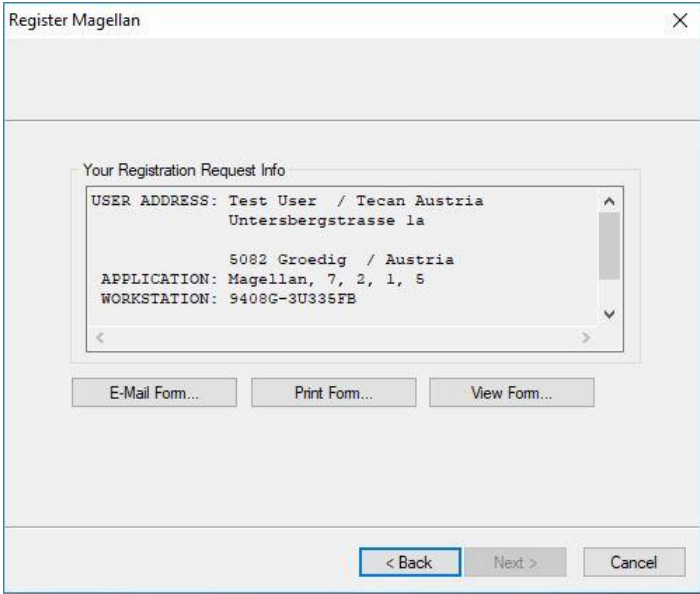
Registration Form

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



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

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



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...

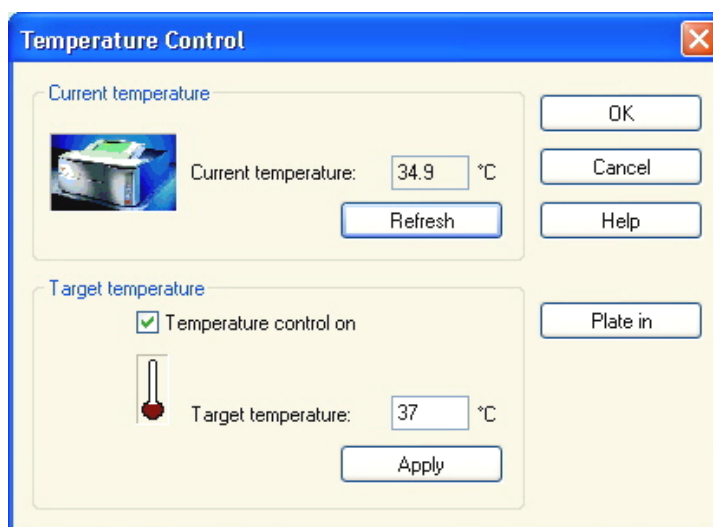
This opens the **Movements** dialog box, in which it is possible to control the movements of the plate carrier and filter slide.

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.

3.2 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:

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

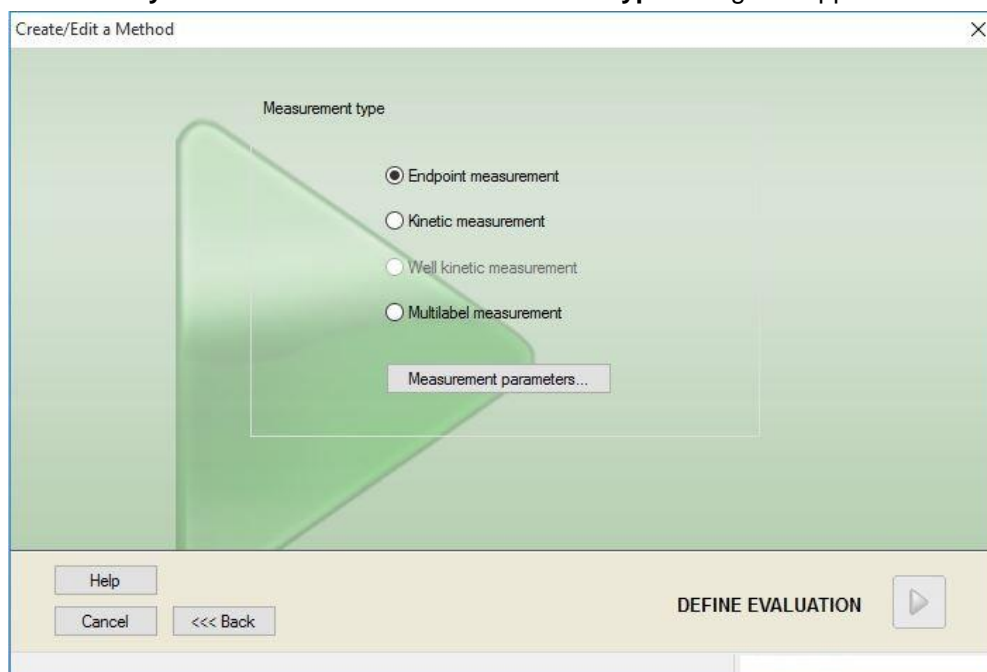
4.2 Define the Measurement Parameters

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.

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

No.	Label	Measurement parameters
1	DEF-1	Measurement mode: Absorbance;Measurerr
2	DEF-2	Measurement mode: Absorbance;Measurerr
3	DEF-3	Measurement mode: Absorbance;Measurerr

Kinetic

Number of cycles:

Interval: hh:mm:ss

Use minimum interval

4. Create/Edit a Method Wizard

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.



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 displays the 'Part of Plate' configuration window. It features a 96-well microplate grid (rows A-H, columns 1-12) with all wells highlighted in yellow. Below the grid, three 'Absorbance' measurement elements are configured:

- Absorbance 3:** Wavelength: 405 nm, Measurement: 405 nm, Reference: 405 nm, Label: Label1.
- Absorbance 4:** Wavelength: 492 nm, Measurement: 492 nm, Reference: 405 nm, Label: Label2.
- Absorbance 5:** Wavelength: 620 nm, Measurement: 620 nm, Reference: 405 nm, Label: Label3.

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 'Kinetic Cycle' configuration window. It features the same 96-well microplate grid. Below the grid, the 'Kinetic Cycle' element is configured:

- Kinetic Cycle:** Cycles: 50, Kinetic Interval: Use kinetic interval (checked), Time: 00:02:30 (hh:mm:ss).

Below the kinetic cycle, an 'Absorbance' measurement element is configured:

- Absorbance 4:** Wavelength: 492 nm, Measurement: 492 nm, Reference: 405 nm, Label: Label1.

4. Create/Edit a Method Wizard

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:

Undo button	Click Undo to undo a previous action.
Redo button	Click Redo to redo an action that was undone.
Select all unused button	Plate Layout mode only: All unused wells of the plate are marked.
Zoom to 10% button	This will set the plate layout view to 10%.
Zoom to 100% button	This will set the plate layout view to 100%.
Zoom mode button	Use the Zoom mode 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.

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
Summary...	Any plate view. The Summary dialog box is displayed. Refer to chapter 7.4.18 Context-Sensitive Menu of a Well/ Summary Dialog for further information on the Summary... dialog box. This option is available if a layout has been assigned to the selected well.
Fill Selection	Plate Layout mode only. 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.
Delete Selection	Plate Layout mode only: This command will delete the IDs and color identifiers of the selected wells and leave them blank.
Select all Unused	Plate Layout mode only: All unused wells of the plate are marked.
Set / Remove Alias...	Plate Layout mode only: 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:

4. Create/Edit a Method Wizard

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

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
Rename transformation	A different name can be assigned to the selected transformation.
Insert transformation	Used to define a new transformation.
Remove transformation	Used to delete a transformation.

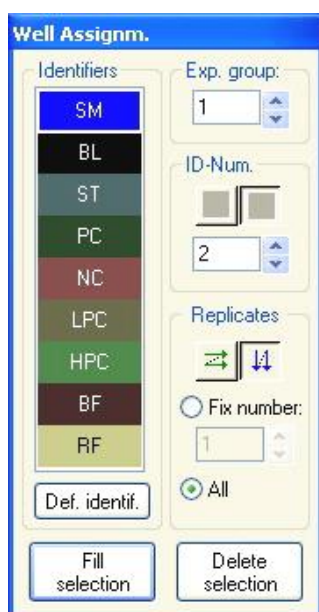
4.3.2 *Method Layout: How to Define a Plate Layout*

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).

4. Create/Edit a Method Wizard

Standard identifiers are:



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

SM1_4	1 st line: sample, experimental group number of 1, sample ID number of 4.
1/14	2 nd line: number of replicate is 1, total number of replicates is 14.
x-BL1	3 rd 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.

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

Identifiers group box	<p>In this group box, corresponding identifiers for the marked wells have to be selected.</p> <ul style="list-style-type: none"> All available identifiers are listed in a drop-down list. Click the Define Identif... button to define additional identifiers. The Define Identifiers dialog box appears, see below for further details.
Exp. group 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 Experiment group selection field, define which experiment the wells belong to.</p>
ID-Num. group box	<p>The ID Number 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"> ID-Num. selection field The ID-Num 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. Arrow buttons 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.
Replicates 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"> Fix number 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. All 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. <p>Two Arrow buttons define the direction of counting up the replicate number.</p>
Fill section 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>
Delete section button	<p>Click Delete or press DEL to delete the IDs and color identifiers of the selected wells and leave them blank.</p>
Define identifier button	<p>Click Def. identif. 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>

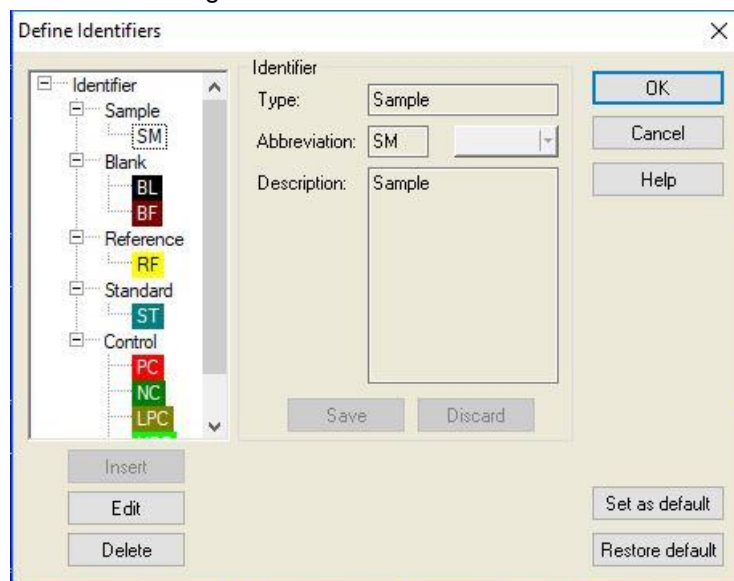
4. Create/Edit a Method Wizard

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

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

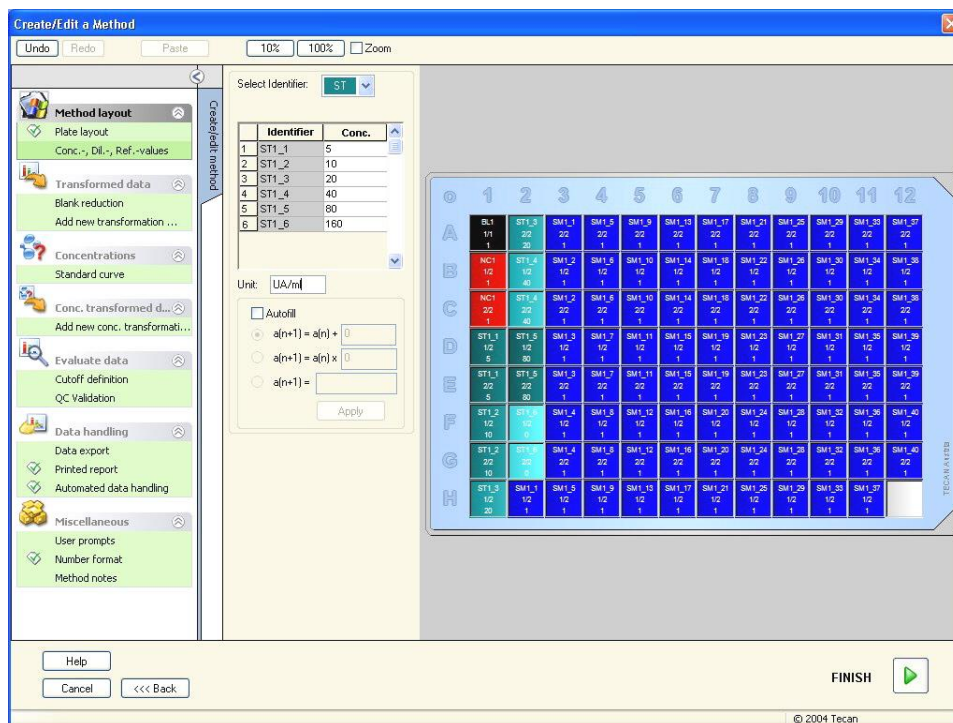
Identifier tree structure	A structured view of all existing identifiers, their colors and abbreviations is offered in a small window. The identifiers are listed under the groups Sample , Blank , Reference , Standard and Control .
----------------------------------	---

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

4. Create/Edit a Method Wizard

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:

<p>Select Identifier drop-down list</p>	<p>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.</p>
<p>Exp. group selection field</p>	<p>Select the respective experimental group. If there is only one experimental group, the field cannot be edited.</p>
<p>Table with Identifier and Concentration/ Dilution columns</p>	<p>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.</p>
<p>Unit text field</p>	<p>The displayed concentration unit can be determined.</p>
<p>Autofill check box</p>	<p>The Autofill function provides the calculation of the corresponding concentrations or dilution factors according to available types of series.</p>

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

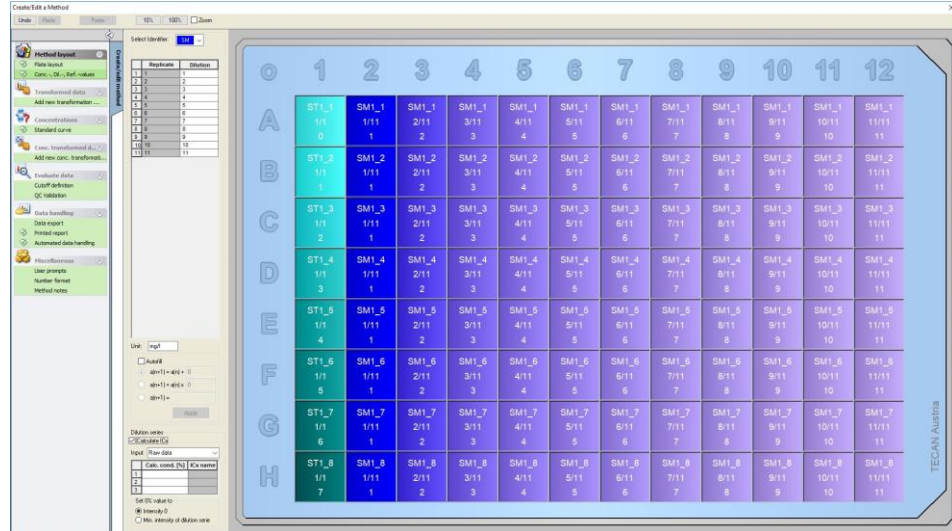
4. Create/Edit a Method Wizard

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 IC_x (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%.

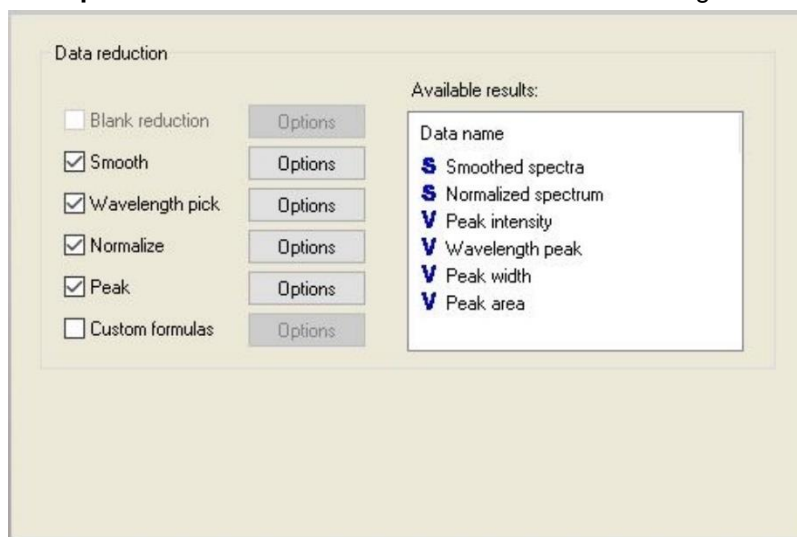
4.3.4 Precalculation: Spectra Data Reduction

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:



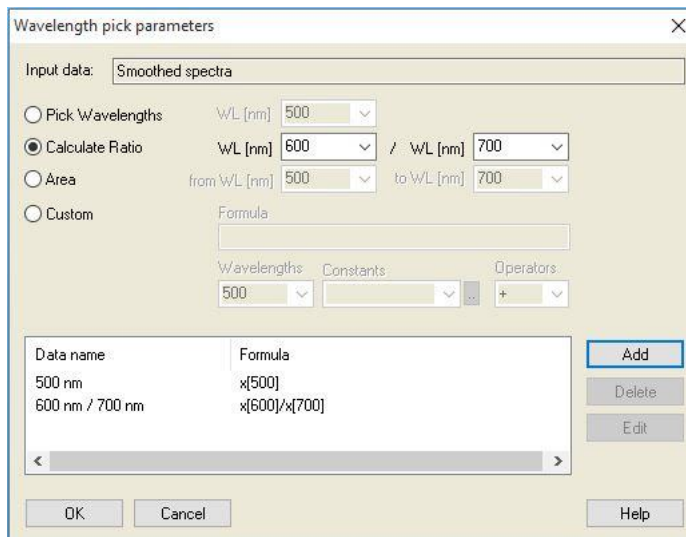
Blank reduction check box	This option is only available if blanks are defined on the layout. The blank reduced spectra is calculated by subtracting the spectrum of the blank well from all other wells. When more blanks are defined on the plate, e.g. when multiple experimental groups are defined, an additional 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.

4. Create/Edit a Method Wizard

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:

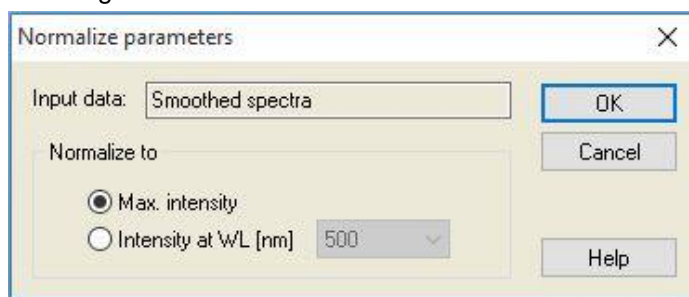


Intensities at a specific wavelength can be extracted, ratios and areas can be calculated and customized formulas can be entered.

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

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.

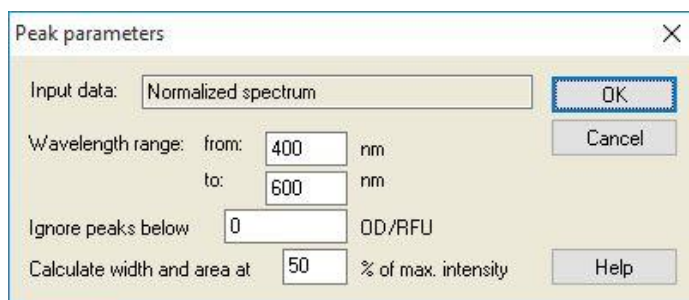
Input data text box: shows the input data to be processed.

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.

4. Create/Edit a Method Wizard

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 in order 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: $1/10^x$.

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:

Input data drop down list	The list contains the measurement values, the results from precalculations and all already defined transformations, as well as the averages. If Mean data is selected as Input data for Transformations , then transformations will be assigned to the first replicate of an identifier only.
Formula text box fx	Formulas can be entered by typing or by selecting the needed function from the Functions&Constants list box.
Formula 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.
Confirm button	Formula edit mode only. Green hook Assigns the transformations to the selected well. Click Confirm button or press ENTER key to assign the formula definition to the well and change to Select mode.
Cancel button	Formula edit mode only. Red cross Click the Cancel button or press the CANCEL key to leave the Edit mode without assigning the formula definition to the well.
Available data 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.
Functions drop down list	Lists all mathematical and Boolean functions for the definition of formulas.
Options 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"> • Identifier average name • Identifier replicate name • Plate well name
Constants button	Click this button to open the Define Constants dialog box where constants for calculation can be defined.

The transformation definition has two modes:

4. Create/Edit a Method Wizard

Select mode	When clicking on a well, the corresponding formula is displayed in the text box. The currently active well is displayed with a red border.
Edit mode	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:

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

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:

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

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

4. Create/Edit a Method Wizard

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 1st and the nth 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):

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

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).

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:

Input data drop down list	Select the input data to be processed.
Mean minimum value check box	Select to open the Points 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.
Mean maximum value check box	Select to open the Points 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.
Area 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"> • Time/Points option buttons: If Time is selected the start and end time is entered in hours, minutes and seconds. If Points is selected the start and end point for the analysis is given through the entered kinetic cycle number.
	<ul style="list-style-type: none"> • Start field: The start time (in hours, minutes and seconds) or cycle number has to be entered here.
	<ul style="list-style-type: none"> • End field: The end time (in hours, minutes and seconds) or cycle number has to be entered here.

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 1st, 2nd, and 3rd kinetic value

average of 2nd, 3rd, and 4th kinetic value

average of 3rd, 4th, and 5th kinetic value

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

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

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

4. Create/Edit a Method Wizard

Available Data Tab

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

Data field	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:

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

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.

Data Tab

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

Exp. group spin control	If several tests are to be performed on one plate the Experiment group must be selected. If the plate contains only one test, then the spin control will not be displayed. For each experiment group the input data can be defined individually.
--------------------------------	--

Input data drop down list	Select the Input data to be used for the standard curve. Select measurement data or any available transformation results.
Standards from layout option button	Calculate the standard curve from the standards on the layout.
Standards from ext. file option button	If the selected experimental group contains no standards, a standard curve can be loaded from a .std file. The Select button must be clicked to select the file.
Standards from exp. group option button	If the selected experimental group contains no standards, a standard curve from another experimental group can be used.
No standard curve 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).
Additional Concentrations button	Click the Additional Concentrations button to open the Calculate Additional Concentration 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:	
Input data drop down list	Select the input data for calculation of additional concentrations.
Selected data list	The list contains the input data names for calculation of additional concentrations.
Add button	Click the Add button to add the currently selected input data in the Input data drop down list to the Selected data list.
Remove button	Click the Remove button to remove the currently selected data from the Selected data 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	<p>Select which interpolation algorithm is to be employed when calculating the standard curve:</p> <p>All offered analysis types are listed and can be selected:</p> <ol style="list-style-type: none"> 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)
-------------------------------------	---

4. Create/Edit a Method Wizard

	10. LogitLog (including the more button for minimum and maximum determination)
Data scaling drop down list	<p>The analysis type is applied to scaled values. Following scaling modes can be selected:</p> <ul style="list-style-type: none"> • 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 0.000001.

More button	<p>Click the More button to view the following options:</p> <ul style="list-style-type: none"> • Standard curve numeric selection field If there is more than one experimental group, for LogitLog and Four Parameters the Min. and Max. value can be selected for each curve individually. • Weighting Select Use weights to use one of the following weighting methods: <ul style="list-style-type: none"> - Automatic using variance - Automatic using relative weight - Manual <p>See chapter 11.4.14 Weighting for Four / Five Parameter Fit – Marquardt / Polynomial Fit</p> • Weighting dialog – select More button if “Automatic using variance” is selected => 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. • Min/Max text fields Min/Max allows the user to define the minimum or the maximum limit of the standard curve for LogitLog and Four Parameters.
Include (0,0) check box	<p>If the Include option is selected, (0,0) will be added as standard point. This is only available if Linear has been selected as the axis division for both axes.</p>

Extrapolation 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 $\text{min}-2*(\text{max}-\text{min})$ and $\text{max}+2*(\text{max}-\text{min})$, where min and max correspond to the minimum and maximum concentration value of the standard curve.
Extrapolation factor numeric field	The factor data field is only active, if the Extrapolation 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.

Exp. group spin control	If a number of experimental groups is available, the appropriate group can be chosen.
Input data drop down list	All data available for calculation is displayed in this list.
Intercept name and formula 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	<p>The selection boxes allow for the easy input of formulas by providing a variety of functions, operators and variables.</p> <ul style="list-style-type: none"> • 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: $(\text{ST1}_1 + \text{ST1}_8) / 2$

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

4. Create/Edit a Method Wizard

Axis Tab

Use this tab to define the appearance of the axes.

X-axis group box	Following elements are available in each group:
Y-axis group box	<ul style="list-style-type: none"> • 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.

Graph Tab

Use this tab to define the appearance of the graph.

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

Input data drop down list	Select the input data which is to be used in the evaluation.
Exp. group 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.
Colors buttons	A color can be allocated to the individual result levels. When displaying the results these colors will be incorporated, representing the qualitative results.
Labels text fields	The result indicators for every value range must be named, for example: positive (pos), negative (neg), intermediate (?), ...
Limits 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 Formula input fields. A maximum of up to nine limits may be defined.
Formula input group box	Formulas to be entered into the Limits 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. <ul style="list-style-type: none"> • Variables drop down list All available variables are 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 Available functions can be selected.

4. Create/Edit a Method Wizard

Competitive Test 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 Low-High arrow will be reversed.
Cutoff results selection... button	Click the Cutoff results selection... button to open the Cutoff Results Selection dialog box.

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:

Cutoff display selection tree structure	All defined identifier names are shown in a tree structure, grouped by identifier types. Each identifier is associated with a check box. 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.
---	--

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:

Input data drop down list	Select the relevant data, to which the validation must apply. For example: Raw data, etc.
Exp group 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.
Validation group selection field	Use Validation groups to define validation criteria for the same experimental group with different input data.
Validation Conditions list field	This one-dimensional list will be filled with the formulas and logical equations, which define the Validation Conditions . 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	<p>Parts of the formulas to be entered into the Validation Conditions field can be selected from the following drop down lists:</p> <ul style="list-style-type: none"> • 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):

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

Available data 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 Available data window and then the arrow pointing towards the Selected data window. Data can be deselected by operating the reverse procedure.
Up and Down buttons	The order of the selected data can be changed by selecting an item and pressing the button Up to move it up or Down to move it down
Selected data list	This list shows all selected data, which has been transferred from the Available data field list.
Export options... button	Click this button to open the Export Options 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

Direction group box	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"> • Horizontal option button The data is collected in rows.
	<ul style="list-style-type: none"> • Vertical option button The data is collected in columns.
Result group box	Select how to export the data in the form of a matrix or of a continuous list:
	<ul style="list-style-type: none"> • Matrix (nested) 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.
	<ul style="list-style-type: none"> • Matrix (separated) option button Data of each selected data set is arranged in a separate matrix.
	<ul style="list-style-type: none"> • Matrix (XFluor style) option button Data of each selected data set is arranged in a separate matrix together with column and well description similar to XFluor.
	<ul style="list-style-type: none"> • Table (well data in rows) option button All data of one well is arranged in horizontal direction starting with data of the well position A1.
	<ul style="list-style-type: none"> • Table (well data in columns) option button All data of one well is arranged in vertical direction starting with data of the well position A1.
	<p>If the Add kinetic timestamps check box is selected, the time stamps of the measurements are added.</p> <p>If the Add Temperatures check box is selected, the temperatures of the measurements are added.</p> <p>If the Insert Data names 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>

Add data group box	<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"> • Date/time of measurement check box • Method filename check box • Method pathname check box • Workspace filename check box • Workspace pathname check box • Filter wavelength value(s) check box • User prompts check box • Current user name check box • Measurement parameters check box • Multiplate plate information check box • Workspace audit trail check box (magellan Tracker only) • Workspace signatures check box (magellan Tracker only)
Set as default button	<p>Settings can be logged as a default for future use.</p>
Restore default button	<p>Settings can be reset to the previously defined default.</p>

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

<p>Matrix (nested), horizontal: 11 81 12 82 13 83 21 91 22 92 23 93</p>	<p>Matrix (separated), horizontal, with timestamps: 0 s 11 12 13 21 22 23 33 s 81 82 83 91 92 93</p>	<p>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</p>
<p>Table (well data in rows), horizontal, with timestamps: 0 s 33 s 11 81 12 82 13 83 21 91 22 92 23 93</p>	<p>Table (well data in columns), horizontal: 11 12 13 21 22 23 81 82 83 91 92 93</p>	<p>Table (well data in columns), vertical: 11 21 12 22 13 23 81 91 82 92 83 93</p>

Export to ASCII File

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

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

Target group box	<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"> • New workbook 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. • New worksheet 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. • Insert into worksheet at cell 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. • Append to current worksheet 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. • Use Insert into Template to export data into a predefined Excel template. Path and name of the Excel template must be entered, clicking the ...-button. The corresponding cell position must be indicated.
Set as default button	The settings can be logged as a default for future use.
Restore default button	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

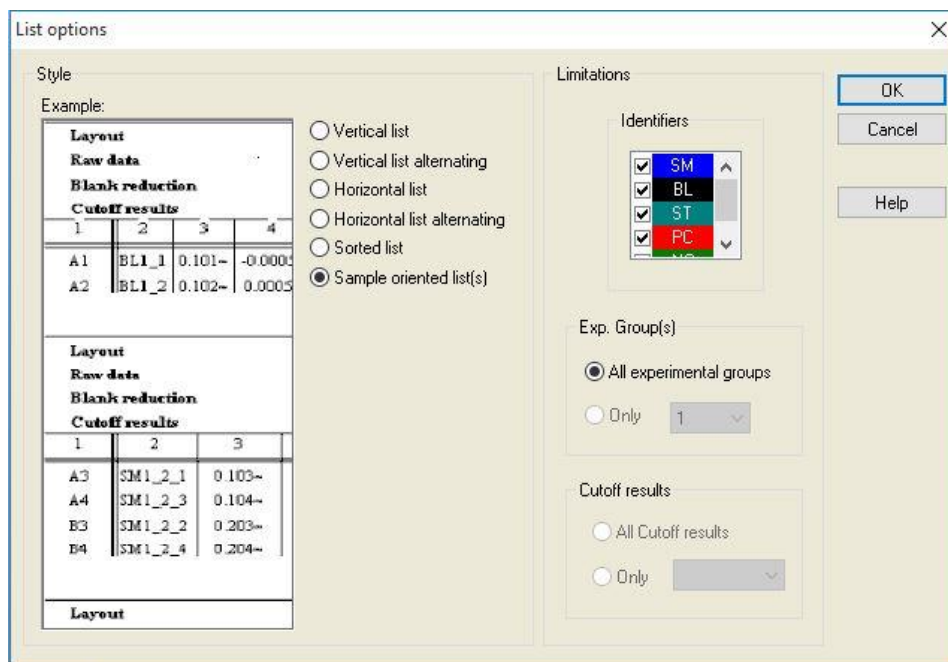
Data Selection Tab

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"> • List The individual list format (horizontal, vertical, sorted and alternating) must be configured in the properties dialog (see below). • Matrix The matrix selection prints the data in a 2 dimensional list (matrix).
Data source and destination lists	<p>Two lists are used to define the printed data:</p> <ul style="list-style-type: none"> • Available data list: List of all available data, which can be printed. Page breaks and dividing lines can be added in order to achieve the preferred layout. Elements to be printed can be selected by double-clicking; they are listed in the selected data list.
	<ul style="list-style-type: none"> • Selected data 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.
Append button	<p>Click this button to transfer data highlighted in the Available data window to the Selected data window. You can also use drag and drop.</p>
Insert button	<p>Use this option to display two pieces of similarly formatted data within the same area. First, data from the Available data list must be selected, then data from the Selected data list. When clicking the Insert 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 Selected data 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	Vertical list option button Prints the data in form of a vertical list (order A1, B1, and so on).
	Vertical list alternating option button The order of the data is alternating for each row or column (order A1, B1, ... H1, H2, G2, ... A2)
	Horizontal list option button Prints the data in form of a horizontal list (order A1, A2, and so on).
	Horizontal list alternating option button The order of the data is alternating for each row or column (order A1, A2, ...A12, B12, B11,...B1).
	Sorted list 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.
	Sample oriented list(s) 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 Sample oriented list(s) with other parameters like Identifiers, Exp. Groups and Cutoff results.

4. Create/Edit a Method Wizard



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 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

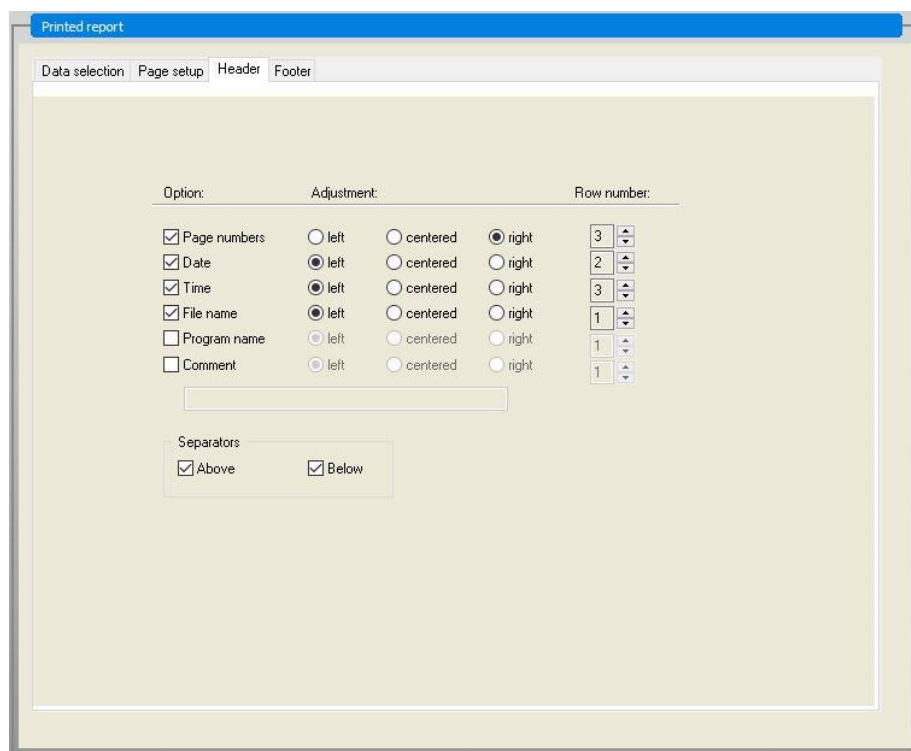
- **Color** option button
The printout is in colors, if supported by the printer. The well specific data is printed in the color of the layout (for example: sample raw data is printed blue). The cutoff results are printed in the color of the range (for example: “pos” wells are printed red). The graph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



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

Adjustment option buttons	Select one of the following options: <ul style="list-style-type: none"> • Left • Centered • Right
Row number list	Row number is a numeric field, where the row for each option can be adjusted.
Separators 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"> • Above check box: Separator line appears above the header. • Below check box: Separator line appears below the header.

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:

Filename group box	Select the filename of the sample ID list to be loaded: <ul style="list-style-type: none"> • Same filename as workspace option button • Filename option button: Enter a filename in the text field.
---------------------------	--

Path group box	Select the path where the sample ID list is stored: <ul style="list-style-type: none"> • Sample ID list default path option button • Use path option button: Select any path.
Format 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"> • Autodetect from the list of supported formats option button • Custom file format option button: Click the File format... button to open the Custom Format dialog box.



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.).

More – Workspace Name

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

Format group box	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: <ul style="list-style-type: none"> • Date (DDMMYYYY) + Counter option button • Date (YYYYMMDD) + Counter option button • Total Counter option button • Use available barcode option button
Prefix text field	The entered text is added at the beginning of the workspace name as defined above.
Example text field	The Example text field shows an example of the current selection.
Set as default button	The settings can be logged as a default for future use.
Restore default button	The settings can be reset to the previously defined default.

4. Create/Edit a Method Wizard

More – Export to LIS

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

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

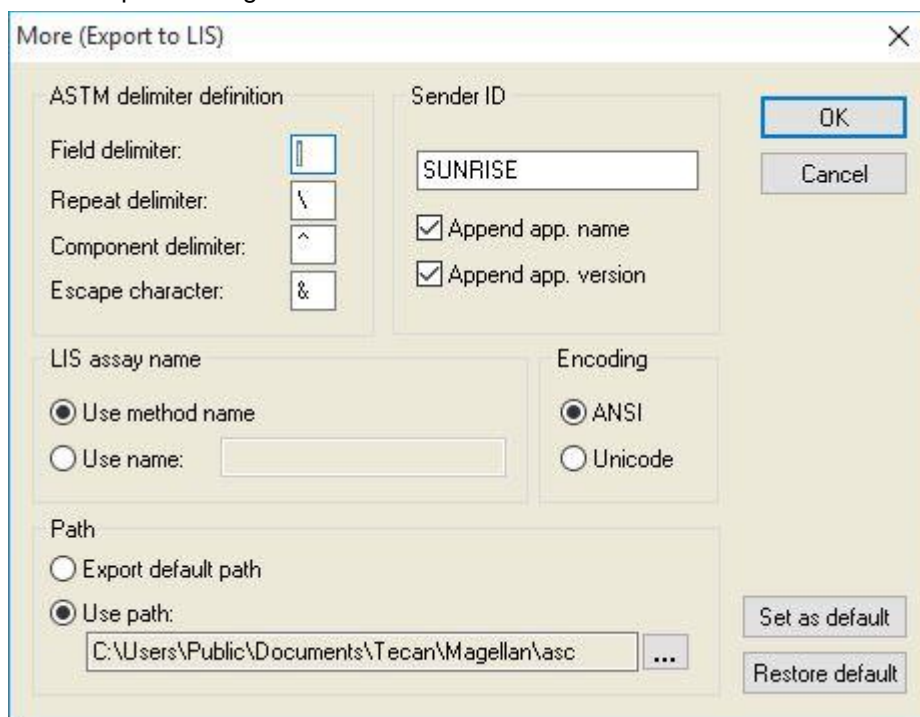
ASTM Export – Example File

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

	<ul style="list-style-type: none"> • Message Header Record: H \^& SUNRISE^Magellan V7.2^Tracker
	<ul style="list-style-type: none"> • Patient Information Record (P): P 1 Sample ID 1 for patient 1
	<ul style="list-style-type: none"> • Test Order Record (O): O 1 SampleID ^method name Date and time of measurement
	<ul style="list-style-type: none"> • Result Record (R): R 1 ^method name^results
	<ul style="list-style-type: none"> • 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|
```

4. Create/Edit a Method Wizard

More – View Results

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

Plate view group box	<p>Select the data to be displayed in the plate view:</p> <ul style="list-style-type: none"> • 1st line in well (fixed) drop down list: Select a name from the available data names. • 2nd line in well (fixed) drop down list: Select a name from the available data names. • 3rd line in well (first selection) 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 3rd line. The first two lines remain unchanged. <p>The 1st and 2nd line can be omitted by selecting not used, which makes the plate view more easily readable.</p>
Text box 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 have to 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.

4.4 Saving the Method

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

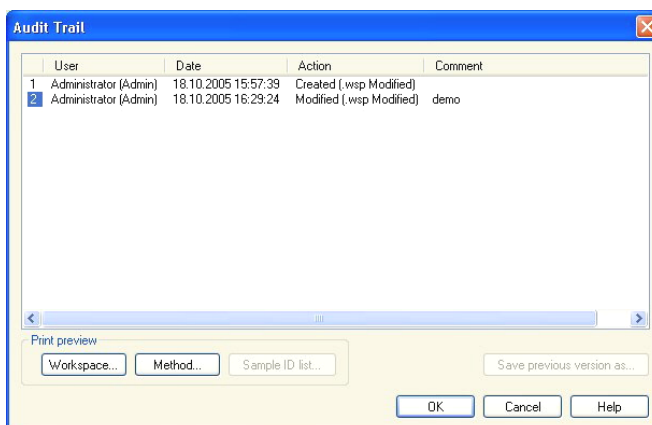
Filename field	Enter or modify the method's file name.
File remarks field	Add some comments to the file name, which will be displayed for example in the Open file dialog boxes.
Audit trail comment field	Add some comment, which will be stored in the audit trail (only available for magellan Tracker).
Organize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

Audit trail... button	<p>Click this button to open the Audit trail 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>
------------------------------	--



Signature... button	<p>Click this button to open the Signature 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 Attach Signature wizard. See chapter 8 Attach Signature Wizard for further details.</p>
Method password 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. Create/Edit a Method Wizard

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

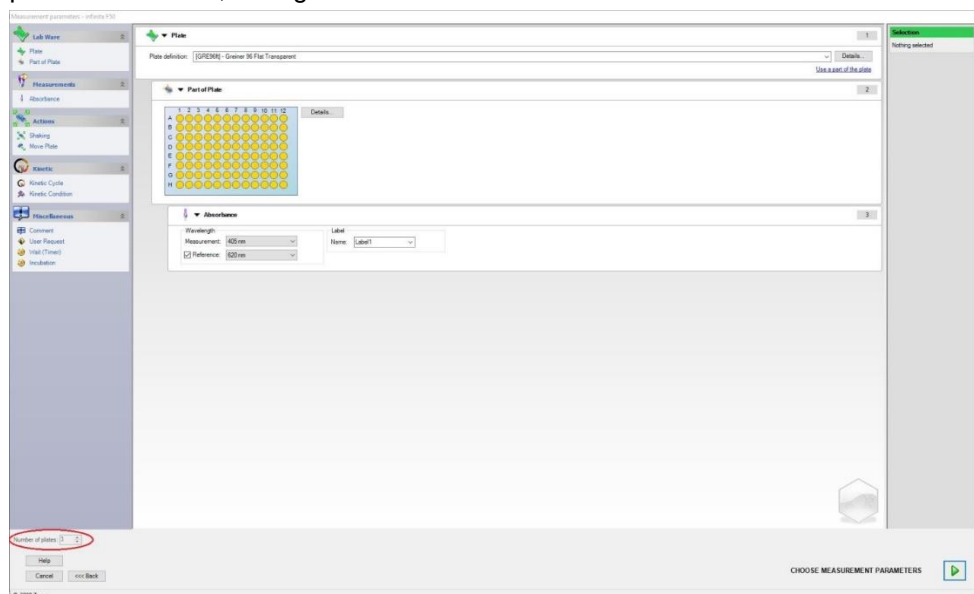
In order to change the password of a password protected method, open the method in **Edit mode** (password entry required) and enter a new password in the **Method password edit field** of the **Save as tab**. Click **Finish**.

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

4.5 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.

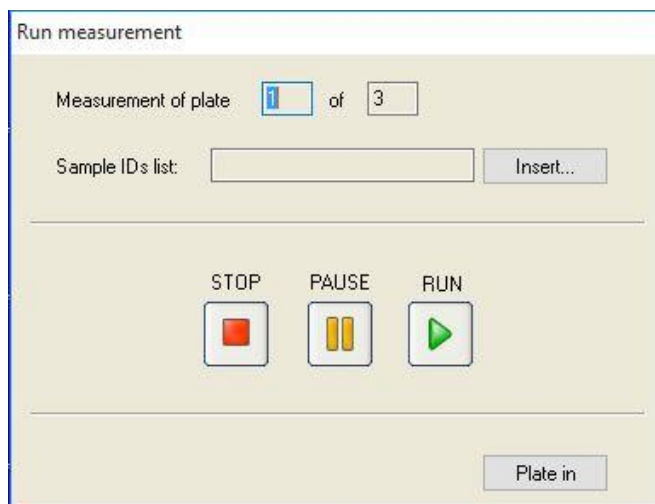


When two or more plates are to be measured, a counter for switching between the plates is available in the **Define Evaluation** window as well.



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

4. Create/Edit a Method Wizard



Sample IDs list	For each single plate a sample ID list can be selected.
STOP button	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.
PAUSE button	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.
RUN button	Measurement of the next plate is started.
Plate in/ Plate out	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) Create new option button	A new sample ID list can be created.
b) Edit option button	An existing sample ID list can be modified.
Show combo box	The files are displayed according to the chosen selection: <ul style="list-style-type: none"> All files My files: This option is available if the user administration is enabled (always enabled in magellan Tracker)
Filename list	The sample ID list to be edited has to be selected. A Remarks 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.
Print Preview... 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

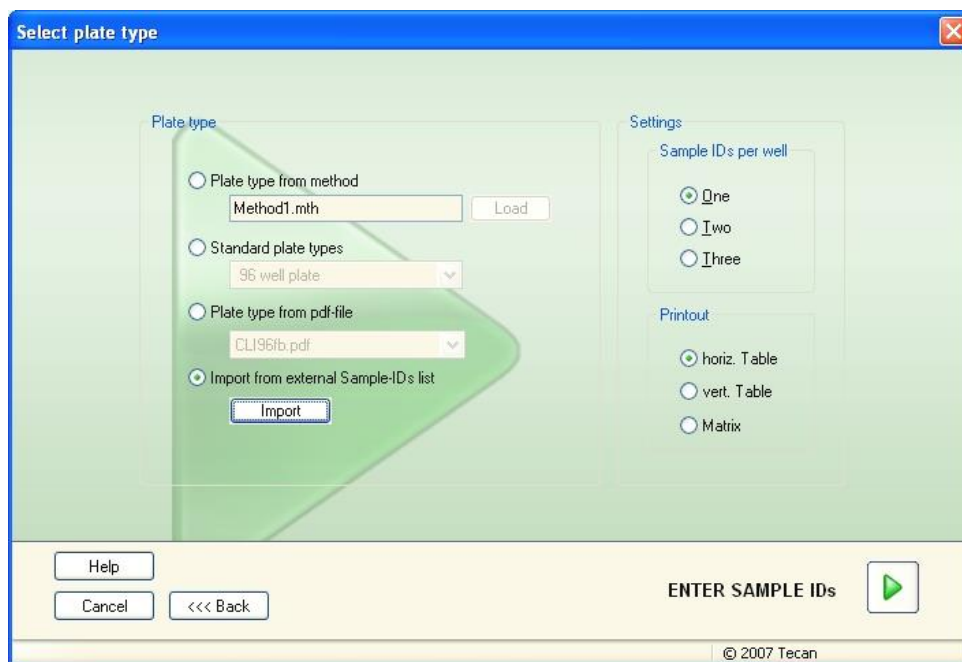
In the **Select Plate Type** window the number of sample IDs per well and the used plate type can be selected. The **Import from external sample ID list** option allows to browse for different types of sample ID files and to import them into **magellan**.



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

Sample IDs per well option buttons

Enter the number of sample IDs required per well (a maximum of three can be entered).

Printout option buttons

Define the layout for printing the sample ID list.

Plate type option buttons

Four option buttons define the plate type to be selected:

- Plate type from method**
 Select a method to load the plate layout. Click **Load** to browse for existing method files. The Windows™ **Open** dialog box appears. Select the desired file and click **Open**.
- Standard plate type**
 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.
- Plate type from pdf-file**
 A predefined pdf file (SUNRISE instruments) or a pdfx file (INFINITE F50 instruments) can be used to define the plate format.
- Import from external Sample ID list**
 An external file type can be selected for import as sample ID list. See chapter 5.2.3 Import a Sample ID List.

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

Settings... button	The button opens the Sample ID List Settings dialog box, where the number of sample IDs per well can be selected.
Edit... button	The Edit button opens the Edit Well dialog box. The sample IDs of the marked well can be edited. See below for further information.
Autofill... button	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 Autofill to open the Autofill Selection dialog box. See below for further information.
Delete button	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 Delete or press the DEL key to delete the sample IDs in the selected wells.
Undo button	Performs an undo of the last action. Click Undo or press CTRL-Z to undo a previous action.
Redo button	Repeats the action, which was performed before the undo step. Click Redo or press CTRL+Y to redo an action that was undone.
Print format	Select the layout for printing the sample ID list: <ul style="list-style-type: none"> • horiz. Table • vert. Table • Matrix
Print preview	Opens the print preview of the printed sample ID list.

5. Create/Edit a Sample ID List Wizard

10% button	This will set the plate layout view to 10%.
100% button	This will set the plate layout view to 100%.
Zoom check box	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 Zoom mode 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 Summary 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 Delete or press DEL 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 Edit option opens the Edit Well 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 Autofill option displays the Autofill Selection 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:

Left, Right, Up and Down 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 Arrow keys can also be used for this kind of navigation.
On Enter move in vertical direction check box	On clicking Enter or Tab , 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.
Edit sample IDs text fields	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 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.
Autoincrement check box	The Autoincrement 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 Enter / Tab key or the arrow buttons. Using Autoincrement , 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.

The Autofill Selection dialog box contains the following elements:

5. Create/Edit a Sample ID List Wizard

Use ID check box	The Use ID 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.
Sample ID text fields	Sample IDs for the marked well can be entered in the Sample ID text fields. The sample IDs can contain letters, numbers or a combination of letters and numbers.
Autoincrement check box	The Autoincrement check box must be selected, if the sample IDs for the wells are to be numbered automatically (incremented by 1).
Start index text field	The Start index text field is only editable, if the Autoincrement check box is selected. The starter value for the automated incrementing of the sample ID has to be entered.
Vertical check box	The Vertical check box can only be accessed, if the Autoincrement 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:

Information tree	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.
Left, Right, Up and Down buttons	The direction buttons can be used to select another well on the plate while leaving the dialog box open.
Expand All / Shrink All	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	alpha numerical, max. 3 characters. If an error occurred during pipetting one of the following characters is displayed here: First character <Space> no liquid error L: no or not enough liquid Second character <Space> no barcode error M: manually entered barcode Third character <Space> no timer overrun O: timer overrun

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.

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

5. Create/Edit a Sample ID List Wizard

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.

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

5. Create/Edit a Sample ID List Wizard

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).

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:

Plate type 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.
Rows	Enter the number of rows.
Columns	Enter the number of columns.
File format group box	In the File format group box the format of the specified file can be defined.
File extension	In the File extension 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.

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

5. Create/Edit a Sample ID List Wizard

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:


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

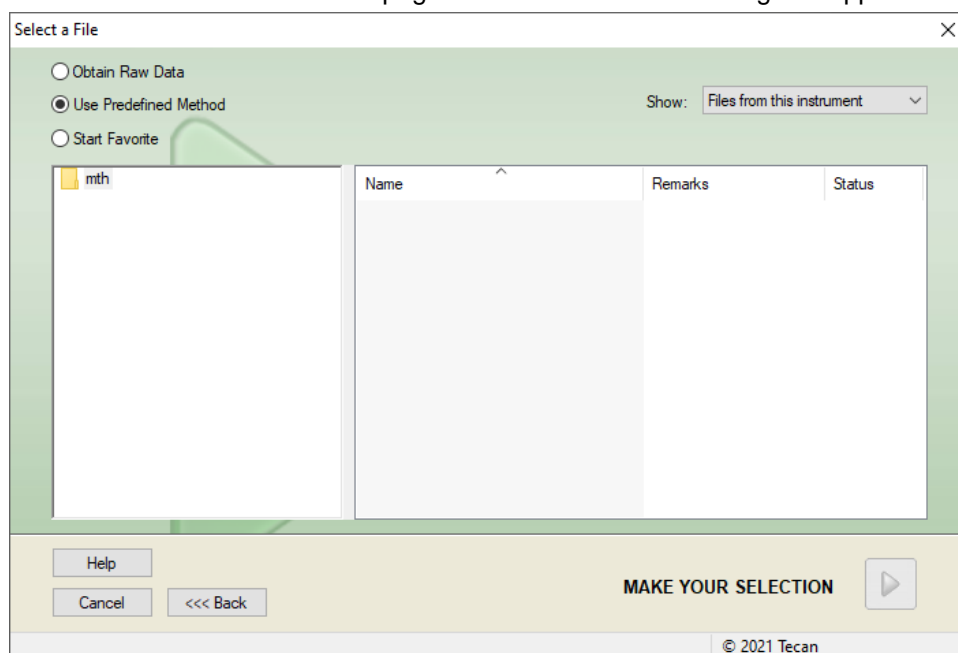
The Save&Finish button is only enabled when a document has been modified. The modified document can be saved under its current file name or under a different name.

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:



Obtain Raw Data	Is used to generate raw data quickly by setting the required measurement parameters.
Use Predefined Method	Is used to perform measurements based on already defined methods.
Start Favorite	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:

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

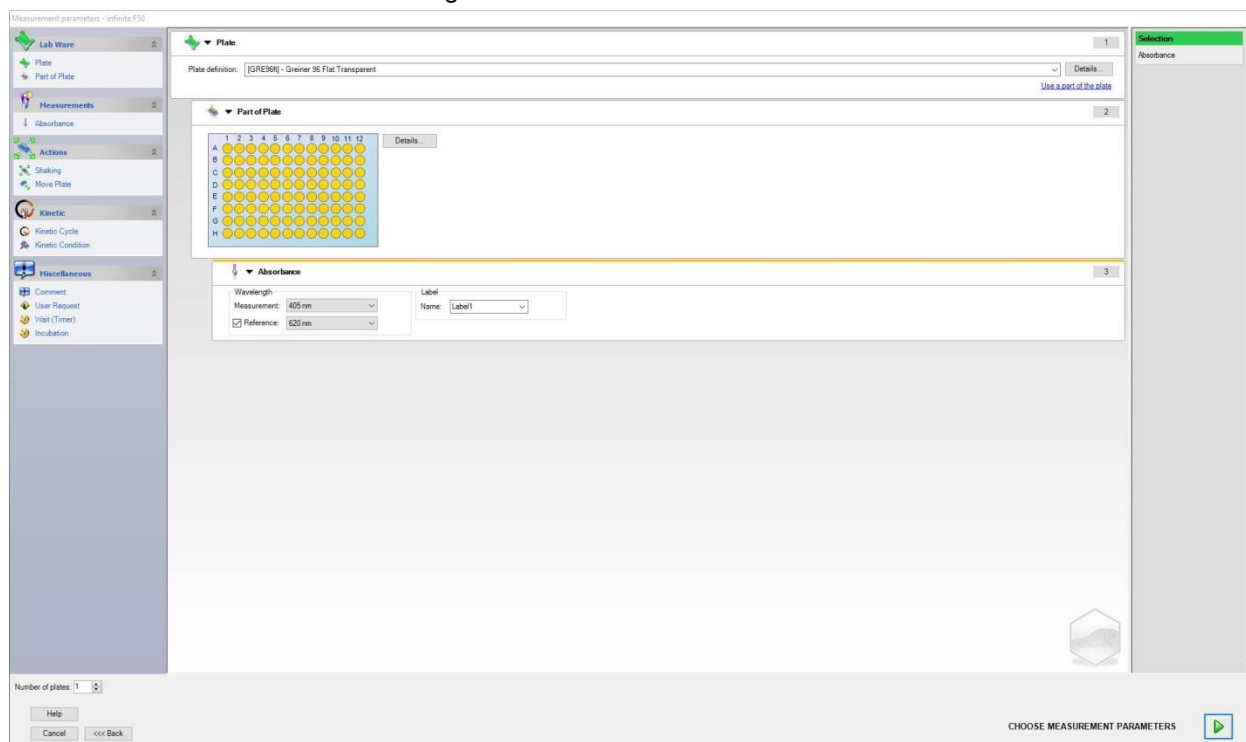


WARNING


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**.

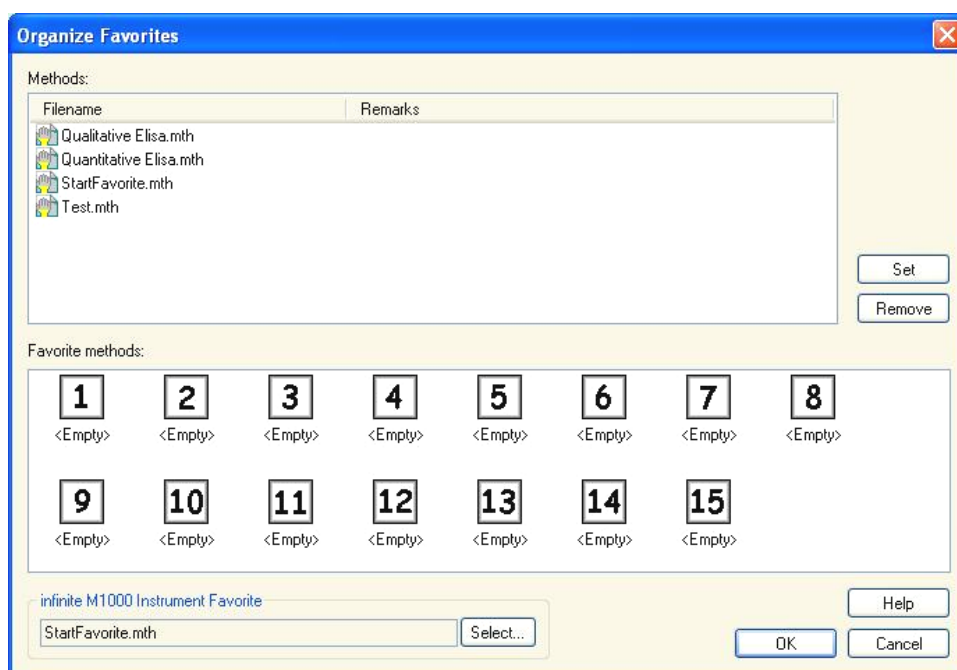
6.4 Start Favorite

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:

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

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:

Prompt Answer list	At each text field of this list any text prompt can be entered.
Req. check box	A Required check box next to every Prompt Answer 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.

Constants list	At each text field of this list the value of the constant or the comment can be modified.
Req. check box	A Required check box next to every Constant value 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

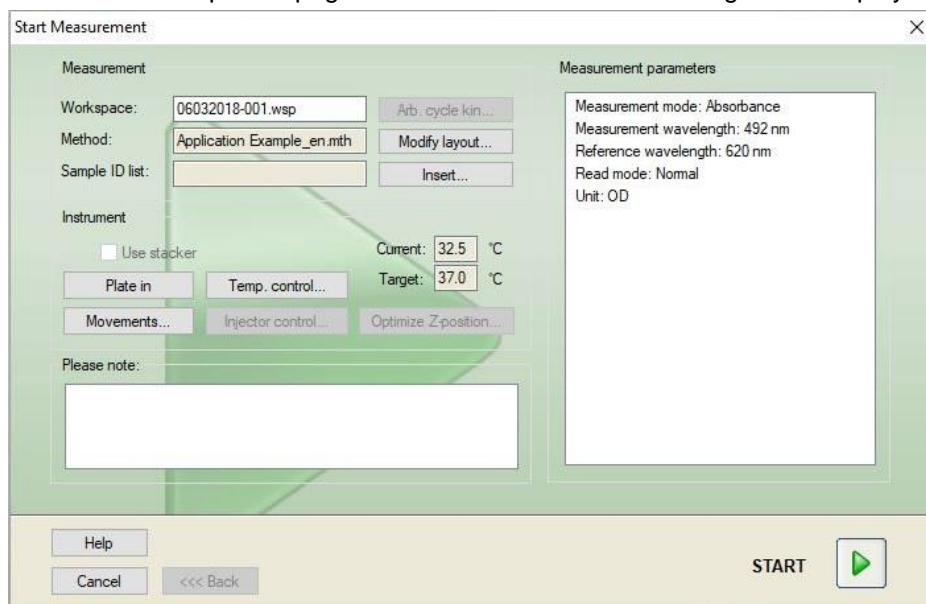
Using magellan Tracker or magellan Standard with User administration, a default magellan Operator (refer to the chapters 9.6 User Rights and 9.5.3 Change User) can edit only the required constants. The constants without required flag set are displayed gray and cannot be edited.

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

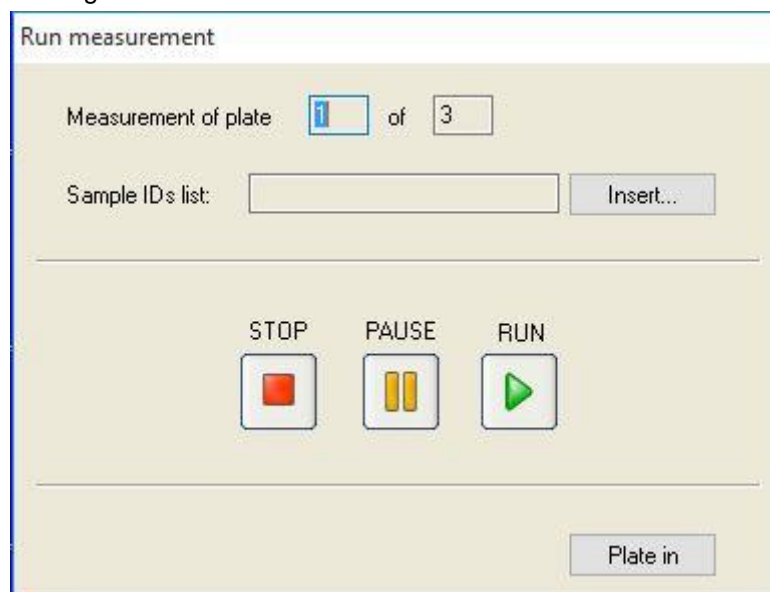
6. Start Measurement Wizard

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

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:

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



Note
Only sample ID lists created in magellan can be inserted. Import of other formats is not supported.

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

Filename field	The list displays all available sample ID list files (.smp). Select a sample ID list by clicking a filename.
Remarks field	Available comments and remarks will be displayed.
Import... button	Click to open a standard Windows Open 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.

6. Start Measurement Wizard

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:

10% button	Click to resize the displayed plate layout to show 10% of the plate layout on the full screen.
100% button	Click to resize the displayed plate layout to show 100% of the plate layout on the full screen.
Zoom check box	When this Zoom 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.
Remove unused samples 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 Remove unused samples 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:

Status text field	The text field is updated during the measurement and contains a measurement status information.
Display in wells group box	Select the mode of representation of data in the wells: Values: The measured value is displayed in the well. If more than one value is measured all values are displayed in one well. Graph: The option is enabled if a kinetic graph can be displayed. The graph is shown as soon as more than one value is available.
Pause button	To pause a kinetic measurement run at the next possible moment, click the Pause button. In the Pausing Kinetic dialog click the Plate out / Plate in button to move the plate transport out of or into the instrument. Click the Continue button to go on with the kinetic run.
Break button	Click this button to break the measurement at the next possible time point.
Plate View display	The Plate View display shows a schematic display of the microplate. According to the Display in wells 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.
Cycle text field	If a kinetic measurement is performed, the Cycle text field displays the current cycle number and the maximum number of kinetic cycles.

Graph 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 Measurement Status dialog box.
Previous cycle group box	As long as the transmission of the data of the current cycle was not started the Raw data and the Temperature text fields contain the value and the temperature of the previous measured cycle of the currently selected well, respectively.
Time group box	The Elapsed time text field displays the time span since the start of the measurement.
	The Exp. run time 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.

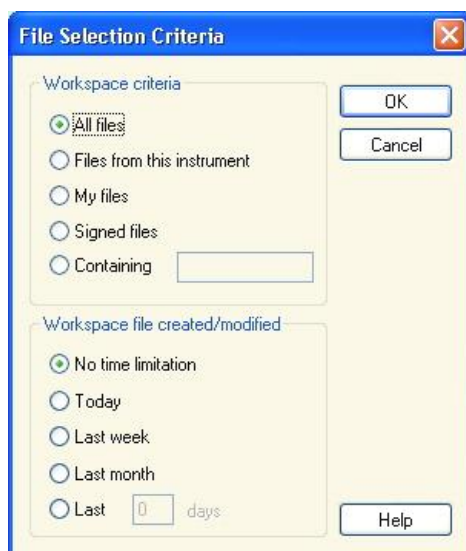
7.2 Select a File

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

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

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

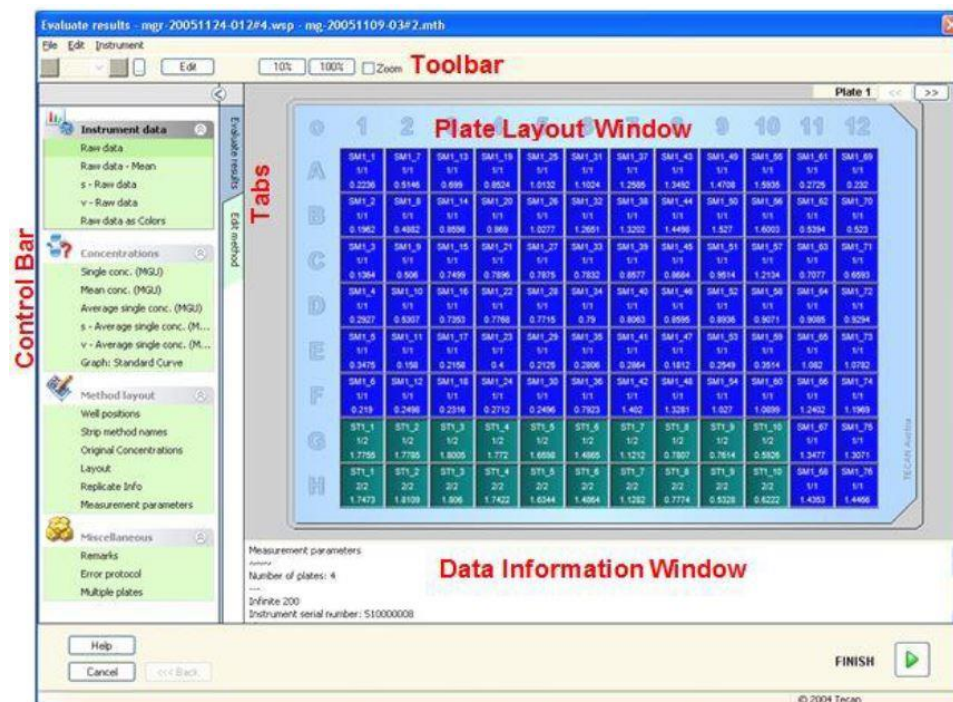
If a SUNRISE instrument is connected, but an INFINITE F50 method is selected, the Instrument Mismatch dialog appears:

- **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.

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.

7. Evaluate Results Wizard

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.

Edit	Click the Edit button to edit or mask raw data.
 button	Click this button to display the Summary dialog box.
10% button	Click this button to resize the displayed plate layout to show 10% of the plate layout on the full screen.
100% button	Click this button to resize the displayed plate layout to show 100% of the plate layout on the full screen.
Zoom check box	When the Zoom 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.
Measurement cycle drop down list	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

File	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...
Edit	Copy to Excel Copy to ASCII Format Paste from ASCII Format Insert Sample ID List... Recalculate with another Method...
Instrument	Movements... Temperature Control... Start Measurement...

7. Evaluate Results Wizard

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.

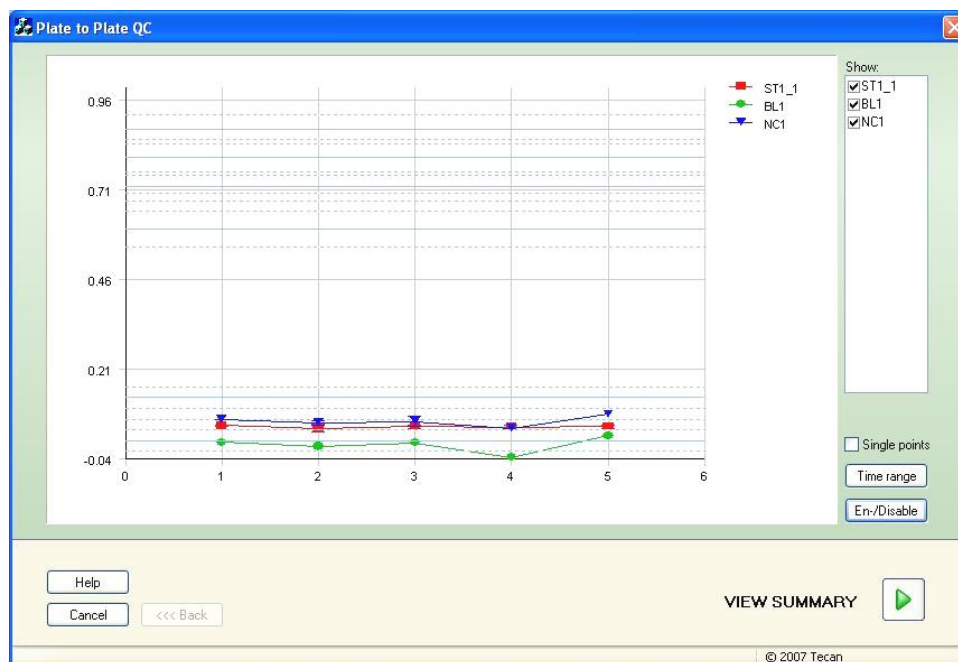
These settings will have no effect on the screen display. Large fonts should be avoided to prevent errors or misrepresentation of data.

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.

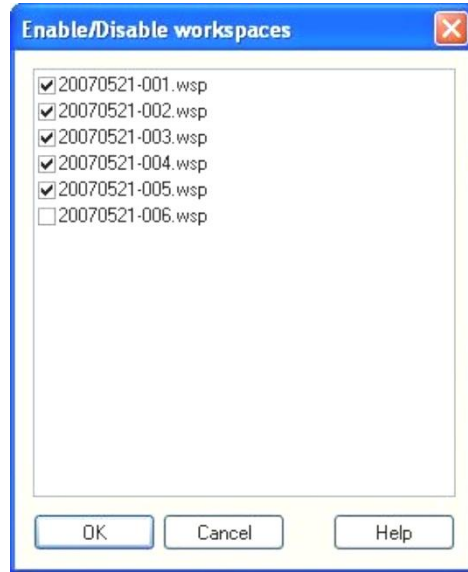
Time Range

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



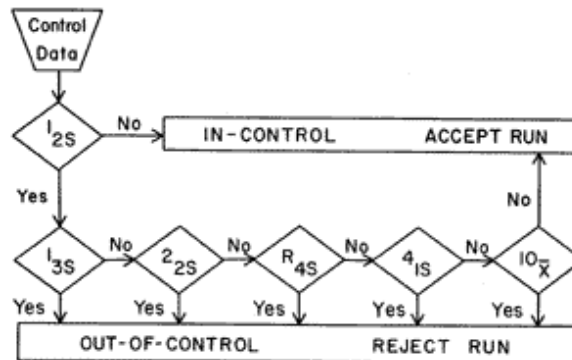
Data Sheet

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

Workspace 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 magellan for further information on Westgards Rules).
Control column	The different controls are listed.
Value column	The mean value of each control is displayed.
Westgard® rule evaluation columns	The individual Westgard® rules are evaluated with OK for a not violated control rule or x for a violated control rule according to the table below (see Westgard rules below).
Comments field	Comments to the evaluation can be entered.
Print Preview button	Print preview with the Levy-Jennings graph, Westgard rules check and comments.

Westgard Rules

The Westgard® rules are a multirule QC model:



Yes = control rule violated

No = control rule not violated

1:2s	<p>Control rule to test whether a control measurement exceeds the control limits of $x + 2SD$ or $x - 2SD$.</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 “in-control”, 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 “out-of-control”.</p>
1:3s	<p>Control rule to test whether a control measurement exceeds the control limits of $x + 3SD$ or $x - 3SD$.</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 $x + 2SD$ or $x - 2SD$.</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 $x + 1SD$ or $x - 1SD$.</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.

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

7. Evaluate Results Wizard

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:

1st line: layout

2nd line: replicate info

3rd 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.

7.4.9 *Control Bar: Transformed Data*

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

7. Evaluate Results Wizard

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.

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

File menu

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.
- **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.

7. Evaluate Results Wizard

- **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. In order 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.

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

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.

7. Evaluate Results Wizard

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

Information tree	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.
Left, right, up and down buttons	The direction buttons can be used to select another well on the plate while leaving the dialog box open.
Expand All / Shrink All	Click this button to display the information tree expanded to the highest level or to shrink to the first level.
OK	Closes the Summary dialog box.

Details Dialog

The **Details** dialog box displays the multiple reads per well results of one well.

File menu	Save & Exit is selected to save all changes and close the dialog box.
Edit menu	The Edit menu contains the following commands: <ul style="list-style-type: none"> Click Copy to copy the single values into the clipboard, which then can be transferred to any Windows application by using the paste function. Select Recalculate to force the recalculation of the statistic data at the bottom of the dialog. This option is disabled if Automatic Recalculation is set. If Automatic Recalculation is set, the statistic data is calculated after every mask/unmask action.
View menu	The View menu contains the following commands: <ul style="list-style-type: none"> Values can be selected to display the reads as values. Use this option to view multiple reads per well coarsely and quickly. Graphic can be selected to display the read values as colors. Brightness uses one color with different brightness to display the values. Pseudo Colors uses different colors to display the values. A color bar with a slide control is displayed to change the intensity.

7. Evaluate Results Wizard

Help menu	Click Help to open the magellan help dialog box.
Click on points	Clicking reads 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.

Edit raw data 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).
Reset button	Resets the well to its original value.
Mask check box	Excludes the value of the well from the calculation. Data is then shown in brackets. Select the Mask check box again to include the value again.
Left, right, up and down buttons	The direction buttons are used to select another well on the plate while leaving the dialog box open.
OK	Closes the Edit 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.

Crosshair cursor	A crosshair cursor is displayed in order to assist in placing the cursor on particular points on the graph.
Copy to Clipboard	Copies the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the paste function.
Save as bitmap	Saves the graph as a bitmap file.
Print...	Opens the Print... dialog box from which the graph can be printed.
Printer setup..	Opens the Printer Setup dialog box in which the printer settings can be defined.
Zoom to 100%	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
Properties...	Select this command to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
Help...	This button opens the magellan help dialog box.

Graph: Kinetics Dialog

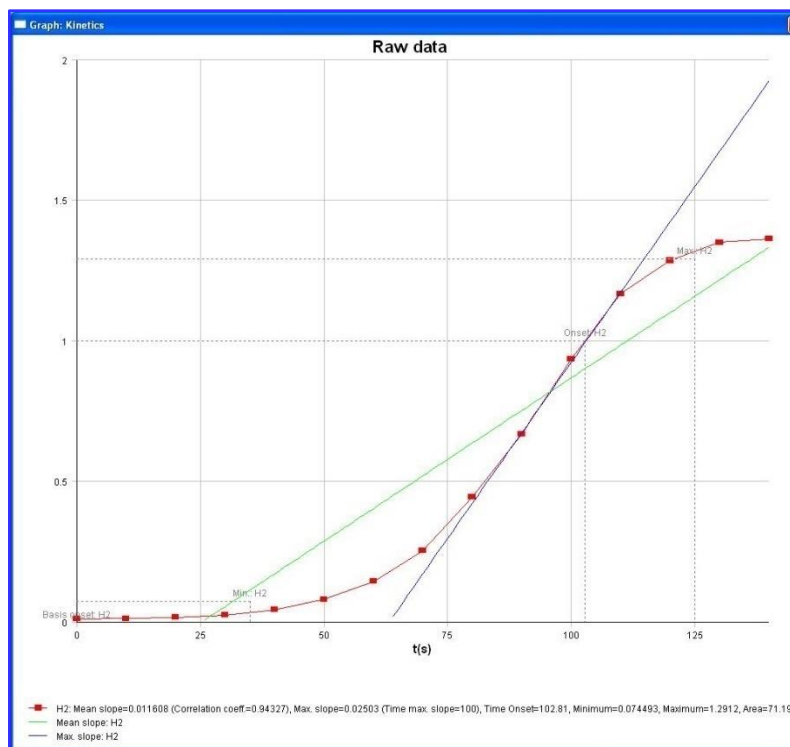
The **Graph: Kinetics** dialog box displays the graphs of kinetic measurements of one or more selected wells. The legend contains the calculated kinetic parameters.

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.

Crosshair Cursor	A crosshair cursor is displayed in order to assist in placing the cursor on particular points on the graph.
Copy to Clipboard	Copies the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the paste function.
Save as bitmap	Saves the graph as a bitmap.
Print...	Opens the Print... dialog box from which the graph can be printed.
Printer Setup...	Opens the Printer Setup dialog box in which the printer settings can be defined.
Zoom to 100%	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
Show Kinetic Reduced Data	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 Show Kinetic Reduced Data in the kinetic graph dialog. The current display state is stored and will be reused for further displays.



Temperature curve	This option shows/hides a curve visualizing the temperature progression during kinetic measurements (if available).
--------------------------	---

7. Evaluate Results Wizard

Kinetic parameters...	Opens the Kinetic parameters dialog box and offers the ability to modify the kinetic settings for the selected well(s).
Kinetic Data...	Select this menu item to show a table of all calculated kinetic data of the selected well(s).
Y-Axis scaling	A range for the Y-axis can be selected.
Properties...	Select this button to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
Help	Opens the magellan 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.

Crosshair cursor	A crosshair cursor is displayed in order to assist in placing the cursor on particular points on the graph.
Copy to Clipboard	Copies the graph to the clipboard as a bitmap, which can be transferred to any Windows application by using the paste function.
Save as Bitmap	Saves the graph as a bitmap.
Save as JCAMP-DX	Select this command to save the graph as a JCAMP-DX 4.24 file.
Save as ASCII	Select this button to save the graph as a tab separated ASCII file.
Print...	Opens the Print... dialog box from which the graph can be printed.
Printer Setup...	Opens the Printer Setup dialog box in which the printer settings can be defined.
Zoom to 100%	Sets the graph display back to 100% if the zoom factor has been changed by selecting rectangular regions of the graph.
Spectra Data Reduction...	Select this command to change the Spectra Data Reduction parameters settings.
Spectra Reduced Data...	Select this command to display a list of reduced spectra data. Note! This command is enabled only when reduced spectra data of type value is available.
Data as Table	Opens a dialog box showing the spectrum as table. This allows copying the data to Excel.

Spectrum masked	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.
Show Prim. Spectrum	The selected spectrum and the raw spectrum are displayed together. Option is available only when reduced spectrum is displayed.
Properties...	Select this command to change the graph display properties. The graph title, the axis styles, the curve style etc. can be customized.
Help...	Opens the magellan 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.*

7.5 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:

Save in group box	Filename text field: a default name for the file will appear, but can be changed if desired.
	File remarks text field: enter remarks if necessary.
Audit trail comment group box	Audit trail comment text field: enter comments to the audit trail as necessary (only available for magellan Tracker).
Save... button:	Saves the workspace file
Export...	Click this button to open the Export dialog
Audit Trail button:	Use to view the Audit Trail of the file (only available for magellan Tracker). Refer to chapter 4.4 Saving the Method – Audit trail for further information.
Signatures button:	Use to view the signatures attached to this file (only available for magellan Tracker). Refer to chapter 4.4 Saving the Method for further information.
Sign this workspace now	Select Sign this workspace now to open the Attach Signature wizard (only available for magellan 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

Review	Can only be signed by a user with the appropriate rights.
Approval	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.
Custom	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.

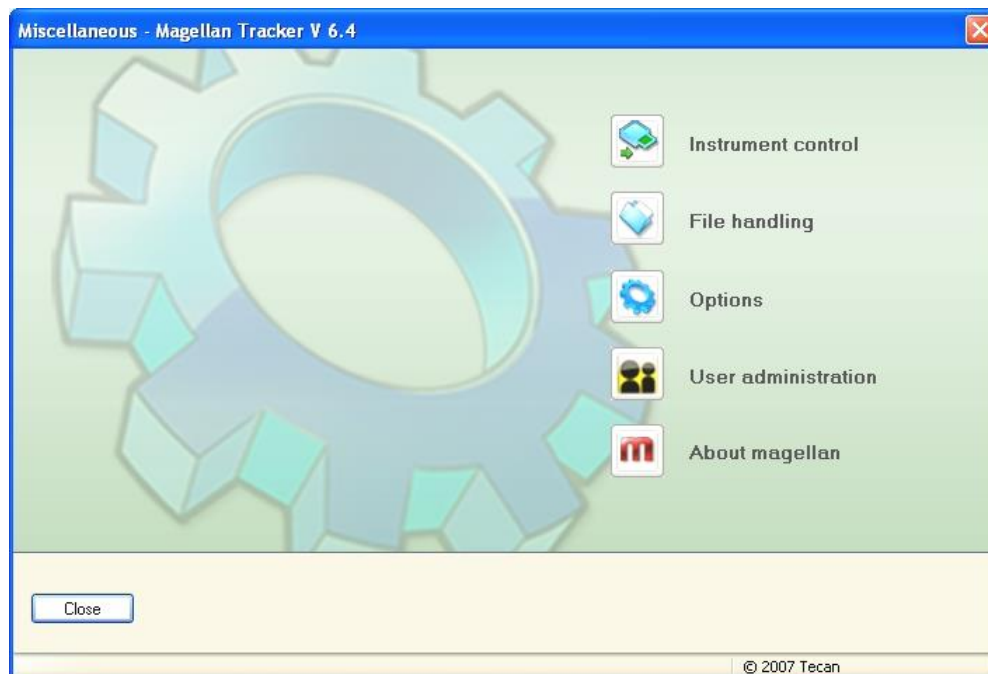


Note

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

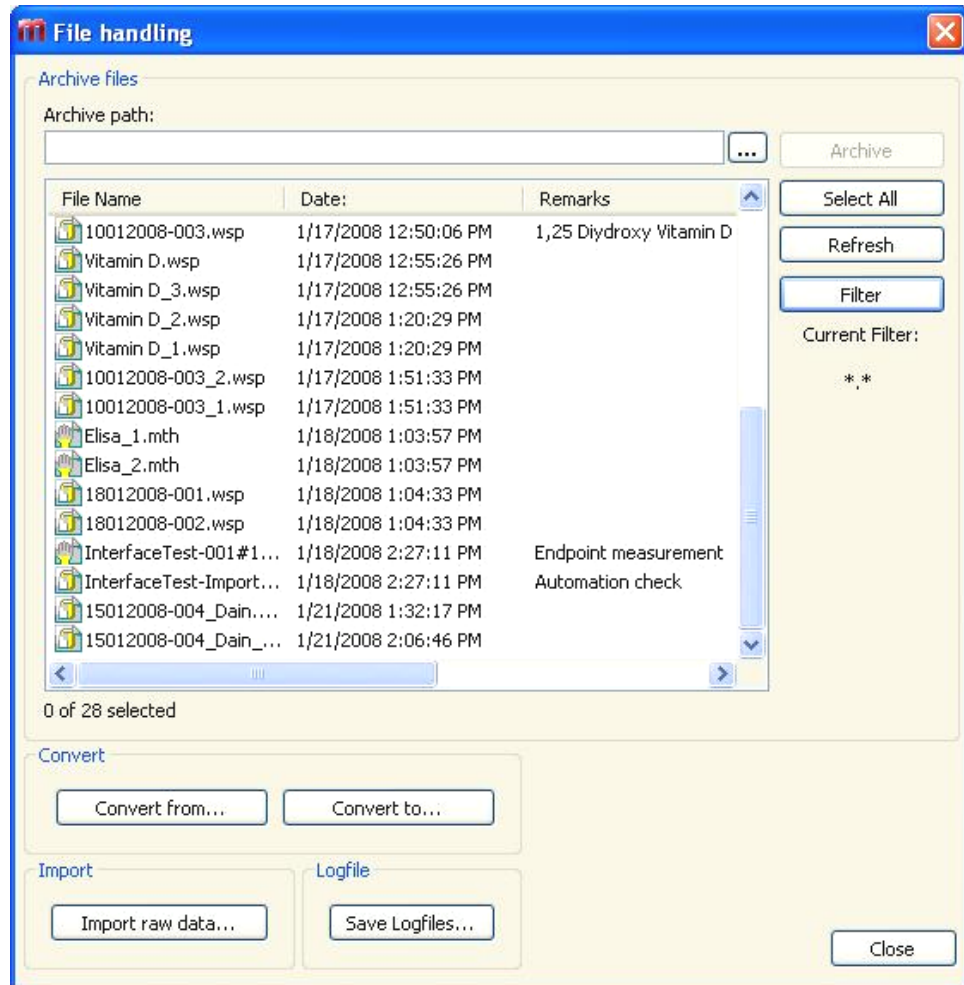
See chapter 3 Instrument Control & Settings.

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.

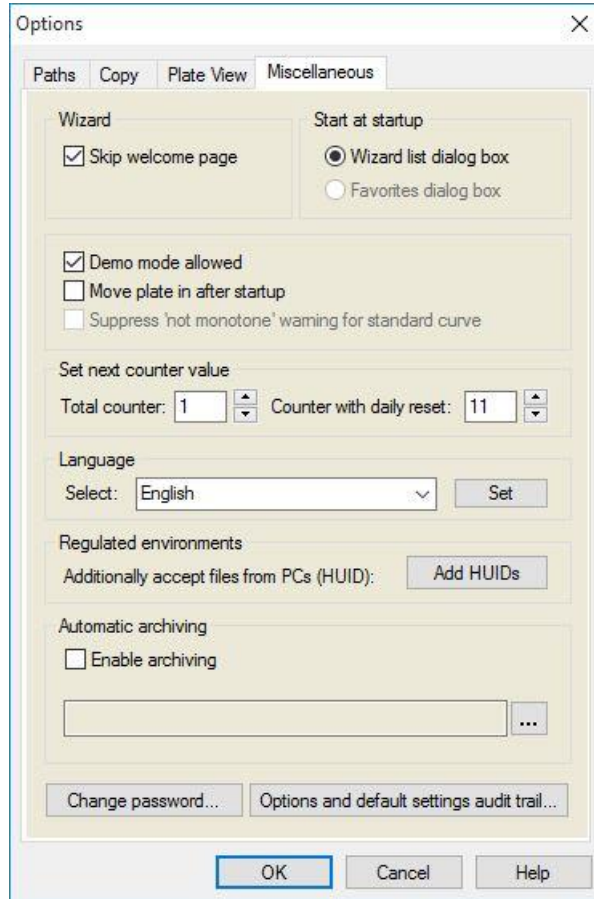
The **Archive Files** group box contains the following elements:

Archive path	Define the archive path. Click the browse  button to change the path.
File Name list	<ul style="list-style-type: none"> Lists all files saved by magellan filtered by the options entered via the Filter button.
Archive button	Click Archive to move all files selected in the File Name list to the backup directory (cut-and-paste function).
Select All button	Click Select All to select all files displayed in the File Name list.
Refresh button	Click the Refresh button to cancel the current Filter option and to refresh the file list.
Filter button	<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"> A question mark ? can be applied as a wildcard for one single character. An asterisk * can be applied as a wildcard for no or many characters.

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:

Format option button	It defines the expected data format Table or Matrix
Separator 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"> • Tabulator if Tabulator is selected. • Any other character entered in the Other text-field.
Orientation option button	It defines the orientation of the data, i.e. either horizontal or vertical .

Measurement Parameters

Info	The box shows the following parameters: <ul style="list-style-type: none"> • Plate format • Data unit • Number of measurements • Measurement interval
Measurement Parameters 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:

Document type group box	Select the document type for conversion
Select all button	Click this button to select all displayed files in the file list
Filename 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.
Source path edit field	The Source path 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.
Destination path edit field	The Destination path 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.
Convert document(s) button	Click this button to start conversion.
Version drop down menu	Select from the drop-down menu the version of magellan the files shall be converted to.
Progress bar	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 in order to be used.



Note
Files from magellan Standard must be converted in order to be used with magellan Tracker.

9. Miscellaneous Icon



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:

Document type group box	Select the document type for conversion, e.g. a method.
Customize new method specific options group box	Several global options – in magellan versions lower than V4.0 – are now method specific. In order to set these options correctly in the method and workspace files, use one of the export buttons or the Workspace name... button.
Select all button	Click this button to select all displayed files in the file list
File name 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. Note! Only workspaces and methods created with the currently connected instrument are displayed.
Source path edit field	The Source path 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.
Destination path edit field	The Destination path 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. magellan Tracker: this path cannot be modified.
Convert document(s) button	Click this button to start conversion.
Progress bar	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

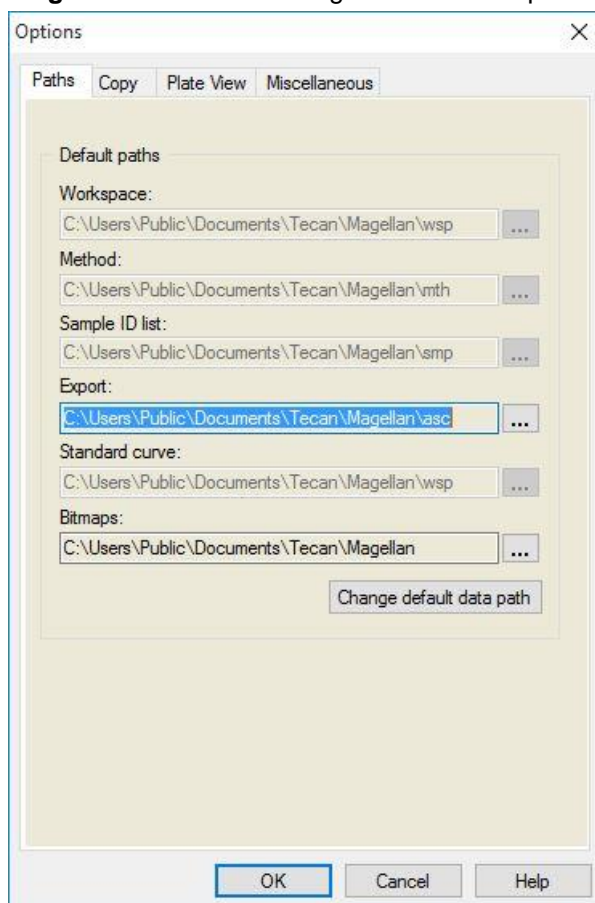


Note

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.

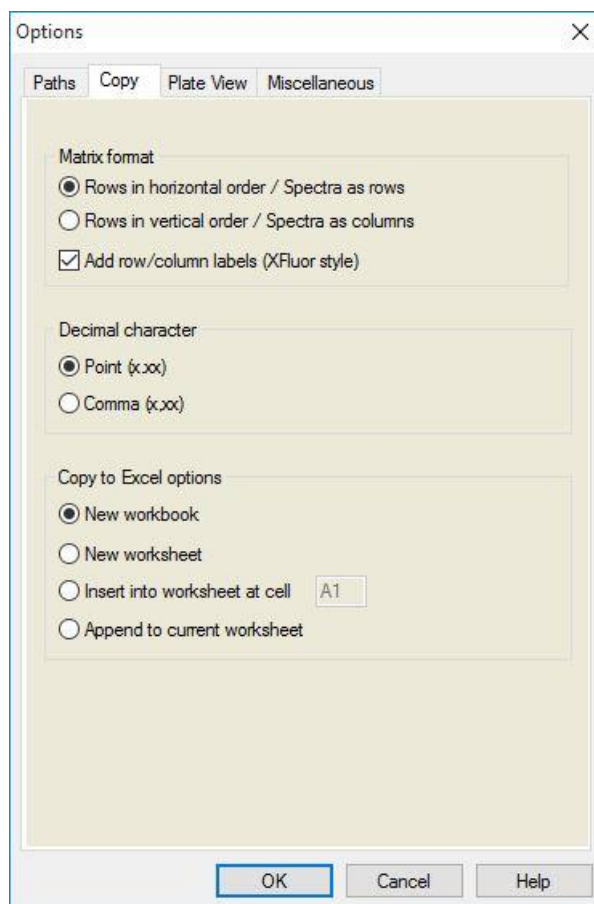


Note

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.



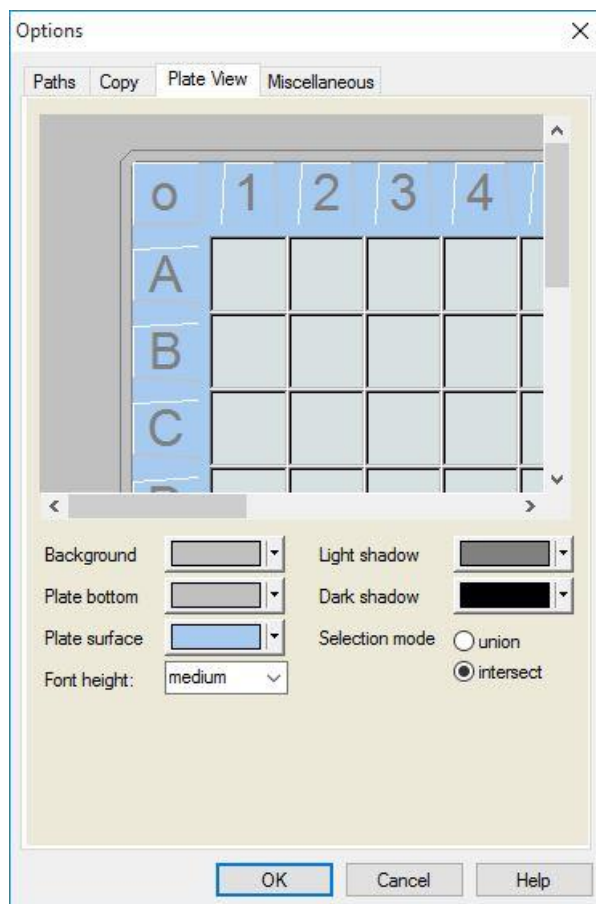
The **Copy** tab contains the following elements:

9. Miscellaneous Icon

Matrix format 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"> • Rows in horizontal order option button Rows of data from the microplate will be copied in horizontal order. • Rows in vertical order option button Rows of data from the microplate will be copied in vertical order. This results in a transposed matrix. • If the Add row/column labels check box is selected, the row and column information like in XFluor is added when copying data.
Copy to clipboard options 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"> • Point (x.xxx) option button Example: 7.893 • Comma (x,xxx) option button Example: 7,893
Copy to Excel options group box	<p>The option buttons enable to define where to position the transferred data within Excel.</p> <ul style="list-style-type: none"> • New workbook 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. • New worksheet 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. • Insert into worksheet at cell option button and cell coordinates text field 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 opened and a new workbook will be created, the requested data is inserted into the first worksheet. • Append to current worksheet 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.

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.

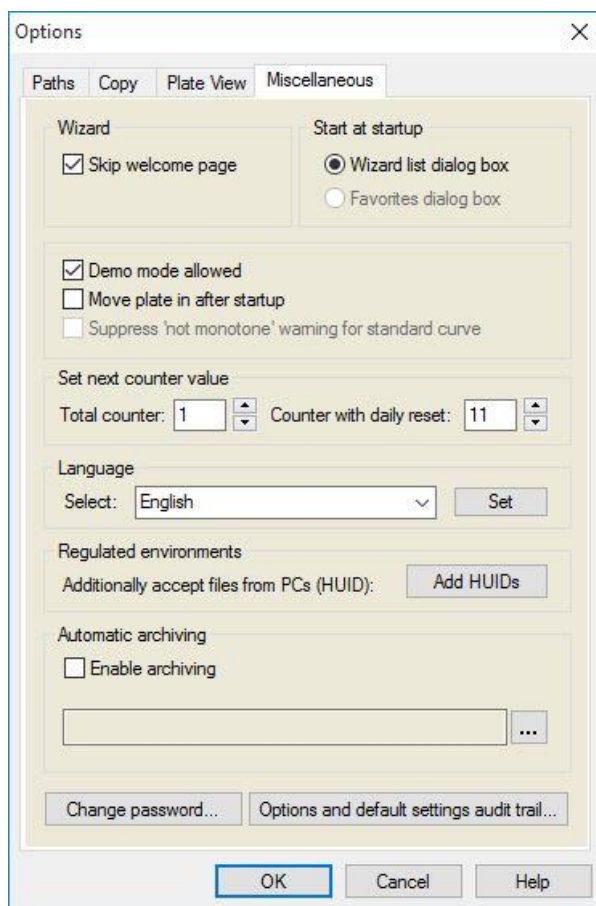


The **Plate View** tab contains the following elements:

<p>Background button</p>	<p>The background color of the <i>Pate view</i> window can be selected.</p>
<p>Plate bottom button</p>	<p>The frame color of the displayed plate can be selected.</p>
<p>Plate surface button</p>	<p>The surface color of the displayed plate can be selected.</p>
<p>Font height drop down list</p>	<p>The font height for the text within the wells can be selected:</p> <ul style="list-style-type: none"> • Small • Medium • Large
<p>Light shadow button</p>	<p>The light-shadow color of the plate frame can be selected.</p>
<p>Dark shadow button</p>	<p>The dark-shadow color of the plate frame can be selected.</p>
<p>Selection mode option buttons</p>	<p>Here the selection mode for marking wells with the mouse is established:</p> <ul style="list-style-type: none"> • Union allows selecting wells only when the mouse has marked the complete area of the well. • Intersect allows for the selection of wells when only a part of the well has been marked with the mouse.

9. Miscellaneous Icon

9.3.4 Miscellaneous



The **Miscellaneous** tab contains the following elements:

Wizard group box	When selecting the Skip welcome page check box, the welcome page of the wizard is not displayed when opening a wizard. The wizard starts at the second of its windows.
Start at startup group box	Selecting the Favorites dialog box check box defines that instead of the <i>Wizard List</i> the <i>Favorite dialog</i> will show up after the start of the magellan software.
Group box	<ul style="list-style-type: none"> • Demo mode allowed check box: Select this option in order to allow connecting to a simulated instrument. This option is helpful if already measured data shall be evaluated. Then, no instrument is needed. • Move plate in after startup check box: If the checkbox is selected and an instrument is connected, the plate carrier is moved in automatically after startup. • Suppress 'not monotone' warning 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). Note! This option is disabled in magellan Tracker.

Set next counter value group box	<p>Two options are offered:</p> <ul style="list-style-type: none"> • Total counter 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. • Counter with daily reset spin control enables to set the counter to any value. Displays the current number of workspace files that have been created during one day.
Language group box	<p>The text field displays the applied language. A different language can be selected from the drop-down list. See Set below.</p>
Set button	<p>Select a different language and click the Set button to restart the program with the selected language</p>
Change password button	<p>Click this button to open a dialog box, where the user can change his password (only available with magellan User Administration activated).</p>
Add HUIDs button	<p>A list of additional HUIDs can be defined which allows the user to open files created on another computer (only available in magellan Tracker).</p>
Automatic archiving	<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>
Options and default settings audit trail... 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 magellan Tracker).</p> <p>Click Save as file to save this information as a .log or .txt file. The text can also be copied to a word processing program for printing.</p>

9.4 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.

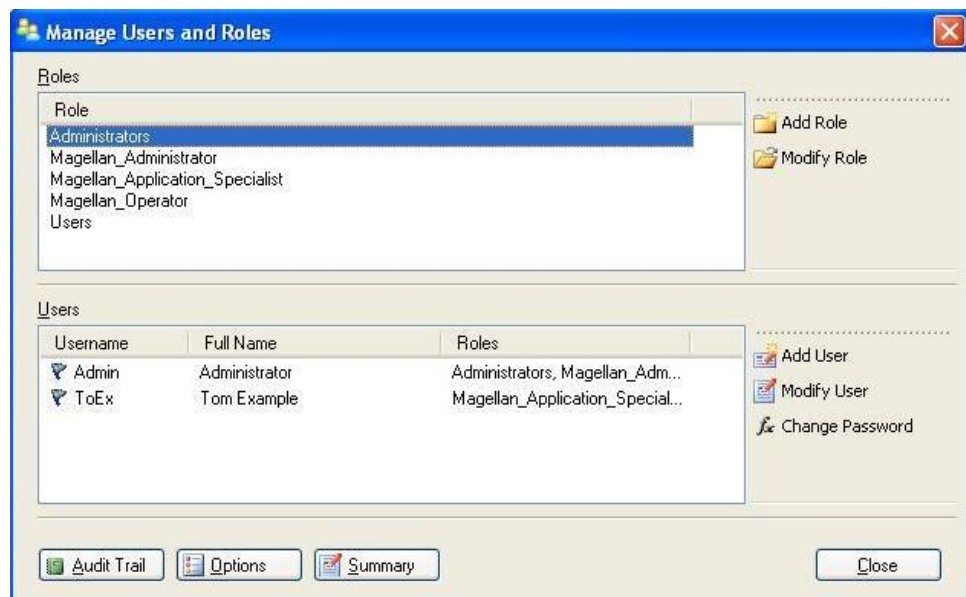


CAUTION

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:



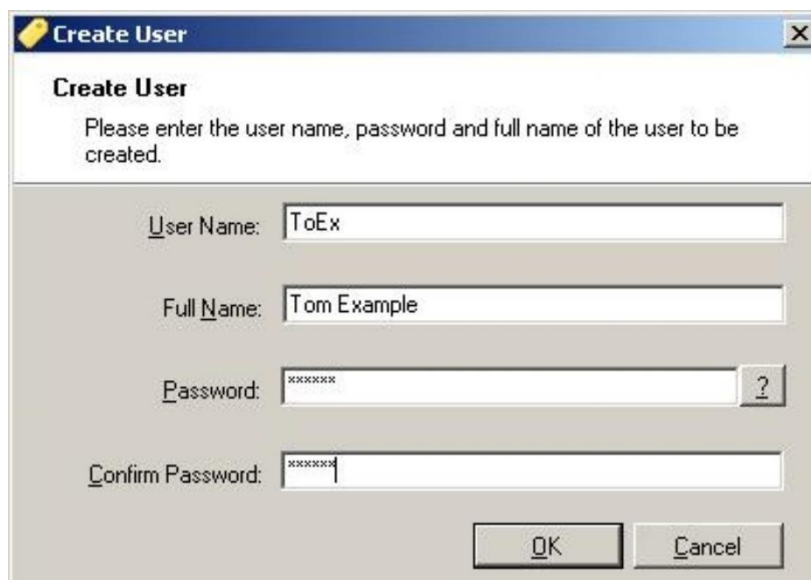
Users and roles can be added and modified; user rights can be defined. The **Manage Users and Roles** dialog box contains the following elements:

Roles	The Roles list shows all existing user groups (user levels).
Add Role	A new group with corresponding rights can be created.
Modify Role	Rights of an existing group can be modified
Users	The user list shows all existing users and which group they are member of.
Add User	A new user can be created.

Modify User	Full name, user level (group) or password of an existing user can be changed.
Lock User	A user account can be enabled / disabled. The button is visible only if a user name is selected.
Audit Trail	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.
Options	General login, password or email options can be modified
Summary	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:

User Name	A unique user name has to be entered when a new user is created. This name cannot be modified afterwards.
Full Name	Enter the full name of the user. This can be changed later.
Password	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:



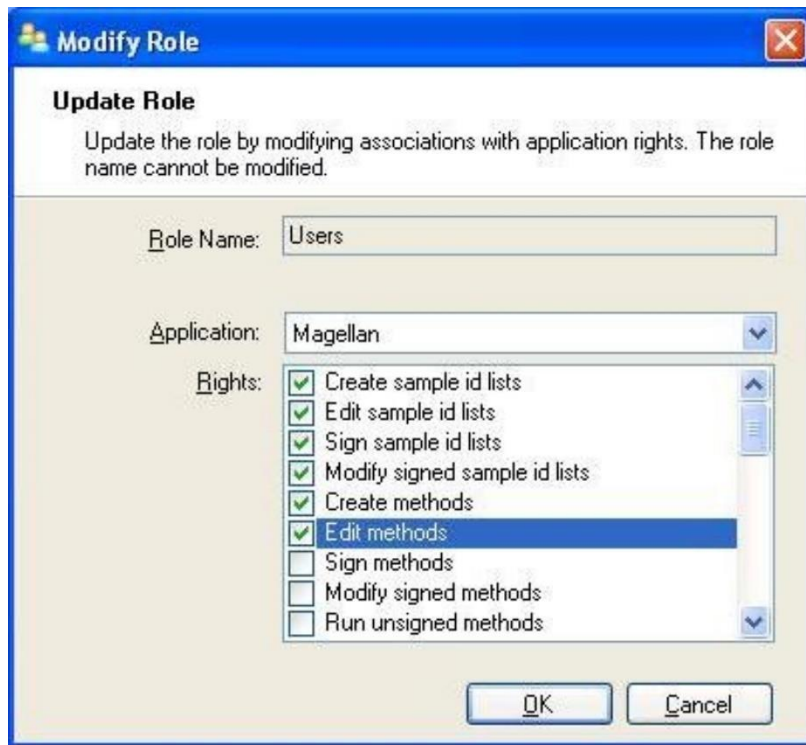
The **Modify User** dialog box contains the following elements:

Full Name	Enter the full name of the user
Roles	Select from one of the existing user groups. The rights associated with that group are assigned to the user.
Change picture	User's picture can be added or changed.
Delete picture	Delete the user's picture.
Change Password	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:



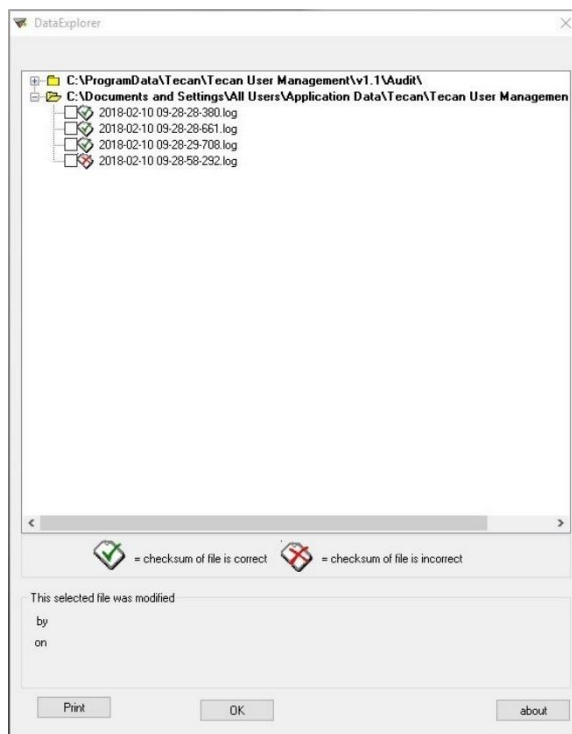
The **Modify Role** dialog box contains the following elements:

Role Name	The role name is defined in the Add Role dialog box.
Application	Tecan software component, i.e. Magellan.
Rights	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.



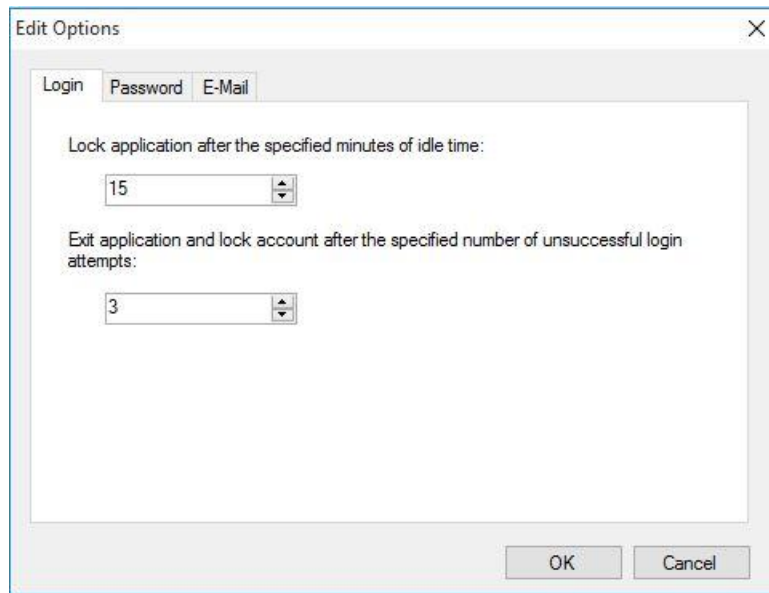
Note

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



Lock application	Lock of application after a specified time (1 min – 36500 h). To unlock the application the user has to reenter the password.
Unsuccessful logins	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. 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.



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).

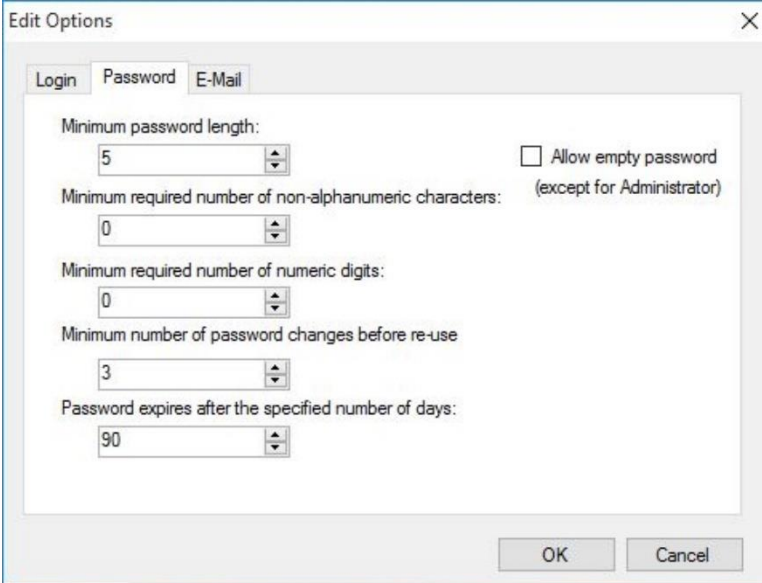


Note

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.

9. Miscellaneous Icon

Password Options



The screenshot shows a dialog box titled "Edit Options" with a close button (X) in the top right corner. It has three tabs: "Login", "Password", and "E-Mail". The "Password" tab is selected. The dialog contains the following settings:

- Minimum password length: 5
- Minimum required number of non-alphanumeric characters: 0
- Minimum required number of numeric digits: 0
- Minimum number of password changes before re-use: 3
- Password expires after the specified number of days: 90
- Allow empty password (except for Administrator)

At the bottom right, there are "OK" and "Cancel" buttons.

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.

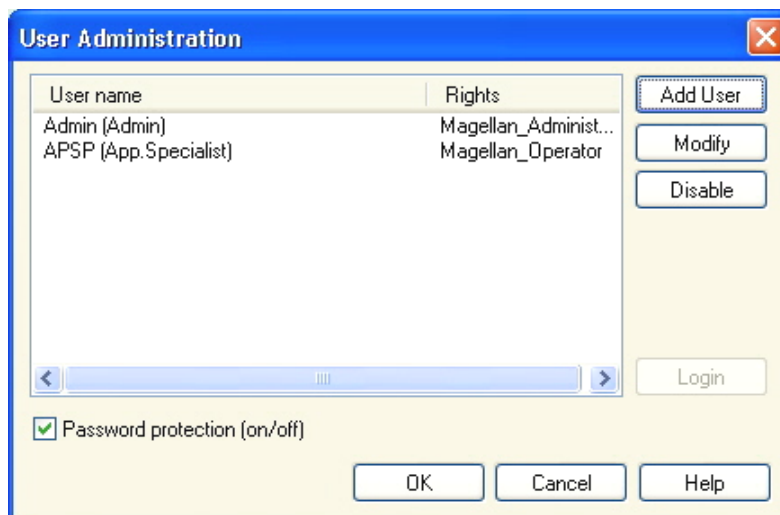
9.4.5 User Administration Summary

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.

9.5 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 of the program's functions and data editing facilities. For **Application Specialist** and **Operator** level, options are increasingly restricted. Only the **User Administrator** has the ability to 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:

Login button	The Login dialog box is displayed. A user can log in with his user name.
User list	<ul style="list-style-type: none"> All currently setup users with their User name and Rights are displayed within this list. Any user to be edited or deleted can be selected here.
Add User button	The Add User button opens the User Rights dialog box, in which a password, name, and user ID can be entered to define a new user.
Modify button	The Modify button opens the User Rights dialog box for modifying the selected user in the user list.
Disable button	The Disable button will disable the selected user in the current user list.
Password protection (on/off) check box	This check box enables to switch on/off the software's password protection facility. If enabled, the Login dialog box will be displayed upon starting magellan .

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:

User name text field	Enter the full name of the user – as it shall be displayed
UserID text field	Define the user ID that the user has to enter for login
User rights option buttons	Define the level of access to the software’s facilities available for the user: <ul style="list-style-type: none"> • Operator • Application Specialist • Administrator
Password text field	Define the user password (at least 5 characters)
Confirm password 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. In order 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.

9.6 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			
Create sample ID lists Create a new sample ID list or save an existing one with a new name.	Yes	Yes	Yes
Edit sample ID lists Edit an existing sample ID list and save it with the same name.	Yes	Yes	No
Sign sample ID lists* Sign an existing sample ID list for review/approval.	Reserved for future use.		
Modify signed sample ID lists* Edit or change sample IDs in a signed sample ID list.	Reserved for future use.		
Method			
Create methods 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
Edit methods Edit an existing method and save it with the same name.	Yes	Yes	No
Sign methods* Sign an existing method for review/approval. Note: The right Sign methods alone is not enough to sign method files. You also need the right Edit methods . Additionally, the Modify signed methods right is also needed to add the Approval signature to files that already have a Review signature .	Yes	No	No
Modify signed methods* Edit a signed method and save it with the same name.	Yes	No	No
Run unsigned methods* With this right alone only approved methods can be used. Note: This right can be used in combination with the right Run not approved methods to allow the user to run all methods.	Yes	Yes	No
Setup favorites Add/Remove methods from the favorite list.	Yes	No	No
Define multilabel measurement Define methods using multilabel measurements.	Yes	Yes	No
Define kinetic transformations Define methods using kinetic transformations.	Yes	Yes	No
Define concentration transformations Define methods using concentration transformations.	Yes	Yes	No
Define alias Define methods using aliases for identifiers.	Yes	Yes	No
Workspace			
Create workspaces Perform a measurement and save the workspace with a new name – or – save an existing workspace with a new name.	Yes	Yes	Yes
Edit workspaces 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
<p>Sign workspaces* Sign an existing workspace for review/approval.</p> <p>Note: The right Sign workspaces alone is not enough to sign workspace files. You also need the right Edit workspaces.</p> <p>Additionally, the Edit signed workspaces right is also needed to add the Approval signature to files that already have a Review signature.</p>	Yes	No	No
<p>Edit signed workspaces* Edit a signed workspace and save it with the same name.</p>	Yes	No	No
<p>Continue evaluation when error Continue calculation after errors have occurred</p>	Yes	Yes	No ¹ /Yes ²
<p>Modify raw data (samples) Edit or mask measurement data of samples.</p>	Yes	No	No
<p>Modify raw data (standards) Edit or mask measurement data of standards, controls, blanks.</p>	Yes	No	No
<p>Import raw data Import raw data from ASCII file in an existing workspace.</p>	Yes	No	No
<p>Modify evaluation Change evaluation (method) settings in an existing workspace.</p>	Yes	Yes	No
<p>Reevaluate with another method Reevaluate an existing workspace with another method.</p>	Yes	Yes	No
<p>Modify layout Change measurement parameters, concentration, and layout before starting a measurement.</p>	Yes	Yes	No
Standard curve			
<p>Create standard curve files Create a new standard curve and save it with a new name.</p>	Yes	Yes	No
<p>Edit standard curve files Edit an existing standard curve and save it with the same name</p>	Yes	Yes	No
<p>Sign standard curve files* Sign an existing standard curve for review/approval.</p>	Reserved for future use.		

User Rights	magellan Administrator	magellan Application Specialist	magellan Operator
Modify signed standard curve files* Edit and change settings in a signed standard curve file.	Reserved for future use.		
General			
Archive files Move files to an archive location	Yes	No	No
Set default paths** Set individual paths for saving workspace, method, sample ID list, export and bitmap files.	Yes	Yes	Yes
Define filter slides Change the filter definition of the instrument	Yes	No	No
Modify general options Select language, suppress not monotone warning, allow demo mode.	Yes	No	No
Print unsigned workspaces* The results of an unsigned workspace can be printed.	Yes	Yes	Yes
Run not approved methods* 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 Run unsigned methods to allow the user to run all methods.	Yes	Yes	No
Edit reviewed method* Reviewed (but not approved) methods can be edited.	Yes	No	No
Edit reviewed workspace* Reviewed (but not approved) workspaces can be edited.	Yes	No	No
Reader Server			
Save plate definition files Create or edit plate definition files.	Yes	No ¹ /Yes ²	No
Save spin profile Create or edit spin profile files.	Yes	No	No


* user rights available in magellan Tracker only

** user rights available in magellan Standard only

¹ magellan Tracker

² magellan Standard

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.

10.2 File Handling

The measured data is always saved directly after the measurement.



Note for magellan Tracker only:
In order 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).

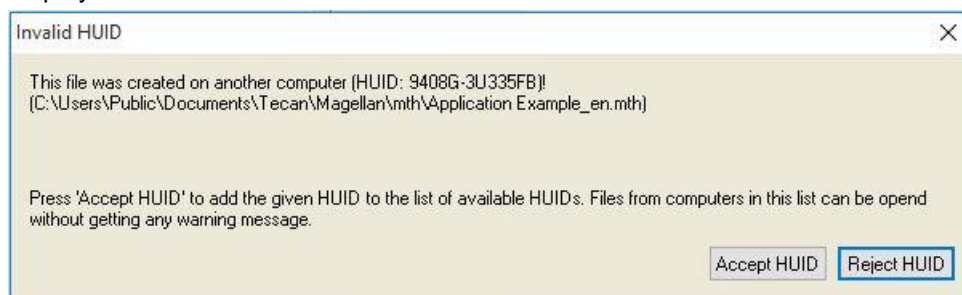
The HUID of a Personal Computer is configured during **magellan** registration and all files created and saved on this PC are linked to this special HUID.

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.

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.

10. Additional Features for magellan Tracker

Event	Event Type	Description
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:

Message text field	The error message and a short explanation is displayed in a text field.
Save as file button	Click the Save as file 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.

11. Calculations

In case values or settings have been changed, a **message box** will appear.

Message	The instrument values have been changed. Do you want to re-start the result calculation?
Yes button	Click the Yes button to re-calculate the evaluation values.
No button	Click the No button to close the message. No re-calculation will be performed.

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 are 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.

11. Calculations



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.



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 `if(i>0) then(x[i]-x[i-1]) 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

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:

11. Calculations

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*x) where x<0 and (x) where x>=0.

Example:

$$\text{abs}(-1) = 1$$

$$\text{abs}(1) = 1$$

exp(argument)

This function raises the Euler (e) value to the power of the argument.

Example: $\text{exp}(1) = e^1 = 2.718$

frac(argument)

This function separates out the fraction section of argument.

frac(): delivers the fraction section of a decimal value.

Example: $\text{frac}(1.7) = 0.7$

int(argument)

This function separates out the integer sections of argument.

int(): delivers the integer section of a decimal value.

Example: $\text{int}(1.7) = 1$

Log(argument)

$$\text{log}(\text{arg1};\text{arg2})$$

This function takes the logarithm of arg2 to the base of arg1.

Example:

The well holds a value of 100.

$$\text{log}(x;10)$$

The result here will be 0.5.

In(argument)

This function takes the natural logarithm of argument.

Example: $\text{In}(10) = 2,303$

Ig(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:

$\text{avg}(SM1)$

The average of all the samples in the first experimental group will be formed. Furthermore, the replicates of a value can be averaged:

$\text{avg}(ST1_1)$

Averages all replicates of the first standard.

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:

$\text{Median}(NC1)$

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.

11. Calculations

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 are valid.

Invalid measurement values will be labeled with an exclamation mark.

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)

11. Calculations

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 in order 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.

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)

Individual values:	NC1_1 = 0.217	$\overline{NC1} = 0.288$
	NC1_2 = 0.439	
	NC1_3 = 0.208	

Step 1: The individual values are sorted by their distance to the average.

$ NC1_1 - \overline{NC1} $	 0.217-0.288 	0.071	→	NC1_2 (0.439)
$ NC1_2 - \overline{NC1} $	 0.439-0.288 	0.151		NC1_3 (0.208)
$ NC1_3 - \overline{NC1} $	 0.208-0.288 	0.08		NC1_1 (0.217)

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. Calculations

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.

peak(threshold;wIStart;wIEnd;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;wIStart;wIEnd)

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:

$$'Label1'!x/'Label2'!x$$

In order 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.

11. Calculations

Conditional result:

If $(x < 0.0)$ then 0 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) 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.

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.

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.

11.4 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

11. Calculations

$$err(A, B) = \sum_{i=1}^n (f(x_i) - y_i)^2$$

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

2nd order: parabolic or quadratic

3rd 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:

$$f : [x_1, x_n] \rightarrow R$$

$$x \mapsto \sum_{i=0}^{order} a_i \cdot x^i, \text{ order} = 2 \text{ or } 3$$

($n > \text{order}$)

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

$$rank \begin{pmatrix} x_1^{order} & \dots & x_1 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ x_n^{order} & \dots & x_n & 1 \end{pmatrix} = order + 1, \text{ which is true if } x_i \neq x_j \forall i, j = 1, \dots, n$$

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 through the use of 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.

11. Calculations

$$\int_{x_1}^{x_n} \left(\frac{d^2 f}{dx^2} \right)^2 dx$$

Minimizes the integral $\int_{x_1}^{x_n} \left(\frac{d^2 f}{dx^2} \right)^2 dx$, 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.

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 $i-1$, $i=2, \dots, n$

$$m_i = \frac{q_i |q_{i+2} - q_{i+1}| + q_{i+1} |q_i - q_{i-1}|}{|q_{i+2} - q_{i+1}| + |q_i - q_{i-1}|}, \quad i=3, \dots, n-2$$

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 $y'_{i-1} = q_i$ (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 3rd 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 3rd 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
- In order 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.

$$X = \log_{10} x$$

$$Y = \ln \left(\frac{\frac{D - y}{D - A}}{1 - \frac{D - y}{D - A}} \right)$$

11. Calculations

$$g : [X_i, Y_i] \rightarrow R$$

$x \mapsto k \cdot x + d$, 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:

$$B = -m \cdot \log_{10}(e)$$

$$C = e^{\frac{b}{B}}$$

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.

11.4.13 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.

11. Calculations

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.

11.5 Calculation of Dilution Series

11.5.1 Detection of Dilution Series

The following criteria have to 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 is able to 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 (OD₄₉₂–OD₆₂₀) are plotted versus the concentration. The regression line that goes through these points is the standard curve.

Interpretation of the test results:

IgM < 18 UA/mL	Negative
18 UA/mL <= IgM < 22 UA/mL	Intermediate
IgM >= 22 UA/mL	Positive

12. Application Example

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.

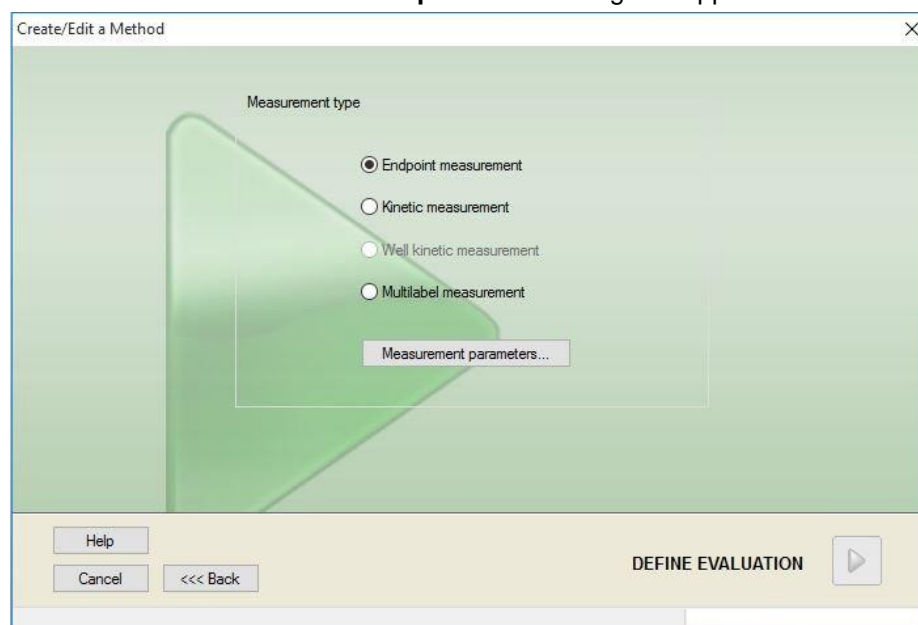
Additionally, the layout and the qualitative results are be stored as ASCII file.

12.1.2 Create a Method

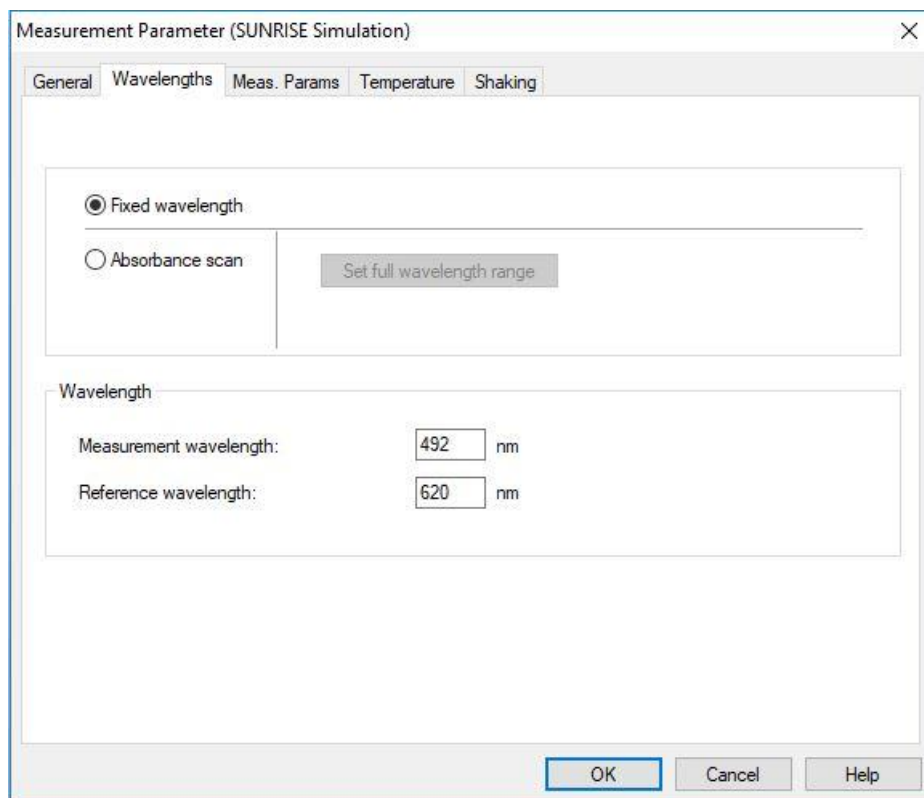
In the **Wizard List** dialog box, select **Create/edit a method** and click **OK**. Click next on the **Welcome** page of the **Create/edit a method wizard** and the **Select a file** dialog box appears. Select **Create new**.

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:

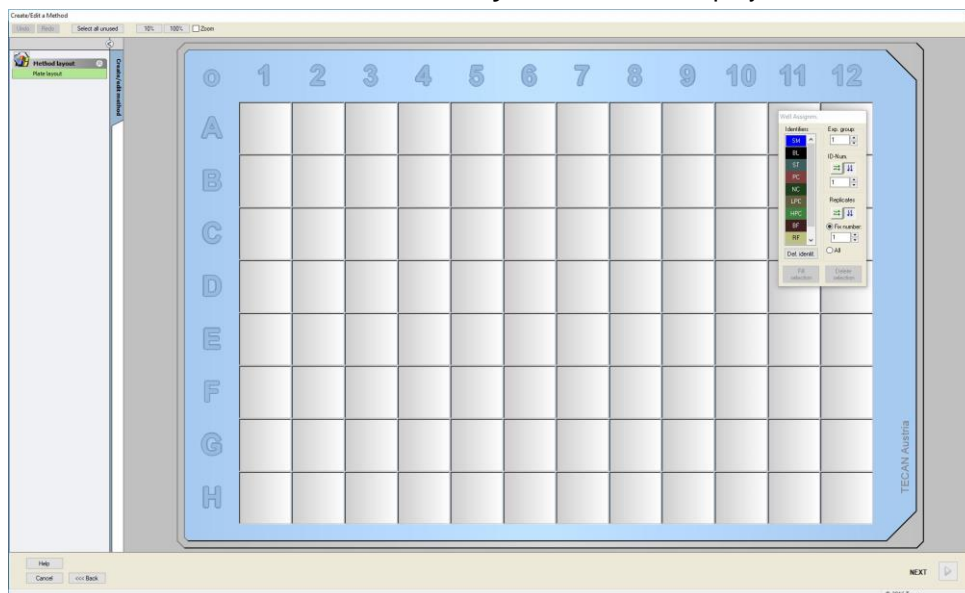


On the **General** tab select **Absorbance**.

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.



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**.

12. Application Example

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**.

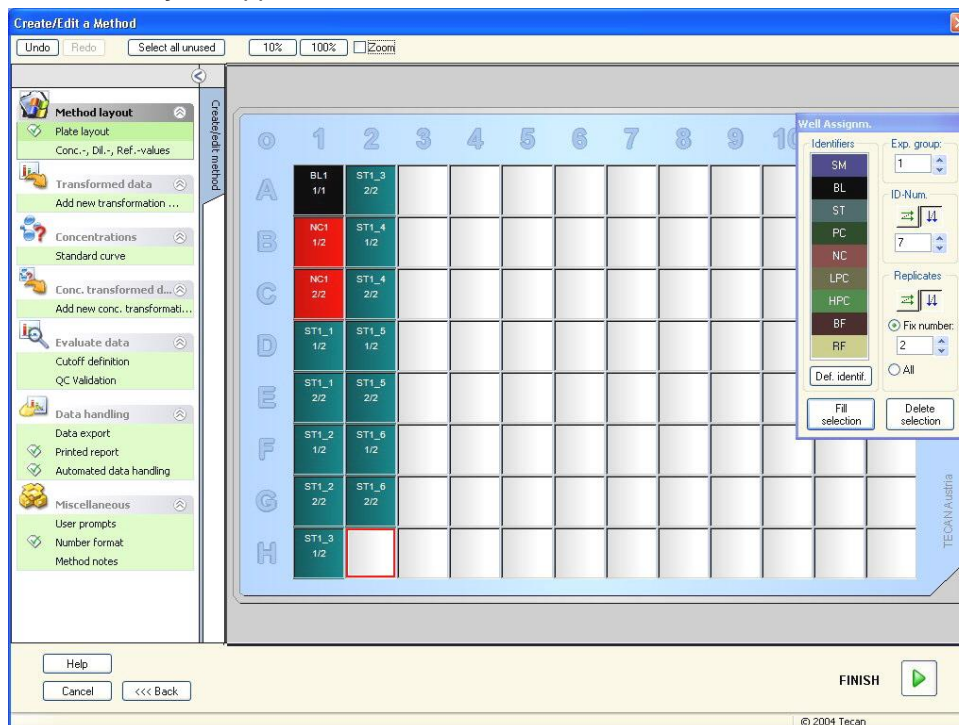
Then select the wells D1 to G2 and click **Fill selection**.



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**.

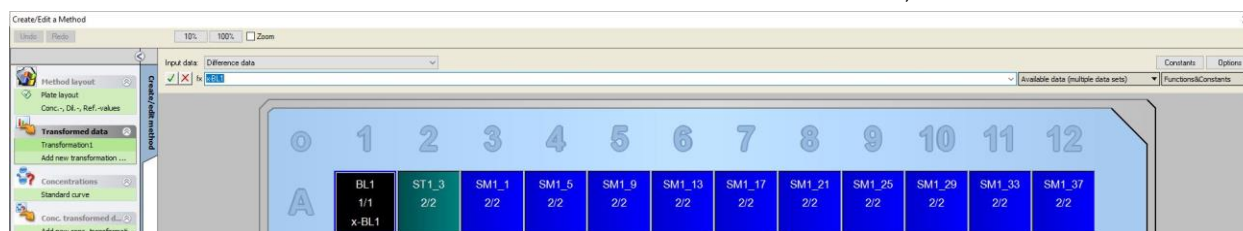
In the **Experimental** group box, the number **1** remains.

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.

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.




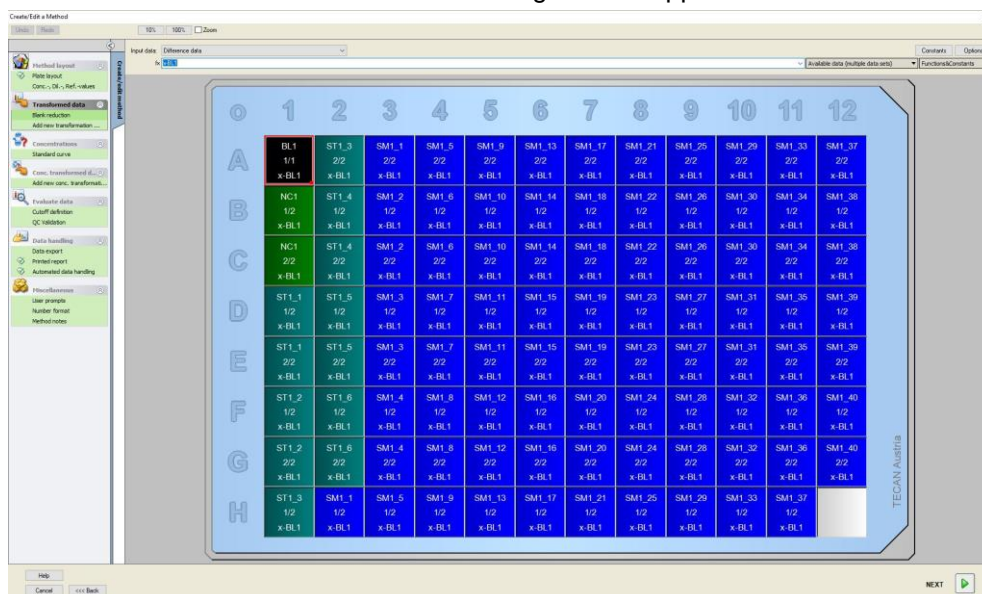
A dialog box appears asking you if you want to define a blank reduction. Click **Yes**.

12. Application Example

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):

SM1_9	Sample, experimental group number 1, sample ID number 4.
2/2	Number of replicate is 2, total number of replicates is 2.
x-BL1 or 1.000	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.

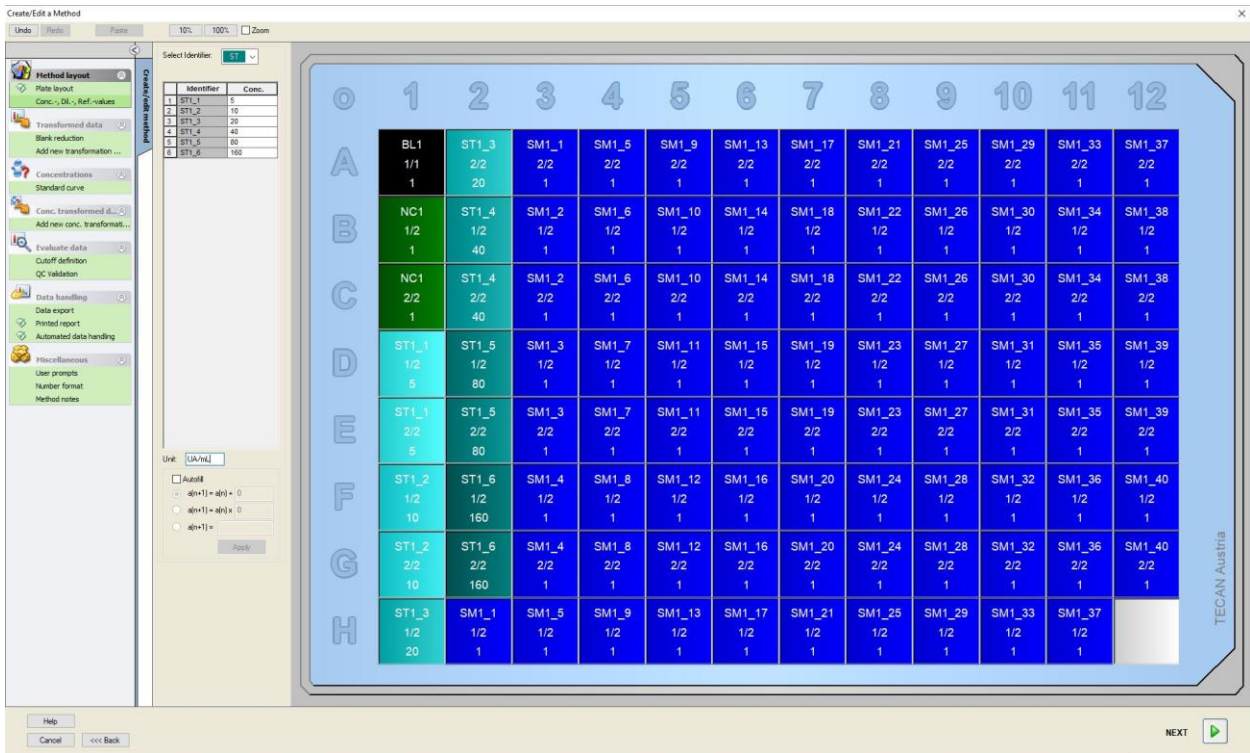
Calibrator 1	5 UA/mL
Calibrator 2	10 UA/mL
Calibrator 3	20 UA/mL
Calibrator 4	40 UA/mL
Calibrator 5	80 UA/mL
Calibrator 6	160 UA/mL

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:



Standard Curve

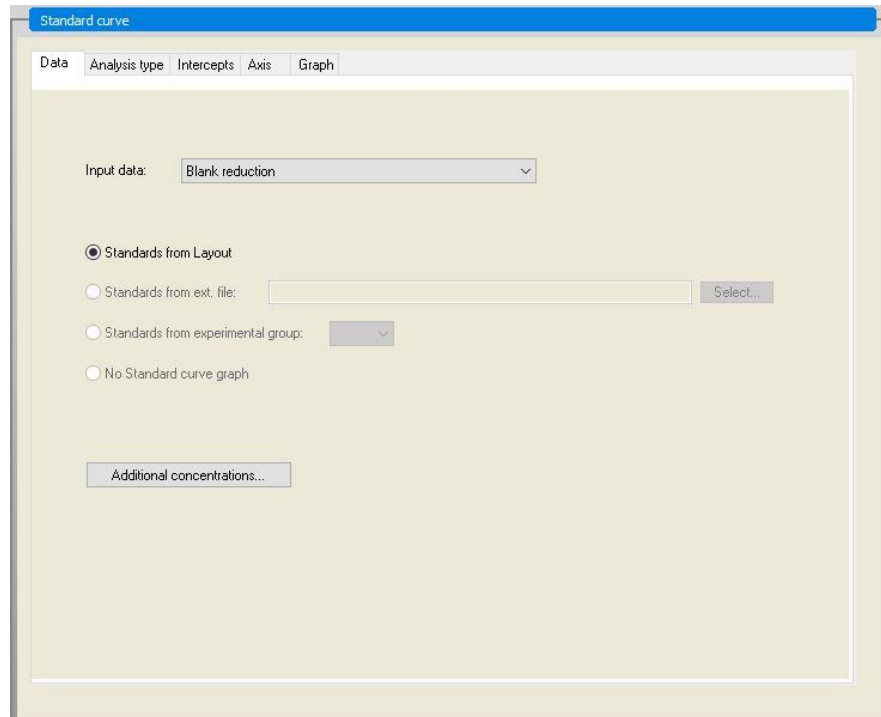
In the control bar click **Standard curve** from the **Concentrations** item to define the appropriate standard curve.

The following is in the test kit description:

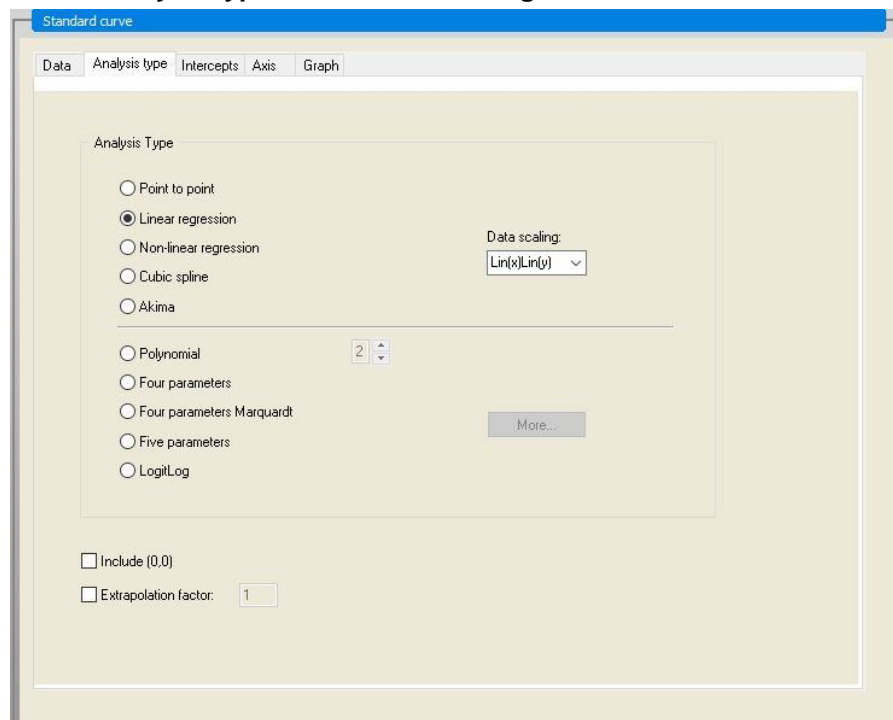
After the blank correction, the optical densities (OD 492 – OD 620) are plotted versus the concentration. The regression line that goes through these points is the standard curve.

On the **Data tab**, select **Blank reduction** as input data.

12. Application Example



On the **Analysis type** tab, select **Linear regression**.



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: Concentration [UA/mL]

Color: [Black] [Log. Scaling]

Auto select range

Range Min.: [] Max.: []

Grid Color: [Grey] Style: [Solid]

Y-axis

Label: Blank reduction

Color: [Black] [Log. Scaling]

Auto select range

Range Min.: [] Max.: []

Grid Color: [Grey] Style: [Solid]

On the **Graph** tab, define the graph title, curves, font and graph display.

Standard curve

Data Analysis type Intercepts Axis Graph

Title

Label: IgM ELISA

Color: [Black]

Curves

Label: Gip. 1

Color: [Red]

Symbol: [Blue Square]

Size: [Medium]

Hide curve

Line width: [1]

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)**.

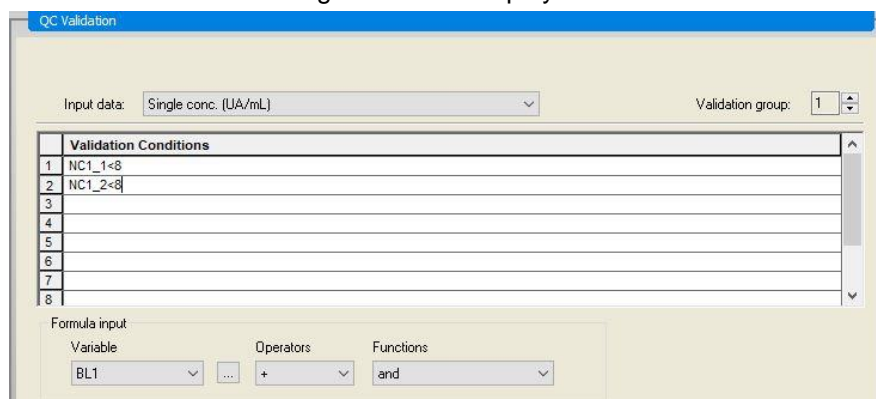
In the first row, type **NC1_1<8**, or enter the formula using the available **variables**, **operators** and **functions**.



Note
NC1_1 means Negative control of experimental group 1, replicate 1.

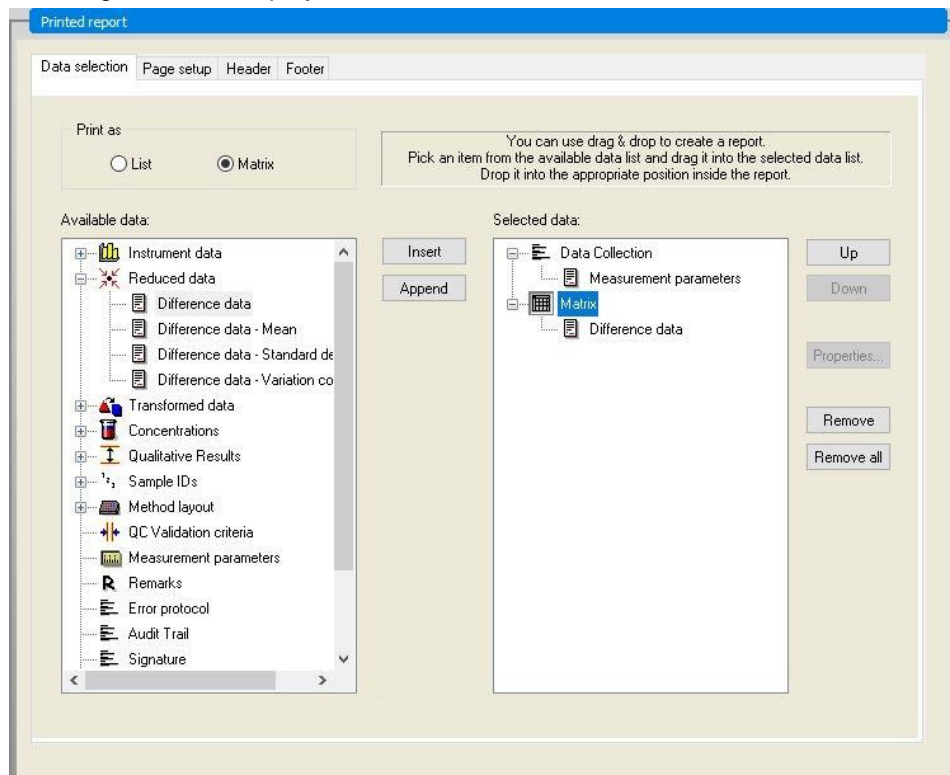
In the second row, type **NC1_2<8**.

The **QC Validations** dialog box is now displayed as follows:



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.

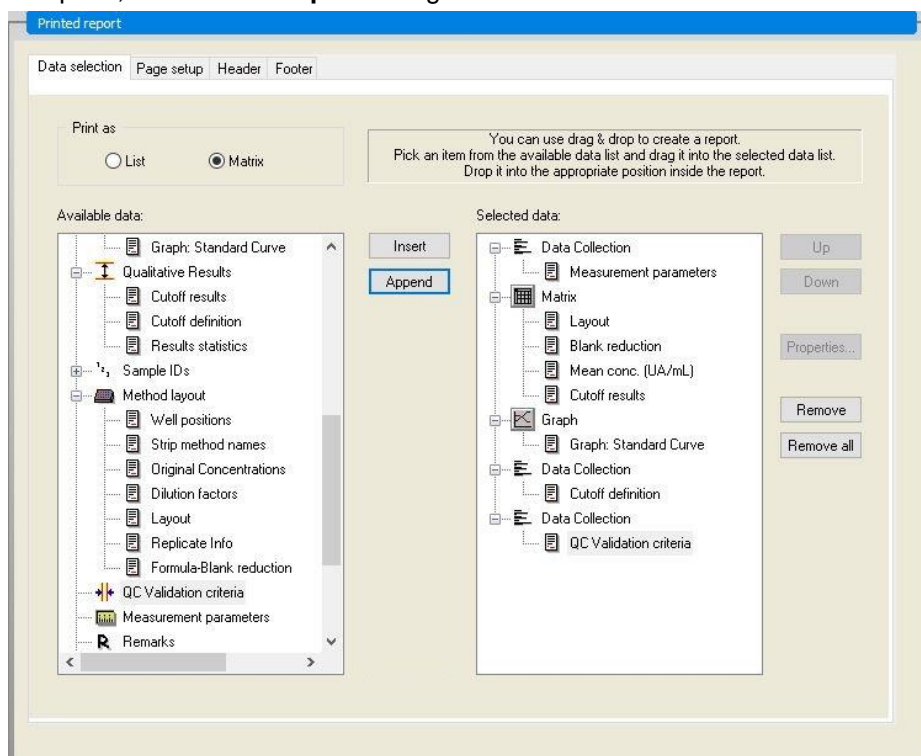
12. Application Example

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**.

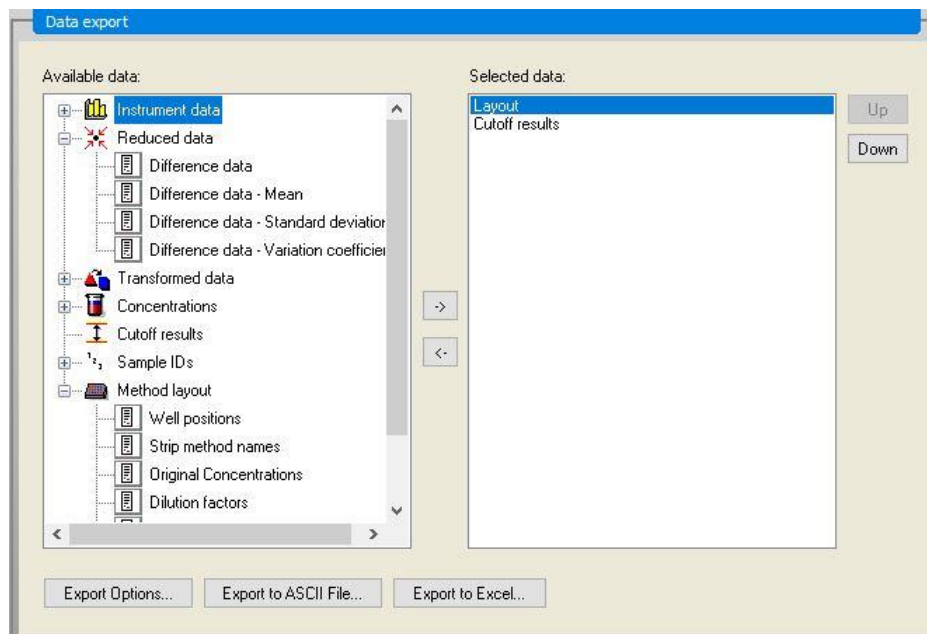
Append Graph: Standard curve, Cutoff definition and QC Validation criteria to the selected data. The data setup part of the report definition procedure is complete; the **Printed Report** dialog box looks like this:



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:

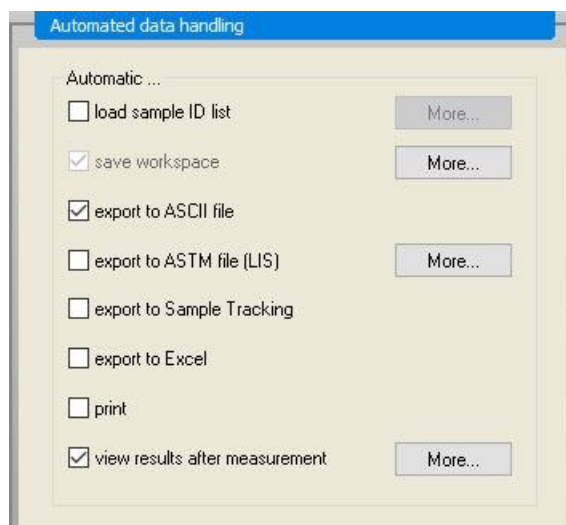


Note

Exported data should always contain the Layout or Sample ID List.

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.

12. Application Example

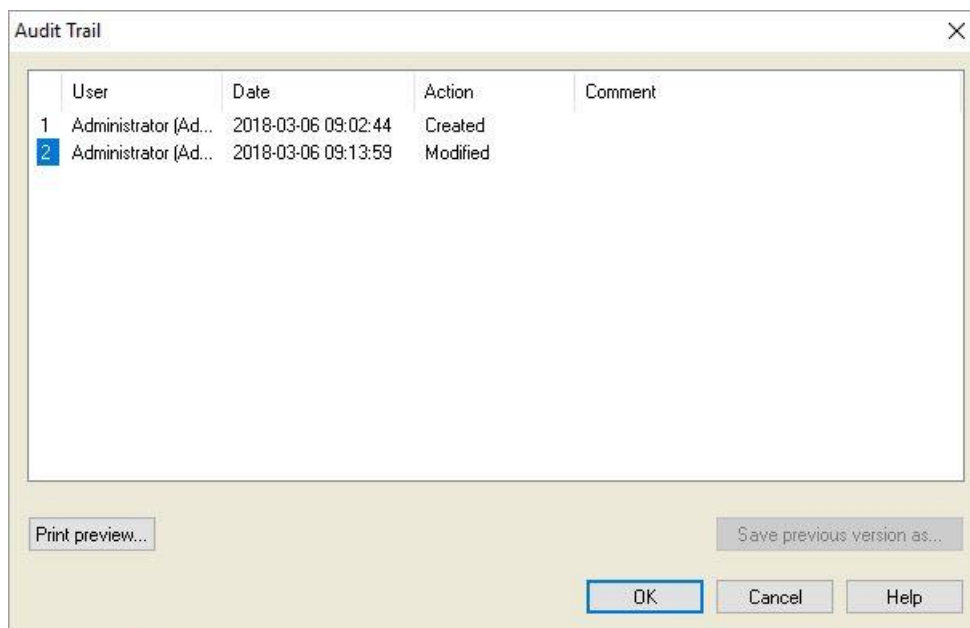
Save the Method

Click **FINISH** to open the **Save as** window. Enter the method filename and complete any other field if appropriate.

Filename text field	A filename must be entered. A default filename is suggested automatically but can be changed.
File remarks text field	Comments entered here will be saved and displayed with the filename.
Audit trail comment text field	Comments entered here will be stored in the audit trail. <i>This option is only available with magellan Tracker.</i>
Audit trail... button	The Audit Trail dialog box appears. <i>This option is only available with magellan Tracker.</i>
Organize Favorites... button	The Organize Favorites dialog box appears. (See chapter 6.4 Start Favorite – Organize Favorites).
Signatures... button	The Signature dialog box appears. <i>This option is only available with magellan Tracker.</i>
Method password	Enter a method password if you want to protect the method to be saved (see chapter 4.4.1 Password Protection of Methods).
Run this method now 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:

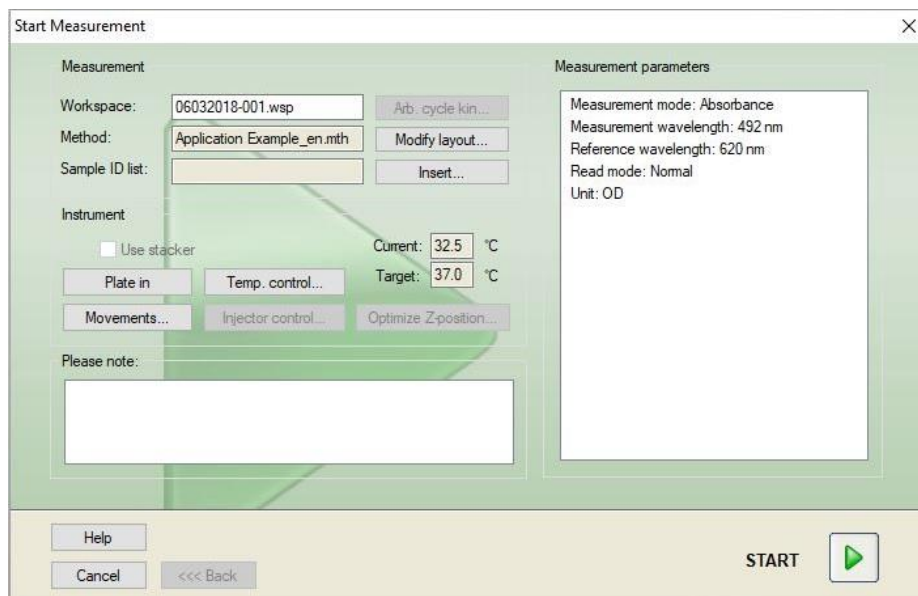


The audit trail shows a list of all modifications made to the method. Each entry consists of the user (name and full name), date and time of change, whether the file was created or modified, and any audit trail comments.

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.

12.1.3 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:



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. Application Example

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.

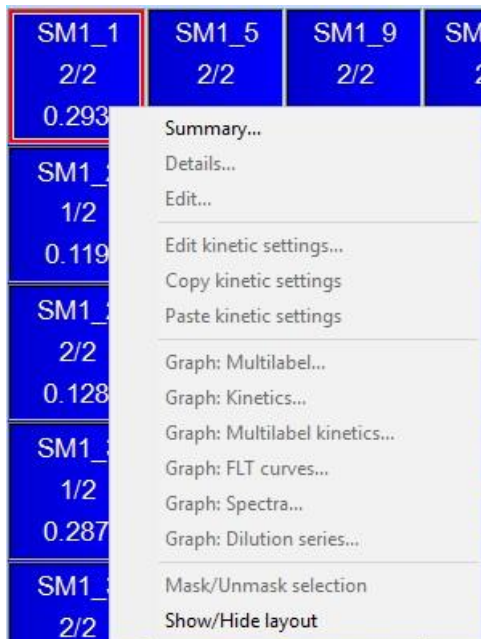
Click **Next** on the **Welcome** page of the **Evaluate Results wizard** and the **Select a file** dialog box appears.

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:

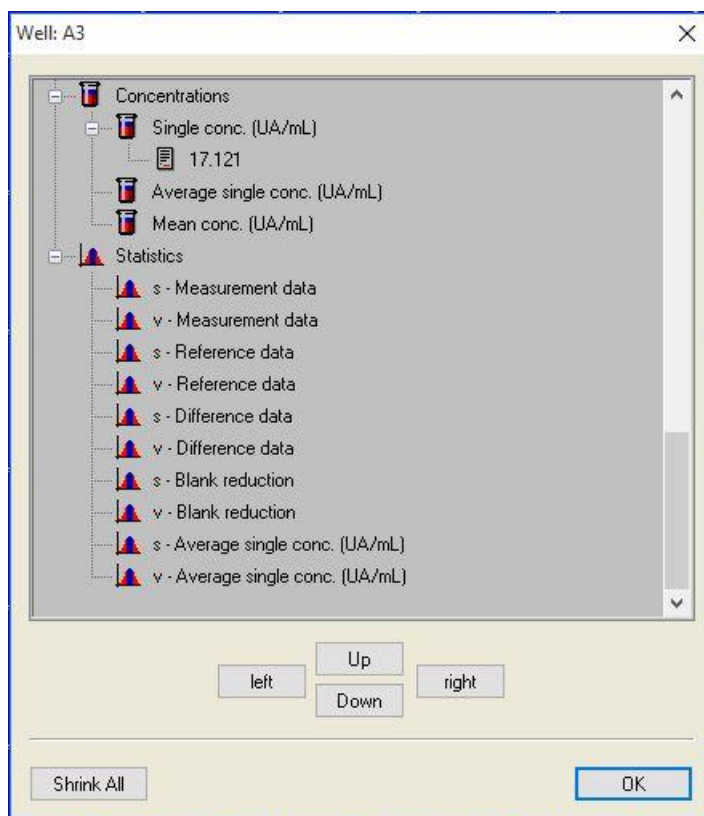
	1	2	3	4	5	6	7	8	9	10	11	12
A	BL1_11 -0.002	ST1_3 0.33	SM1_1 0.293	SM1_5 0.2974	SM1_9 -0.002	SM1_13 0.597	SM1_17 0.41	SM1_21 -0.003	SM1_25 0.489	SM1_29 0.553	SM1_33 0.38	SM1_37 -0.003
B	NC1_1 0.134	ST1_4 0.657	SM1_2 0.119	SM1_6 0.271	SM1_10 -0.001	SM1_14 0.19	SM1_18 -0.002	SM1_22 0.257	SM1_26 0.901	SM1_30 -0.002	SM1_34 -0.001	SM1_38 0.327
C	NC1_1 0.131	ST1_4 0.646	SM1_2 0.128	SM1_6 0.289	SM1_10 -0.001	SM1_14 0.123	SM1_18 -0.001	SM1_22 0.312	SM1_26 0.129	SM1_30 -0.002	SM1_34 -0.001	SM1_38 0.327
D	ST1_1 0.098	ST1_5 1.265	SM1_3 0.287	SM1_7 0.48	SM1_11 0.485	SM1_15 0.305	SM1_19 -0.001	SM1_23 0.487	SM1_27 0.411	SM1_31 0.287	SM1_35 0.413	SM1_39 0.404
E	ST1_1 0.083	ST1_5 1.266	SM1_3 0.293	SM1_7 0.501	SM1_11 0.488	SM1_15 0.289	SM1_19 -0.002	SM1_23 0.477	SM1_27 0.482	SM1_31 0.291	SM1_35 0.385	SM1_39 0.391
F	ST1_2 0.176	ST1_6 2.369	SM1_4 -0.002	SM1_8 0.27	SM1_12 0.291	SM1_16 -0.001	SM1_20 0.298	SM1_24 0	SM1_28 0.4	SM1_32 -0.001	SM1_36 0.379	SM1_40 0.12
G	ST1_2 0.178	ST1_6 2.346	SM1_4 -0.002	SM1_8 0.278	SM1_12 0.303	SM1_16 -0.002	SM1_20 0.275	SM1_24 -0.002	SM1_28 0.394	SM1_32 -0.002	SM1_36 0.402	SM1_40 0.41
H	ST1_3 0.322	SM1_1 0.272	SM1_5 0.294	SM1_9 -0.001	SM1_13 0.512	SM1_17 0.419	SM1_21 -0.001	SM1_25 0.404	SM1_29 0.488	SM1_33 0.398	SM1_37 -0.001	

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:



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. Application Example

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
Average single conc. (???)	Concentration calculated by averaging the single concentrations
Basis OD	Kinetic Parameter: Basis OD value of the onset calculation
Basis OD %	Kinetic Parameter: Basis value of the onset calculation in %
Clipboard	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.
Correlation coeff.	Correlation coefficient, indicates the strength and direction of a linear relationship between two random variables.
Cutoff limit	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.
Cutoff results	Name of the cutoff range the value lies in as defined under cutoff definition
Cutoff definition	Definition of all cutoff ranges and calculated limits
Dilution factors	Defined dilution factors of the samples and controls. A dilution factor of 2 represents a 1:2 dilution.
Dilution series	A sample with replicates in different dilutions.
Goodness of fit	1 minus average relative square deviations of the base points from the curve
Graph	Graphs can be displayed for kinetic measurements, enzyme kinetics, multilabel measurements, dilution series or standard curves.
Hidden	Displayed if well data is hidden when printing
HUID	H ardware U nit I dentification Number
IC 50	The dilution/concentration which results in 50% of the maximum response
Invalid	Value is invalid, no calculation possible
Graph: Kinetic	Graph of kinetic measurements
Lamp low	No values from measurement because of absorbance instrument error.
Layout, Plate Layout	Defines where samples or controls are placed on the microplate
Max. slope OD/hr	Kinetic Parameter: Maximum slopes of the kinetic curves per hour
Max. slope OD /min	Kinetic Parameter: Maximum slopes of the kinetic curves per minute
Max. slope OD /sec	Kinetic Parameter: Maximum slopes of the kinetic curves per second
Maximum OD	Kinetic Parameter: Maximum value of the kinetic curves
Mean slope OD /hr	Kinetic Parameter: Average slopes of the kinetics curves per hour
Mean slope OD /min	Kinetic Parameter: Average slopes of the kinetics curves per minute
Mean slope OD /sec	Kinetic Parameter: Average slopes of the kinetics curves per second

13. Glossary of Terms

Term	Definition
Mean. conc (???)	Concentration calculated from the mean of the replicates of the input data
Measurement data	Dual wavelength absorbance measurement: Data measured using the measurement filter
Measurement parameters	Defines measurement mode, wavelength, plate size, shaking, etc.
Measurement type	The measurement type can be endpoint measurement, kinetic measurement, multilabel measurement or well-kinetic measurement.
Method	Methods contain of the measurement parameters and the evaluation definition. Running a method leads to a workspace that contains the measured and calculated data.
Minimum OD	Kinetic Parameter: Minimum value of the kinetic curves
MultPt	The standard curve is not monotone and delivers more than one concentration at the given input data.
NoCalc	No value returned from the calculation.
Original Concentrations	Concentrations of the standard curve defined in the method.
Pipetting status	If a sample ID list is imported from a pipetting software, the pipetting status can be displayed.
QC Validation	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.
Raw data	Data measured by the instrument.
Reference data	Dual wavelength absorbance measurement: Data measured using the reference filter
Results statistics	Summary of the number of values in the different cutoff ranges
Sample ID List	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.
Sample IDs	IDs of the samples
Single. conc (???)	Concentration calculated from the input data of each replicate
Test	In previous versions a test contained the evaluation settings but not the measurement parameters. Tests are no longer supported in magellan and are replaced by the more powerful methods.
Time Basis OD	Kinetic Parameter: Time until the basis value is reached
Time Basis OD %	Kinetic Parameter: Time until the basis value % is reached
Time Basis to Onset OD	Kinetic Parameter: Time between basis value and onset value
Time Basis to Onset OD %	Kinetic Parameter: Time between the basis and the onset value %
Time max. slope sec	Kinetic Parameter: Kinetic Parameter: Time point of the maximum slope
Time maximum OD	Kinetic Parameter: Time until the maximum is reached
Time minimum OD	Kinetic Parameter: Time until the minimum is reached
Time Onset OD	Kinetic Parameter: Time until the defined onset value is reached

Term	Definition
Time Onset OD %	Kinetic Parameter: Time until the defined onset in % is reached
Time points	Time stamps of the single measurements of a kinetic measurement
Unavailable	Requested data is not available
Unused	No data measured; no layout defined in this well
User Prompts	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.
Validation criteria	Summary of validation condition results
Well position	Name of the well, for example: A1, A2, ...
Workspace	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.
!	Precedes values that have been eliminated during calculation
#	Precedes concentration values that have been calculated using extrapolation and lie outside the range of the standard curve
()	Parenthesis surround values that have been masked
*	An asterisk marks values that have been measured using the "Use gain regulation" option, which corrects (=lowers) the gain.
??? – Mean	Calculated averages (for example: Raw data – Mean)
??? – Standard deviation s - ???	Calculated standard deviations (for example: Raw data – Standard deviation or s – Raw data)
??? – Variation coefficient v - ???	Calculated variation coefficients (for example: Raw data – Variation coefficient or v – Raw data)
~	Added to values that have been edited or simulated
<Min	Calculated concentration is lower than minimum
>Max	Calculated concentration exceeds maximum
<Blank>	Printed report: Insert empty matrix or table printout
<Page break>	Printed report: Print next item on the next page
<Separator>	Printed report: Print line between two items
x	Symbol x refers to the current value within a well
concX	Symbol concX refers to the concentration of the standard in the current well.
dilX	Symbol dilX refers to the dilution of the sample or control in the current well.
'???'	Available data set if more than one set of input data shall be used for calculations
[]	Indices access the different cycles of a kinetic measurement whereas [0] indicates the first cycle
*	The asterisk marks identifiers that have been set as aliases.

Index

A

About magellan.....	158
abs(argument)	168
Absorbance Multilabel Measurement	37
Add HUIDs.....	160
Add New Transformation.....	52
Add/Modify Role	147
Add/Modify User (magellan Standard).....	153
Add/Modify User (magellan Tracker)	145
Akima	180
and – logical expression	167
Application Examples	187
Application Locked	24
Approval	130
Arbitrary Cycle Kinetic	101
Archive Files.....	131
area under the kinetic curve	57
ASCII File Export.....	112
Assign Alias	39, 44
ASTM delimiter definition.....	76
ASTM Export Settings	77
ASTM file.....	76, 77
ASTM File Export	74, 76, 77, 111, 112
ASTM File Export (LIS).....	112
Attach signature.....	129
Audit Trail	159
Autofill Selection	87
Automated Data Handling	74
Automatic Archiving.....	133
Available Data	58
avg(argument)	169

C

calcAlways(argument)	174
Calculations	163
Spectra Data Reduction.....	164
Calculations	163
Change Password	24
Components & Terms.....	19
Conc., Dil. and Ref. Values	46
Concentrations	118
Connecting an Instrument	24
Context Sensitive Menu of a Well of Evaluate Results	
Tab.....	123
Details Dialog.....	123
Edit Dialog	124
Graph-Kinetics Dialog	124
Graph-Multilabel Dialog	124
Graph-Spectra Dialog	126
Summary of a well	39, 123
Convert Documents	135
Convert From.....	135
Convert To.....	134
Copy in ASCII-Format	115
Copy Tab.....	139
Copy to Excel	115
Copy/Export Options	139
correlation coefficient.....	183, 184
countDeleted(arg1; arg2).....	172
Create/Edit a Method.....	33
Create/edit a sample ID	83
Cubic Spline	179
Cutoff.....	63

Cybersecurity.....	16
--------------------	----

D

Data Export.....	65
Data Handling.....	65
Default paths	138
Define a new identifier	44
Define a Plate Layout	41
Define Constants	54
Define Evaluation	38
Define Filter Slides	32
Dilution Series	121

E

Edit Constants	100
Edit user prompts	100
Edit well	87
eliminate (arg1; arg2; arg3; arg4)	171
eliminatePerc (arg1; arg2; arg3; arg4).....	171
eliminateRange (arg1; arg2; arg3; arg4).....	172
Email Options	151
End Point Measurements	36
Enzyme Kinetics	58
Enzyme Kinetics Graph	118
Evaluate Data	63
Evaluate Results.....	107, 128
Excel Export	112
exp(argument)	168
Export	
to ASCII	68
to Excel.....	69
Export to ASTM file.....	74
Export to LIS.....	76

F

File Handling.....	160
File Selection Criteria.....	108
file type symbols	20
File Types Used with magellan.....	19
Five Parameters – Marquardt.....	183
Folder Handling	20
Formula	165
Basic Functions	168
Elimination Functions.....	171
Functions	167
How to write a formula	165
Logical Expressions	167
Operators.....	167
Other Functions	174
Spectra Functions.....	174
Statistical Functions	169
Variables.....	165
Four Parameters.....	182
Four Parameters – Marquardt	183
frac(argument)	168

G

Glossary of Terms	205
-------------------------	-----

H

Help Button.....	21
HUID.....	14, 27, 160

Index

I	
Icons	18
ICx calculation	48
identifiers	44, 45
if(...) then(...) else(...) – logical expression	167
ignore()	174
Import Raw Data	134
Import sample ID list	89
Import/edit a sample ID list	85
ln(argument)	168
Initial Password	24
Insert Sample ID List	103
Installation	
Software	12
Installation Qualification	13
Instrument Control	31
Instrument Data	117
int(argument)	168
isInvalid()	174
K	
Kinetic Data Reduction	55
Kinetic Measurements	37
Kinetic Parameters	118
Kinetic transformations	58, 63
Kinetics Graph	125
L	
Levenberg-Marquardt algorithm	183
Levenberg-Marquardt method	183
Levy-Jennings-Graph	113
lg(argument)	168
Licensing magellan	27
LIS - Laboratory Information System	74
Lock application	149
Log(argument)	168
Logical Expressions	
and	167
if(...) then(...) else(...)	167
or	167
login	153
Login	24
logins	
unsuccessful	149
M	
magellan Standard	12
magellan Tracker	12
Manufacturer	2
max(argument)	170
maxAvg(argument)	170
mean(argument)	169
Measurement Parameters	34
Measurement Status	104
Measurement Types - SUNRISE	34
median(argument)	169
medianPlate()	169
Menus of the Evaluate Results Tab	111
Method Export	112
Method Layout	122
Method Notes	78
min(argument)	170
Min./Max.	57
minAvg(argument)	170
Miscellaneous Icon	131
Options	137
Miscellaneous of Evaluate Results Tab	122
Miscellaneous Tab	142
Movements	
plate carrier, filter slide	31
Multilabel Graph	124
Multilabel Measurement	35
Multiplate Methods	81
N	
Number Format	78
O	
Obtain Raw Data	97, 98
Onsets	56
Operation Qualification OQ	13, 16
or – logical expression	167
Organize Favorites	99
P	
Password	
Options	150
Paste from ASCII-Format	115
Paste in ASCII-Format	88
Paths Tab	138
Plate layout	41
Plate Layout Window	39, 116
Plate to Plate QC	65, 113
Plate View Settings	140
Plate View Tab	140
PointwiseCV(argument)	170
Print	112
Print Preview	112
Printed Report	70
Printer Setup	112
Printout Font	112
Q	
QC Validation	64, 122
Qualitative Results	122
Quantitative ELISA Example	187
R	
Reader Compatibility	12
Recalculate with Another Method	116
Reduced Data	117
Register Wizard	158
Registration form	29
Review	130
round(argument)	169
S	
sample ID list	
importing	83, 89
Sample ID List Settings	83
Sample IDs	122
Saving the Evaluated Results	128
Saving the Method	79
Saving the Sample ID List	96
Shortcuts List	22
Sign a File	129
Signature	129
Approval	130
Review	130
Slopes	55
SMTP server	151
Software	
Installation	12
Removal	15
Special Characters	117
Spectra Data Reduction	49, 164

Spectra Dialog	126	User Administration	
spectrum of a scan measurement	126	Options	149
sqr(argument)	169	User Administration (magellan Tracker)	
sqrt(argument)	169	Change User	153
Standard Curve	58, 119	Login	153
Standard Curve Analysis Types	176	User Administration Audit Trail	148
Standard Curve Graph	121	User Administration Summary	151
Standard Elements	21	User Interface	17
Start Favorite	97	User Prompts	78
Start Measurement	97, 100	User Rights	154
Starting magellan	23	User Rights (magellan Standard)	154
stddev(argument)	170	W	
Sum(argument)	170	Weighting	
System Audit Trail	161	Four / Five Parameter Fit – Marquardt / Polynomial	
System Recovery	14	Fit	60, 184
T		Welcome Dialog box	22
Temperature Control	19, 31, 102	Well Summary	88
Test Mail	151	Westgard® rules	114
Transformed Data	117	Wizard	
U		Standard Elements	21
Unsuccessful logins	149	Wizard List	17
Use Predefined Method	97, 99	Workspace Overview	109

Trademarks

The following product names and any registered or unregistered trademarks mentioned in this document are used for identification purposes only and remain the exclusive property of their respective owners:

- **[Product Name]TM** (infinite[®])
Tecan[®] and the Tecan Logo are registered trademarks of Tecan Group Ltd., Männedorf, Switzerland
- DNA ExpertTM is a registered trademark of Techcomp Ltd., Hong Kong, China
- Agilent[®] is a registered trademark of Agilent Technologies, Inc., Santa Clara, CA, USA
- AIR LIQUIDETM is a registered trademark of AIR LIQUIDE, S.A., Paris, France
- Aseptisol[®] is a registered trademark of BODE Chemie GmbH & Co. KG, Hamburg, Germany
- Bacillo[®] is a registered trademark of BODE Chemie GmbH & Co. KG, Hamburg, Germany
- Costar[®], Corning[®] and NBSTM are registered trademarks of Corning Incorporated, Corning, NY, USA
- Greiner[®], µClear[®], LumitracTM and FluotracTM are registered trademarks of Greiner Labortechnik GmbH, Frickenhausen, Germany
- HTRF[®] is a registered trademark of Cisbio International, France
- InvitrogenTM is a registered trademark of Invitrogen Corporation, Carlsbad, CA, USA
- Lysetol[®] and Gigasept[®] (formerly Lysetol) are registered trademarks of Schülke & Mayr GmbH, Norderstedt, Germany
- Microcide[®] is a registered trademark of Global Biotechnologies Inc., Portland, Maine, USA
- Microman[®] is a registered trademark of Gilson, Inc., Middleton, WI, USA
- Pentium[®] is a registered trademark of Intel Corporation, Santa Clara, CA, USA
- Invitrogen[®] and PanVera[®] are registered trademarks of Invitrogen Corporation Carlsbad, CA, USA
- Windows[®], MS DOS[®], Visual Basic[®] and Excel[®] are registered trademarks of Microsoft Corporation, Redmond, WA, USA
- Hamamatsu[®] is a registered trademark of HAMAMATSU Photonics K.K. [IR], Hamamatsu City, Japan
- NUNCTM and Matrix are registered trademarks of Thermo Fisher Scientific, Waltham, MA, USA
- Polyfiltronics[®] is a registered trademark of Whatman International Ltd.
- Dynex[®] is a registered trademark of Magellan Biosciences, Chelmsford, MA, USA
- Labsystem[®] is a registered trademark of Labsystem kft., Budapest, Hungary
- BRET^{2®}, DeepBlueC[®] and PerkinElmer[®] are registered trademarks of PerkinElmer, Inc., Waltham, Massachusetts, USA
- Chroma-GloTM is a registered trademark of Promega Corporation, Madison, WI 53711 USA
- MycoAlert[®] is a registered trademark of Cambrex Corporation, East Rutherford, NJ, USA

Tecan Customer Support

If you have any questions or need technical support for your Tecan product, contact your local Tecan Customer Support organization. Go to <http://www.tecan.com/> for contact information.

Prior to contacting Tecan for product support, prepare the following information for the best possible technical support (see name plate):

- Model name of your product
- Serial number (SN) of your product
- Software and software version (if applicable)
- Description of the problem and contact person
- Date and time when the problem occurred
- Steps that you have already taken to correct the problem
- Your contact information (phone number, fax number, e-mail address, etc.)

End User Software License Agreement

IMPORTANT - READ CAREFULLY: This End-User License Agreement ("EULA") is a legal agreement between you (either an individual or a legal entity) and Tecan Austria GmbH ("Tecan") for the proprietary software product identified above, which includes computer software ("SOFTWARE PRODUCT") and may include associated media, printed materials, and "online" or electronic documentation ("DOCUMENTATION"). This SOFTWARE PRODUCT is made available to you only on the terms and conditions of this EULA. By installing, copying, or otherwise using the SOFTWARE PRODUCT (whichever occurs first), you agree to be bound by the terms of this EULA. If you do not agree with the terms of this EULA, you are not authorized to install and/or use the SOFTWARE PRODUCT.

SOFTWARE PRODUCT LICENSE

The SOFTWARE PRODUCT and the DOCUMENTATION are protected by copyright laws and international copyright treaties, as well as other intellectual property laws and treaties. The SOFTWARE PRODUCT is licensed, not sold.

1. GRANT OF LICENSE

This EULA grants you the non-exclusive and non-transferable right to use the SOFTWARE PRODUCT in accordance with the instructions and procedures in the DOCUMENTATION for your own internal purposes only. You may install and use the number of copies of the SOFTWARE PRODUCT on the number of computers or workstations connected to the number of devices as specified in the documentation to this EULA in accordance with the software installation procedure described in the documentation.

You may either make one copy of the SOFTWARE PRODUCT solely for archival purposes in support of your use of the SOFTWARE PRODUCT on a single computer or transfer the SOFTWARE PRODUCT to a single hard disk provided that you keep the original only for backup or archival purposes. You may not reproduce or distribute the SOFTWARE PRODUCT in any other way, including rental or leasing.

The SOFTWARE PRODUCT shall be used exclusively with the devices specified in the documentation and must not be used on any other devices.

2. LICENSE FEE

The license fee for the right to use the SOFTWARE PRODUCT is set forth in the documentation.

3. DESCRIPTION OF OTHER RIGHTS AND LIMITATIONS

You may not reverse engineer, decompile, or disassemble the SOFTWARE PRODUCT, except and only to the extent that such activity is expressly permitted by applicable law notwithstanding this limitation.

The SOFTWARE PRODUCT is licensed as a single product. Its component parts may not be separated for use on more than one computer or workstation.

Tecan may provide you with support services related to the SOFTWARE PRODUCT ("SUPPORT SERVICES"). Use of SUPPORT SERVICES is governed by Tecan's policies and programs described in the user manual, in "online" documentation, and/or in other materials provided by Tecan. Any supplemental software code provided to you as part of the SUPPORT SERVICES shall be considered part of the SOFTWARE PRODUCT and subject to the terms and conditions of this EULA. With respect to technical information, you provide to Tecan as part of the SUPPORT SERVICES, Tecan may use such information for its business purposes, including for product support and development. Tecan will not utilize such technical information in a form that personally identifies you.

You may not transfer any of your rights under this EULA without the prior written consent of Tecan to a third party.

Without prejudice to any other rights, Tecan may terminate this EULA if you fail to comply with the terms and conditions of this EULA. In such event, you may not use the SOFTWARE PRODUCT any longer and you must destroy all copies of the SOFTWARE PRODUCT and the DOCUMENTATION and all its component parts within a period of fourteen days.

4. COPYRIGHT

All title and copyrights in and to the SOFTWARE PRODUCT (including but not limited to any charts, images, photographs, animations, video, audio, music, text, and "applets" incorporated into the SOFTWARE PRODUCT), the DOCUMENTATION and any copies of the SOFTWARE PRODUCT and the DOCUMENTATION are owned by Tecan Austria GmbH or its suppliers and licensed to Tecan. The SOFTWARE PRODUCT and the DOCUMENTATION are protected by copyright laws and international treaty provisions. Therefore, you must treat the SOFTWARE PRODUCT and the DOCUMENTATION like any other copyright protected material.

5. TERMS AND CONDITIONS FOR USE

Use of the SOFTWARE PRODUCT shall be subject to compliance with the following terms and conditions relating thereto:

- The SOFTWARE PRODUCT shall be used exclusively on devices specified in the documentation;
- only the latest version of the SOFTWARE PRODUCT shall be used;
- the SOFTWARE PRODUCT shall not be modified nor caused to be modified.

It shall be your responsibility to personally effect any requisite declarations to the authorities with a view to using SOFTWARE PRODUCTS.

6. PRECAUTIONS OF USE

Before being commercialized, the SOFTWARE PRODUCT underwent a series of tests to measure the reliability of results obtained.

However, taking into account the high number of possible applications for which the SOFTWARE PRODUCT can be used, it has not been possible to carry out said tests in a real work situation.

The contracting parties agree that it is not possible in practice to produce data processing programs which will be 100% suitable for all applications.

Therefore, you are strongly advised to verify and to validate results obtained before using the SOFTWARE PRODUCT in a real work situation every time it is used in a new application.

Should there be any doubt as to the results, or in the case of erroneous results, you are requested to immediately contact Tecan.

For the perfect use of SOFTWARE PRODUCTS, you are reminded that:

- You must have the requisite knowledge;
- you must, in a regular fashion, write-protect and backup, in particular, to protect the data files from incidents such as deletion, overwriting, virus infection, etc.

7. LIMITED WARRANTY

The SOFTWARE PRODUCT is under warranty for a period of 90 days as of the date of delivery thereof.

During said period, Tecan shall use reasonable efforts to deliver, as quickly as possible and by any means it chooses an updated version or a copy of the said version of the program free of any significant defect appeared.

The provisions mentioned above determine the extent of the warranty granted to you.

Note on Java Support. The SOFTWARE PRODUCT may contain support for programs written in Java. Java technology is not fault tolerant and is not designed, manufactured, or intended for use or resale as online control equipment in hazardous environments requiring fail-safe performance, such as in the operation of nuclear facilities, aircraft navigation or communication systems, air traffic control, direct life support machines, or weapons systems, in which the failure of Java technology could lead directly to death, personal injury, or severe physical or environmental damage. Sun Microsystems, Inc. requires the addition of this disclaimer.

8. RESTRICTED LIABILITY

Tecan shall be subject to an undertaking to exercise due-care.

Said undertaking shall concern the supply of the software conforming to the functionalities described in the documentation thereof, no guarantee whatsoever being given either with regard to results obtained or the fitness of the SOFTWARE PRODUCT for your purposes.

You shall be solely liable for the use of the SOFTWARE PRODUCT and results obtained. In particular, you shall be responsible for verifying the contents and the consistency thereof, as the SOFTWARE PRODUCT shall be used under your sole management, control and responsibility.

TECAN SHALL NOT BE HELD LIABLE FOR ANY INDIRECT OR CONSEQUENTIAL DAMAGES OR ANY LOSS OF PROFIT, SHORTFALL IN EARNINGS OR LOSS OF DATA INCURRED BY YOU EVEN IF TECAN HAS BEEN INFORMED THAT THE SAID LOSS OR PREJUDICE COULD OCCUR.

The SOFTWARE PRODUCT has undergone an anti-virus test. However, Tecan shall not be liable should a virus be present that was undetectable by the anti-virus utility used to run the test mentioned above.

SHOULD FOR ANY REASON WHATSOEVER, TECAN BE HELD LIABLE BY THE COURTS, THE AMOUNT OF ANY DAMAGES EFFECTIVELY OWED AND ORDERED TO BE PAID SHALL, WITH THE EXCEPTION OF INTENTIONAL MISCONDUCT OR

GROSS NEGLIGENCE, NOT EXCEED THE TOTAL AMOUNT OF THE SUMS RECEIVED BY TECAN BY VIRTUE OF THE PRESENT EULA.

9. CONFIDENTIALITY

You hereby acknowledge and agree that you will not disclose the SOFTWARE PRODUCT and the DOCUMENTATION to any of your employees (except to those responsible for the application) or to any third party without the prior written consent of Tecan and that this duty of confidentiality survives the term of this EULA. You will safeguard the SOFTWARE PRODUCT and the DOCUMENTATION with the highest degree of care.

10. TERMINATION

If you fail to comply with any of your obligations hereunder, Tecan shall have the right, at any time, to terminate the EULA and take immediate possession of the SOFTWARE PRODUCT and the DOCUMENTATION and of all copies wherever located without demand or notice.
