TECAN.

Instructions for Use for

magellan

Reference Guide

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WARNING

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

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We would appreciate any comments on this publication.

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Declaration for EC Certificate

Provided upon request.

magellan Intended Use

See 1.2 Intended Use 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.

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Warnings, Cautions and Notes

The following types of notices are used in this publication and 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.

Table of Contents

1. Introduction

1.1 Area of Application

magellan is a universal **reader control and data reduction software** for analyzing data generated from microplate tests using Tecan measuring devices.

magellan is available in two versions:

- magellan **Tracker** and
- magellan **Standard**.

magellan **Standard** software is intended for endpoint, kinetic and multilabel assays in pharmaceutical, biotechnological and life science industry, for research use, for food analysis and veterinary applications.

magellan **Tracker** offers all functionality to become compliant with the FDA Regulation 21 CFR part 11 and with the European In vitro diagnostic directive 98/79/EC.

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.***

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.

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

Three default levels of user rights can be selected: **Administrator, Application Specialist** and **Operator**. The Administrator must always be trained by Tecan or a Tecan authorized organization.

1. The **Administrator** is responsible for procedural and technical laboratory issues and for compliance with federal regulations. It is recommended this individual be a Laboratory Supervisor.
   For detailed description of the Rights of an **Administrator** refer to chapter 10.4.4 User Rights (magellan Tracker) and 10.5.4 User Rights (magellan Standard).
2. The **Application Specialist** is responsible for performance of routine tests and examinations and assistance in the setup of experiments. magellan allows the Application Specialist to define specifications containing measurement parameters and evaluation settings and carry out measurements accordingly. The Application Specialist must be trained by the Administrator. It is recommended this individual meet the minimum requirements necessary to be a Laboratory Technician.
   For a detailed description of the rights of an Application Specialist refer to chapter 10.4.4 User Rights (magellan Tracker), respectively to chapter 10.5.4 User Rights (magellan Standard).

3. The **Operator** performs routine analysis under immediate supervision. It is recommended this individual meet the minimum requirements necessary to be a Laboratory Assistant. magellan allows the Operator to carry out measurements according to the specifications given by the Application Specialist or Administrator. The Operator cannot change those specifications. The Operator must be trained by the Administrator.
   For a detailed description of the user rights of an Operator refer to chapter 10.4.4 User Rights (magellan Tracker) respectively to chapter 10.5.4 User Rights (magellan Standard).

magellan **Tracker** is designed for use with the operating systems and Microsoft Office versions specified in chapter 1.4.3 Software Requirements. If additional programs are installed, functionality in accordance with IVD for Europe and FDA Regulations cannot be guaranteed.

Note

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

1.2 Intended Use of magellan

magellan software is a reader control and data reduction software for analyzing data generated from microplates using a Tecan absorbance, fluorescence and/ or luminescence microplate reader. The software is intended for endpoint, kinetic, multilabel, fluorescence lifetime, and spectral scanning assays.

magellan software is intended for professional use according to the software specifications described in the manual (Instructions for Use for magellan).

magellan Tracker software offers all functionality for compliance with the FDA regulation 21 CFR part 11 for electronic records and signatures in addition to the functionality of magellan Standard. magellan Tracker software is also intended for in vitro diagnostic use in Europe according to the In vitro diagnostic directive 98/79/EC as an accessory together with a Tecan Sunrise absorbance reader. magellan cannot be used for agglutination assays.

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 is able to recognize and avoid dangers.

The administrator has extensive skills and is able to 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 is able to recognize and avoid dangers.

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

1.4 Specifications

1.4.1 *General*

magellan software is available in two different versions:

- magellan **Standard** software is intended for endpoint, kinetic and multilabel assays in pharmaceutical, biotechnological and life science industry, for research use, for food analysis and veterinary applications. It supports a basic user administration.
- magellan **Tracker** software is designed to support FDA 21 CFR part 11 regulated environments. It offers all functionality to become compliant with the FDA Regulation 21 CFR part 11 and with the European In Vitro diagnostic directive 98/79/EC.

1.4.2 *Hardware Requirements*

The following requirements have to be met for using magellan:

Hardware	**Minimum**	**Recommended**	**Advanced (FLT/Scanning)**
Memory	512 MB	1024 MB	1024 MB
CPU	Pentium III or Atom	Pentium IV	Pentium Core2Duo
Resolution	1024 x 600	1280 x 1024	1280 x 1024
Serial/ USB ports	1 (USB 2.0 or higher)	2 (USB 2.0 or higher)	2 (USB 2.0 or higher)

Note

When an Infinite instrument is connected, we recommend at least 512 MB memory and Pentium III.

1.4.3 *Software Requirements*

The following requirements have to be met for using magellan:

Operating system	
Microsoft Windows	Windows XP Professional/SP2 Windows Vista 32Bit Windows 7

Additionally supported software	
	Microsoft Excel 2000 Microsoft Excel XP Microsoft Excel 2003 Microsoft Excel 2007 Microsoft Excel 2010

1.4.4 Reader Compatibility

The following Tecan readers can be used with magellan:

Instrument Types	Measurement Mode
DNA Expert	Fluorescence / Absorbance / Luminescence
GENios	Fluorescence / Absorbance / Luminescence
GENios FL	Fluorescence
GENios Plus	Fluorescence / Absorbance / Luminescence
GENios Pro	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization
SPECTRAFluor	Fluorescence / Absorbance
SPECTRAFluor Plus	Fluorescence / Absorbance / Luminescence
SAFIRE	Fluorescence / Absorbance
SAFIRE^2	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization
SUNRISE	Absorbance
ULTRA Evolution	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization / FLT
ULTRA	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization
ULTRA 384	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization
Infinite M200	Fluorescence / Absorbance / Luminescence
Infinite F50	Absorbance
Infinite F200	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization
Infinite F500	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization
Infinite M1000	Fluorescence / Absorbance / Luminescence / Fluorescence Polarization

Note

The* Connect *stacker can be used together with Tecan instruments in order to measure batches of plates. Please refer to the Instruction for Use for* Connect *for more information.

1.5 Software Installation Procedure

1.5.1 Automatic Software Setup Program

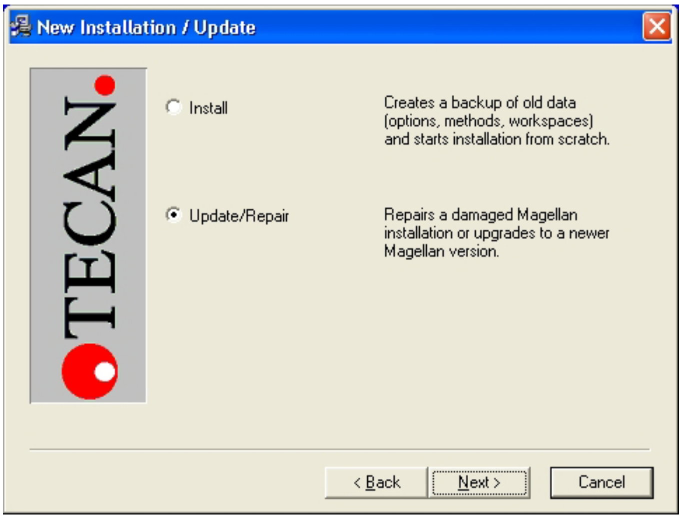
magellan is installed by an automatic software setup program. All necessary components are installed automatically.

Start **Setup.exe** to begin the installation procedure. Some components of this software are using the Microsoft .NET Framework technology. Click **I agree** in the window which appears immediately after having started the setup to continue. The setup program then starts inspecting your current configuration, this may take some seconds.

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 setup program automatically detects a previous installation of magellan. In the next window the user has to decide whether he wants to reuse existing data files (select **Update/Repair**) or make a new installation (select **Install** - existing files will be moved to a backup folder). Select according to your needs and click **Next**.


New Installation / Update

○ Install — Creates a backup of old data (options, methods, workspaces) and starts installation from scratch.

● Update/Repair — Repairs a damaged Magellan installation or upgrades to a newer Magellan version.

The **Choose Destination Location** window appears next. The default installation path is displayed. Click **Browse** to change the default destination path, if desired. Click **Next** to continue.

In the next window, a name for the program group, in which the program will be stored, can be entered or chosen from the list. The default group name is Tecan. Click **Next** to continue.

The serial number 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 2.6 Licensing magellan).

In the next window, select magellan **Standard** or magellan **Tracker**, depending on which version you have ordered, to install the software. Click **Next** to continue.

Example files will be installed with the setup if this option is selected in the next window. Example files are installed only when installation is executed from scratch. They are not installed when updating the software. If examples have been forgotten during the first installation, repeat the installation selecting **Install**.

In the current window, the preferred language version can be selected from a drop down list.

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**6** in the program group defined above.

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 dealer 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 11.2.4 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 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 10.2.2 Automatic Archiving.

Magellan Paths – Windows XP

Magellan.ini	C:\Documents and Settings\All Users\Documents\Tecan\Magellan
Methods	C:\Documents and Settings\All Users\Documents\Tecan\Magellan\mth or as set in the **Options** dialog box
Workspaces	C:\Documents and Settings\All Users\Documents\Tecan\Magellan\mth or as set in the "**Options** dialog box
Sample ID lists	C:\Documents and Settings\All Users\Documents\Tecan\Magellan\wsp or as set in the **Options** dialog box
Exported data	C:\Documents and Settings\All Users\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 chapter 11.2.4 Opening a File Created on Another PC – Add HUIDs

Magellan Paths – Windows Vista, Windows 7

Magellan.ini	C:\Users\Public\Documents\Tecan\Tecan\Magellan
Methods	Standard path: C:\Users\Public\Documents\Tecan\Tecan\Magellan\mth or as set in the **Options** dialog box
Workspaces	C:\Users\Public\Documents\Tecan\Tecan\Magellan\smp or as set in the **Options** dialog box
Sample ID lists	C:\Users\Public\Documents\Tecan\Tecan\Magellan\wsp or as set in the **Options** dialog box
Exported data	C:\Users\Public\Documents\Tecan\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 11.3 System Audit Trail

1.5.5 *Automatic Software Removal*

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

magellan must be closed.

Select **Add/Remove Programs** from the **Settings - Control Panel** in the **Windows Start menu**.

Select the magellan icon and click **Remove**.

The Uninstall wizard is started. Select the preferred uninstall method (**Automatic** or **Custom**) and click **Next** to continue.

In the next window, click **Finish** to uninstall magellan.

In the next window, decide whether or not shared components should be removed. If **Yes** is selected, magellan will be completely uninstalled and other Tecan programs such as XFluor, HS Control Manager or Gemini 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 any more and must be re-installed.

2. Start Working with magellan

Note
Before starting to work with magellan***, we suggest reading the document*** **Notice Anomalies magellan** ***for any malfunctions in the application.***

2.1 User Interface

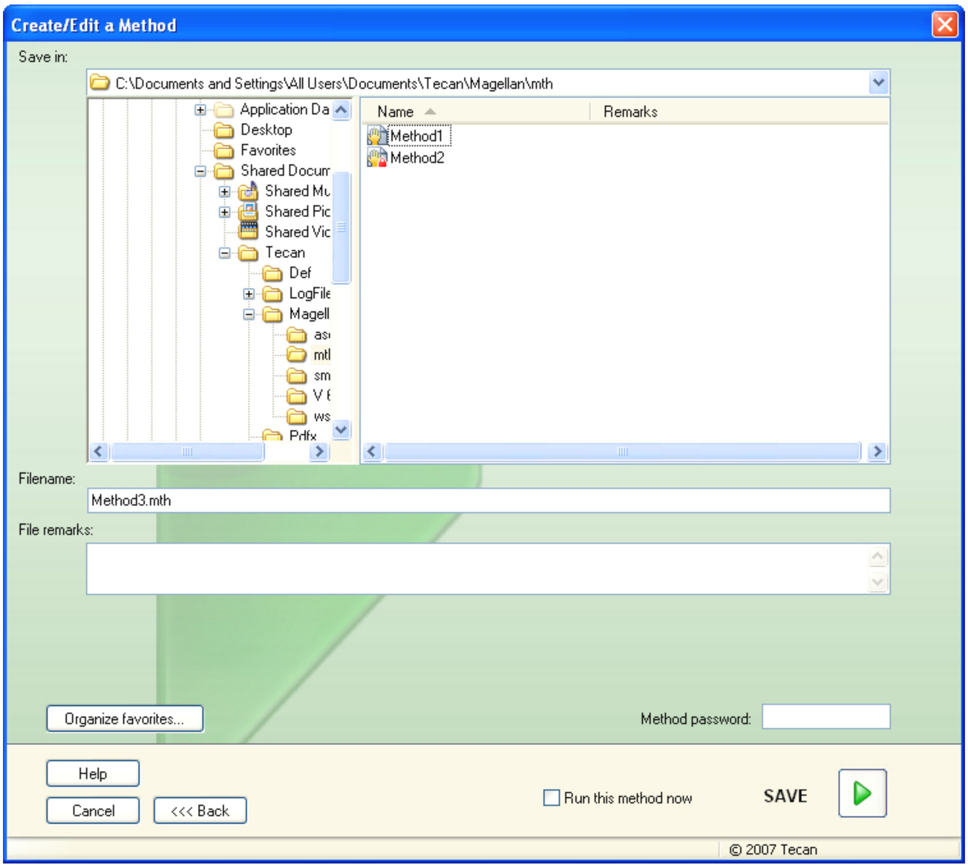
The main type of the user interface in magellan is the wizard.

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.

2.1.1 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.



Save in: C:\Documents and Settings\All Users\Documents\Tecan\Magellan\mth

Filename: Method3.mth

☐ Run this method now

New folders can be created by right-clicking and selecting **New folder** from the context sensitive menu. Files and folders can be moved easily from one folder to another by drag and drop or cut/copy/paste respectively, 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

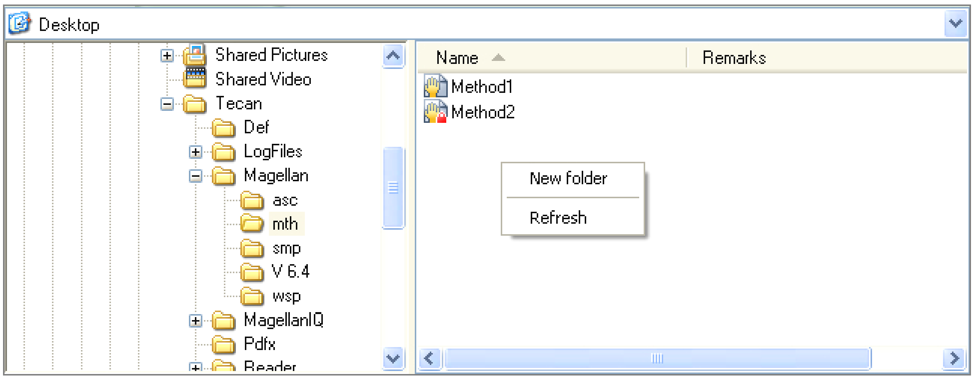
Password protected method

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. If the user administration is activated, users can define individual default paths.

When the **Create/edit a method, Create/edit a sample ID list**, **Evaluate results** wizards, or **Use predefined method** of **Start measurement** wizard are started, the specified default path is opened automatically. Users can create new folders in any folder of the Windows Explorer during the saving process.

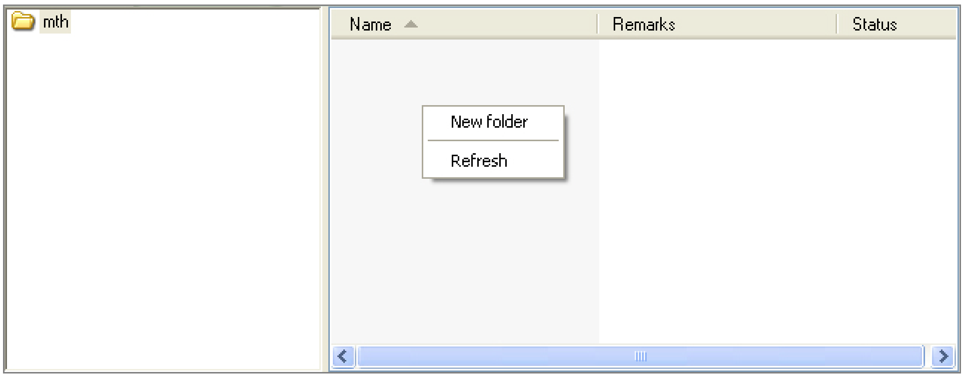


In the **Save** window, the folder, specified by the default path of the method, workspace, standard curve or sample ID list, is opened automatically, whenever a new file is created. If an already existing file is modified, the path to the current location of the file will be opened. However, it is possible 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.

When the **Create/edit a method, Create/edit a sample ID list**, **Evaluate results** wizards, or **Use predefined method** of **Start measurement** wizard are started, the specified default path is opened automatically. Users can also create new subfolders 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 method, workspace, standard curve or sample ID list, 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 Components & Terms – Basic Logic of magellan

magellan supports four file types:

- **Methods (.mth)**
- **Sample ID Lists (.smp)**
- **Workspaces (.wsp)**
- **Standard curves (.std)**

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

The magellan main window contains the **window area** and a **status bar** at the bottom of the page. Depending on the data selected, a **toolbar** (e.g. plate view, graph) and a **menu bar** (plate view – evaluate results) in the header are displayed.

2.2.1 Method (.mth)

With the Create/edit a method wizard **methods** are created which combine all of the necessary parameters for the measurement, evaluation and data handling of an assay: measurement parameters, evaluation settings, a printed report setup, data export setup, number format, and automated data handling settings. They do not, however, contain any measurement data (refer to chapter 4 Create/Edit a Method Wizard).

Methods accelerate data evaluation and can be customized for assays which are processed regularly.

When a new method is created, at first all wells of the plate layout will be empty.

When defining the layout, transformations etc., the identifiers, formulas etc. are displayed in the corresponding wells.

Data can be analyzed with different methods.

2.2.2 Sample ID List (.smp)

With the Create/edit a sample ID list wizard **sample ID lists** are created which contain the alphanumeric IDs of each sample in the microplate. magellan supports the import of various sample ID list formats (see chapter 5.2.3 Import a Sample ID List generated by pipetting software applications. It is also possible to generate sample ID lists for the corresponding analysis plates by allocating names to the individual wells. Up to three sample IDs per well can be defined. Barcodes can be read or well numbers can be generated automatically.

2.2.3 Workspace (.wsp)

A **Workspace** is created whenever a measurement is performed (Run a Method or Obtain raw data without method) and **contains measured and calculated data as well as all method settings**.

The Workspace stores **all of the information** gathered during a measurement run: the used method with measurement parameters, raw data, evaluation settings, printed report setup, automated data handling, etc. A **Sample ID List** can also be included.

Data display settings (numbers, graphs, colors, etc.) can be defined in the workspace.

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

In the Edit method tab of a workspace method, settings can be changed for the currently opened workspace which results in a re-calculation of data but has no influence on the saved method file itself.

2.2.4 Standard Curve (.std)

A measured standard (calibration) curve can be saved as a **.std** file and used for subsequent evaluations of other measurements (refer to chapter 4.3 Define Evaluation / Control Bar of Create/Edit Method Tab).

2.2.5 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\Magellan

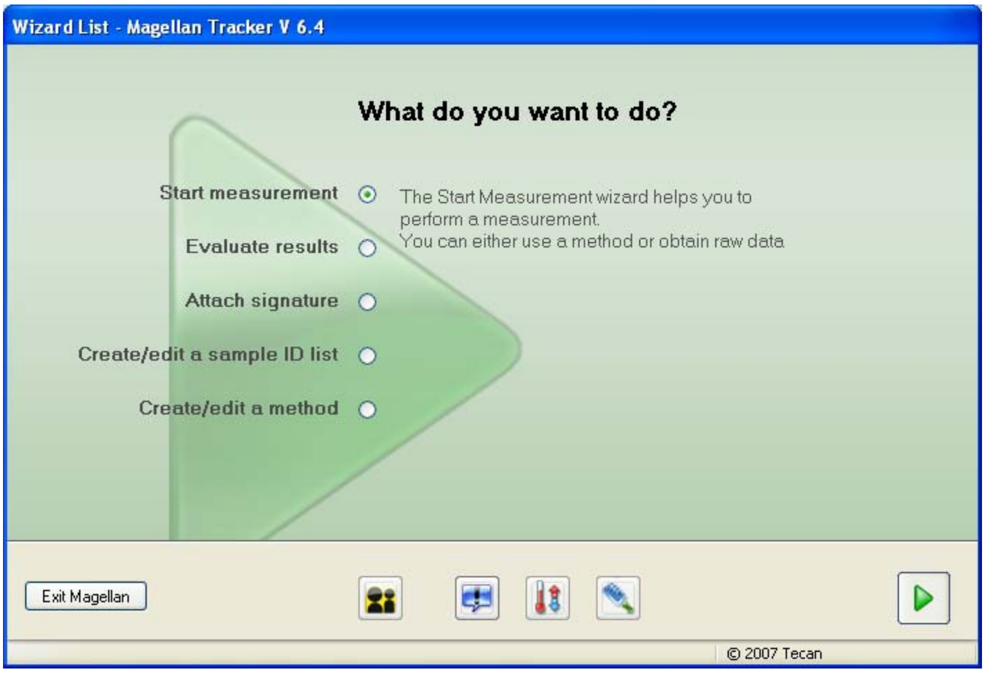
The subdirectories are displayed in the table below:

Type of File	**File Extension**	**Directory** magellan
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 \Reader\pdfx

Note
The difference between plate definition files with .pdf extension and .pdfx extension is that Infinite Series instruments use the .pdfx format files, whereas all other Tecan instruments use .pdf files.

2.3 User Interface – Wizard List

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



Wizard List - Magellan Tracker V 6.4

What do you want to do?

Start measurement ●
Evaluate results ○
Attach signature ○
Create/edit a sample ID list ○
Create/edit a method ○

The Start Measurement wizard helps you to perform a measurement.
You can either use a method or obtain raw data

The displayed screenshot shows the wizard list page when magellan **Tracker** is installed. With magellan **Standard** the Attach signature wizard is not available.

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

2.3.1 Start Measurement Wizard

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

The following choices are available:

- **Obtain Raw Data** is used to generate raw data quickly and easily by setting the required measurement parameters and starting a measurement. The Obtain raw data wizard creates a new workspace in which the obtained values are presented and stored.
- **Run Strip Layout** is used to collect strips from different methods, combine the strips to one method and run this method.
- **Use Predefined Method** is used to perform measurements based on previously defined methods. The wizard creates a new workspace containing the selected method (which consists of all measurement parameters and evaluation definitions) and enables you to insert a sample ID list. After the measurement, the workspace is completed with the obtained raw data that will be evaluated.
- **Start Favorite** is used to select one of the most frequently used methods from the list of numbered icons.

After the measurement is finished a workspace file is created (.wsp; refer to chapter 2.2 Components & Terms – Basic Logic of magellan).

2.3.2 Evaluate Results Wizard

For a detailed description, refer to chapter 7 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. All this information is stored in workspace file (.wsp; refer to chapter 2.2 Components & Terms – Basic Logic of magellan.

2.3.3 Attach Signature Wizard

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

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

The **Attach signature** wizard is only available with magellan Tracker.

2.3.4 Create/Edit a Sample ID List Wizard

For a detailed description, refer to chapter 5 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. Up to three sample IDs per well can be entered or imported. The sample ID lists are saved as .smp files (refer to chapter 2.2 Components & Terms – Basic Logic of magellan).

2.3.5 Create/Edit a Method Wizard

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

The **Create/edit a method wizard** is used to define or edit methods. Methods contain all necessary parameters for measurement, evaluation and data handling according to the performed assay. Methods are saved as .mth files (refer to chapter 2.2 Components & Terms – Basic Logic of magellan).

2.3.6 Icons

Icon: Change Current User

If the user administration is active (refer to chapter 10.4 User Administration (magellan Tracker) and to chapter 10.5 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 10.2 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 10.3 Options.
- **User administration** is used to add or disable users and to set or modify user rights. See chapter 10.4 User Administration (magellan Tracker), respectively chapter 10.5 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 2.6 Licensing magellan).

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

Icon: Temperature control

For detailed description, refer to chapter 3.1.2 Temperature Control... .

Use this icon to set the target temperature for the connected instrument.

Icon: Move plate

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

2.3.7 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. The following buttons are used in the individual windows of a wizard:

Back button	The **Back** button is used to navigate back to the previous window within a wizard. When the window is the active area click **<<< Back** or press **SHIFT+B** to navigate back to the previous window.
Next button	The **Next** button is the large green arrow in the bottom right corner and is used to navigate forward to the next window within a wizard. When the window is the active area click **Next** or press **SHIFT+N** or **ENTER** to navigate forward to the next window.
Finish button	The **Finish** button is the large green arrow in the bottom right corner and is used to navigate forward to the save window of the wizard. When the window is the active area click **Next** or press **SHIFT+N** or **ENTER** to navigate forward to the next window.
Save button	The **Save** button is only found in the last window of a wizard and replaces the **Next** button. The **Save** button is a large green arrow in the bottom right corner. It is used to close the wizard and save all changes or to start a process. When the window is the active area click **Save** or press **ENTER** to close a wizard and to save all changes.
Cancel button	The **Cancel** button is used to close a wizard without saving any changes to settings or documents. When the window is the active area click **Cancel** or press **ESC** to close a wizard without saving any changes.
Help button	The **Help** button opens the help window. When the window is the active area click **Help** or press **F1** to open 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

2.3.8 *The Help Button*

Click the **Help** button or press 'F1' to open the magellan online help. The tabs Contents, Index and Search are available. For further details on using the Windows Help function refer to your Windows instructions of use.

2.3.9 *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.

2.3.10 *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)

2.4 Starting magellan

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 2.5 Connecting an Instrument), switch the instrument on before starting*** magellan***.***

2.4.1 Starting Standard Version

Perform the following steps to start magellan:

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

2.4.2 Starting Tracker Version

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.

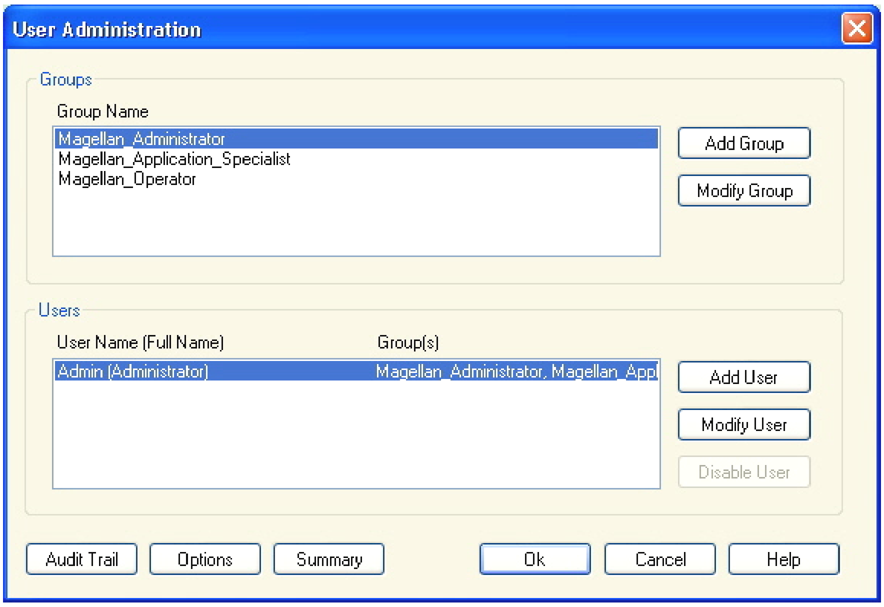
Caution

If the User Administrator password is forgotten, User Administration settings cannot be changed and magellan **must be completely reinstalled.**

Note

We recommend to create at least two User Administrators.

After clicking **OK**, the **User Administration** dialog box appears:



Users and groups can be added, edited or disabled and user rights can be defined. Options for login, password, and email can be edited. See chapter 10.4 User Administration (magellan Tracker) and chapter 10.5 User Administration (magellan Standard).

Change 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.

The old password has to be entered. The new password must comply with the defined password rules and has to be entered twice to prevent typing errors. Old passwords cannot be reused. The new password will expire after a defined period of time. See chapter 10.4.5 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 close the dialog box and the user is logged in. Only those user actions can be performed, that correspond to the user's rights.

Click the **Cancel** button to close the dialog box and magellan is terminated.

The user account will be disabled after the maximum number of consecutive unsuccessful logins has been reached (see chapter 10.4.5 User Administration Options/ Login Options).

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.

2.5 Connecting an Instrument

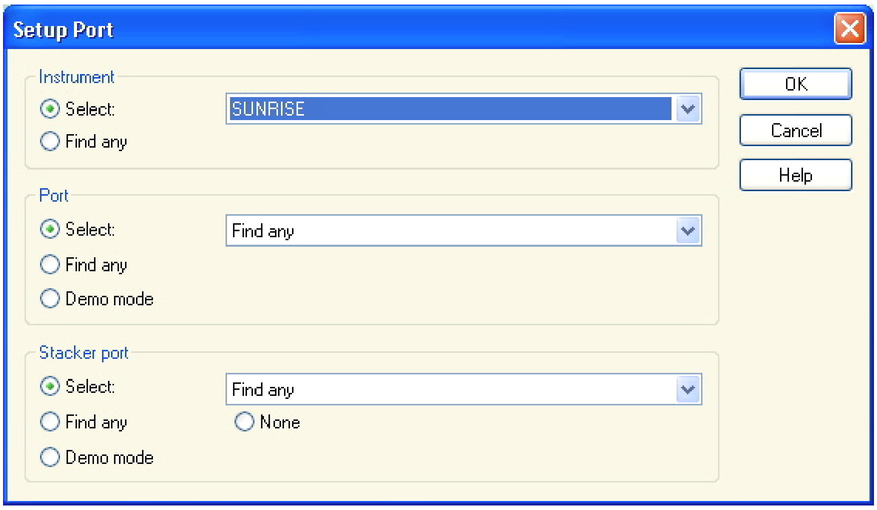
magellan can be run either with an instrument connected or in a demo mode, simulating an instrument connected.

2.5.1 Instrument Connected

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:



Setup Port

Instrument
● Select: SUNRISE
○ Find any

Port
● Select: Find any
○ Find any
○ Demo mode

Stacker port
● Select: Find any
○ Find any
○ None
○ Demo mode

Instrument	In the **Instrument** group box, 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**. If the connection was successful a Dialog is displayed with Information, which instrument is connected to which port. The instrument is now connected and ready for operation using the magellan software.
Stacker Port	If a Tecan **Connect** stacker is used together with the instrument, select the connecting port from the drop down list or select **Find any**. If no stacker is used select **None** for the stacker port.

Change Instrument

Click the **miscellaneous** icon in the wizard list and **instrument control** in the miscellaneous list. The instrument control window is displayed showing two group boxes: **Instrument** and **Setup & Service**. Select **Change instrument** from Setup & Service to connect an instrument or to change the currently connected instrument.

2.5.2 Demo Mode

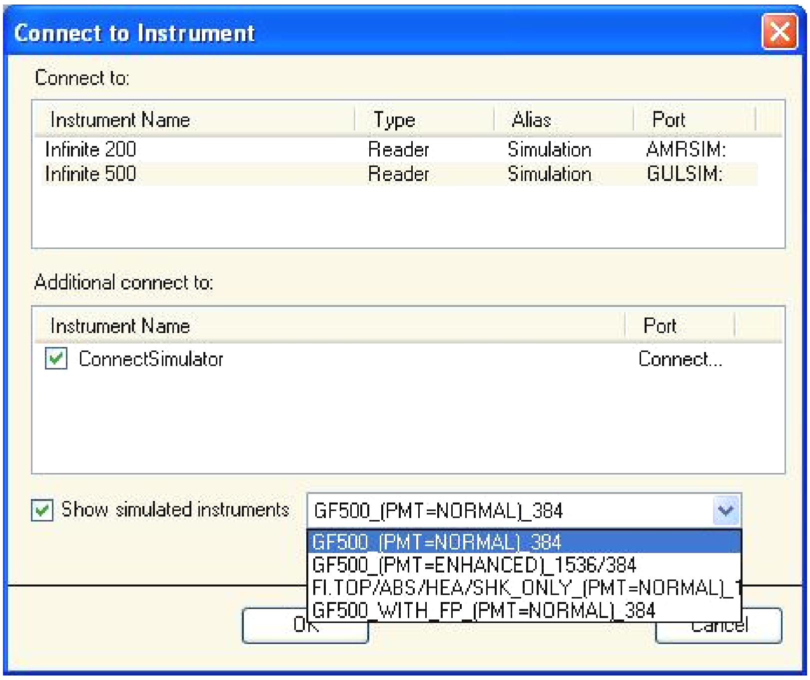
If **no instrument** is connected, select the instrument to be simulated from the drop down list in the **Instrument** group box and select **Demo mode** in the **Port** group box and Click **OK**. magellan is now in demo mode.

Demo mode allowed (in the **Options** dialog) is selected by default (see chapter 10.3.4 Miscellaneous to change this default setting).

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

2.5.3 Connecting an Instrument of the Infinite Series

Select **Infinite Series** in the **Instrument** group box in the **Setup Port** dialog box. Click **OK** to display the **Connect to Instrument** dialog box, select the instrument and click **OK**. For demo mode select the **Show simulated instruments** checkbox and the preferred instrument from the drop down list and click OK.



Connect to:

Instrument Name	Type	Alias	Port
Infinite 200	Reader	Simulation	AMRSIM:
Infinite 500	Reader	Simulation	GULSIM:

Additional connect to:

Instrument Name	Port
☑ ConnectSimulator	Connect...

☑ Show simulated instruments: GF500_(PMT=NORMAL)_384

2.5.4 Connecting a Stacker

The Tecan **Connect** stacker can be used additionally. See chapter 9 Batch Processing for further details.

2.6 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.***

For licensing magellan there are two possibilities:

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

Note
It is very important that the person who registers the software has administrator rights on the computer with operating system Win XP.

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 over the **miscellaneous** icon in the wizard list starting page. (**miscellaneous** → **About** magellan → **Register**).

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

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 serial number and the license number you have to start the registration wizard again and enter both numbers. 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.

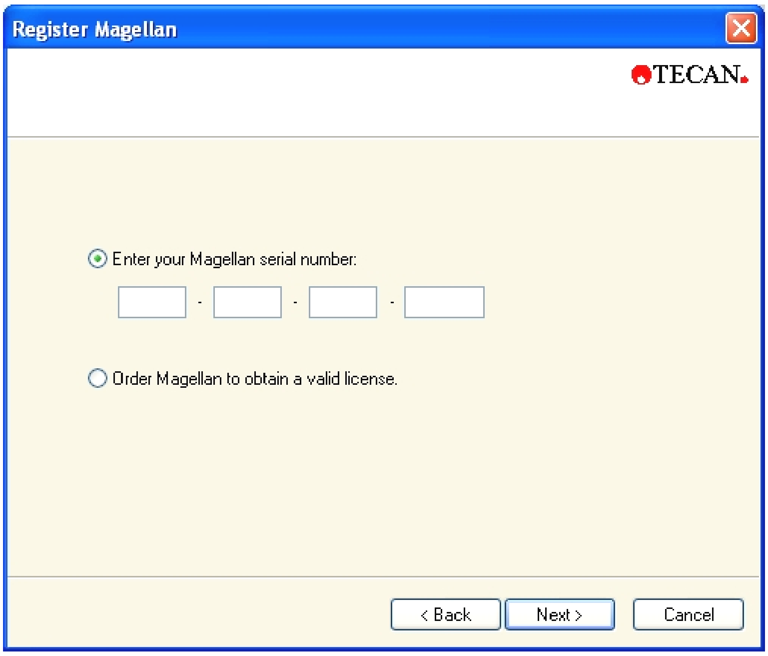
2.6.1 Registration Wizard

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

Serial and License Number

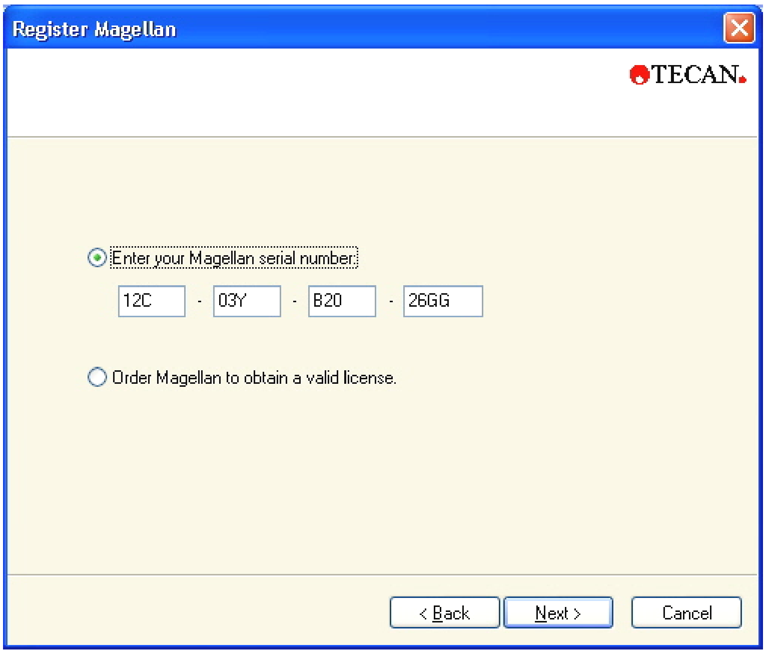
Order a Serial Number for magellan

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



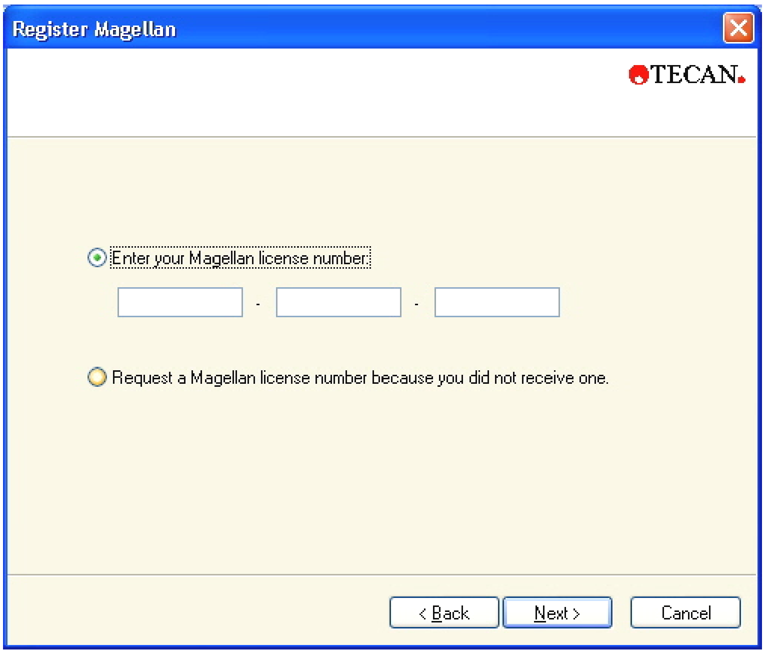
magellan **Has Already Been Purchased**

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



● Enter your Magellan serial number:
12C - 03Y - B20 - 26GG

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



● Enter your Magellan license number:

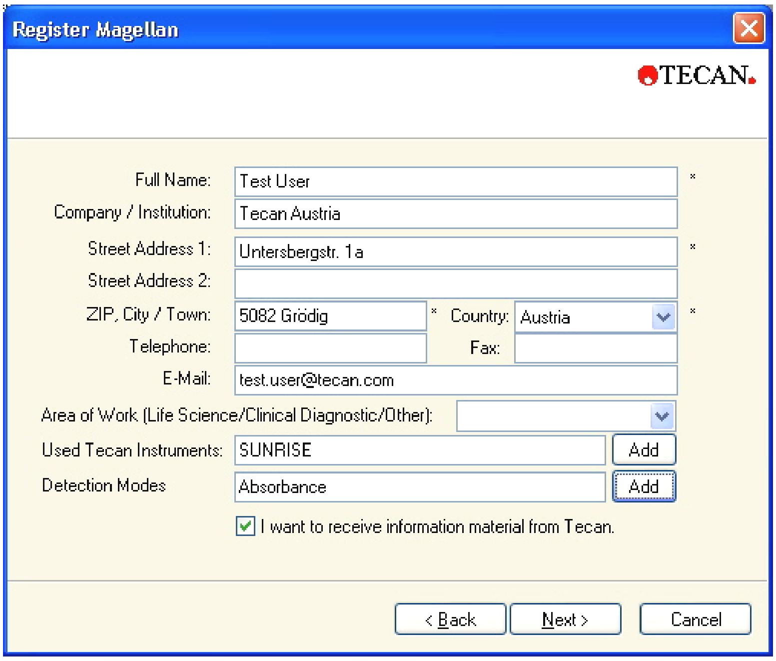
☐ - ☐ - ☐

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

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

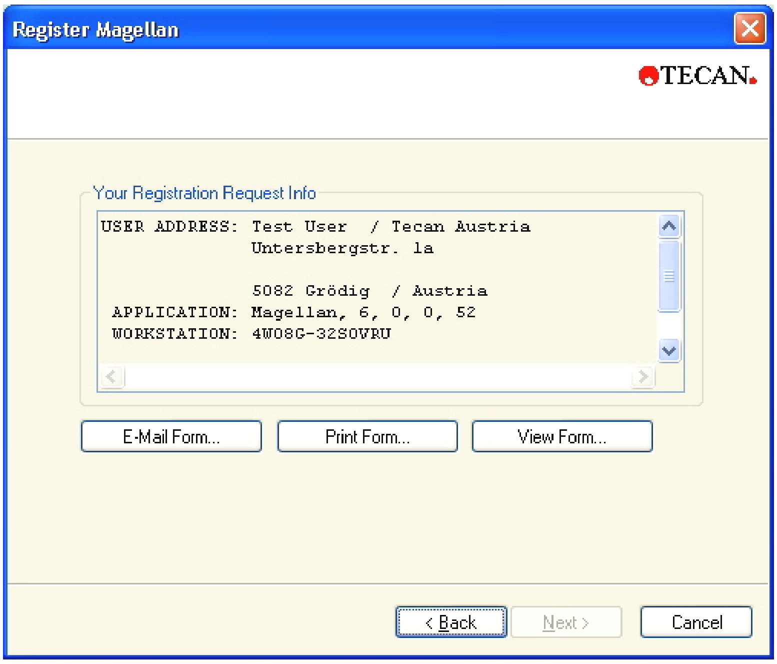
Complete the registration form. Fields marked with an asterisk are mandatory.



Full Name: Test User *
Company / Institution: Tecan Austria
Street Address 1: Untersbergstr. 1a *
Street Address 2:
ZIP, City / Town: 5082 Grödig * Country: Austria *
Telephone: Fax:
E-Mail: test.user@tecan.com
Area of Work (Life Science/Clinical Diagnostic/Other):
Used Tecan Instruments: SUNRISE
Detection Modes: Absorbance
☑ I want to receive information material from Tecan.

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.



```
USER ADDRESS: Test User  / Tecan Austria
              Untersbergstr. 1a

              5082 Grödig  / Austria
 APPLICATION: Magellan, 6, 0, 0, 52
 WORKSTATION: 4W08G-32S0VRU
```

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.

Click **Next** and the Registration requested window appears:

Registration requested!

You successfully created and sent a Magellan registration form. When you have received your license number start the Registration wizard again and register Magellan on your computer.

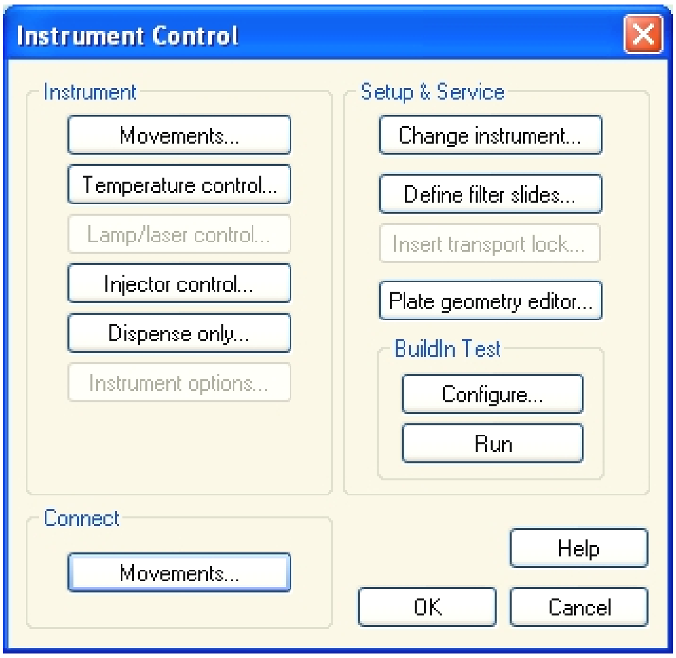
Finishing Licensing magellan

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 the filter slides.

In the **Movements** dialog box, specific **In** and **Out** buttons can be used to move the plate carrier or filter slides into the reader or out of it.

Refer to the Instructions for Use for the Reader Server, document number 30008897, for further information on the **Movements** dialog box.

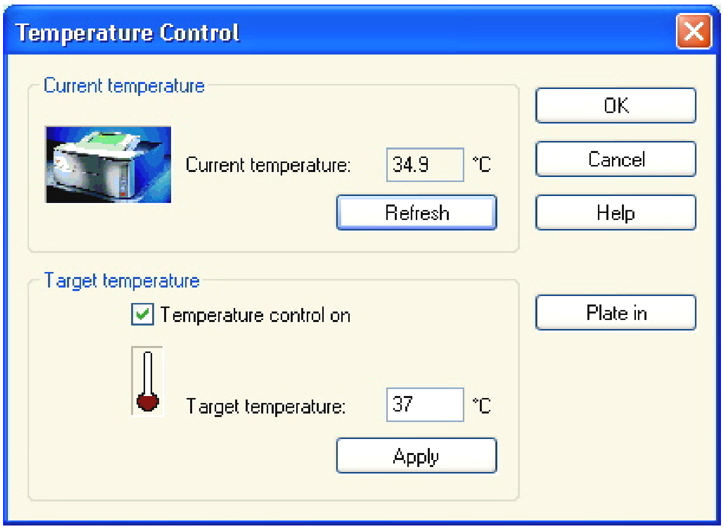
3.1.2 Temperature Control...

Only available for instruments equipped with temperature control.

In the **Instrument Control** dialog box, click the **Temperature Control** button.

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 6.6 Start Measurement with a Predefined or Favorite Method).



Temperature Control

Current temperature

Current temperature: 34.9 °C

Target temperature

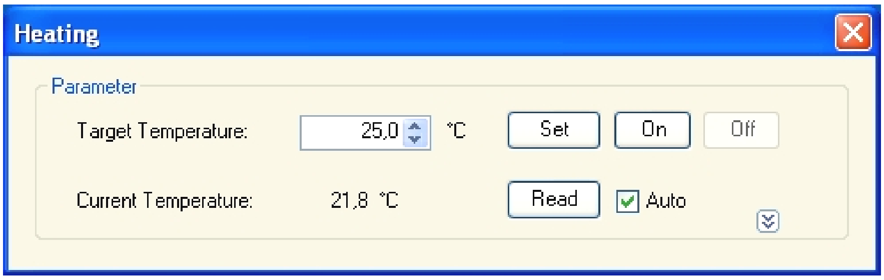
☑ Temperature control on

Target temperature: 37 °C

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. To set the temperature of the instrument, click the **Apply** button. The temperature is sent to the instrument, but the dialog box is still displayed. Click **OK**, the target temperature is sent to the instrument and the dialog box disappears.

Refer to the **Reader Server** Instructions for Use, document number 30008897, for further information on the **Temperature Control** dialog box.

3.1.3 Heating Dialog (Temp Control for Infinite Series Readers)



Heating

Parameter

Target Temperature: 25,0 °C

Current Temperature: 21,8 °C

☑ Auto

Target temperature	This command is used to set the target temperature of the instrument manually. Select or enter the **Target temperature** and click **Set**. Click **On/Off** to start/stop instrument heating.
Current temperature	Click the **Read** button to display the current temperature of the instrument or click the **Auto** check box to have it read automatically. Click **Off** to stop heating. Click the down button, ︾, to display the heating graph and click the up button, ︽, to collapse. Click the close button, ☒ , to exit the **Heating** dialog box.

3.1.4 Lamp/Laser Control...

Instrument feature (see the corresponding Instructions for Use of the instrument connected for more information).

3.1.5 Injector Control...

This option is only applicable for instruments equipped with injectors. See the respective Instructions for Use of the instrument for further details.

3.1.6 Dispense Only…

This option is only applicable for instruments equipped with Injectors. See the respective Instructions for Use of the instrument for further details.

Instrument features – baud rate, power down. See the corresponding Instructions for Use of the instrument for further details.

3.2 Setup & Service Options

3.2.1 Change Instrument...

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.

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 2.5 Connecting an Instrument for further details.

Click the **Change instrument…** menu option and the currently connected instrument will be disconnected. In the **Setup Port** dialog box, the desired instrument and the communication port can be selected and thus be connected to magellan.

Refer to the **Reader Server** instructions for use, document number 30008897, for further information on the **Setup Port** dialog box.

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

3.2.2 Define Filter Slides...

Standard and custom filter slides can be defined.

3.2.3 Insert Transport Lock...

Instrument feature (see the corresponding Instructions for Use for more information).

3.2.4 Optimize Z-Position

Only applicable for instruments with z-positioning option.

In the **Instrument Control** dialog box, click **Optimize Z-Position...**

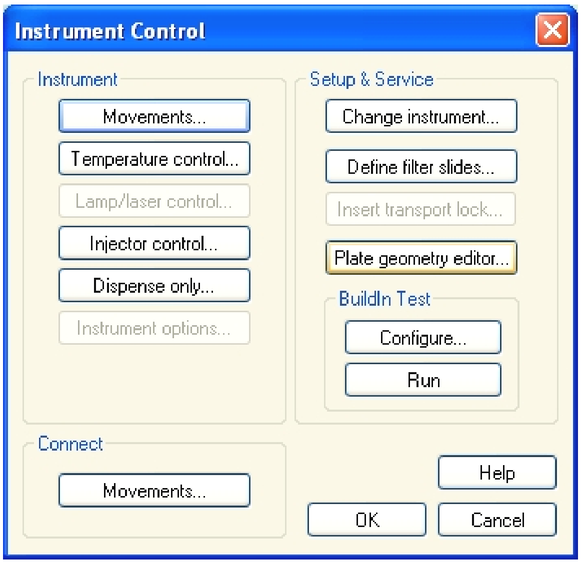
This option can be used to find the optimum Z-position of the plate transport in relation to the measuring head for specific instruments. Therefore, the **Optimize Z-Position** dialog box is displayed.

Refer to the **Reader Server** instructions for use, document number 30008897, for further information on the **Optimize Z-Position** dialog box.

3.2.5 Plate Geometry Editor...

Click the **Miscellaneous** icon from the wizard list.

Select **Instrument Control** and connect to an instrument (button **Change instrument**). Then click the button **Plate geometry editor** in the **Instrument Control** dialog box and **Continue** (green arrow) on the wizard welcome page.



magellan offers a wide selection of predefined plate geometry files for standard plate formats to choose from. Use the **Plate geometry editor** to create plate geometry files for not listed plates in order to use them with magellan or to validate existing plate geometry files.

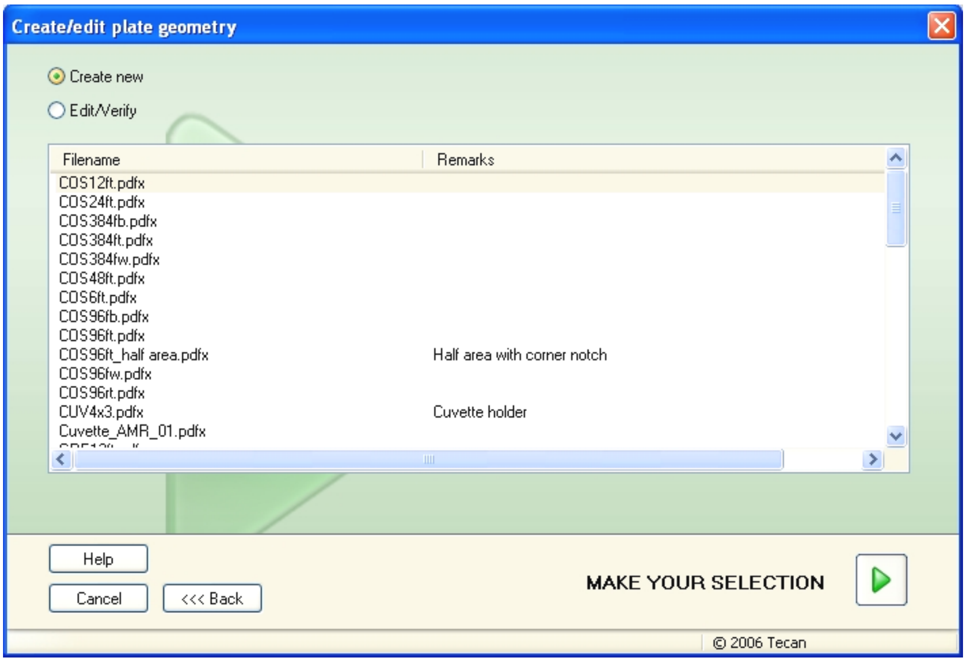
The **Plate geometry editor** is a software application accessible via magellan. The following commands and options are available.

Create/ edit plate geometry	A new plate definition file can be created or an existing plate definition file can be edited or verified.
Basic dimensions	Basic dimensions of the plate and the wells can be set (e.g. number of rows and columns, well shape, well diameter, well depth).
Scan plate / Enter well position	Select between 2, 4 or whole plate scan or enter the corresponding distance of top left well and bottom right well.
Measurement parameters	When **Scan plate** is selected, the measurement parameters can be inserted, clicking the corresponding button.
Save	The newly created or modified plate geometry can be saved entering a name (and remarks).

Note
We recommend not to use the functions* Gain from Well *and* Z from Well *with scanning. Use* Manual Gain *and* Manual Z *instead.

Create New Plate Definition File or Validate an Existing Plate Definition File

Select **Create new** in the **Create/edit plate geometry** dialog box and click on the green arrow **Make Your Selection** to open the editor.



● Create new
○ Edit/Verify

Filename	Remarks
COS12ft.pdfx	
COS24ft.pdfx	
COS384fb.pdfx	
COS384ft.pdfx	
COS384fw.pdfx	
COS48ft.pdfx	
COS6ft.pdfx	
COS96fb.pdfx	
COS96ft.pdfx	
COS96ft_half area.pdfx	Half area with corner notch
COS96fw.pdfx	
COS96rt.pdfx	
CUV4x3.pdfx	Cuvette holder
Cuvette_AMR_01.pdfx	

Plate Definition

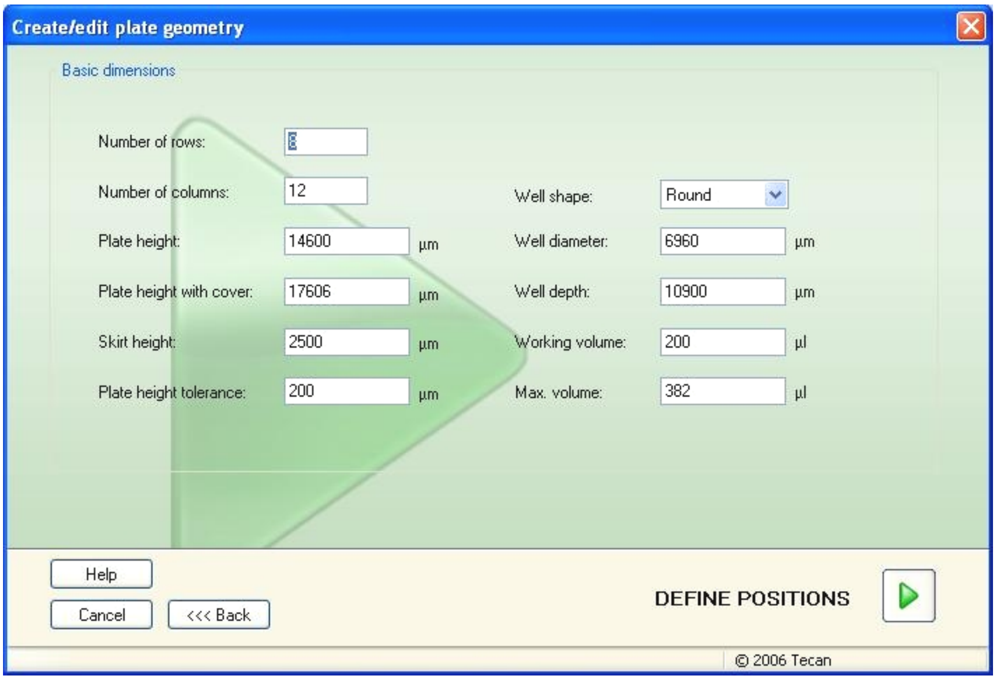
Insert the **Basic dimensions:**

Number of rows	Skirt height
Number of columns	Well shape
Plate height	Well diameter
Plate height with cover	Well depth

Note
Be careful with settings of µm and µl values!

Measure with a caliper ruler or better use values from the plate design drawings, given by the plate manufacturer. Be aware, that when you manually measure the plate height, any plate tolerances caused by the production process of the plate will not be covered!

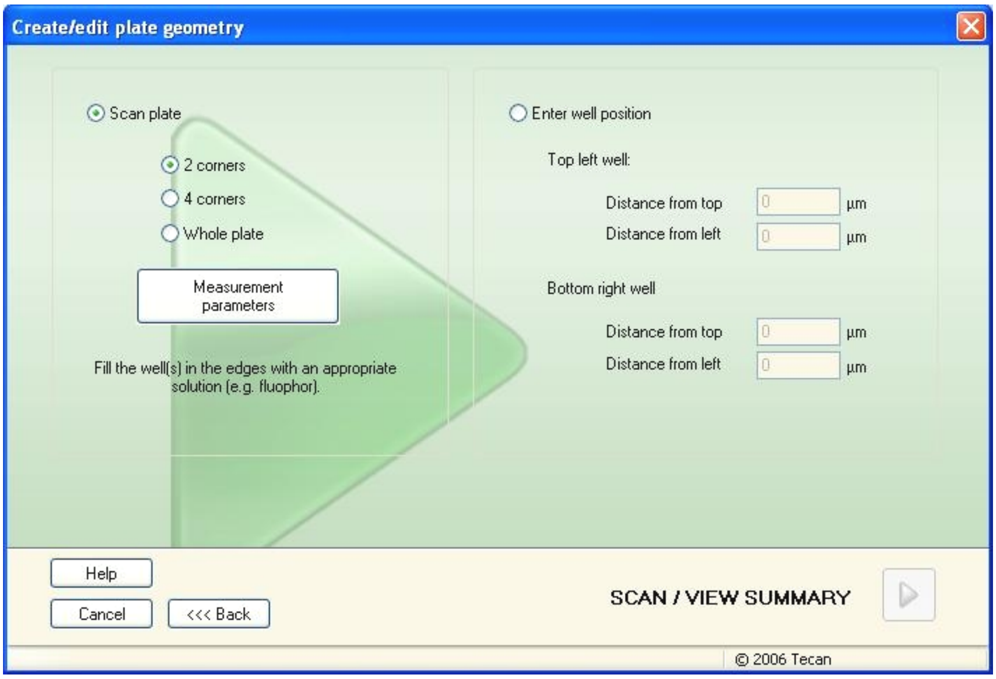
Select **Define Positions** by clicking on the green arrow button (example when connected to an Infinite F500 instrument).



Number of rows: 8
Number of columns: 12
Plate height: 14600 µm
Plate height with cover: 17606 µm
Skirt height: 2500 µm
Plate height tolerance: 200 µm
Well shape: Round
Well diameter: 6960 µm
Well depth: 10900 µm
Working volume: 200 µl
Max. volume: 382 µl

magellan allows scanning of plates on 2 or 4 corners, depending on the instrument connected. With an instrument of the Infinite Series connected, also a whole plate can be scanned.

Note
Usually a scan of 2 corners is sufficient. In case of a strip plate we recommend to use 4 corners. Select the number of corners and continue with the measurement parameters.

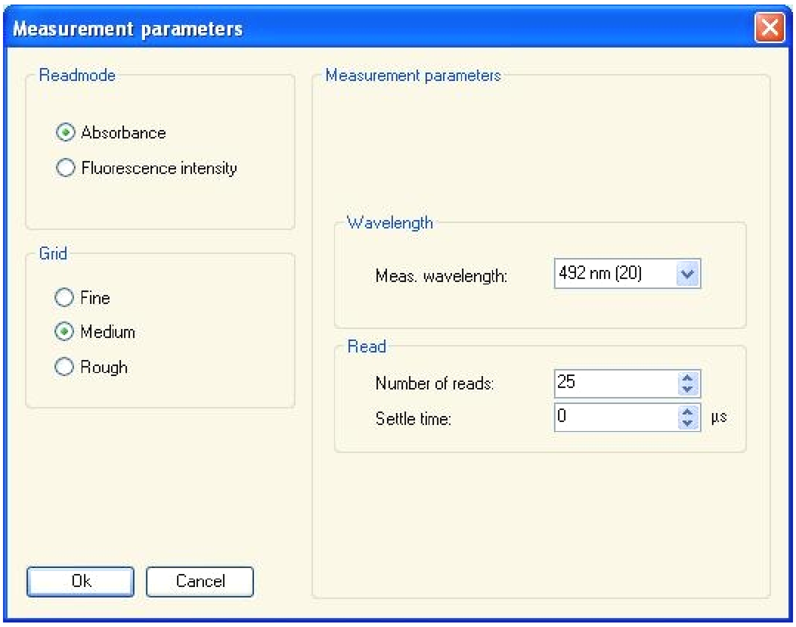


● Scan plate
● 2 corners
○ 4 corners
○ Whole plate

Fill the well(s) in the edges with an appropriate solution (e.g. fluophor).

○ Enter well position
Top left well:
Distance from top 0 µm
Distance from left 0 µm
Bottom right well
Distance from top 0 µm
Distance from left 0 µm

Click the button **Measurement parameters** to setup the measurement (example when connected to an Infinite F500).



Readmode
● Absorbance
○ Fluorescence intensity

Grid
○ Fine
● Medium
○ Rough

Measurement parameters

Wavelength
Meas. wavelength: 492 nm (20)

Read
Number of reads: 25
Settle time: 0 µs

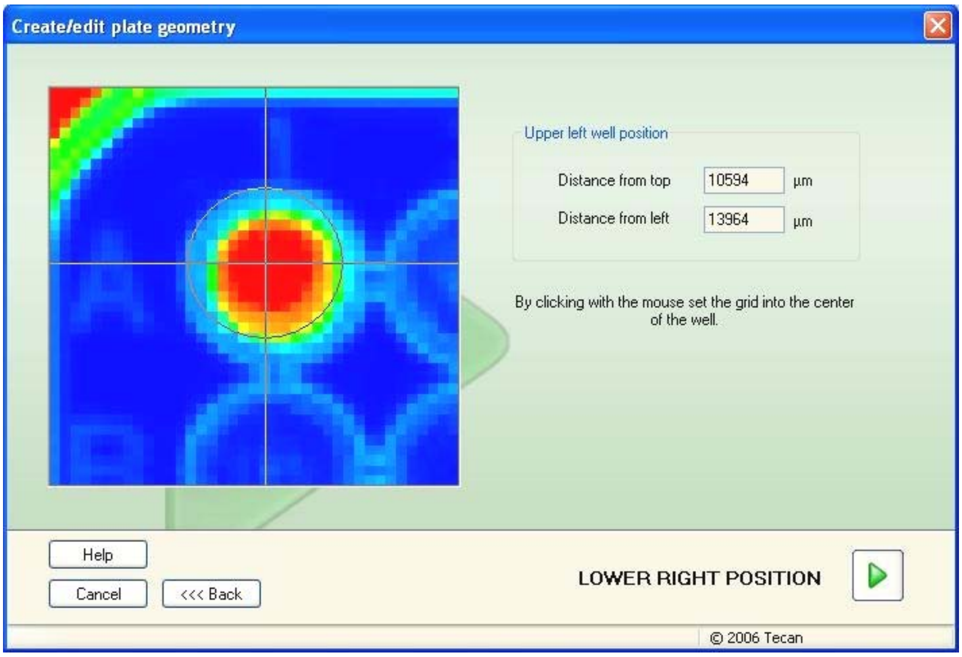
Scanning a Black Plate

If you scan a black plate you have to fill in an appropriate reagent into the upper left well (in this case A1) and the lower right well (here H12) (in case of 2 corners) and in case of 4 corners into the upper left well, upper right well (here A12); lower left well (here H1) and lower right well (here H12).

Click **OK** to close the measurement parameter dialog.

Put the microplate on the plate transport and start the scanning by clicking on the green arrow button **Scan / View Summary**.

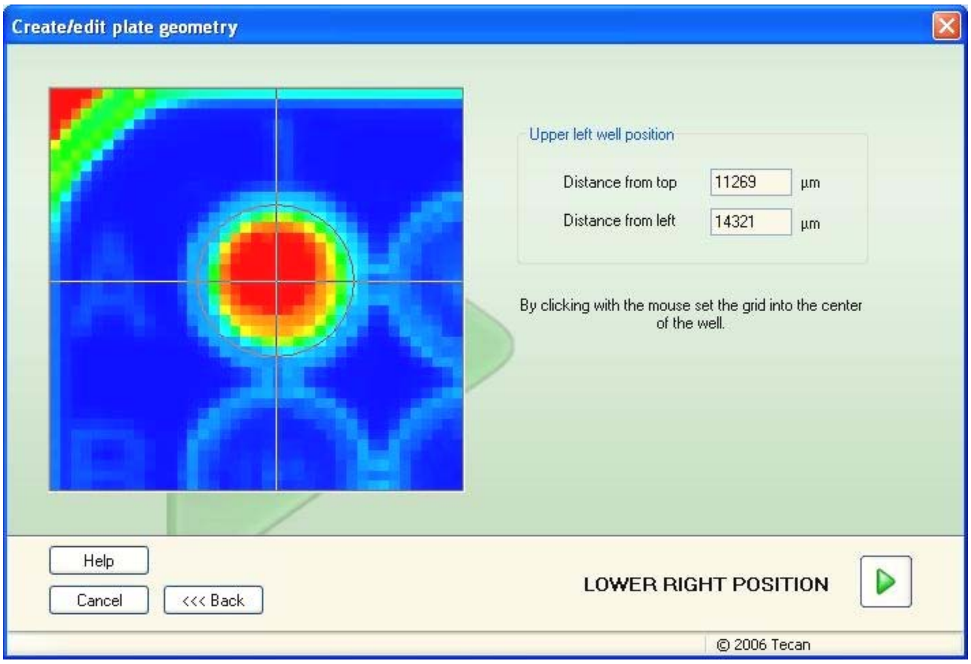
Next adjust the position of 2 of the 4 scanned wells starting with the upper left position (example when connected to an Infinite F500).



Upper left well position
Distance from top 10594 µm
Distance from left 13964 µm

By clicking with the mouse set the grid into the center of the well.

Click on the cursor and adjust the grid to the scanned image:



Create/edit plate geometry

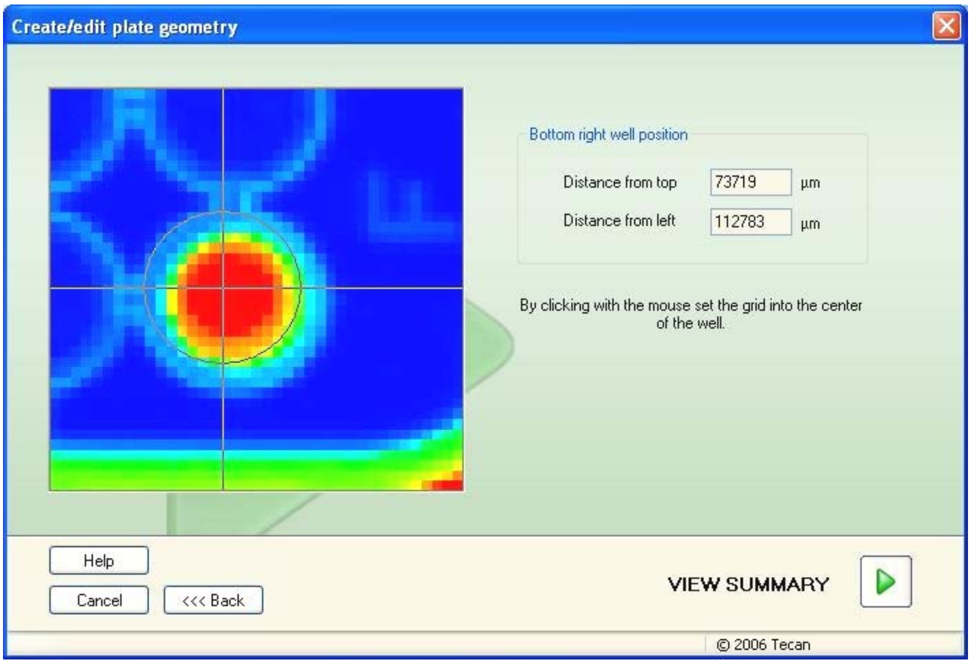
Upper left well position

Distance from top: 11269 µm

Distance from left: 14321 µm

By clicking with the mouse set the grid into the center of the well.

Continue with the remaining well (lower right position) by clicking on the green arrow button **Lower Right Position** and also adjust the grid.



Create/edit plate geometry

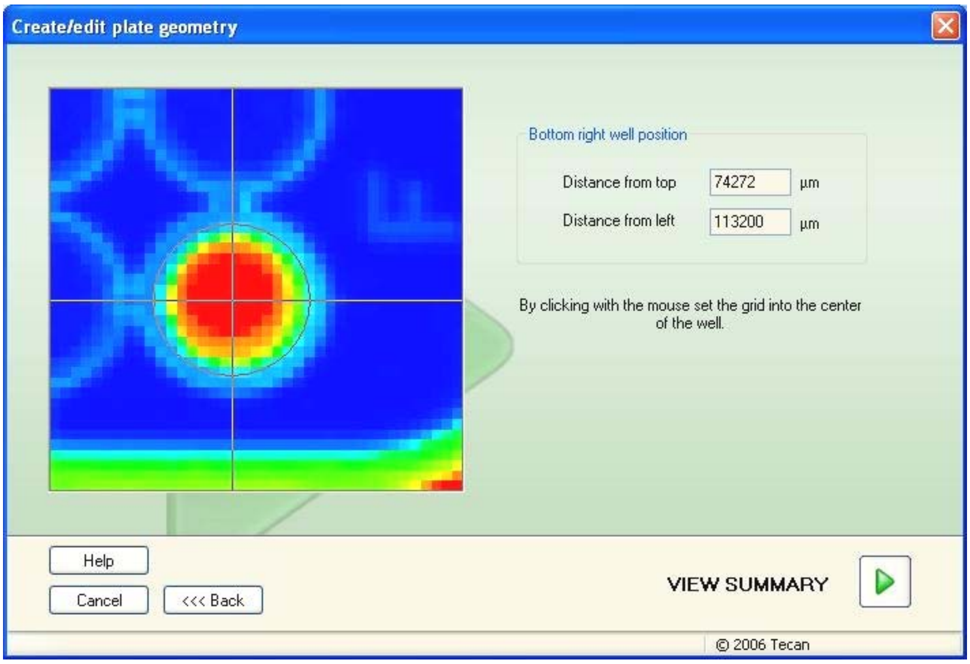
Bottom right well position

Distance from top: 73719 µm

Distance from left: 112783 µm

By clicking with the mouse set the grid into the center of the well.

Click on the cursor and adjust the grid to the scanned image:



Create/edit plate geometry

Bottom right well position

Distance from top: 74272 µm

Distance from left: 113200 µm

By clicking with the mouse set the grid into the center of the well.

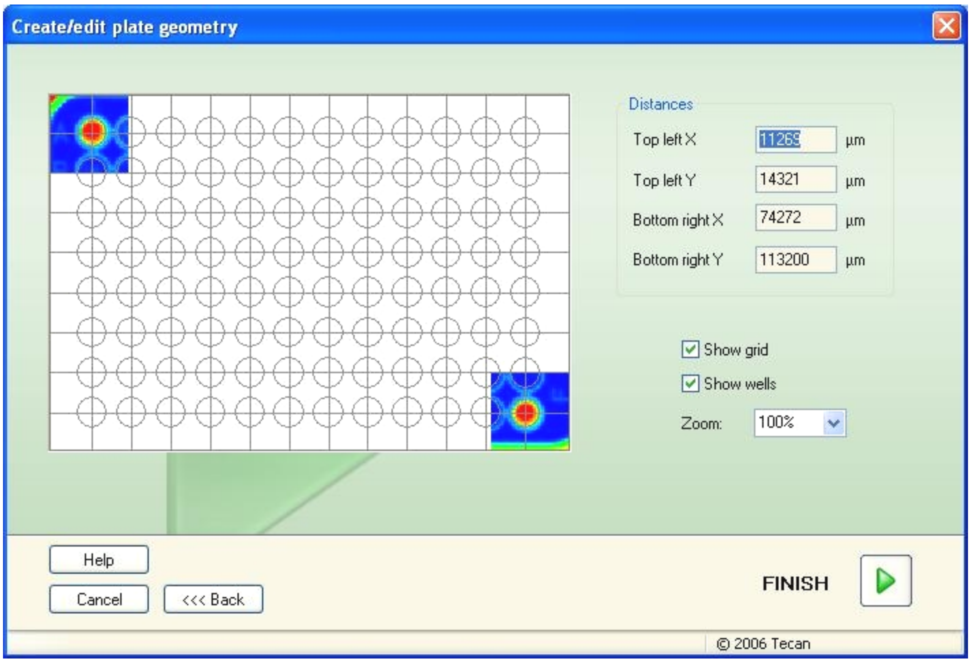
In case the picture does not show an acceptable result, go back to **Measurement Parameters** and enter different gain settings.

Note
When using a fluorescent reagent for performing this plate definition scan, it is recommended to measure this sample first in a comparable but known microplate using a typical filling volume to determine the gain and z-position for the measurement in the unknown plate.

Continue by clicking on the green arrow button **View Summary** to see the summary.

Finish and Save

In the summary dialog you can finally check the grid for the new microplate. A zoom function allows a more detailed view of the plate. In case you are not fully satisfied you can use the **Back** button to do further optimizations (example when connected to an Infinite F500).



Distances
Top left X 11269 µm
Top left Y 14321 µm
Bottom right X 74272 µm
Bottom right Y 113200 µm

☑ Show grid
☑ Show wells
Zoom: 100%

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):
  C:\Documents and Settings\AllUsers\Documents\Tecan\LogFiles
- Infinite Series Log files (communication between magellan and Infinite series instrument):
  C:\Documents and Settings\All Users\Documents\Tecan\LogFiles\Magellan\V x.y
- Rdr.OLE Log files (communication between magellan and Rdr.ole Instrument) by default:
  C:\Documents and Settings\CurrentUser\Local Settings\Temp
- 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 Expertline-at@tecan.com for support request. For further information please refer to chapter 10.2 File Handling – Save Log Files.

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 the Quantitative Elisa example in chapter
13.2 Step-by-Step Example: Quantitative ELISA.

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 appears.

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

Create new button	The **Create New** button must be selected 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: • 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 10.3.1 Default Data Paths).

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 the proper instrument for the selected file is not connected, the Instrument Mismatch dialog box appears. The dialog offers two options:

- ***Connect to the proper instrument***
- ***Convert the measurement parameters to those compatible with the connected instrument.***

This option** is not available **if the measurement mode is not supported by the connected instrument, for example, a Sunrise does not support Fluorescence measurements.

It is highly recommended to review the measurement parameters.

Note

After the** magellan **30-day demo license has expired, printing and saving will not be possible.

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.

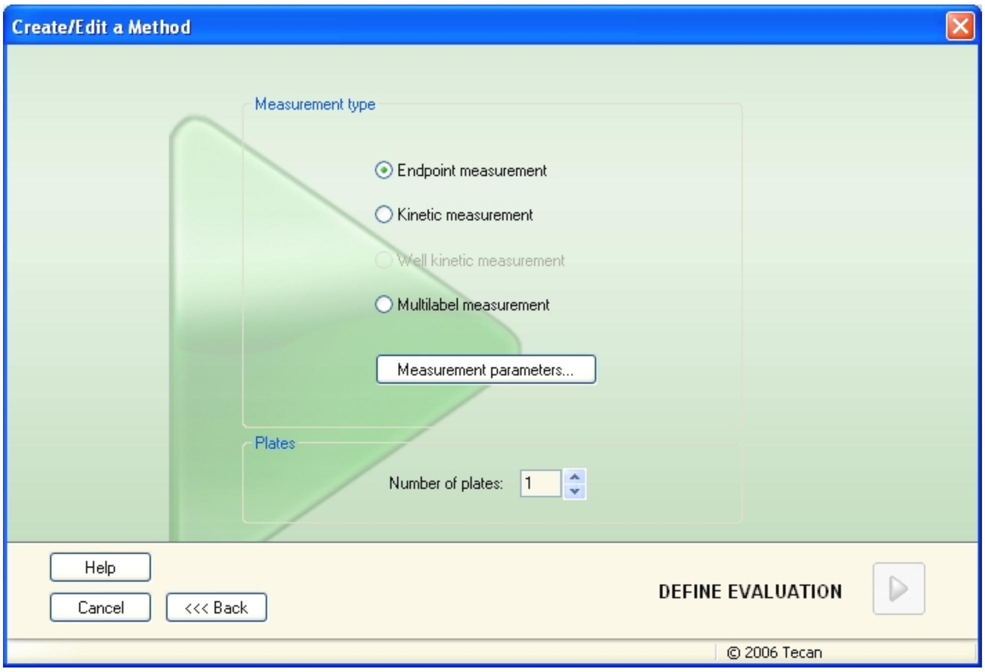
When connected to an Infinite instrument, refer to the Instructions for Use for i-control for further details on defining measurement parameters.

Note

The available parameters to be defined depend on the instrument connected.

4.2.1 Measurement Types

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 **Well kinetic (injector) measurement** to perform kinetic measurements per well with a specified interval time and injector control. • Select **Multilabel measurement** to perform multilabel measurements with different measurement parameters.
Plates group box	• Select a number of plates in the edit box for Multiplate measurements (only available with Safire II instrument).

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

4.2.2 Measurement Parameters

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

- General measurement parameters,
- Plate format,
- Stacker,
- Wavelength,
- Measurement parameters (gain, integration time, number of reads, Z-position),
- 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.

Refer to the Instructions for Use for the **Reader Server**, document number 30008897, for further information.

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

Multilabel Measurement

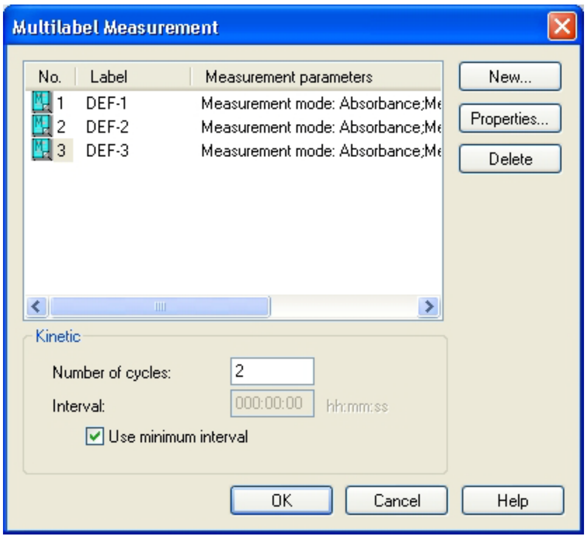
If the measurement type multilabel measurement was selected, the **Multilabel Measurement** dialog box is displayed.
To create a list of parameter windows the **New** button must be clicked. The **Measurement Parameters** dialog box will appear where a new set of measurement parameters can be defined. 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;Me
2	DEF-2	Measurement mode: Absorbance;Me
3	DEF-3	Measurement mode: Absorbance;Me

Kinetic

Number of cycles: 2

Interval: 000:00:00 hh:mm:ss

☑ Use minimum interval

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).

Note

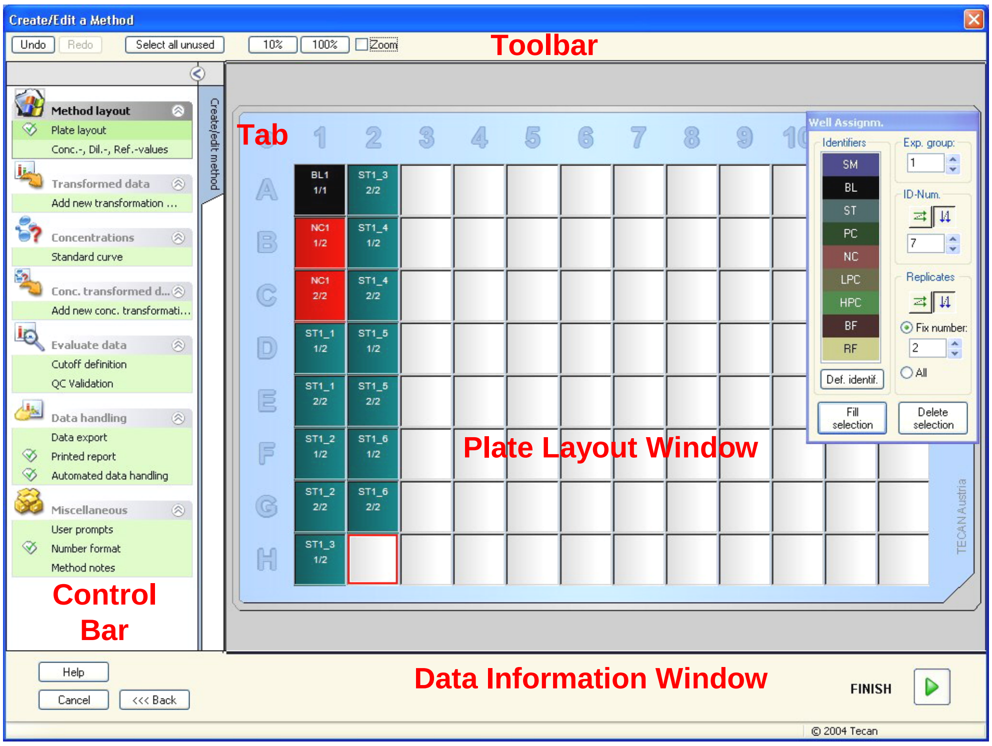
Defining multilabel measurements with Safire2:

It is not allowed to define absorbance dual wavelength labels. On closing the measurement parameter dialog any defined reference wavelength will be set to 0. A message box will inform the user about this change.

4.3 Define Evaluation

4.3.1 The Create/Edit Method Overview Window

In the **Define Evaluation** window the user defines the plate layout, he inserts 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.

In the central area of the window the **Plate Layout** window displays a schematically layout of a microplate. Rows are marked alphabetically, columns numerically.

If a new method has been generated, all wells are empty. A mouse click selects an individual well.

Wells that will not be measured, as given by the part of the plate settings, are displayed in grey color.

When defining the layout, transformations etc., the identifiers, formulas etc. are displayed in the corresponding wells.

Toolbar Buttons

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.
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	In case the well plate consists of a large number of wells, the individual well assignments cannot be displayed in the 100% zoom mode. 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

The **Plate Layout** window shows the defined parameters and/or procedures depending on the selection in the control bar (see chapter below Control Bar of Create/Edit Method Tab).

Parameters and procedures are:

- **Method Layout**: plate layout; concentration-, dilution- and reference values
- **Precalculation**: polarization, FLT, spectra and cuvette data reduction
- **Transformed Data**: add new transformation…
- **Kinetic**: kinetic data reduction
- **Kinetics Transformation**: add new kinetic transformation…
- **Concentrations**: standard curve
- **Conc. Transformation**: add new concentration transformation…
- **Evaluate data**: cutoff definition, QC validation
- **Data Handling**: data export, printed report, automated data handling
- **Miscellaneous**: user prompts. number format, method notes.

Each of these inputs is invoked with a separate option, preferably in this sequence.

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.

Menu	Description
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:

Method layout group	• **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	• **Polarization data reduction** for fluorescence polarization measurements • **Spectra data reduction** for wavelength scans • **Cuvette data reduction** for combined plate and cuvette measurements
Transformed data group	• **Add new transformation …** item The *Plate layout* window is opened, displaying the plate layout and the *Transformations* dialog input field.
Kinetic group	• **Kinetic data reduction** item The *Kinetics Calculation Parameters* window is opened. The evaluation of the kinetics measurement data can be defined.

Kinetics transformation	• **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	• **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	• **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	• **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	• **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.

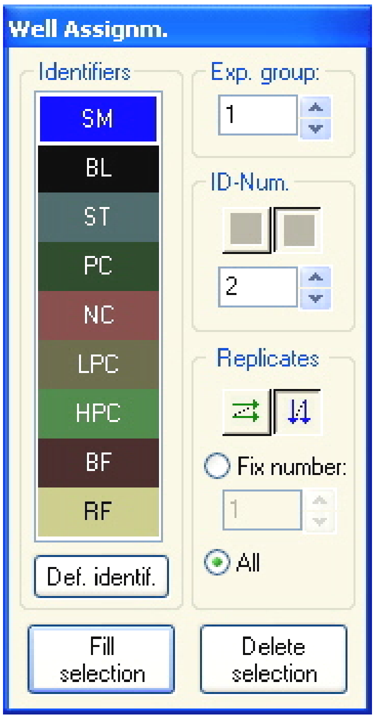
Control Bar – Create/Edit Method Tab: Context-Sensitive Menu

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).

Assign an Identifier to the Required Well

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

The desired settings have to be made in the **Well Assignment** dialog box. There are several ways to select the wells:

- Clicking the individual well.
- Dragging the mouse over the required wells.
- Click one of the letters (A – H) or numbers (1 – 12) to select a row or column.
- Click the **O** symbol in the upper left corner of the microplate to select the whole plate.
- Add wells in a certain area: After selecting a single well, hold the Shift-key and click and drag the previously selected well to the currently selected well.
- Toggle selection state of a well: When holding the Ctrl-key, the selection state of the selected well is toggled. For example: a click on an already selected well removes the well from the current selection.

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	1st line: sample, experimental group number of 1, sample ID number of 4.
1/14	2nd line: number of replicate is 1, total number of replicates is 14.
x-BL1	3rd line: primary empty – filled with the transformation formula after Transformations are defined and selected: reduce the value of this well (x) by the mean of the blanks (refer to chapter 12.4 How to Write a Formula).
1.000	or 3rd line: Concentration, dilution or reference value if Conc.-Dil.-Ref.-values is selected in the control bar: dilution factor value of 1.0.

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

Identifiers group box	In this group box, corresponding identifiers for the marked wells have to be selected. • 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	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.
ID-Num. group box	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. • **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	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: • **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. Two **Arrow buttons** define the direction of counting up the replicate number.
Fill section button	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.
Delete section button	Click **Delete** or press **DEL** to delete the IDs and color identifiers of the selected wells and leave them blank.
Define identifier button	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)

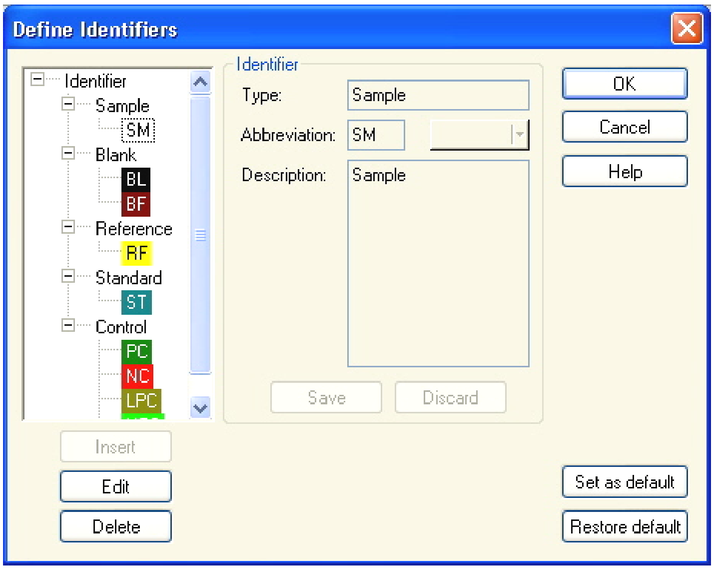
Assign Alias to the Required Well

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.

EXPERT'S KNOW HOW

DEFINE A NEW IDENTIFIER

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



Type: Sample
Abbreviation: SM
Description: Sample

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)

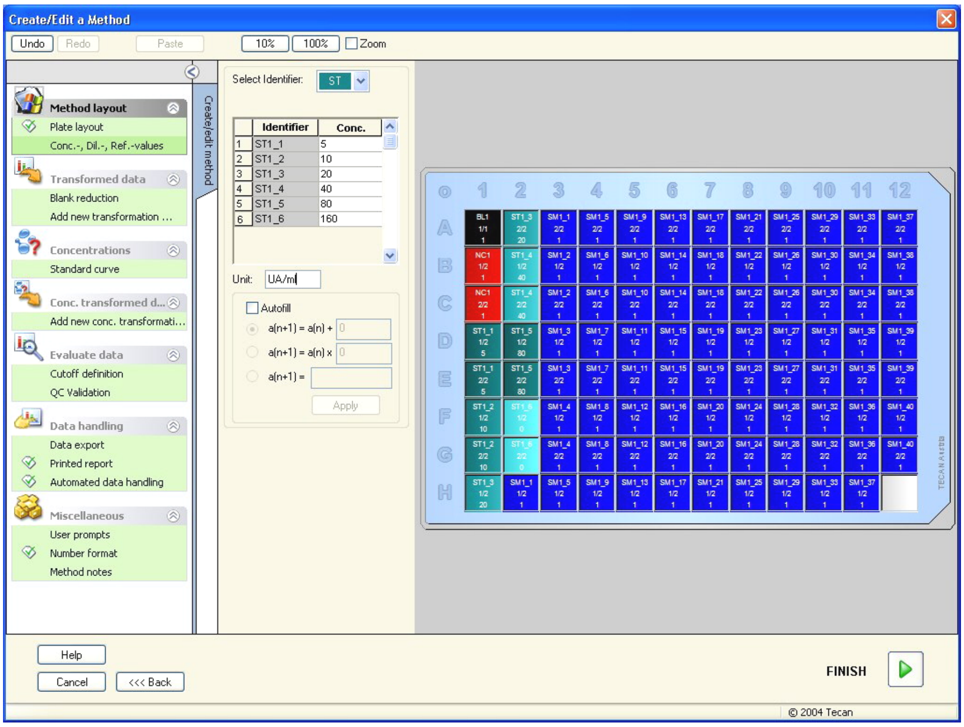
The **Define Identifiers** dialog box contains the following elements:

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	The criteria held by the various identifiers used in the program will be displayed. If new identifiers are required, they can be inserted here. In the **Identifier** group box the type, abbreviation, well color and description of the identifier selected in the tree structure is displayed.

	The **Identifier** group box is only activated for entering data, when • 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. Then, in this group box, the type, abbreviation, well color and description of the new identifier need to be defined.
	Type text field: The type of identifier is displayed. No changes are possible.
	Abbreviation text field: The identifier's abbreviation will be used in the analysis plate display.
	Color drop down list: The color of the identifier on the plate layout has to be selected here.
	Description text field: A text description can be entered for each identifier.
	Use one of these two buttons to save changes of newly entered data or to discard any changes:
	Save button: The **Save** button saves the entered color, abbreviation and description of the relevant identifier.
	Discard button**:** The **Discard** button will cancel any changes.
Insert button	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.
Edit button	A selected identifier can be modified.
Delete button	Click **Delete** or press **DEL** to delete any selected identifier.
Set as default button	Using this option, the settings can be defined as default for future use.
Restore default button	Using this option, the settings can be reset to the previously defined default.

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.



Select Identifier: ST

	Identifier	Conc.
1	ST1_1	5
2	ST1_2	10
3	ST1_3	20
4	ST1_4	40
5	ST1_5	80
6	ST1_6	160

Unit: UA/ml

☐ Autofill

● a(n+1) = a(n) + 0

○ a(n+1) = a(n) x 0

○ a(n+1) =

Apply

o	1	2	3	4	5	6	7	8	9	10	11	12
A	BL1 1/1 1	ST1_3 2/2 20	SM1_1 2/2 1	SM1_5 2/2 1	SM1_9 2/2 1	SM1_13 2/2 1	SM1_17 2/2 1	SM1_21 2/2 1	SM1_25 2/2 1	SM1_29 2/2 1	SM1_33 2/2 1	SM1_37 2/2 1
B	NC1 1/2 1	ST1_4 1/2 40	SM1_2 1/2 1	SM1_6 1/2 1	SM1_10 1/2 1	SM1_14 1/2 1	SM1_18 1/2 1	SM1_22 1/2 1	SM1_26 1/2 1	SM1_30 1/2 1	SM1_34 1/2 1	SM1_38 1/2 1
C	NC1 2/2 1	ST1_4 2/2 40	SM1_2 2/2 1	SM1_6 2/2 1	SM1_10 2/2 1	SM1_14 2/2 1	SM1_18 2/2 1	SM1_22 2/2 1	SM1_26 2/2 1	SM1_30 2/2 1	SM1_34 2/2 1	SM1_38 2/2 1
D	ST1_1 1/2 5	ST1_5 1/2 80	SM1_3 1/2 1	SM1_7 1/2 1	SM1_11 1/2 1	SM1_15 1/2 1	SM1_19 1/2 1	SM1_23 1/2 1	SM1_27 1/2 1	SM1_31 1/2 1	SM1_35 1/2 1	SM1_39 1/2 1
E	ST1_1 2/2 5	ST1_5 2/2 80	SM1_3 2/2 1	SM1_7 2/2 1	SM1_11 2/2 1	SM1_15 2/2 1	SM1_19 2/2 1	SM1_23 2/2 1	SM1_27 2/2 1	SM1_31 2/2 1	SM1_35 2/2 1	SM1_39 2/2 1
F	ST1_2 1/2 10	ST1_6 1/2 0	SM1_4 1/2 1	SM1_8 1/2 1	SM1_12 1/2 1	SM1_16 1/2 1	SM1_20 1/2 1	SM1_24 1/2 1	SM1_28 1/2 1	SM1_32 1/2 1	SM1_36 1/2 1	SM1_40 1/2 1
G	ST1_2 2/2 10	ST1_6 2/2 0	SM1_4 2/2 1	SM1_8 2/2 1	SM1_12 2/2 1	SM1_16 2/2 1	SM1_20 2/2 1	SM1_24 2/2 1	SM1_28 2/2 1	SM1_32 2/2 1	SM1_36 2/2 1	SM1_40 2/2 1
H	ST1_3 1/2 20	SM1_1 1/2 1	SM1_5 1/2 1	SM1_9 1/2 1	SM1_13 1/2 1	SM1_17 1/2 1	SM1_21 1/2 1	SM1_25 1/2 1	SM1_29 1/2 1	SM1_33 1/2 1	SM1_37 1/2 1	

The concentrations for the standards, the reference values for the Reference (used with Fluorescence Polarization measurements) and the dilution factors for all other identifiers can be entered or edited in the table next to the **Plate View** window. The values can be defined for each well individually. By default the dilution factors are set to 1, the concentrations are set to 0 and the reference value is set to 22. Entering a dilution factor of 2 means that the sample has been diluted by half. The calculated concentration will therefore be multiplied by 2.

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

Select Identifier drop down list	The values are co-related within the individual well types; this field provides all wells currently included in the measurement. Select an identifier to edit the corresponding dilution or concentration factors. All wells, which match the selected well type identifier, are listed.
Exp. group selection field	Select the respective experimental group. If there is only one experimental group, the field cannot be edited.
Table with **Identifier** and **Concentration/ Dilution** columns	This table displays all wells in the **Identifier** column, which match the selected identifier (as from the **Select Identifier** list). The corresponding dilutions, concentrations or reference values are listed in the **Dilution/Concentration/Reference** column, where they can be edited individually.
Unit text field	The displayed concentration unit can be determined.

Autofill check box	The **Autofill** function provides the calculation of the corresponding concentrations or dilution factors according to available types of series. This is useful when the dilution series is quite large and the concentrations are in a clear mathematical relationship to each other.
Option buttons for the mathematical concentration calculation	If the **Autofill** check box has been selected, the following options are available: • Arithmetic series: a (n+1) = a (n) + ... • Geometric series: a (n+1) = a (n) x ..... • User defined series a(n+1) = ... Example 1: Each subsequent concentration should contain twice + 0.5 of the previous concentration: Formula 1: a(n+1) = 2 * n + 0.5 Example 2: Each subsequent concentration should contain one third of the previous concentration: Formula 2: a(n+1) = n/3
Apply button	The **Apply** button applies the selected mathematical concentration calculation to the wells as displayed in the table with **Identifier** and **Concentration/ Dilution** columns.
Dilution series group box	**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 (see chapter Expert's Know How below for further details).
	Input Data drop down list Select from the drop down list the input data.
	Calculation Condition text field The intercept will be calculated with the entered percentage of the maximum value respectively maximum value minus minimum value (see chapter **Expert's Know How** below for further details).
	ICx name text field Data can be selected for ICx calculation. The name is filled in automatically based on the calculation condition.
	Set 0% value to Intensity 0: (see chapter **Expert's Know How** below for further details). Min. intensity of dilution series: (see chapter **Expert's Know How** below for further details).

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.

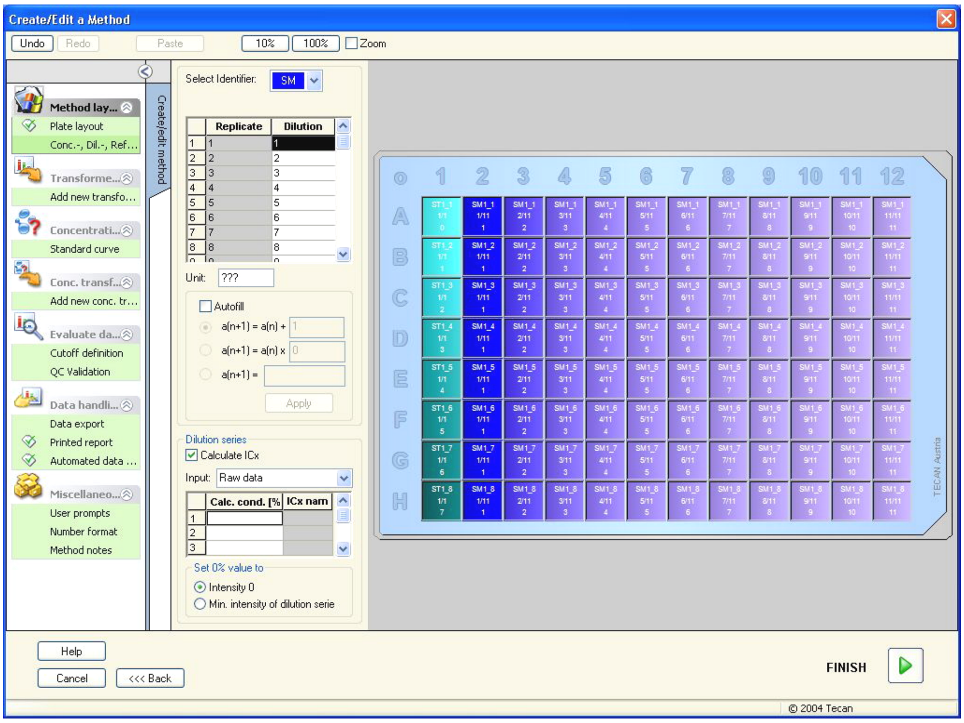
EXPERT'S KNOW HOW

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.



Select Identifier: SM

	Replicate	Dilution
1	1	1
2	2	2
3	3	3
4	4	4
5	5	5
6	6	6
7	7	7
8	8	8

Unit: ???

☐ Autofill

○ a(n+1) = a(n) + 1

○ a(n+1) = a(n) x 0

○ a(n+1) =

Dilution series

☑ Calculate ICx

Input: Raw data

	Calc. cond. [%	ICx nam
1		
2		
3		

Set 0% value to

● Intensity 0

○ Min. intensity of dilution serie

o	1	2	3	4	5	6	7	8	9	10	11	12
A	ST1_1 1/1 0	SM1_1 1/11 1	SM1_1 2/11 2	SM1_1 3/11 3	SM1_1 4/11 4	SM1_1 5/11 5	SM1_1 6/11 6	SM1_1 7/11 7	SM1_1 8/11 8	SM1_1 9/11 9	SM1_1 10/11 10	SM1_1 11/11 11
B	ST1_2 1/1 1	SM1_2 1/11 1	SM1_2 2/11 2	SM1_2 3/11 3	SM1_2 4/11 4	SM1_2 5/11 5	SM1_2 6/11 6	SM1_2 7/11 7	SM1_2 8/11 8	SM1_2 9/11 9	SM1_2 10/11 10	SM1_2 11/11 11
C	ST1_3 1/1 2	SM1_3 1/11 1	SM1_3 2/11 2	SM1_3 3/11 3	SM1_3 4/11 4	SM1_3 5/11 5	SM1_3 6/11 6	SM1_3 7/11 7	SM1_3 8/11 8	SM1_3 9/11 9	SM1_3 10/11 10	SM1_3 11/11 11
D	ST1_4 1/1 3	SM1_4 1/11 1	SM1_4 2/11 2	SM1_4 3/11 3	SM1_4 4/11 4	SM1_4 5/11 5	SM1_4 6/11 6	SM1_4 7/11 7	SM1_4 8/11 8	SM1_4 9/11 9	SM1_4 10/11 10	SM1_4 11/11 11
E	ST1_5 1/1 4	SM1_5 1/11 1	SM1_5 2/11 2	SM1_5 3/11 3	SM1_5 4/11 4	SM1_5 5/11 5	SM1_5 6/11 6	SM1_5 7/11 7	SM1_5 8/11 8	SM1_5 9/11 9	SM1_5 10/11 10	SM1_5 11/11 11
F	ST1_6 1/1 5	SM1_6 1/11 1	SM1_6 2/11 2	SM1_6 3/11 3	SM1_6 4/11 4	SM1_6 5/11 5	SM1_6 6/11 6	SM1_6 7/11 7	SM1_6 8/11 8	SM1_6 9/11 9	SM1_6 10/11 10	SM1_6 11/11 11
G	ST1_7 1/1 6	SM1_7 1/11 1	SM1_7 2/11 2	SM1_7 3/11 3	SM1_7 4/11 4	SM1_7 5/11 5	SM1_7 6/11 6	SM1_7 7/11 7	SM1_7 8/11 8	SM1_7 9/11 9	SM1_7 10/11 10	SM1_7 11/11 11
H	ST1_8 1/1 7	SM1_8 1/11 1	SM1_8 2/11 2	SM1_8 3/11 3	SM1_8 4/11 4	SM1_8 5/11 5	SM1_8 6/11 6	SM1_8 7/11 7	SM1_8 8/11 8	SM1_8 9/11 9	SM1_8 10/11 10	SM1_8 11/11 11

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/RFU

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

  or

- **Minimum intensity of the dilution series**

  Using the minimal intensity of the dilution series

Note

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

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

4.3.4 Precalculation: Polarization Data Reduction

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

This option is only available for Fluorescence Polarization (FP) measurements. FP measurements consist of two fluorescence intensity measurements, one with polarizers in parallel and one with polarizers in perpendicular position. The G-factor compensates for differences in optical components between parallel and perpendicular measurement. The G-factor can be established by a calibration measurement using a reference solution with known polarization value and a corresponding reference blank solution.

The appropriate entries for fluorescence polarization measurements must be made under the **G-factor** and **Sample blank reduction** group boxes of the **Polarization Settings** dialog box. Under **Reference** the appropriate reference value has to be typed in mP units. It is recommended to use a reference blank for the G-factor calibration. The reference blank check box has to be activated and the appropriate identifier (which has been defined in the plate layout) has to be selected from the list box.

In the **Sample blank reduction** group box it has to be determined if the blank reduction is applied to the samples measurement values or not. If the blank reduction is selected, a blank reduction is performed before the calculation of the polarization values.

The option **Automatically precalculate polarization data** can be disabled for further custom evaluation of parallel and perpendicular raw data.

The **Polarization Settings** dialog box contains the following elements:

Automatically precalculate polarization data check box	Select this option in order to use automatic precalculation of polarization data. This option cannot be enabled for multilabel measurements.
G-factor group box	A G-factor must be established when measuring with polarization. • **Use** option button and text field: If the G-factor is known, it can be directly entered in the text field attached to the option button.
	• **Confirm at runtime** check box: If this box is selected, the user is prompted to confirm or modify the G-factor.
	• **Request from instrument** check box: If this box is selected, the G-factor is read directly from the reader and cannot be entered manually.
	• **Calibrate** option button: The G-factor is determined by calibration measurement. Select under **Reference** the appropriate reference identifier and enter the polarization value.
	• **Reference blank** check box and drop down list: If blanks are to be used in the calculation, the **Reference blank** check box has to be selected and the correct identifier has to be chosen from the list.
Blank reduction group box	• **Exp. group** list: If the method contains a number of individual experimental groups, the desired group can be selected using this option.

- **No blank reduction** option button:
  This option button has to be selected if blank reduction is not to be applied at the measurement.
- **Reduce** option button:
  Before calculating the polarization values a blank reduction is used.
- **All by** check box and **Identifier** drop down list:
  If **all by** is checked, all measurement values will be reduced by the value of the well as defined by its identifier in the drop down list.
- **Except .... by** check box:
  The **except by** check box defines, whose value (identifier) is to be deducted from the first selected identifier (drop down list).
  This setting is used for individual Sample blanking. Create a new identifier (e.g.: SMB: Sample Blank) under the identifier group samples in the **Identifiers Definition** dialog box to use this function.

Note
It is recommended to use always a reference on the plate to calculate the G-factor.

For more information on calculation refer to chapter 12 Calculations.

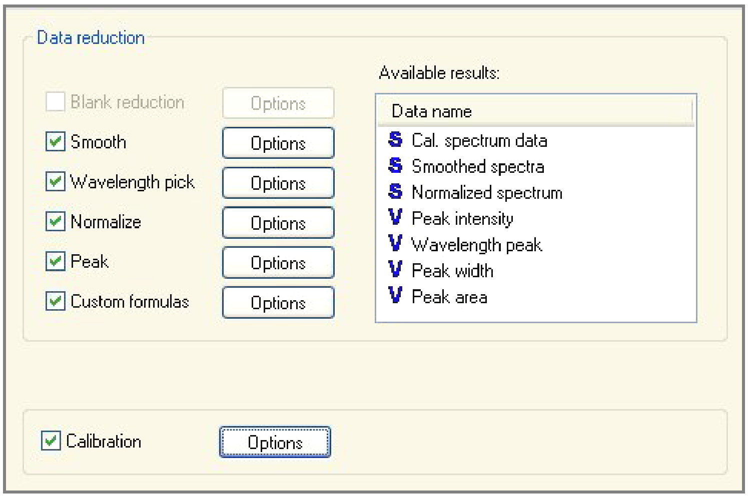
4.3.5 Precalculation: Spectra Data Reduction

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

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

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:



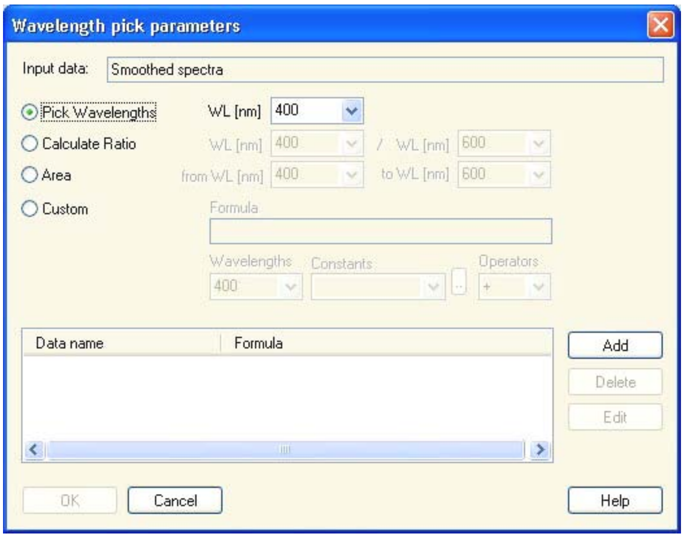
Data reduction

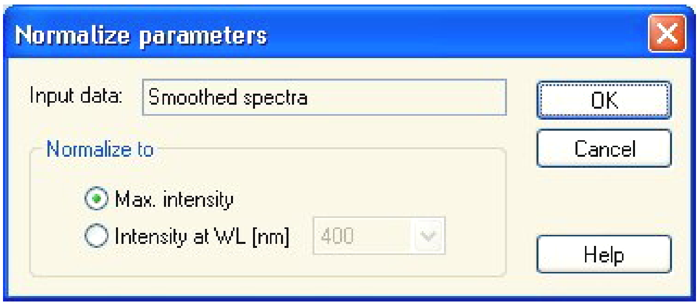
☐ Blank reduction
☑ Smooth
☑ Wavelength pick
☑ Normalize
☑ Peak
☑ Custom formulas

Available results:

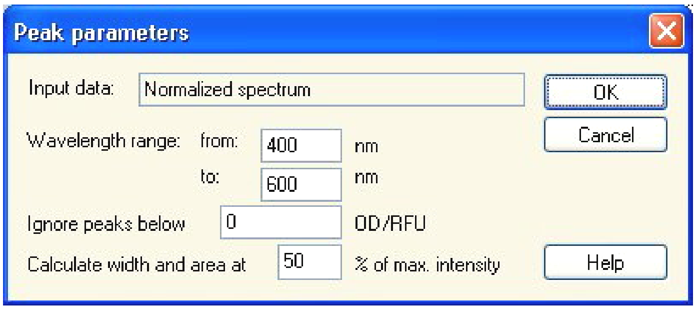
Data name
S Cal. spectrum data
S Smoothed spectra
S Normalized spectrum
V Peak intensity
V Wavelength peak
V Peak width
V Peak area

☑ Calibration

Blank reduction check box	This option is only available if blanks are defined on the layout. The blank reduced spectra is calculated by subtracting the spectrum of the blank well from all other wells. When more blanks are defined on the plate, e.g. when multiple experimental groups are defined, an additional options button appears. This allows to define the blank to be used.
	Input data text box: shows the input data to be processed.
	Blank reduction option button: select, if a blank reduction should be performed on the selected experimental group.
	Reduce all by dropdown list: select to define the identifier to be used for blank reduction.
Smooth check box	A spectrum containing a lot of noise can be smoothed. A smooth factor can be set in the options part. This factor defines the degree of smoothing.
	Input data text box: shows the input data to be processed.
	Smooth factor: to define the smooth factor.
Wavelength pick check box	**Wavelength pick** is used to extract intensities at specific wavelengths and calculate results like ratios. It is mandatory to set the options. The **Wavelength pick** parameters dialog box contains the following elements:  Wavelength pick parameters Input data: Smoothed spectra ● Pick Wavelengths WL [nm] 400 ○ Calculate Ratio WL [nm] 400 / WL [nm] 600 ○ Area from WL [nm] 400 to WL [nm] 600 ○ Custom Formula Wavelengths 400 Constants Operators + Data name Formula Add Delete Edit OK Cancel Help 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:



Input data: Normalized spectrum

Wavelength range: from: 400 nm

to: 600 nm

Ignore peaks below 0 OD/RFU

Calculate width and area at 50 % of max. intensity

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

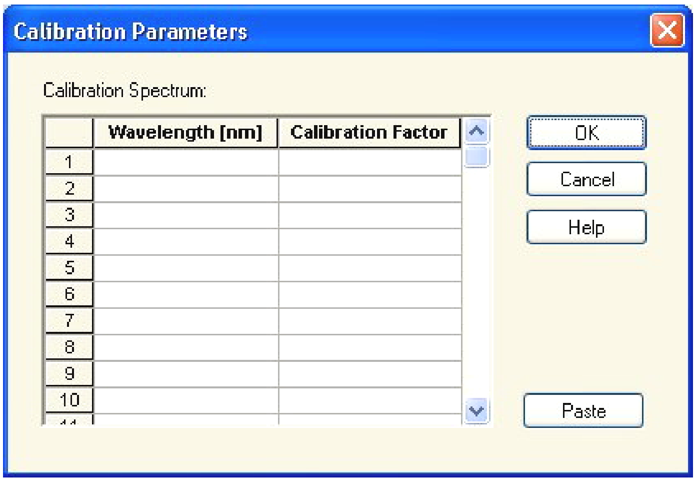
Custom formulas check box

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

Refer to chapter 12.3 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.

Calibration check box

Use this check box to calibrate the curve at a certain wavelength using a calibration factor.



Calibration Spectrum:

	Wavelength [nm]	Calibration Factor
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		

See Note below when connected to a Safire instrument.

Available results

Available results of all data are listed.

S is a spectrum

V is a value.

Note
For the* Safire *instrument the calibration factor for each wavelength has to be defined.

For the* Safire^2 *instrument only the check box for calibration has to be selected. The calibration spectrum is stored in the instrument and the calibration is done automatically.

This check box is not available for the* Infinite M200 *because calibration is always performed automatically.

4.3.6 Precalculation: Cuvette Data Reduction

If you are using an **Infinite M200** with **Cuvette option** you can define methods with a combination of plate and cuvette measurements. For the cuvette Absorbance ratio, Absorbance scans and Absorbance kinetic measurements can be defined. Using the Precalculation - cuvette data reduction dialog it is possible to define formulas to get single values from a scan or a kinetic measurement.

Examples:

For scan:

Formula x[698]/x[600] gives you as result the ratio between the value at 698 nm and the value at 600 nm.

For kinetic:

Formula x[5]-x[0] means that the value of the 6th kinetic cycle is reduced by the value of the 1st kinetic cycle.

4.3.7 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 click **Add new transformation…** . The new transformation with a default name will be inserted.

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.

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
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.

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 12.4 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: • 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.

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
('Lable1'!x-'Label1'!BL1)/('Label2'!x-'Label2'!BL1) ... predefined ratio caculation with blank reduction
('Lable2'!x-'Label2'!BL1)/('Label1'!x-'Label1'!BL1) ... predefined ratio caculation 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.

The transformation definition has two modes:

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.

EXPERT'S KNOW HOW

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: • **Name** In the **Name** text field an appropriate identifier name for the constant, for example: a code or an abbreviation, must be entered. Only letters can be used. • **Value** In the **Value** text field a numerical value must be allocated to the constant. • **Comment** Enter a short comment to the constant. • **Req.** ("required") The **Req.** check box indicates, that a measurement can only be launched on receipt or confirmation of the value for the constant.

4.3.8 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).

Use the **Slopes** tab to establish the evaluation of the kinetic curve's slope behavior.

The **Onsets** tab defines calculation of the time by which a certain OD/RFU value is reached.

Use the **Min./Max./Area** 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.

Use the **Enzyme kinetics** tab to define the evaluation of enzyme kinetics.

Use the **Available output data** tab to display the data, calculated using the kinetics evaluation.

> ***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.

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

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 12 Calculations).
Mean slope check box	The start and end time can be typed into the provided text fields, otherwise the whole kinetic is analyzed.
	• **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	The start and end time can be typed into the provided text fields, otherwise the whole kinetic is analyzed.
	• **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 and an end time must first be entered. All measurement points that fall within the interval of the slope will be determined and then, from these details, 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 point (OD/RFU/Polarization value).

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

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.
	• Text field: An **absolute** value for the onset must be entered.
	• **Basis mean of the first n points** option button and text field: If the option button is selected, the points text field is active and the desired number of points can be entered here.
	• **Basis** option button and text field: If the **Basis** option button is 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.
	• Text field: A **percentage** value for the onset must be entered.
	• **Basis mean of the first n points** option button and text field: If the option button is clicked, the points text field is active and the desired number of points can be entered here.
	• **Basis** option button and text field: If the **Basis** option button is 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.

The **Min./Max./Area** tab contains the following elements:

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.
	• **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.

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:

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

Available Data Tab

A list of the results is displayed in the **Available output data** tab. This gives an overview of the results of the selected calculations.

The **Available output data** tab contains the following elements:

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.

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

The **Enzyme kinetics** tab contains the following elements:

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 from: • Hanes • Eadie-Hofstee • Lineweaver-Burk The calculation type can be selected as Hanes (concentration versus concentration/input data), Eadie-Hofstee (input data/concentration versus input data) and 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.

4.3.9 Kinetics Transformations: Add New Kinetics Transformations

Select **Add new kin. transform…** from the control bar.

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 4.3.7 Transformed Data: Add New Transformation for further information.

4.3.10 Concentrations: Standard Curve

In the control bar expand **Concentrations** and click **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. This option can save time by allowing the user to evaluate a number of plates on the basis of one saved standard curve. 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 (is set per default in this case).
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 12.5 Standard Curve Analysis Types for a detailed description of the analysis types.

Analysis type option buttons	Select which interpolation algorithm is to be employed when calculating the standard curve: All offered analysis types are listed and can be selected: 1. Point to point 2. Linear Regression 3. Non-linear Regression 4. Cubic spline 5. Akima 6. Polynomial (including the field for selection of the polynomial order and including weight options) 7. Four Parameters (including the more button for minimum and maximum determination) 8. Four Parameters Marquardt (including the more button for definition of the weighting options) 9. Five parameters (including the more button for definition of the weighting options) 10. LogitLog (including the more button for minimum and maximum determination)
Data scaling drop down list	The analysis type is applied to scaled values. Following scaling modes can be selected: • Lin(x)Lin(y): x and y axis are scaled linear • Lin(x)Log(y): x axis is scaled linear, y axis is scaled logarithmically • Log(x)Lin(y): x axis is scaled logarithmically, y axis is scaled linear • Log(x)Log(y): x and y axis are scaled logarithmically

Note

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

More button	Click the **More** button to view the following options: • **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: ∗ Automatic using variance ∗ Automatic using relative weight ∗ Manual See chapter 12.5.14 Weighting for Four / Five Parameter Fit – Marquardt / Polynomial Fit • 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	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.
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 min-2*(max-min) and max+2*(max-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	The selection boxes allow for the easy input of formulas by providing a variety of functions, operators and variables. • **Variables** All variables accepted by the software are available using in the list box. • **... button** Click this button to open the **Define constants** dialog box. • **Operators** All operators accepted by the software are displayed here. • **Functions** All functions accepted by the software are displayed here.

Example

IC50 for standard curve:

Formula: (ST1_1+ST1_8)/2

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

Axis Tab

Use this tab to define the appearance of the axes.

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

Graph Tab

Use this tab to define the appearance of the graph.

Title group box	Following elements are available: • **Label** text field: Enter a label for the graph. • **Color** button: Select a color for the label of the graph.
Curves group box	Following elements are available: • **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	Following elements can be selected to be viewed: **Legend**: The curve color, base point style, and label are viewed together with additional information (analysis type parameters, correlation coefficient, and so on). **Base points** **Intercepts**: If intercepts are specified, the intercepts can be displayed and labeled in the graph. **Error bars**: If standards are defined as replicates, a bar showing the range plus/minus standard deviation is displayed for each base point.

4.3.11 Concentrations Transformations: Add New Concentration Transformations

Select **Add new conc. transform…** from the control bar.

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 4.3.7 Transformed Data: Add New Transformation for further information.

4.3.12 Evaluate Data: Cutoff Definition

In the control bar expand **Evaluate data** and select **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 results will be generated on the basis of these settings and displayed in the corresponding color.

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.

In the **Cutoff** list, up to ten cutoff ranges can be defined. The limits for each range can be entered.

The highest limit value must be entered on top of the list. The next lower will be placed beyond and so on. A displayed Low-High arrow shows the level. The limit values itself belong to the upper ranges (greater and equal condition).

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 12.4 How to Write a Formula for further details. • **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.
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.

4.3.13 Evaluate Data: QC Validation

In the control bar expand **Evaluate data** and select **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 chapters 10.4.4 User Rights (magellan Tracker and 10.5.4 User Rights (magellan Standard).

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, Mean concentration and so on.
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	Parts of the formulas to be entered into the **Validation Conditions** field can be selected from the following drop down lists: • **Variables** drop down list All available variables displayed. • **... button** Click this button to open the **Define constants** dialog box. • **Operators** drop down list All available operators are displayed. • **Functions** drop down list Using the given palette, available functions can be chosen. Refer to chapter 12.4 How to Write a Formula for further details.

Plate to Plate QC

Use this option to define a long-term QC validation. For different controls a mean value and a standard deviation can be entered. Every measured workspace using this method will be correspondingly evaluated (refer to chapter 7.4.2 Toolbar Menu: File/ Plate to Plate QC).

The **Plate to Plate QC** dialog box contains the following elements:

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

4.3.14 Data Handling: Data Export

This dialog box provides options for organizing data export.

In the control bar expand **Data handling** and select **Data export**.

Data to be exported into an ASCII or Excel file can be selected using this dialog box. A list of all available data, according to the method definition is displayed. The actual exporting of data only occurs using automated data handling (see 4.3.16 Data Handling: Automated Data Handling).

The **Data export** dialog box contains the following elements:

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.

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.
	• **Horizontal** option button The data is collected in rows.
	• **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:
	• **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.
	• **Matrix (separated)** option button Data of each selected data set is arranged in a separate matrix.
	• **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.
	• **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.

	• **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.
	If the **Add kinetic timestamps** check box is selected, the time stamps of the measurements are added. If the **Add Temperatures** check box is selected, the temperatures of the measurements are added. 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.
Add data group box	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: • 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	Settings can be logged as a default for future use.
Restore default button	Settings can be reset to the previously defined default.

Example

Raw data, kinetic cycle 1, timestamp 0 s

11 12 13

21 22 23

Raw data, kinetic cycle 2, timestamp 33 s

81 82 83

91 92 93

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

Export of Multiple Reads per Well Data

Note

When multiple reads per well data are available, it is possible to export the single values of such a measurement beside the averages by selecting the* Data name – Multiple Reads per Well *in the export data list. A separate data block in fix format is generated. Multiple reads per well is exported in the following format only:

Well name followed by a block of Value separator Value separator and so on.

Export to ASCII File

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

Decimal character group box	The decimal character may be a point or a comma: • **Point (x.xx)** option button • **Comma (x,xx)** option button
Delimiter group box	This option sets a delimiter to separate the individual values within the data in the lines of an ASCII file. TAB is the default delimiter. A different symbol can be used:
	• **Tabulator** option button This check box is selected by default, and specifies, that tabulators are used as delimiters.
	• **Other symbol** text field This text field is only active, if the **Other symbol** option button is selected. Then, a user-defined delimiter character can be entered.
Path group box	This option sets the path where the ASCII file will be stored: • **Export default path** option button **Use path** option button: Select any path where the ASCII file shall be stored
Encoding group box	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	Using this option, the settings can be logged as a default for future use.
Restore default button	Using this option, the settings can be reset to the previously defined default.

STOP

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	The option buttons define where to position the transferred data within Excel. This option is also valid for automatic Excel export. • **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	Using this option, the settings can be logged as a default for future use.
Restore default button	Using this option, the settings can be reset to the previously defined default.

4.3.15 Data Handling: Printed Report

In the control bar expand **Data handling** and select **Printed report**.

This dialog box provides options for defining the printed report.

The **Printed report** dialog box provides formatting features for hardcopy printouts to customize the contents and the appearance of the printout. Output for reporting or presentation needs can be created.

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

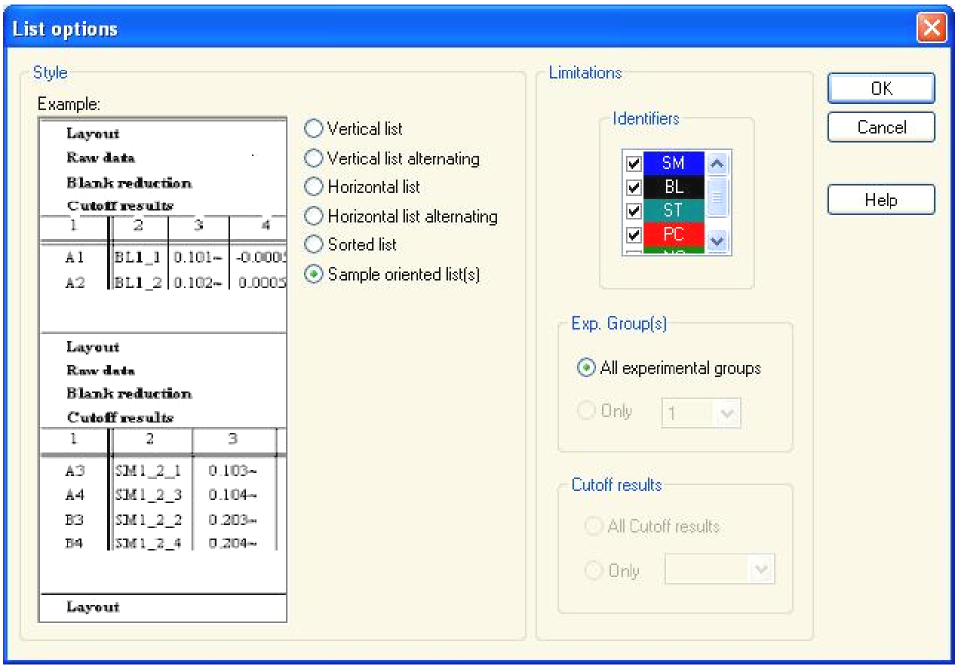
1. Data Selection tab
2. Page Setup tab
3. Header tab
4. Footer tab

Data Selection Tab

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

Print as group box	Select whether the data is to be printed in the form of a matrix or in the form of a list: • **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	Two lists are used to define the printed data: • **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.
	• **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	Click this button to transfer data highlighted in the **Available** data window to the **Selected** data window. You can also use *drag and drop*.
Insert button	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.
Import… button	This button provides the possibility to import the selected data list from another method. If this button is clicked, the **Open a file** (method) window appears and another method can be selected.
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.



○ Vertical list
○ Vertical list alternating
○ Horizontal list
○ Horizontal list alternating
○ Sorted list
● Sample oriented list(s)

☑ SM
☑ BL
☑ ST
☑ PC

● All experimental groups
○ Only 1

○ All Cutoff results
○ Only

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.

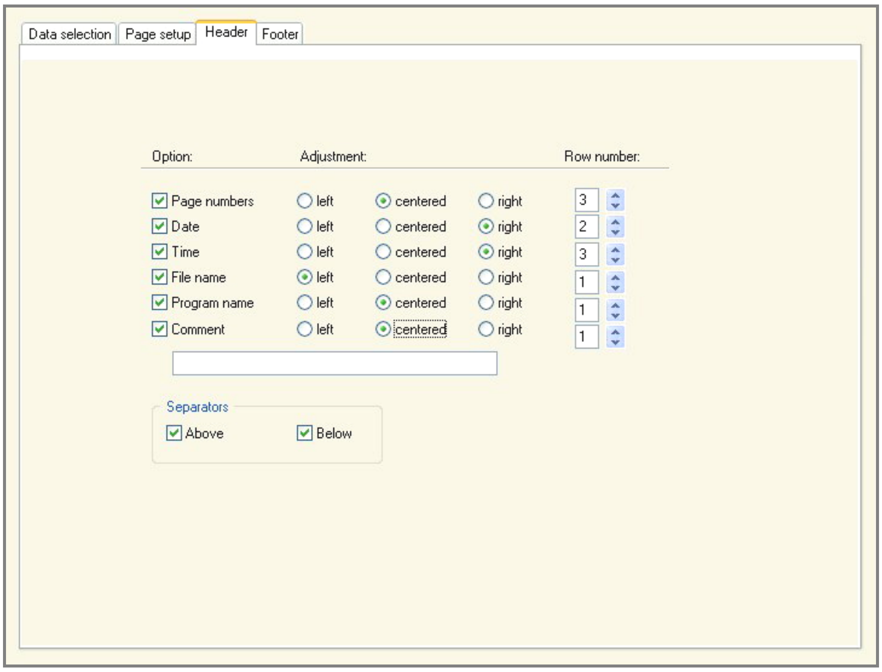
Page Setup Tab

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:	Adjustment:			Row number:
☑ Page numbers	○ left	● centered	○ right	3
☑ Date	○ left	○ centered	● right	2
☑ Time	○ left	○ centered	● right	3
☑ File name	● left	○ centered	○ right	1
☑ Program name	○ left	● centered	○ right	1
☑ Comment	○ left	● centered	○ right	1

Separators
☑ Above ☑ Below

Option check boxes	Use **Option** to select any of the following check boxes to be printed in the header: • Page numbers • Date (current) • Time • File name • Program name • Comment The **Comment** text field is active, supposed the Comment check box has been selected.
Adjustment option buttons	Select one of the following options: • 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. • **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.

4.3.16 Data Handling: Automated Data Handling

In the control bar expand **Data handling** and select **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, when running the method a sample ID list is automatically loaded.
- If the **save workspace** check box is selected (always selected in magellan Tracker), after running the method the created workspace is automatically saved.
- If the **export to ASCII file** check box is selected, after running the method the data selected for export is 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, after running the method the data selected for export is automatically exported to Excel.
- If the **print** check box is selected, after running the method the data selected for the printed report is automatically printed on the default printer.
- If the **view results after measurement** check box is selected, after running the method, the measurement data and the calculated data are displayed for reviewing.

More – Load Sample ID List

Click on the **More** button next to the check box **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: • **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: • **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): • **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 appears. It contains the following elements:

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: • **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	Using this option, the settings can be logged as a default for future use.
Restore default button	Using this option, the settings can be reset to the previously defined default.

More – Export to LIS

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

<table>
<tr><td>ASTM delimiter definition group box</td><td>Define the ASTM delimiters:
• 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).</td></tr>
<tr><td>Sender ID group box</td><td>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. Infinite 200, the name is displayed in the header of the ASTM file (e.g. H|\^&|||Infinite 200^Magellan V6.55^Standard).
• Append app. name: If selected, application name, i.e. magellan, is exported in the header of the ASTM file (e.g. magellan V6.55).
• Append app. version: If selected, the magellan version number is exported in the header of the ASTM file (e.g. <i>Standard</i> or <i>Tracker</i>).</td></tr>
</table>

LIS assay name group box	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**: ELISA Test order record: O|1|Sample ID||^^^ELISA||Date and time of measurement Result record: R|1|^^^ ELISA^results
Encoding group box	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	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	• Using this option, the settings can be logged as a default for future use.
Restore default button	• Using this option, the settings can be reset to the previously defined default.

EXPERT'S KNOW HOW

ASTM EXPORT – EXAMPLE FILE

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

- **Message Header Record:**
  |\^&|||Infinite 200^Magellan V6.55^Standard
- **Patient Information Record (P):**
  P|1||Sample ID 1 for patient 1

P|2||Sample ID 2 for patient 2

P|3||Sample ID 3 for patient 3.

- **Test Order Record (O):**
  O|1|SampleID||^^^method name||Date and time of measurement

O|2|SampleID||^^^method name||Date and time of measurement

O|3|SampleID||^^^method name||Date and time of measurement

- **Result Record (R):**
  R|1|^^^ method name^results

R|2|^^^ method name^results

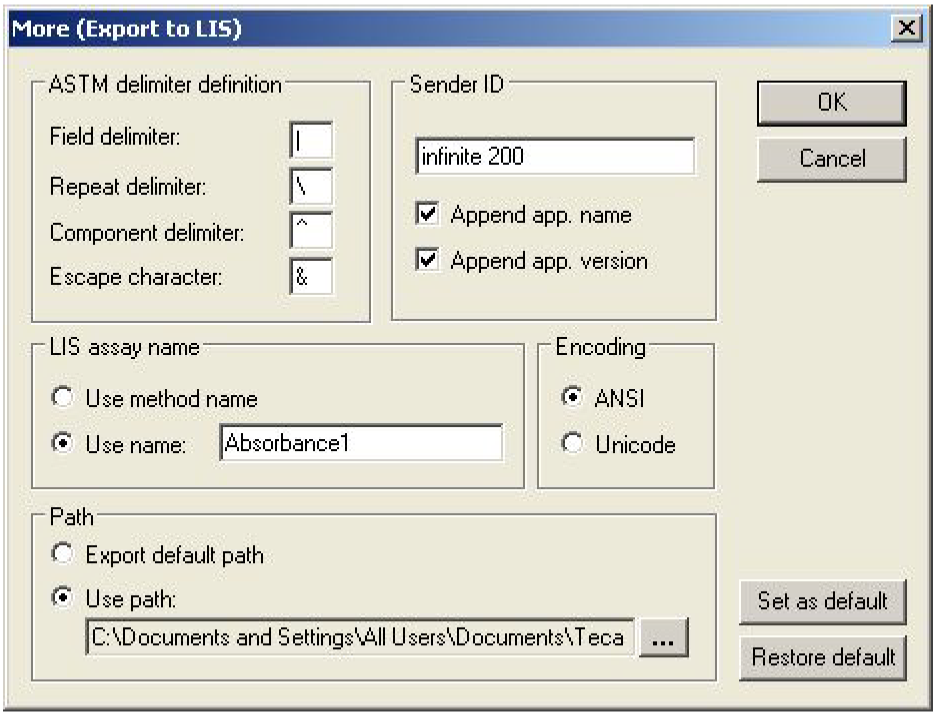
R|3|^^^ method name^results

- **Message Terminator Record:**

L|1|N

Example:

ASTM Export Settings:



ASTM delimiter definition
Field delimiter: |
Repeat delimiter: \
Component delimiter: ^
Escape character: &

Sender ID
infinite 200
☑ Append app. name
☑ Append app. version

LIS assay name
○ Use method name
● Use name: Absorbance1

Encoding
● ANSI
○ Unicode

Path
○ Export default path
● Use path:
C:\Documents and Settings\All Users\Documents\Teca

The corresponding ASTM file:

```
|\^&|||Infinite 200^Magellan V6.55^Standard
P|1||a0
O|1|a0||^^^Absorbance1||20090114124953
R|1|^^^Absorbance1^Raw data^A1|0.1015~|OD|
P|2||a1
O|1|a1||^^^Absorbance1||20090114124953
R|1|^^^Absorbance1^Raw data^B1|0.1015~|OD|
P|3||a2
O|1|a2||^^^Absorbance1||20090114124953
R|1|^^^Absorbance1^Raw data^C1|0.1015~|OD|
P|4||a3
O|1|a3||^^^Absorbance1||20090114124953
R|1|^^^Absorbance1^Raw data^D1|0.1015~|OD|
P|5||a4
O|1|a4||^^^Absorbance1||20090114124953
R|1|^^^Absorbance1^Raw data^E1|0.1015~|OD|
P|6||a5
O|1|a5||^^^Absorbance1||20090114124953
R|1|^^^Absorbance1^Raw data^F1|0.1015~|OD|
L|1|N
```

More – View Results

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

Plate view group box	Select the data to be displayed in the plate view: • **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. The 1st and 2nd line can be omitted by selecting **not used**, which makes the plate view more easily readable.
Text box group box	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.

4.3.17 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.

4.3.18 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 ca 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.

4.3.19 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

Once all the data relevant to a method is set as desired, click **Finish** and the **Save as** window appears, in which the created or modified method can be saved.

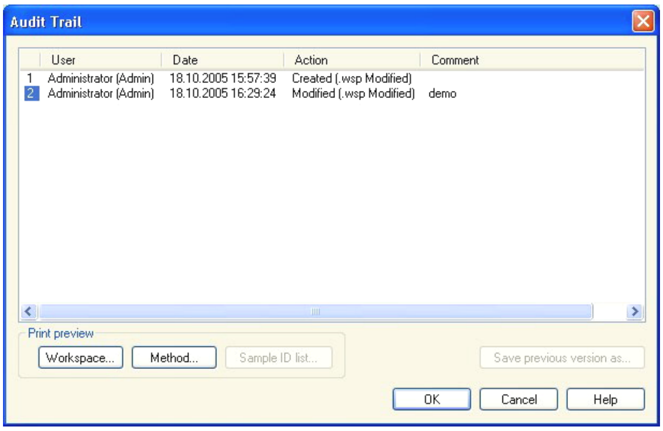
The **Save as** window contains the following elements:

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 6.5 Start Favorite for further information.
Run this method now check box	When this check box is selected the method run will be started immediately after finishing this wizard.

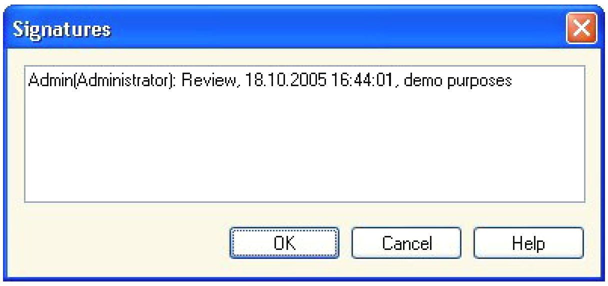
The modified document can be saved under its current file name or under a different name.

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

Additional buttons in magellan **Tracker:**

Audit trail... button	Click this button to open the **Audit trail** dialog box where the user, the date, the executed action and a comment are displayed. 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. Additionally it is possible to save a previous version of the method under another name. 

	User	Date	Action	Comment
1	Administrator (Admin)	18.10.2005 15:57:39	Created (.wsp Modified)	
2	Administrator (Admin)	18.10.2005 16:29:24	Modified (.wsp Modified)	demo

Signature... button	Click this button to open the **Signature** dialog box, where user, date, action and comment are displayed.  Signatures Admin(Administrator): Review, 18.10.2005 16:44:01, demo purposes OK Cancel Help 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.
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!

4.4.1 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

When you open a password protected method, a dialog box is displayed, asking for the method password.

Enter the correct method password and the method is opened in **Edit mode**. It is possible to edit and save the method. No additional password entry is needed.

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**. The password has been changed.

4.5 Multiplate Methods

When connected to a Tecan instrument from the Infinite series or to a Safire^2 instrument, **multiplate methods** can be defined using magellan, version 6.0 or higher.

When connected to an instrument from the Infinite series, the number of plates to be measured can be set in the measurement parameters editor, during method definition (see the Instructions for Use for i-control:

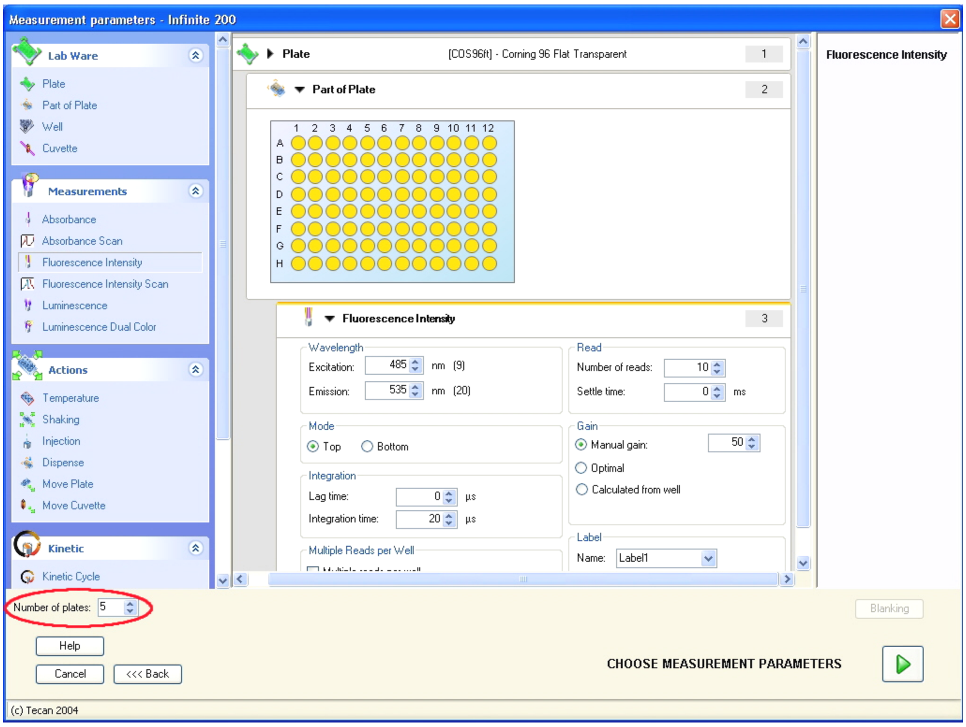


Plate [COS96ft] - Corning 96 Flat Transparent

Part of Plate

Fluorescence Intensity

Wavelength
Excitation: 485 nm (9)
Emission: 535 nm (20)

Read
Number of reads: 10
Settle time: 0 ms

Mode
● Top ○ Bottom

Gain
● Manual gain: 50
○ Optimal
○ Calculated from well

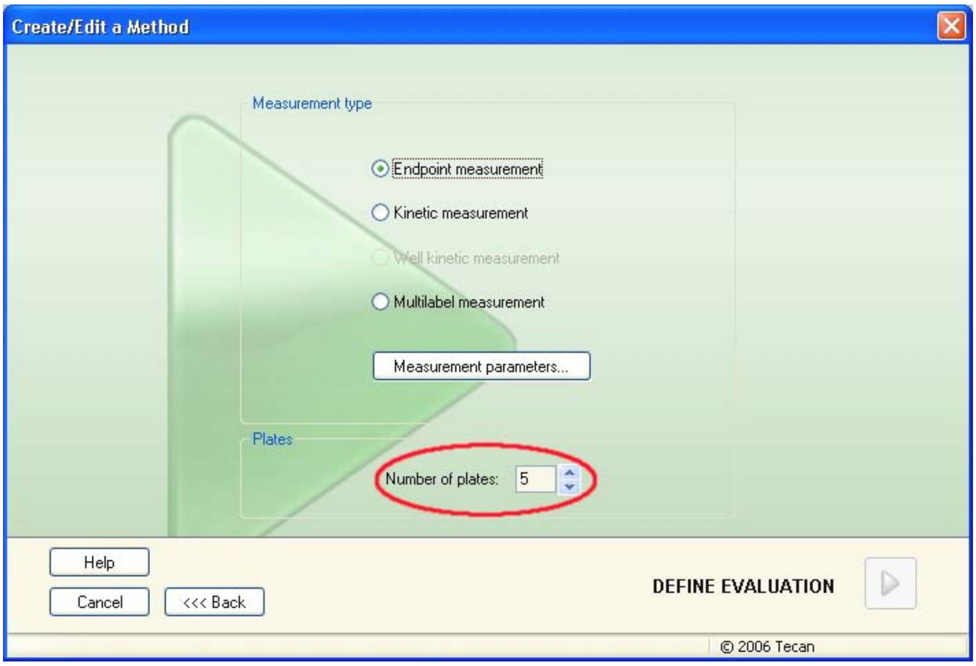
Integration
Lag time: 0 µs
Integration time: 20 µs

Multiple Reads per Well

Label
Name: Label1

Number of plates: 5

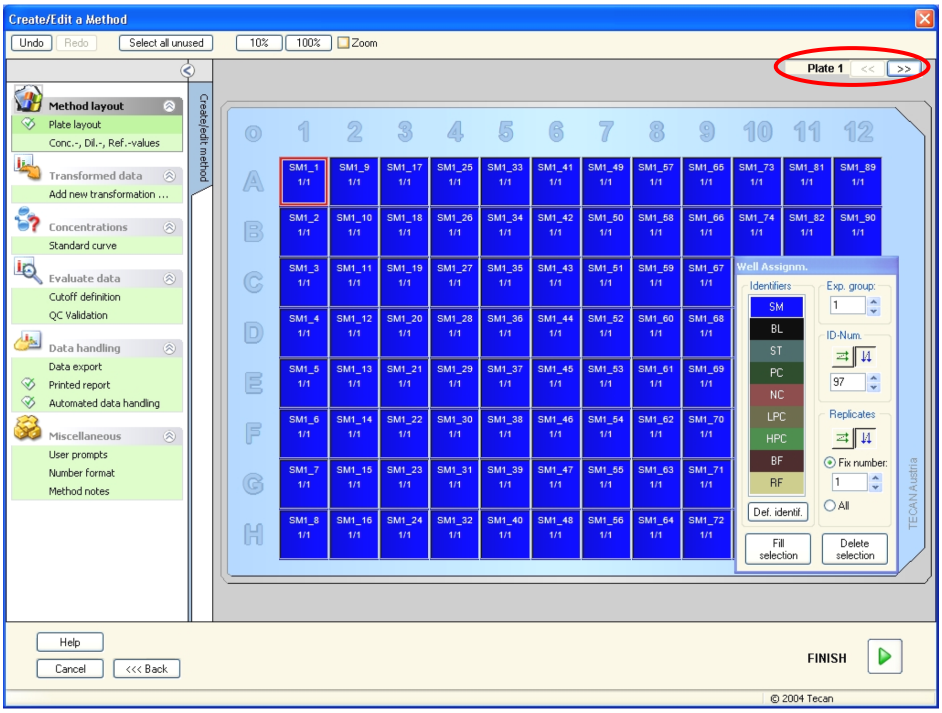
When connected to a Safire^2 instrument, the option can be selected from the Create/ Edit a Method wizard page:



Measurement type
● Endpoint measurement
○ Kinetic measurement
○ Well kinetic measurement
○ Multilabel measurement

Plates
Number of plates: 5

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.

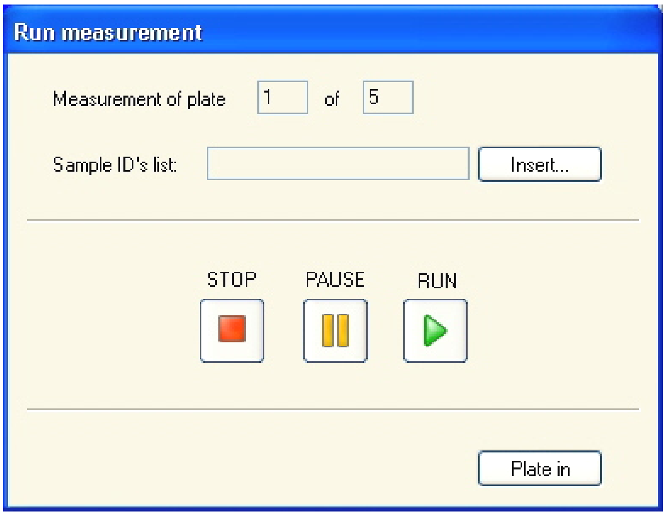


0	1	2	3	4	5	6	7	8	9	10	11	12
A	SM1_1 1/1	SM1_9 1/1	SM1_17 1/1	SM1_25 1/1	SM1_33 1/1	SM1_41 1/1	SM1_49 1/1	SM1_57 1/1	SM1_65 1/1	SM1_73 1/1	SM1_81 1/1	SM1_89 1/1
B	SM1_2 1/1	SM1_10 1/1	SM1_18 1/1	SM1_26 1/1	SM1_34 1/1	SM1_42 1/1	SM1_50 1/1	SM1_58 1/1	SM1_66 1/1	SM1_74 1/1	SM1_82 1/1	SM1_90 1/1
C	SM1_3 1/1	SM1_11 1/1	SM1_19 1/1	SM1_27 1/1	SM1_35 1/1	SM1_43 1/1	SM1_51 1/1	SM1_59 1/1	SM1_67 1/1			
D	SM1_4 1/1	SM1_12 1/1	SM1_20 1/1	SM1_28 1/1	SM1_36 1/1	SM1_44 1/1	SM1_52 1/1	SM1_60 1/1	SM1_68 1/1			
E	SM1_5 1/1	SM1_13 1/1	SM1_21 1/1	SM1_29 1/1	SM1_37 1/1	SM1_45 1/1	SM1_53 1/1	SM1_61 1/1	SM1_69 1/1			
F	SM1_6 1/1	SM1_14 1/1	SM1_22 1/1	SM1_30 1/1	SM1_38 1/1	SM1_46 1/1	SM1_54 1/1	SM1_62 1/1	SM1_70 1/1			
G	SM1_7 1/1	SM1_15 1/1	SM1_23 1/1	SM1_31 1/1	SM1_39 1/1	SM1_47 1/1	SM1_55 1/1	SM1_63 1/1	SM1_71 1/1			
H	SM1_8 1/1	SM1_16 1/1	SM1_24 1/1	SM1_32 1/1	SM1_40 1/1	SM1_48 1/1	SM1_56 1/1	SM1_64 1/1	SM1_72 1/1			

Exp. group: 1
ID-Num.: 97
Replicates: ● Fix number: 1

All further parameters can be defined as is done for single plate methods.

At starting a multiple plate method the following dialog box appears:



Measurement of plate 1 of 5

Sample ID's list:

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. Up to three sample IDs can be entered or imported per well.

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.

When **Create new** sample ID list is selected, the **Select plate type** page appears, in which the plate type and sample IDs per well or the import settings can be set.

Then the **Import/edit a sample ID list** page appears where the sample ID for the wells can be entered individually or automatically using the **Autofill…** function.

Finally, in the **Save as** page the created or modified sample ID list is saved.

5.2 Create/Edit a Sample ID List

In the wizard list, click **Create/edit a sample ID list**. After the welcome page, select **Create new** to create a new sample ID list or select **Edit** to edit an existing sample ID list from the file selection window.

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

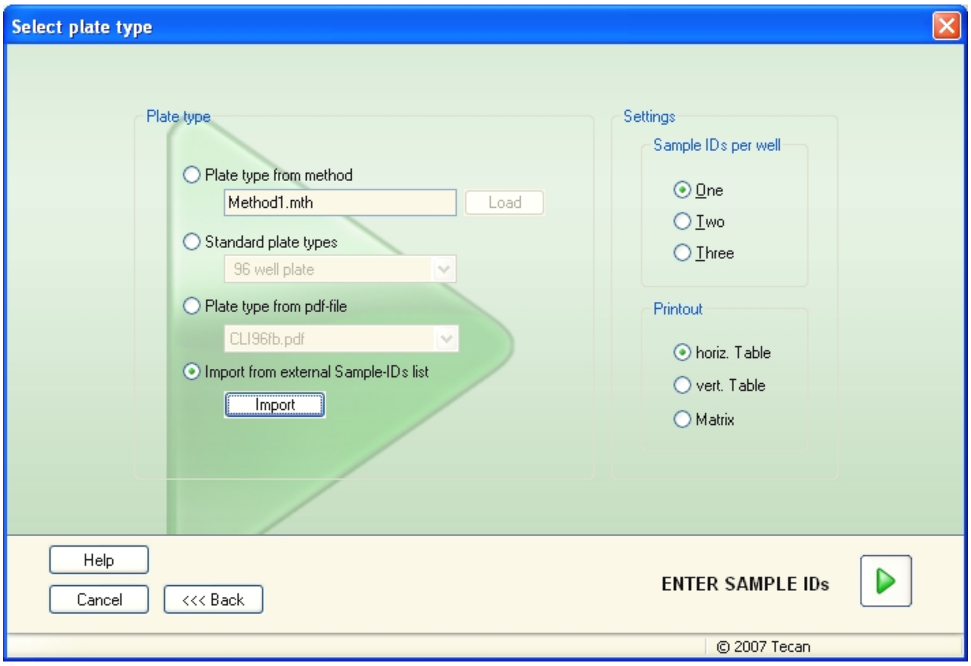
a) Create new option button	When the **Create new** option was selected, a new sample ID list can be created. The user will be guided to the **Select plate type** window where plate type and number of sample IDs per well are defined.
b) Edit option button	When the **Edit** option was selected the **Import/edit a sample ID list** window is displayed where an existing sample ID list can be modified. Sample IDs can be inserted in the wells.
Show combo box	In the **Show** combo box the displayed list of files can be modified according to the selection: • All files • My files: This option is available if the user administration is enabled (always enabled in magellan Tracker)
Filename list	In the **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.

> ***Note***
> ***After the** magellan **30-day demo license has expired, printing will not be possible.***

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.***



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): • One • Two • Three
Printout option buttons	Define the layout for printing the sample ID list: • horiz. Table • vert. Table • Matrix

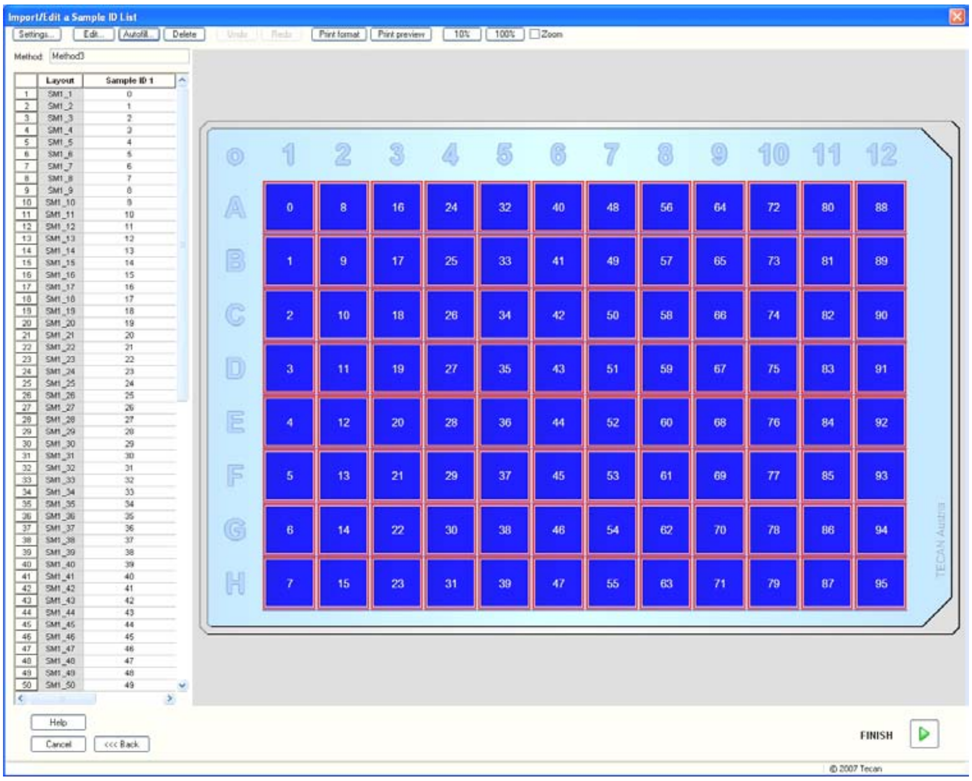
Plate type option buttons	Four option buttons define the plate type to be selected: • **Plate type from method** Select a method to load the plate layout. Click **Load** to browse for existing method files. The Windows^{TM} **Open** dialog box appears. Select the desired file and click **Open**. • **Standard 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 (or .pdfx file for infinite series instruments) can be used to define the plate format. magellan offers a wide selection of predefined plate formats to choose from. Plates that are not listed can be created using the **Plate geometry editor** option, which is a software application accessible via magellan. For more information refer to chapter 3.2.5 Plate Geometry Editor... . When activated, a predefined *.pdf* file can be chosen from an associated drop down list. • **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 (method has been loaded, standard plate type or pdf-file has been selected.) have been defined.

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. It contains the following elements:

- Toolbar
- Plate view
- Sample ID list (when **Plate type from method** has been selected)

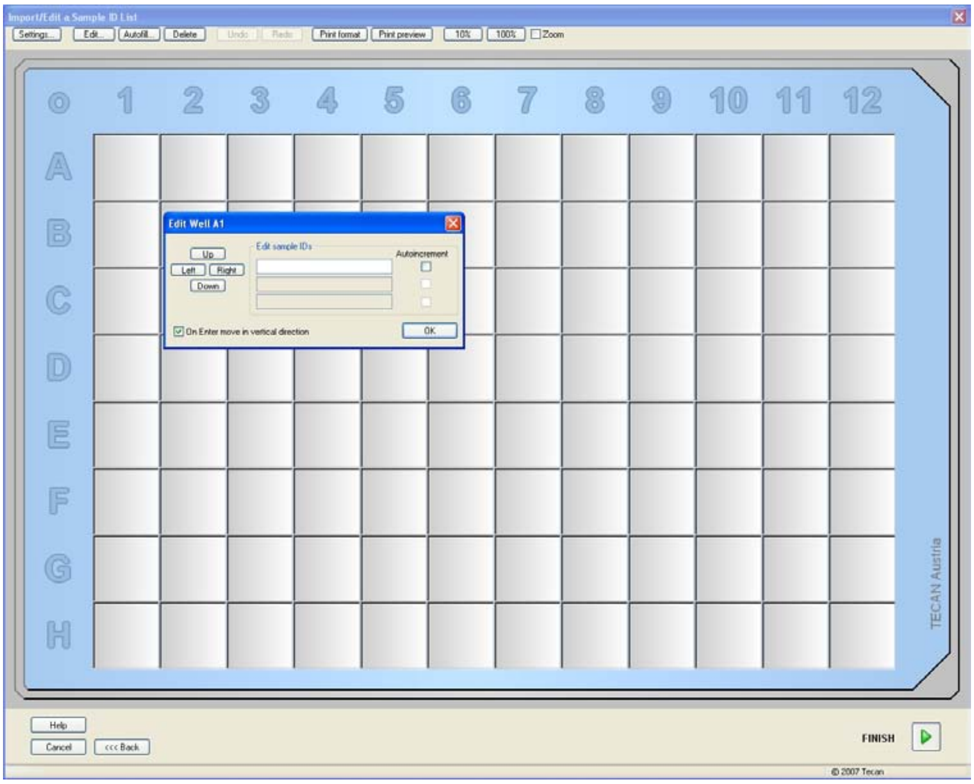


Method: Method3

	Layout	Sample ID 1
1	SM1_1	0
2	SM1_2	1
3	SM1_3	2
4	SM1_4	3
5	SM1_5	4
6	SM1_6	5
7	SM1_7	6
8	SM1_8	7
9	SM1_9	8
10	SM1_10	9
11	SM1_11	10
12	SM1_12	11
13	SM1_13	12
14	SM1_14	13
15	SM1_15	14
16	SM1_16	15
17	SM1_17	16
18	SM1_18	17
19	SM1_19	18
20	SM1_20	19
21	SM1_21	20
22	SM1_22	21
23	SM1_23	22
24	SM1_24	23
25	SM1_25	24
26	SM1_26	25
27	SM1_27	26
28	SM1_28	27
29	SM1_29	28
30	SM1_30	29
31	SM1_31	30
32	SM1_32	31
33	SM1_33	32
34	SM1_34	33
35	SM1_35	34
36	SM1_36	35
37	SM1_37	36
38	SM1_38	37
39	SM1_39	38
40	SM1_40	39
41	SM1_41	40
42	SM1_42	41
43	SM1_43	42
44	SM1_44	43
45	SM1_45	44
46	SM1_46	45
47	SM1_47	46
48	SM1_48	47
49	SM1_49	48
50	SM1_50	49

0	1	2	3	4	5	6	7	8	9	10	11	12
A	0	8	16	24	32	40	48	56	64	72	80	88
B	1	9	17	25	33	41	49	57	65	73	81	89
C	2	10	18	26	34	42	50	58	66	74	82	90
D	3	11	19	27	35	43	51	59	67	75	83	91
E	4	12	20	28	36	44	52	60	68	76	84	92
F	5	13	21	29	37	45	53	61	69	77	85	93
G	6	14	22	30	38	46	54	62	70	78	86	94
H	7	15	23	31	39	47	55	63	71	79	87	95

- Dialog to insert sample IDs (when **Standard plate type** has been selected)



On top of the window a **Toolbar** is displayed: Settings, Edit, Autofill, Delete, Undo/Redo, Print format, Print preview and Zooming can be accessed clicking the corresponding button (see below for details).

In the main area of the window the **Plate View** displays a schematically layout of a microplate. Rows are marked alphabetically, columns numerically.

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: • horiz. Table • vert. Table • Matrix
Print preview	Opens the print preview of the printed sample ID list.
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.

First the whole plate or parts of the plate must be selected. The desired sample IDs and increment settings for the marked wells must be entered 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:

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.

STOP

Important

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^{TM} **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^{TM} ***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).

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

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. The final layout will be handled like strip methods.

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	L R	05-20-199919:12:53
990520S1D1	2	test1_2	PC1		05-20-199919:12:53
990520S1E1	2	test1_2	00000000010		05-20-199919:12:53
990520S1F1	2	test1_2	00000000010	V	05-20-199919:12:53

Interpretation

When magellan is processing an .apl-file

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

Gemini-Files .csv

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

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

The file format is defined as follows:

The first line contains the column headers, which are the same for all formats, except for some which support only upper-case characters. The second line shows information about the rack / striprack, 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 striprack.

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 stripracks 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 striprack, 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.

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

EXPERT'S KNOW HOW

IMPORT SAMPLE-IDS FROM SAMPLE TRACKING (.CSV)

The option **Investigate Checksum** is available for the import of Sample IDs from sample tracking (*.csv) only.

Note
These Sample ID files have to be imported as custom format files. The checksum is part of the file.

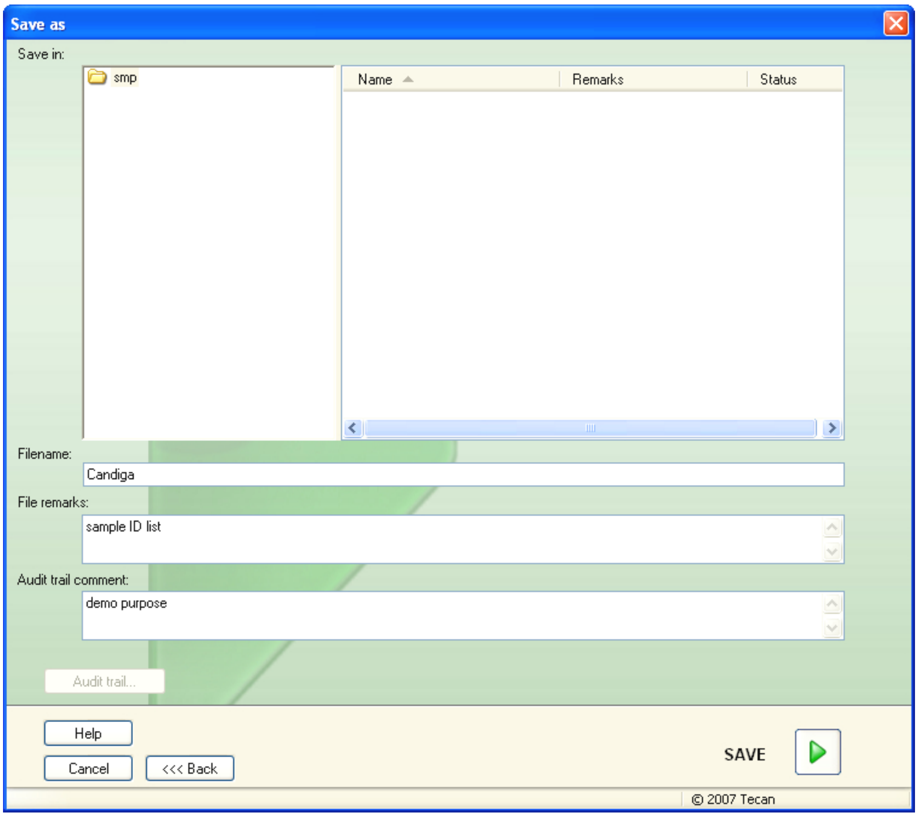
When importing such a list, the checksum is verified by magellan. The import fails if the list has been manipulated in some way afterwards (error: "Failed to load: … Checksum incorrect.)

For performing the checksum verification, select **Investigate checksum** in the **Custom Format** dialog.

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.

magellan Tracker:



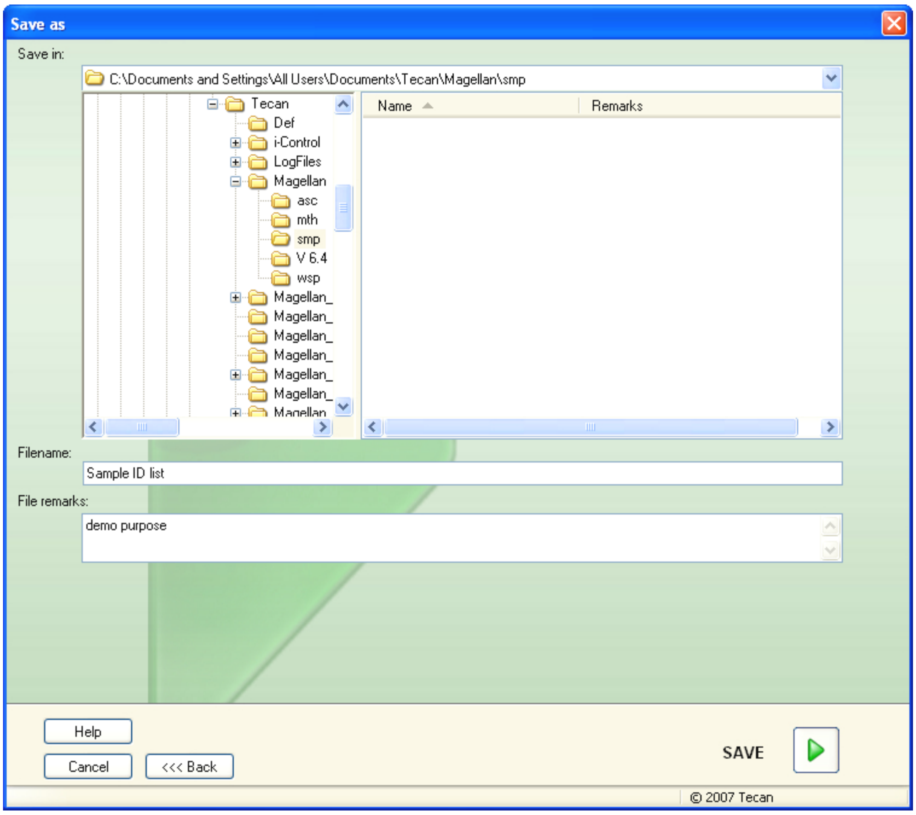
Save in: smp

Filename: Candiga

File remarks: sample ID list

Audit trail comment: demo purpose

magellan Standard:



Save in: C:\Documents and Settings\All Users\Documents\Tecan\Magellan\smp

Filename: Sample ID list

File remarks: demo purpose

The **Save as** window contains the following elements:

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.

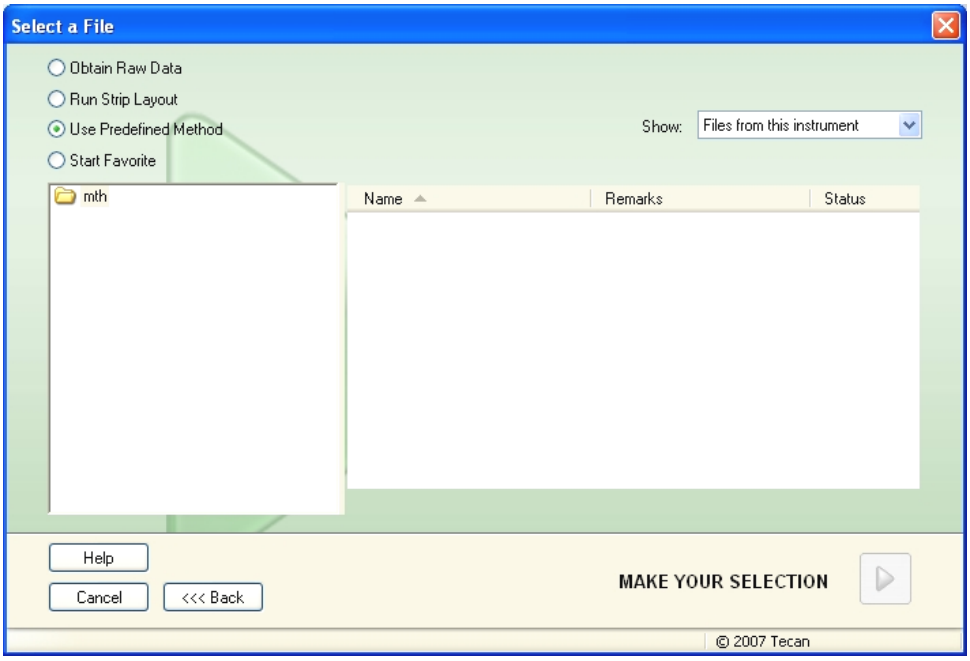
The **Save&Finish** button is only enabled when a document has been modified. The modified document can be saved under its current file name or under a different name.

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

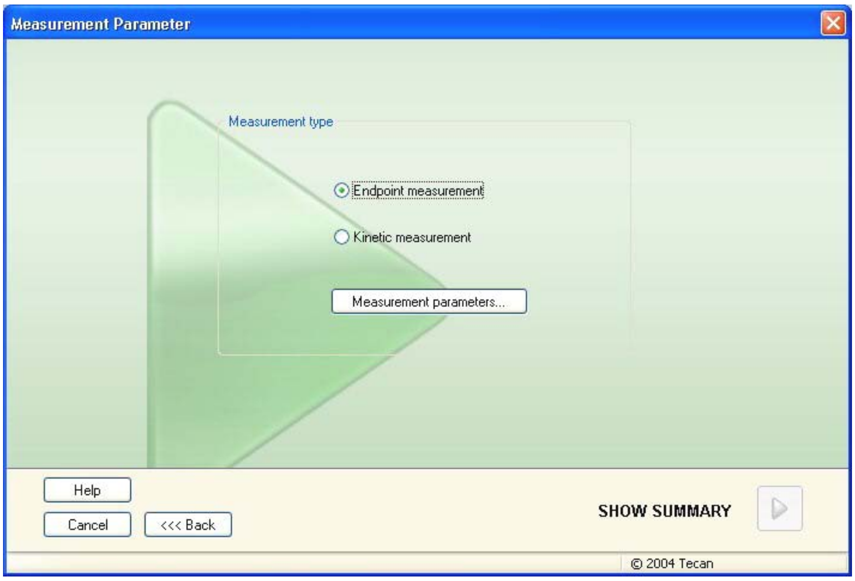
In the **Wizard List** window, click **Start Measurement** to open the wizard. Click **Continue** ▷ on the welcome page and the **Select a file** dialog box appears:



Obtain Raw Data	Is used to generate raw data quickly by setting the required measurement parameters. This wizard is designed to create a new workspace, to set the measurement parameters and to obtain measured values.
Run Strip Layout	Enables the user to create one strip method from different methods and to run this combined method.
Use Predefined Method	Is used to perform measurements based on already defined methods. The wizard creates a new workspace, that contains the selected method (which consists of all measurement parameters and definitions for evaluation) and enables you to insert a *Sample ID list*. After the measurement, the workspace is completed with the obtained raw data which will be evaluated.
Start Favorite	Is used to select one of the most frequently used methods from the list of numbered icons.

6.2 Obtain Raw Data

Select **Obtain Raw Data** and click **Next**; the following wizard page appears:



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.

Refer to the **Reader Server** instructions for use, document number 30008897, for further information on 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.

6.2.1 *Obtain Raw Data with the* Infinite *Instrument*

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

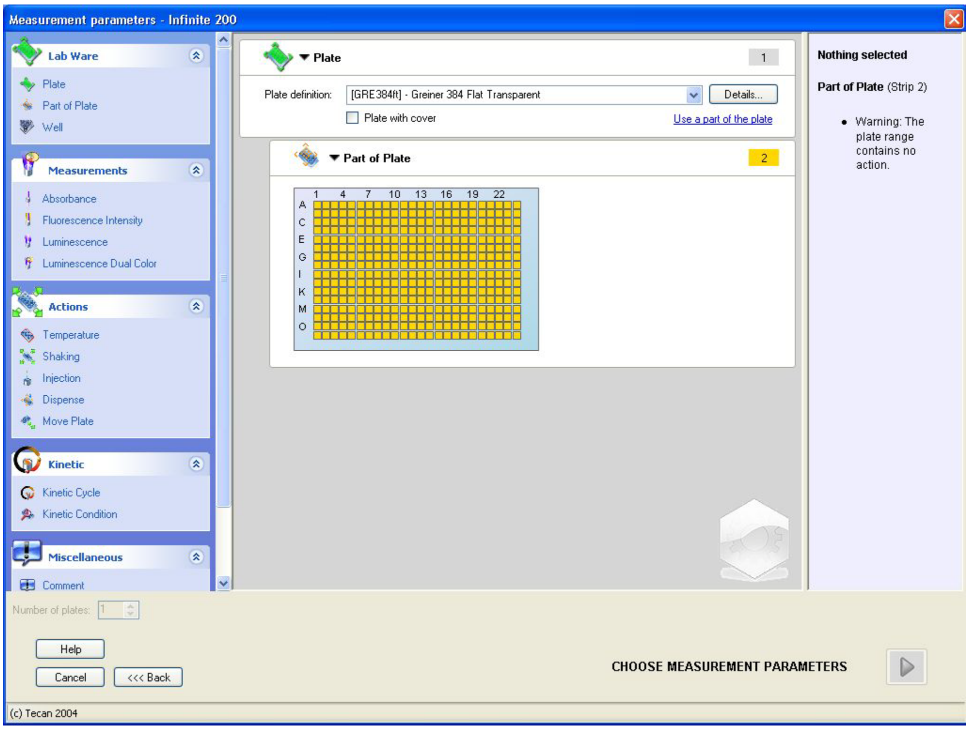


Plate definition: [GRE384ft] - Greiner 384 Flat Transparent

☐ Plate with cover

Nothing selected

Part of Plate (Strip 2)

- Warning: The plate range contains no action.

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

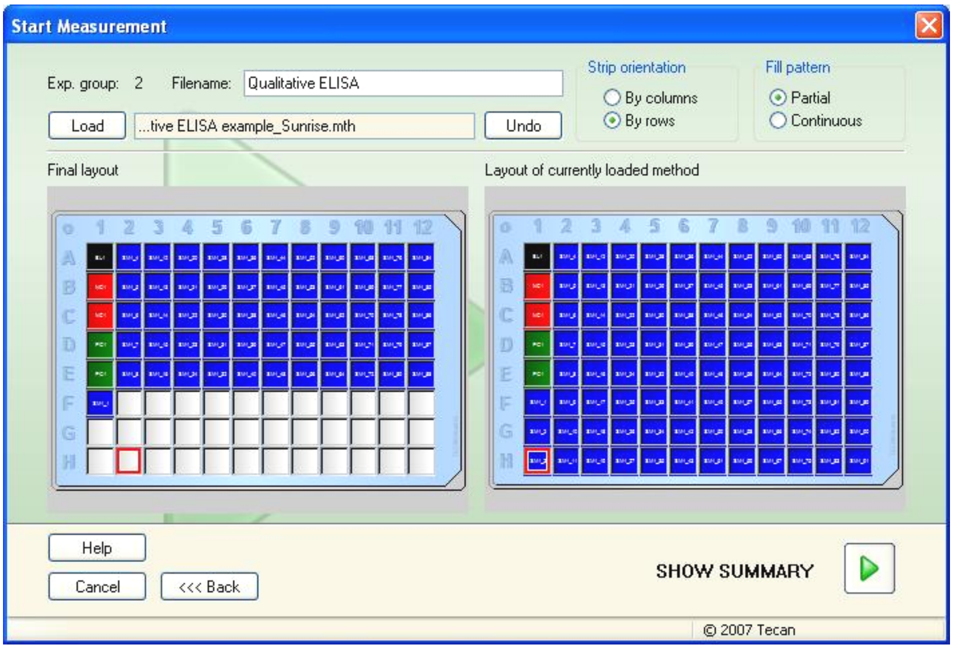
Click **Choose Measurement Parameters** ▷ to finish the definition. Refer to the i-control instructions for use for further information.

6.3 Run Strip Layout

The **Strip Method...** option allows the user to create one method composed of strips from different methods containing different parameters and to run this combined method.

Observe the criteria for combining strips of methods. The methods involved must be defined with:

- exactly the same measurement parameters
- transformations, concentration and kinetic transformations must have the same name.



Exp. group: 2

Filename: Qualitative ELISA

...tive ELISA example_Sunrise.mth

Strip orientation
○ By columns
● By rows

Fill pattern
● Partial
○ Continuous

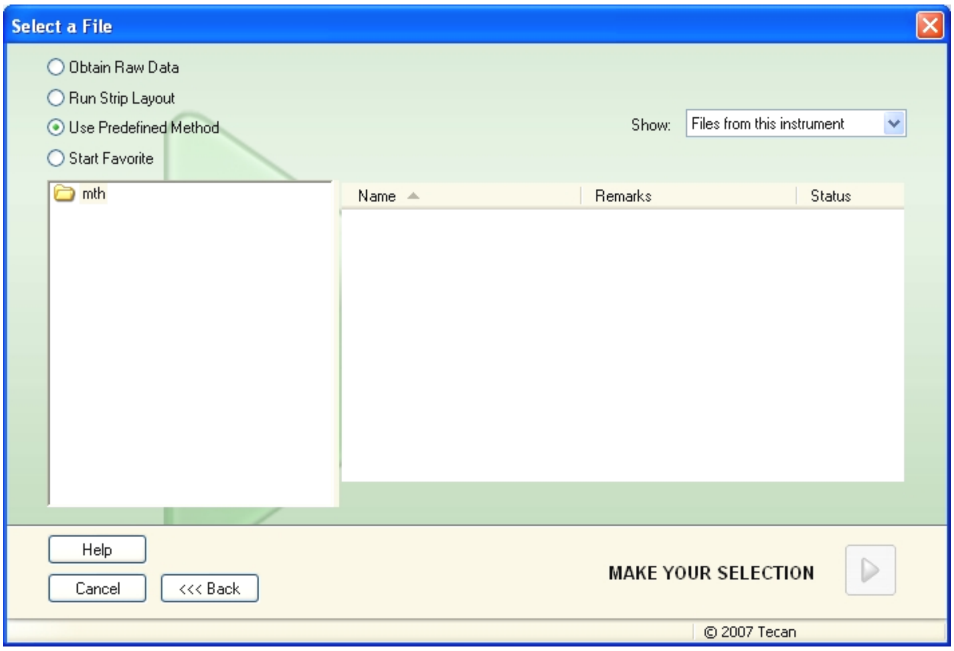
The **Strip Method Definition** dialog box contains the following elements:

Exp. group field	This field displays the experimental group number that is assigned to the next inserted strip method.
Load button	Click the **Load** button to open a file selection dialog box where all available method files are displayed. Select the required single strip method from the file list and click **Open**.
File name text field	This field displays the name of the currently selected method file.
Text field	In this field the complete path of the method file name is displayed.
Undo button	This option cancels the last strip method insertion.
Strip orientation option buttons	Determine how the strips are to be allocated to the plate. • **By columns**: If this option is selected, the strips must be allocated in columns to the plate. • **By rows**: If this option is selected, the strips must be allocated in rows to the plate.

Fill pattern option buttons	This option allows the users to decide between allocating every new strip to a new row or column or allocating it to the next available well in the plate. • **Partial**: If this option is selected, the strips will be allocated to complete new rows or columns in the plate. • **Continuous**: If this option is selected, the strips will be allocated to the next available well in the plate.
Final layout graphical display	The graphical display shows the layout of the composition of strip methods. The way, in which wells are transferred from the **Layout of currently loaded method** area to the **Final layout** area depends on the settings of the option buttons **Strip orientation** and **Fill pattern**.
Layout of currently loaded method graphical display	The graphical display shows the layout of the currently loaded method. Double-clicking on the last available well will add the strip method at this position to the plate. This will be displayed in the **Final layout** area on the left side. Replicates, which are not selected, are automatically added. This step can be repeated by loading another strip method.

6.4 Use Predefined Method

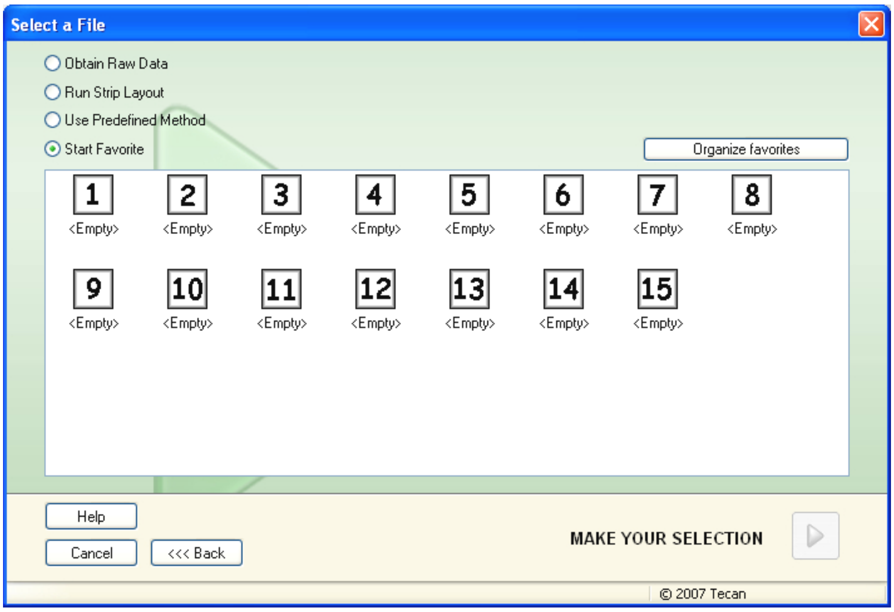
Select **Start measurement** from the wizard list. Click **Continue** on the welcome page and the **Select a file** dialog box appears. Select **Use Predefined Method** and select the required method from the **Filename** list:



The **Show** drop down list is a filter. **All files, Files from this instrument, My files, Signed files** or **Last selected methods** can be selected.

6.5 Start Favorite

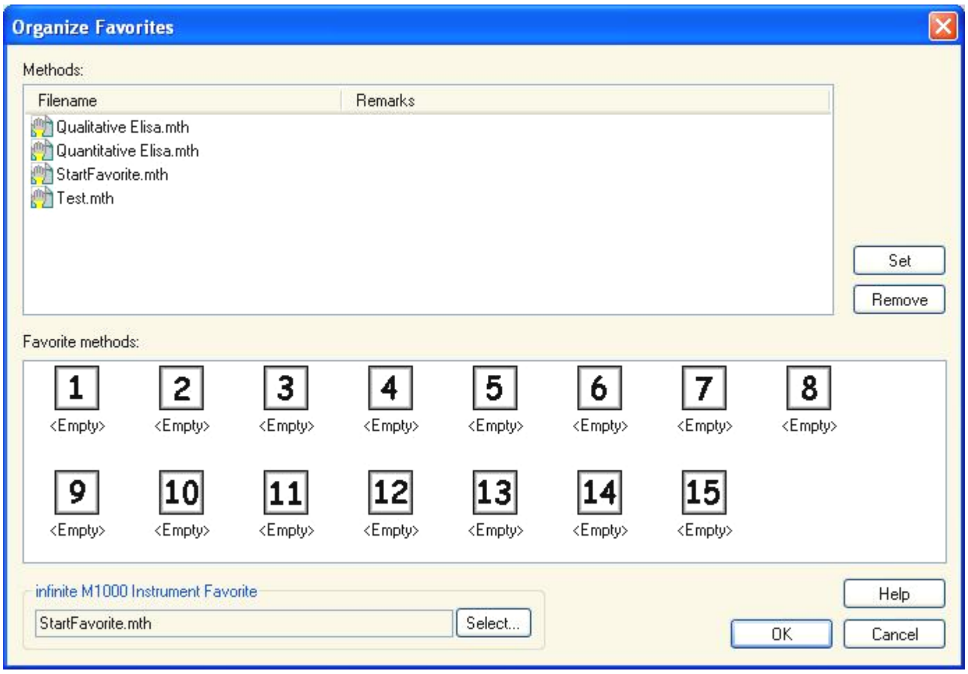
In the **Select a file** dialog box click **Start Favorites.** Select one of the most frequently used methods from the list of numbered icons:



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**.
Infinite M1000 Instrument Favorite group box	With the Infinite M1000 instrument, it is possible to start a measurement run with a favorite method directly via the instrument's **Start** button. To define a favorite method click the **Select…** button and select a method. This method will remain the favorite one as long as another method is selected.

6.6 Start Measurement with a Predefined or Favorite Method

Click **Make your selection** respectively **Show Summar**y 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. If evaluation settings are defined, the calculation is started right after the measurement.

Edit Prompts Dialog

If user prompts were specified in the method, the **Edit user prompts** dialog box is displayed. It contains the following elements:

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.

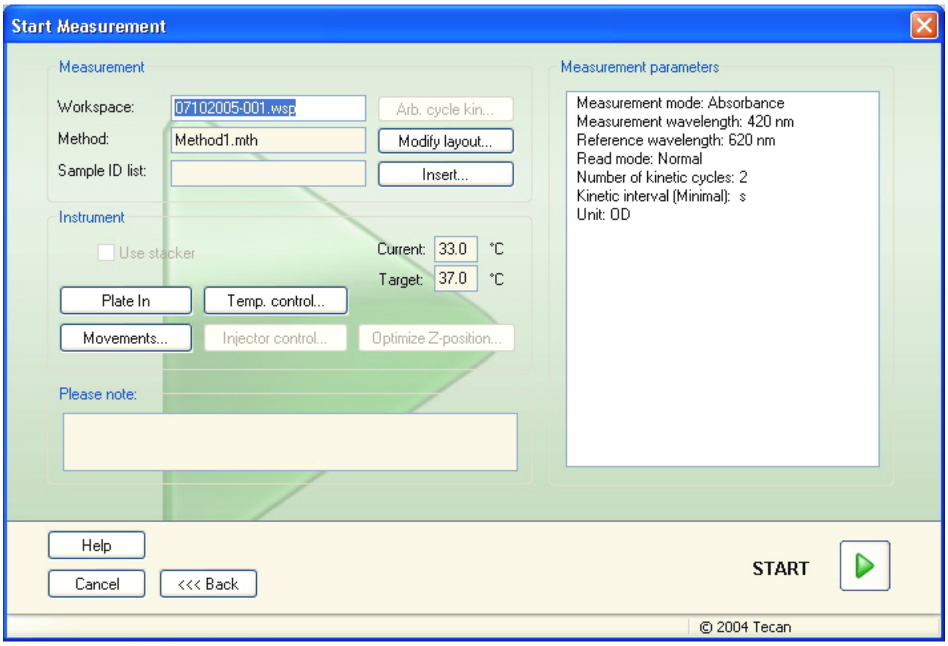
Note

Using magellan **Tracker** ***or*** magellan **Standard** ***with User administration, a default*** magellan ***Operator (refer to chapters 10.4.4 User Rights (***magellan ***Tracker and to chapter 10.5.3 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 edit also 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.



Workspace: 07102005-001.wsp
Method: Method1.mth
Sample ID list:
☐ Use stacker
Current: 33.0 °C
Target: 37.0 °C

Measurement mode: Absorbance
Measurement wavelength: 420 nm
Reference wavelength: 620 nm
Read mode: Normal
Number of kinetic cycles: 2
Kinetic interval (Minimal): s
Unit: OD

It contains the following elements:

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 Series instruments.

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

	Insert... button: see also below. Click this button to open the **Insert Sample ID List** dialog box. After selection of a sample ID list file the **Sample ID List with Plate Layout Preview** dialog appears in which the user has to confirm the selection.
Instrument group box	**Use stacker:** This option is available whenever the **Connect** stacker is used together with the instrument. Check this option in order to measure all plates in the stacker with this method. Refer to the **Connect** Instructions for Use for further information. 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.**
	Plate In/Out button: Click to move the plate carrier. This button changes its text depending on the position of the plate carrier.

Note

When* Use stacker *is selected while using* magellan*, make sure that the overall runtime does not exceed the time set in the Auto Lock option (see chapter 10.4.5 User Administration Options/ Login Options).

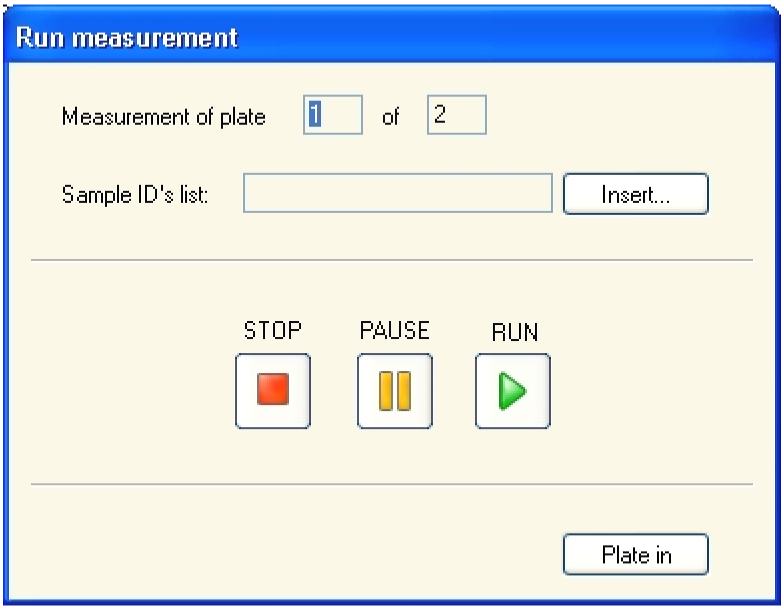
When* magellan *is locked, the stacker run will stop even if the measurements are not finished.

	Movements button: Further movements of the instrument can be invoked (filter slide, mirror carriage and so on.)
	Optimize Z-Position button: The user can optimize the z-position of the reader. Refer to the **Reader Server** instructions for use, document number 30008897, for further information.
	Injector control: Refer to the respective instrument's instructions for use.
	Current Temperature text field: The current temperature of the instrument is displayed.
	Target Temperature text field: The target temperature, set in the **Temperature Control** dialog box, is displayed.
	Temperature Control button: Click this button to open the **Temperature Control** dialog box. See chapter 3.1.2 Temperature Control... .
Measurement parameters group box	In a text field all configured measurement parameters are listed and can be double-checked.
Please note group box	Important information is displayed. Read this information and start appropriate actions before running the method.

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

Click **Start** to start the measurement. 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.

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.

The **Insert Sample ID List** dialog box contains the following elements:

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.

If the method and the sample ID list have different plate formats, then an error message is displayed.

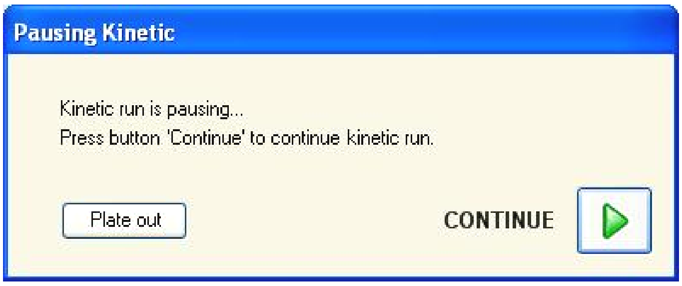
When the sample ID list is selected in the printed report setup then it is displayed on the printout.

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

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.

6.7 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** option button: The measured value is displayed in the well. If more than one value is measured (for example: polarization measurement) all values are displayed in one well.
	Graph option button: 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.  Kinetic run is pausing... Press button 'Continue' to continue 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. Some instruments support row-wise or even well-wise data transmission; other instruments only plate-wise data transmission. 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** text field contains the value of the previous measured cycle of the currently selected well. As long as the transmission of the data of the current cycle was not started the **Temperature** text field contains the temperature of the previous measured cycle.

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**. After a welcome dialog box, the **Select a File** dialog box appears. Select an existing workspace file containing the measurement data to be evaluated.

Click **Make your selection** and the **Results** dialog box appears, in which the results can be viewed or printed (**Evaluate Results** tab).

If necessary, the used method can also be modified (**Edit Method** tab).

Click **Finish** and the **Save** dialog box appears, in which a file name and remarks about the measurement can be entered and saved as 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

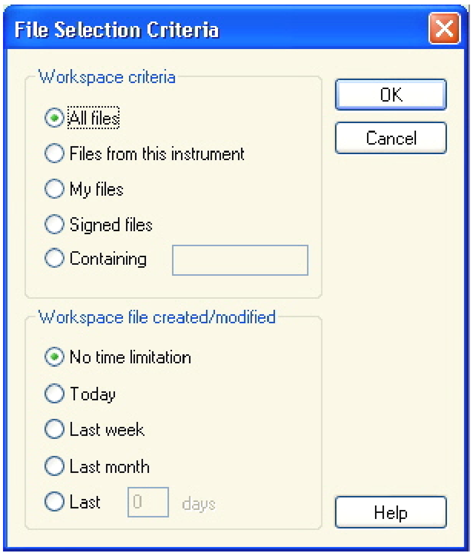
On the **Wizard List** page, click **Evaluate Results**.

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

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

Filename list	The **Filename** list contains the names of all files within the standard workspace directory. Remarks entered for that measurement are displayed.
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 • 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.

7.2.1 File Selection Criteria



File Selection Criteria

Workspace criteria

● All files
○ Files from this instrument
○ My files
○ Signed files
○ Containing

Workspace file created/modified

● No time limitation
○ Today
○ Last week
○ Last month
○ Last 0 days

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

Select one of the options under **Workspace Criteria***:* **All files**, **Files from this instrument**, **My files**, **Signed files** or enter characters in the **Containing** text field which must appear in the **Filename**. The files filtered can be further limited to a specific period of time by selecting one of the options under **Workspace file created/modified***:* **No time limitation**, **Today**, **Last week**, **Last month** 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 the proper instrument for the selected file is not connected, the Instrument Mismatch dialog box appears.
The dialog offers two options:

- ***Connect to the proper instrument***
- ***Convert the measurement parameters to the connected instrument.***

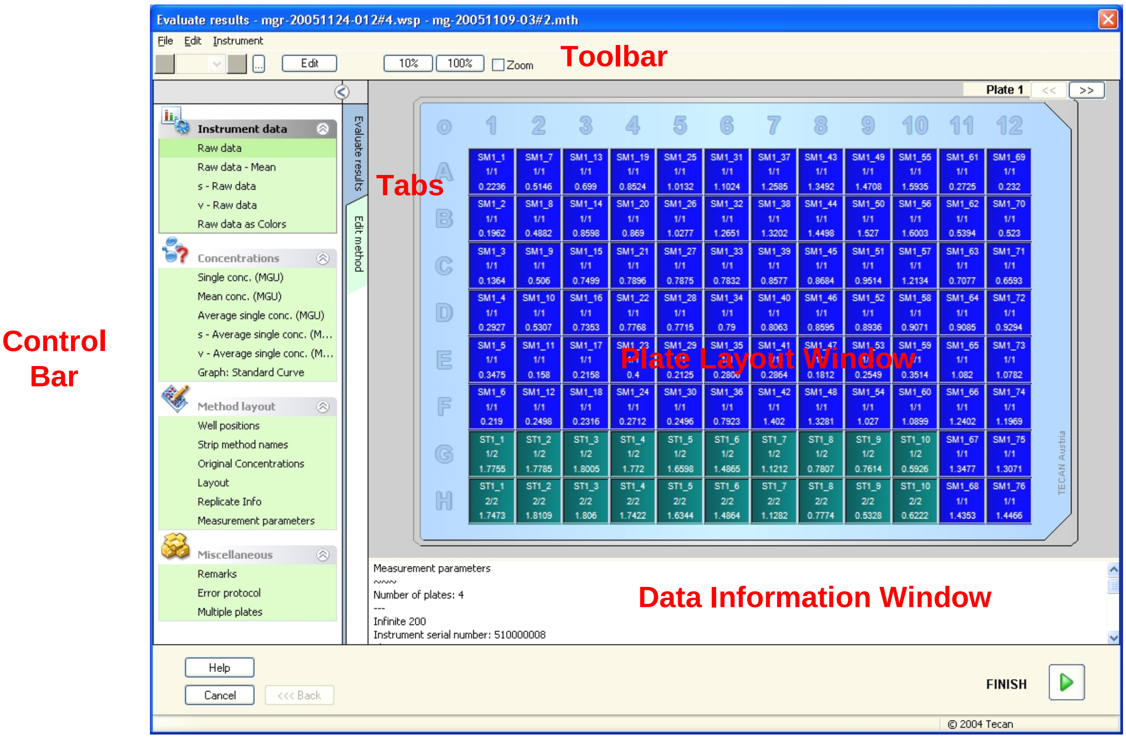
This option is not available if the measurement mode is not supported by the connected instrument, for example: a Sunrise does not support fluorescence measurements.

7.3 The Workspace Overview Window

Click the **Next** button and the **Workspace Overview** window of the **Evaluate Results** wizard appears. It displays all available data of the currently selected workspace and helps to easily locate and view instrument data, calculated data, cutoff results, measurement parameters, etc.

If the currently working user has the appropriate rights (refer to chapter 10.4.4 User Rights (magellan Tracker and chapter 10.5.4 User Rights (magellan Standard), 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.

For more detailed information on the calculation procedure and sequence of calculations, refer to chapter 12 Calculations.



o	1	2	3	4	5	6	7	8	9	10	11	12
A	SM1_1 1/1 0.2236	SM1_7 1/1 0.5146	SM1_13 1/1 0.699	SM1_19 1/1 0.8524	SM1_25 1/1 1.0132	SM1_31 1/1 1.1024	SM1_37 1/1 1.2585	SM1_43 1/1 1.3492	SM1_49 1/1 1.4708	SM1_55 1/1 1.5935	SM1_61 1/1 0.2725	SM1_69 1/1 0.232
B	SM1_2 1/1 0.1962	SM1_8 1/1 0.4882	SM1_14 1/1 0.8598	SM1_20 1/1 0.869	SM1_26 1/1 1.0277	SM1_32 1/1 1.2651	SM1_38 1/1 1.3202	SM1_44 1/1 1.4498	SM1_50 1/1 1.527	SM1_56 1/1 1.6003	SM1_62 1/1 0.5394	SM1_70 1/1 0.523
C	SM1_3 1/1 0.1364	SM1_9 1/1 0.506	SM1_15 1/1 0.7499	SM1_21 1/1 0.7896	SM1_27 1/1 0.7875	SM1_33 1/1 0.7832	SM1_39 1/1 0.8577	SM1_45 1/1 0.8684	SM1_51 1/1 0.9514	SM1_57 1/1 1.2134	SM1_63 1/1 0.7077	SM1_71 1/1 0.6593
D	SM1_4 1/1 0.2927	SM1_10 1/1 0.5307	SM1_16 1/1 0.7353	SM1_22 1/1 0.7768	SM1_28 1/1 0.7715	SM1_34 1/1 0.79	SM1_40 1/1 0.8063	SM1_46 1/1 0.8595	SM1_52 1/1 0.8936	SM1_58 1/1 0.9071	SM1_64 1/1 0.9085	SM1_72 1/1 0.9294
E	SM1_5 1/1 0.3475	SM1_11 1/1 0.158	SM1_17 1/1 0.2158	SM1_23 1/1 0.4	SM1_29 1/1 0.2125	SM1_35 1/1 0.2800	SM1_41 1/1 0.2864	SM1_47 1/1 0.1812	SM1_53 1/1 0.2549	SM1_59 1/1 0.3514	SM1_65 1/1 1.082	SM1_73 1/1 1.0782
F	SM1_6 1/1 0.219	SM1_12 1/1 0.2498	SM1_18 1/1 0.2316	SM1_24 1/1 0.2712	SM1_30 1/1 0.2496	SM1_36 1/1 0.7923	SM1_42 1/1 1.402	SM1_48 1/1 1.3281	SM1_54 1/1 1.027	SM1_60 1/1 1.0899	SM1_66 1/1 1.2402	SM1_74 1/1 1.1969
G	ST1_1 1/2 1.7755	ST1_2 1/2 1.7785	ST1_3 1/2 1.8005	ST1_4 1/2 1.772	ST1_5 1/2 1.6598	ST1_6 1/2 1.4865	ST1_7 1/2 1.1212	ST1_8 1/2 0.7807	ST1_9 1/2 0.7614	ST1_10 1/2 0.5926	SM1_67 1/1 1.3477	SM1_75 1/1 1.3071
H	ST1_1 2/2 1.7473	ST1_2 2/2 1.8109	ST1_3 2/2 1.806	ST1_4 2/2 1.7422	ST1_5 2/2 1.6344	ST1_6 2/2 1.4864	ST1_7 2/2 1.1282	ST1_8 2/2 0.7774	ST1_9 2/2 0.5328	ST1_10 2/2 0.6222	SM1_68 1/1 1.4353	SM1_76 1/1 1.4466

```
Measurement parameters
~~~~
Number of plates: 4
---
Infinite 200
Instrument serial number: 510000008
```

The Workspace Overview is composed of the following elements:

- **Plate Layout** window: data for each well is displayed in the plate layout (for example: raw data). 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.

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… Optimize Z-Position… Injector Control… Start Measurement…

7.4.2 Toolbar Menu: File

ASCII File Export

In the **File** menu, click **ASCII File Export** to export data as ASCII (.asc) files so that other programs can read and process the data provided by magellan.

Before data can be exported, 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.

The **Save as** dialog box is a standard Windows dialog box, with file navigation elements, a text field for entering a file name, a drop down list for the selection of a file type (*.asc) and **Save** and **Cancel** buttons.

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

In the **File** menu, 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

In the **File** menu, click **Method Export...**.

In some cases the user will request to save the method definition of a workspace as a method file. These method files can be opened and modified.

The folder to save the method in must be selected and the desired file name needs to be entered. Additionally some comments can be added in the **Remarks** text field.

Click the **Save** button to save the current measurement data into a method file. **Cancel** will cancel the current operation.

The **Save as** dialog box is a standard Windows dialog box, with file navigation elements, a text field for entering a file name, a drop down list for the selection of a file type (*.tst), **Save** and **Cancel** buttons.

An additional **Remarks** text field provides a possibility to add useful information or remarks to the method file.

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.

> ***Note***
>
> ***After the*** magellan ***30-day demo license has expired, printing will not be possible.***

Print Preview

In the **File** menu, click **Print Preview....**to see exactly how a print-out will appear without actually having to print the document.

The **Print Preview** window contains the following elements:

Print... button	Click this button to close the print preview window and the **Print** dialog box appears. The current document can be printed.
Next Page button	Click this button to view additional page(s).
Prev. Page button	Click this button to view previous page(s).
One Page / **Two Page** button	Toggle switch: shows either a single page or two pages of the document.
Zoom In button	The shown page is zoomed in.
Zoom Out button	The shown page is zoomed out.
Close button	Closes the print preview window.
Document area	In the main area, the pages of the document are shown as they would look when printed.

Printer Setup

In the **File** menu, 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

In the **File** menu, click **Printout Font…** to select a specific font, font style, font size, font color etc. for future printouts.

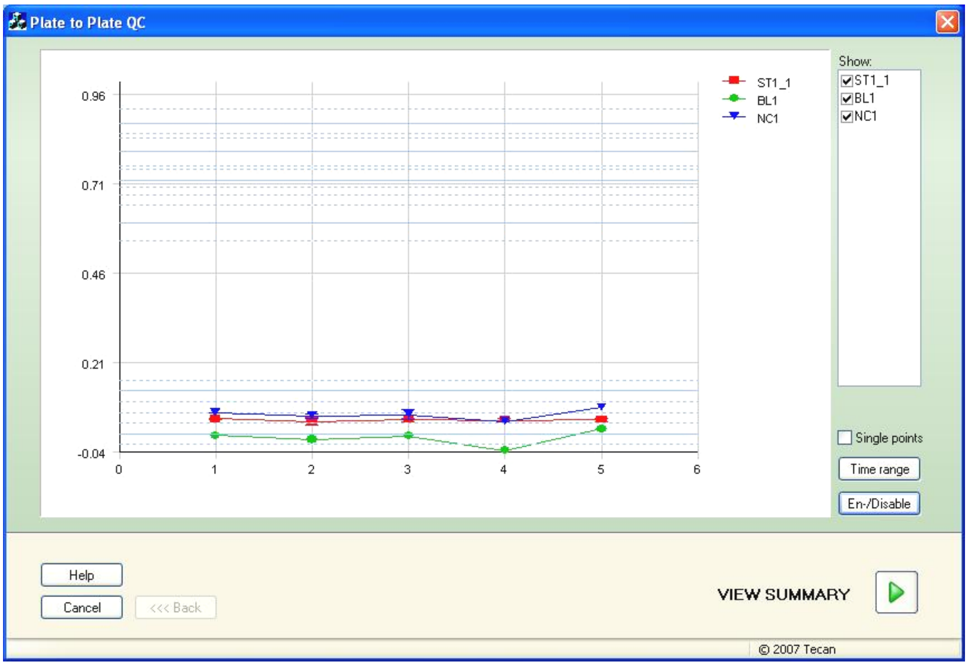
These settings will have no effect on the screen display, so it will be difficult to judge the effect these setting have on the printout. Large fonts should be avoided to prevent errors or misrepresentation of data.

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

In the **File** menu, click **Plate to Plate QC** and the *Levy-Jennings-Graph* window appears. The Levy-Jennings-Graph displays the trend of the control values.



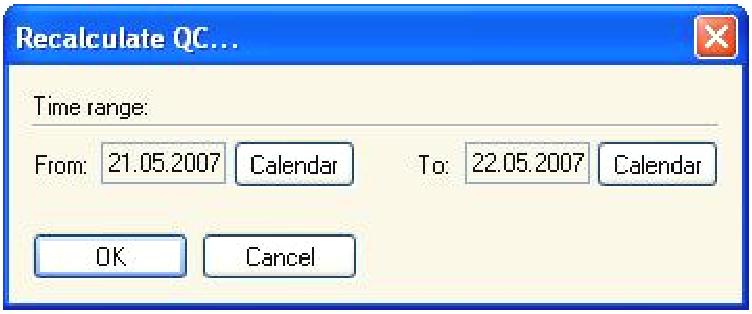
On the y-axes, the data values (raw data, concentrations, etc.) as set in the method definition) are applied and on the x- axes, the time range in days is applied.

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, measurement date and time and rule violated, if any). Use the check boxes of the single elements of the **Show** list to select various controls to be displayed.

Time Range

Beside the graph, next to **Show**, various controls can be selected to be displayed. Click **Time range** and the following window appears:



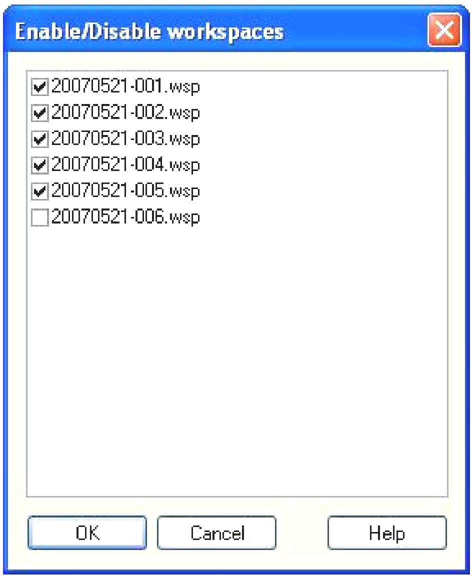
From: 21.05.2007

To: 22.05.2007

Select an appropriate time range to be displayed.

Select Workspaces

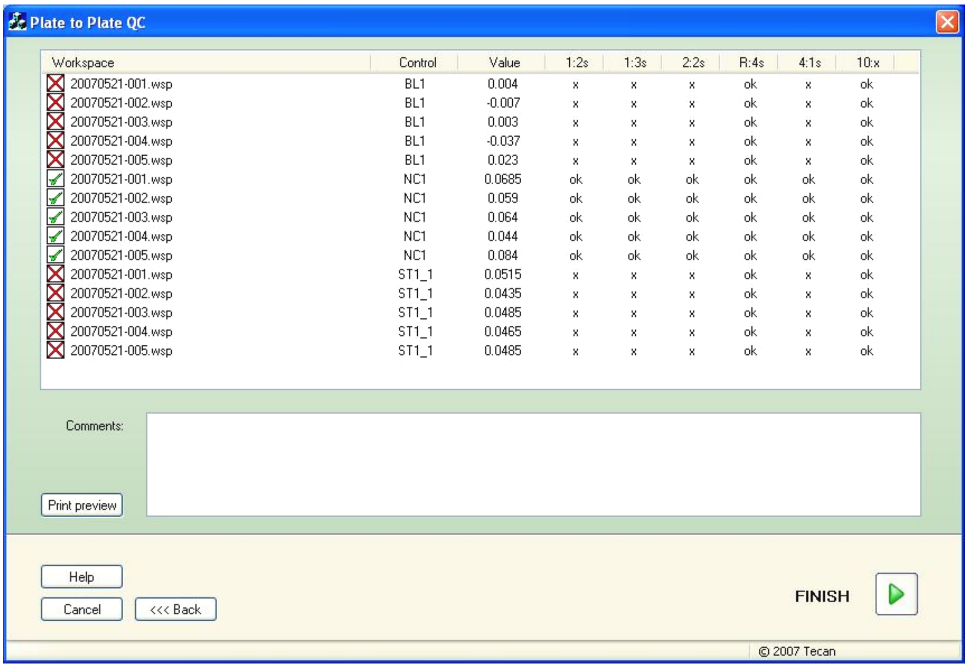
Click **En-/Disable** to enable or disable certain workspaces for evaluation.



☑ 20070521-001.wsp
☑ 20070521-002.wsp
☑ 20070521-003.wsp
☑ 20070521-004.wsp
☑ 20070521-005.wsp
☐ 20070521-006.wsp

Data Sheet

Click **View summary** and the **Data sheet** window appears:



Workspace	Control	Value	1:2s	1:3s	2:2s	R:4s	4:1s	10:x
☒ 20070521-001.wsp	BL1	0.004	x	x	x	ok	x	ok
☒ 20070521-002.wsp	BL1	-0.007	x	x	x	ok	x	ok
☒ 20070521-003.wsp	BL1	0.003	x	x	x	ok	x	ok
☒ 20070521-004.wsp	BL1	-0.037	x	x	x	ok	x	ok
☒ 20070521-005.wsp	BL1	0.023	x	x	x	ok	x	ok
☑ 20070521-001.wsp	NC1	0.0685	ok	ok	ok	ok	ok	ok
☑ 20070521-002.wsp	NC1	0.059	ok	ok	ok	ok	ok	ok
☑ 20070521-003.wsp	NC1	0.064	ok	ok	ok	ok	ok	ok
☑ 20070521-004.wsp	NC1	0.044	ok	ok	ok	ok	ok	ok
☑ 20070521-005.wsp	NC1	0.084	ok	ok	ok	ok	ok	ok
☒ 20070521-001.wsp	ST1_1	0.0515	x	x	x	ok	x	ok
☒ 20070521-002.wsp	ST1_1	0.0435	x	x	x	ok	x	ok
☒ 20070521-003.wsp	ST1_1	0.0485	x	x	x	ok	x	ok
☒ 20070521-004.wsp	ST1_1	0.0465	x	x	x	ok	x	ok
☒ 20070521-005.wsp	ST1_1	0.0485	x	x	x	ok	x	ok

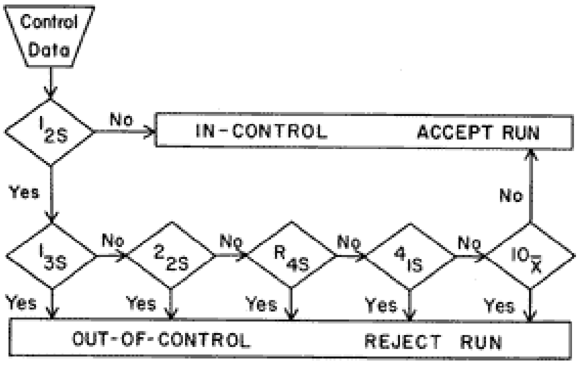
The **Data sheet** dialog box contains the following elements:

Workspace column	Contains a list of the evaluated workspace files. On the left hand side of the workspace name, the result of the multirule Westgard® evaluation is displayed (see below). A green checkmark indicates fulfillment, a red cross indicates failure.
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 non 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, which will appear on the printout .
Print Preview button	Preview of the printout, which contains 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	Control rule to test whether a control measurement exceeds the control limits of **x + 2SD or x - 2SD**. This rule is used as a warning rule to trigger careful inspection of the control data by the following control rules. 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. 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**“.
1:3s	Control rule to test whether a control measurement exceeds the control limits of **x + 3SD or x - 3SD**. A run is rejected if a single control measurement exceeds the mean plus 3s or the mean minus 3s control limit.
2:2s	Control rule to test whether two consecutive control measurements exceed the same control limit of either **x + 2SD or x - 2SD**. A run is rejected if 2 consecutive control measurements exceed the mean plus 2s or the mean minus 2s control limit.
R:4s	Control rule to test whether the range, or difference, between control measurements exceeds 4SD. 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.
4:1s	Control rule to test whether four consecutive control measurements exceed the same control limit of either **x + 1SD or x - 1SD**. A run is rejected if 4 consecutive control measurements exceed the mean plus 1s or the mean minus 1s control limit.
10:x	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.

7.4.3 Toolbar Menu: Edit

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

Copy to Excel

In the **Edit** menu, click **Copy to Excel** or press **CTRL-X**.

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

The necessary options, regarding the copying of the data to Excel, can be defined in the **Options** dialog box. Refer to chapter 10.3.2 Copy/Export Options.

First the relevant wells must be selected with the mouse. If more than one non-adjacent well field must be selected, press the **Control** key while clicking the requested fields. If no wells are selected, all wells will be copied.

Once all wells are selected, the **Copy to Excel** function transfers the well data into an Excel worksheet.

Copy in ASCII-Format

In the **Edit** menu, click **Copy in ASCII format** or press **CTRL+C**. Additionally, in sample ID list documents **Copy in ASCII format** can be accessed via the context-sensitive menu.

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. The copied data can be pasted into any suitable kind of file.

The necessary options, regarding the style of the data which is copied to the clipboard, can be defined in the **Options** dialog box. Refer to chapter 10.3.2 Copy/Export Options.

First the relevant wells must be selected with the mouse. If more than one non-adjacent well field must be selected, press the **Control** key while clicking on the requested fields.

Once all desired wells are selected, the **Copy in ASCII format** function transfers the well data into the clipboard.

The data can be pasted into any other software application if the application provides the paste function and accepts data in ASCII format.

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 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.

For polarization measurement, the parallel and perpendicular RFU values can be changed.

Insert Sample ID list

For detailed information see 6.6 Start Measurement - Insert Sample ID List.

Recalculate with another Method

In the **Method** menu, click **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

Movements

For detailed information see 3.1.1 Movements... .

Temperature Control

For detailed information see 3.1.2 Temperature Control... .

Optimize Z-Position

For detailed information see 3.2.4 Optimize Z-Position.

Injector Control

For detailed information see 3.1.5 Injector Control... .

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 6.6 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 mean values or statistics of the replicates:

- Raw data (absorbance, fluorescence intensity or luminescence, single wavelength measurement)
- Measurement data/Reference data (absorbance dual wavelength only)
- RFU – parallel/perpendicular
- Raw data statistics (mean, standard deviation, variation coefficient)
- Raw data as colors
- Single raw data as colors for multiple reads per well measurements
- Kinetic graph for kinetic measurements. The graphs are displayed in the plate layout.
- Spectrum data (for scans)
- Label 1, 2 … (for multilabel measurements)
- Count rate (for FLT measurements)

7.4.8 Control Bar: Reduced Data

- Difference data (Reference data subtracted from Measurement data)
- Polarization, Anisotropy, Total Intensity, Intensity – parallel/perpendicular, Blank Reduction – parallel/perpendicular
- Blank-reduced spectra, smoothed spectra, peak intensity, wavelength peak

7.4.9 Control Bar: Transformed Data

The user can select the required transformation to display the calculated results:

- Transformation[n] results
- Transformation[n] – statistics (mean, standard deviation, variation coefficient)
- Transformation[n] as colors
- Transformation[n] kinetic graph for kinetic measurements and transformations with kinetic results

7.4.10 Control Bar: Kinetic Parameters

The user can select the kinetic evaluation as defined:

- Mean slope OD/RFU/RLU/mP / sec
- Mean slope OD/RFU/RLU/mP / min
- Mean slope OD/RFU/RLU/mP/ hr
- Goodness of fit (Mean slope)
- Correlation coeff.
- Max slope OD/RFU/RLU /mP/ sec
- Max slope OD/RFU/RLU /mP/ min
- Max slope OD/RFU/RLU /mP/ hr
- Time max. slope sec
- Time Onset OD/RFU/RLU/mP, Basis OD/RFU/RLU/mP, Time Basis OD/RFU/RLU/mP, Time Basis to Onset OD/RFU/RLU/mP and the same for percentage calculation
- Minimum OD/RFU/RLU/mP, Time minimum OD/RFU/RLU/mP
- Maximum OD/RFU/RLU/mP, Time maximum OD/RFU/RLU/mP
- Area OD/RFU/RLU/mP*sec
- Graph: Enzyme Kinetics
  Click this option to open the **Graph: Enzyme Kinetics** dialog box
- If kinetic transformations have been defined the results of the kinetic transformations can be selected.

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

EXPERT'S KNOW HOW

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 4.3.8 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
- If concentration transformations have been defined the results of the concentration transformations can be selected.
- 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 options displays the **Printer Setup** dialog box.
- **Exit** is selected to exit the standard curve dialog box.
  If any modifications have been made, for example a change of interpolation process, a new calculation will be performed.

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

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	Cancels 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.

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. This overview is particularly useful, if the cutoff limits are defined as formulas.

In the data information window on the bottom of the screen, the list of cutoff definitions is displayed. The list contains the experimental groups, the input data for each experimental group, the cutoff ranges, the cutoff formulas, and the calculated cutoff limits.

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.

- Sample ID 1
- Sample ID 2
  if available
- Sample ID 3
  if available
- Pipetting status
  if available

7.4.14 Control Bar: Method Layout

The user can view the method layout.

- Well positions
  for example: A1, B1
- Strip method names
  Available if a strip method was used
- Original concentrations
  Concentrations originally assigned to standards
- Dilution factors
  Dilution factors previously assigned to samples
- Layout
  Layout of the identifiers
- Replicate Info
  Replicate number and maximum number of replicates of the corresponding identifiers.
- Measurement parameters

7.4.15 Control Bar: QC Validation

The validations are the criteria that determine the validity of a test. They are defined in the method.

In the data information window, the list of validations is displayed. The list contains the experimental groups, the input data for each validation group, the validation formulas and their results (TRUE or FALSE) are displayed.

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.

- Remarks
- Error protocol
- Constants
- Results

7.4.17 Color Scale Dialog 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, offering the following commands:

Summary	The **Summary** dialog box is displayed.
Details	The **Multipoint Measurement** dialog box is displayed to show the single measurement points per well.
Edit	The **Edit** dialog box is displayed (for Raw Data only).
Edit kinetic settings	Opens the **Kinetic parameters** dialog box and offers the ability to modify the kinetic settings for the selected well(s).
Copy kinetic settings	Copies the kinetic settings of the selected well(s) into the clipboard.
Paste kinetic settings	Assigns the kinetic settings from the clipboard to the selected well(s).
Graph: Multilabel…	The graph displays data of selected well(s). The raw data versus well IDs is displayed.
Graph: Kinetics…	The graph of the **kinetic** measurement is displayed for the selected well(s).
Graph: Multilabel kinetics…	The graph of the **multilabel kinetics** measurement is displayed for the selected well(s).
Graph: Spectra…	The graph of the **spectra** is displayed for the selected well(s).
Graph: Dilution Series…	The graph of the **dilution** series is displayed for the selected well(s).
Mask/Unmask selection	Toggle switch that masks or unmasks measurement values in the selected well. If the user selects to mask a well in a kinetic or multilabel measurement, a dialog box appears asking whether the user wants to mask/unmask all data of the well. No calculations are performed for the masked well.
Show/Hide layout	Toggle switch to show or hide the graph or measurement values in the individual wells. The information will not be printed or exported. Where information has been blanked out, the word **Hidden** will appear on the relevant well. The **Show/Hide Layout** button opens no window or dialog box; the **Show/Hide Layout** process is executed instantly as a background process.

EXPERT'S KNOW HOW

Setting different kinetic parameters for different wells is only possible when using the context sensitive menu of a well in the plate layout window or when using the context sensitive menu in the kinetic graph dialog. By editing the kinetic parameters on the Edit method tab, the kinetic parameters are set equal for all wells.

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: • 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: • **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.
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). For polarization measurements only the RFU values can be edited.
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

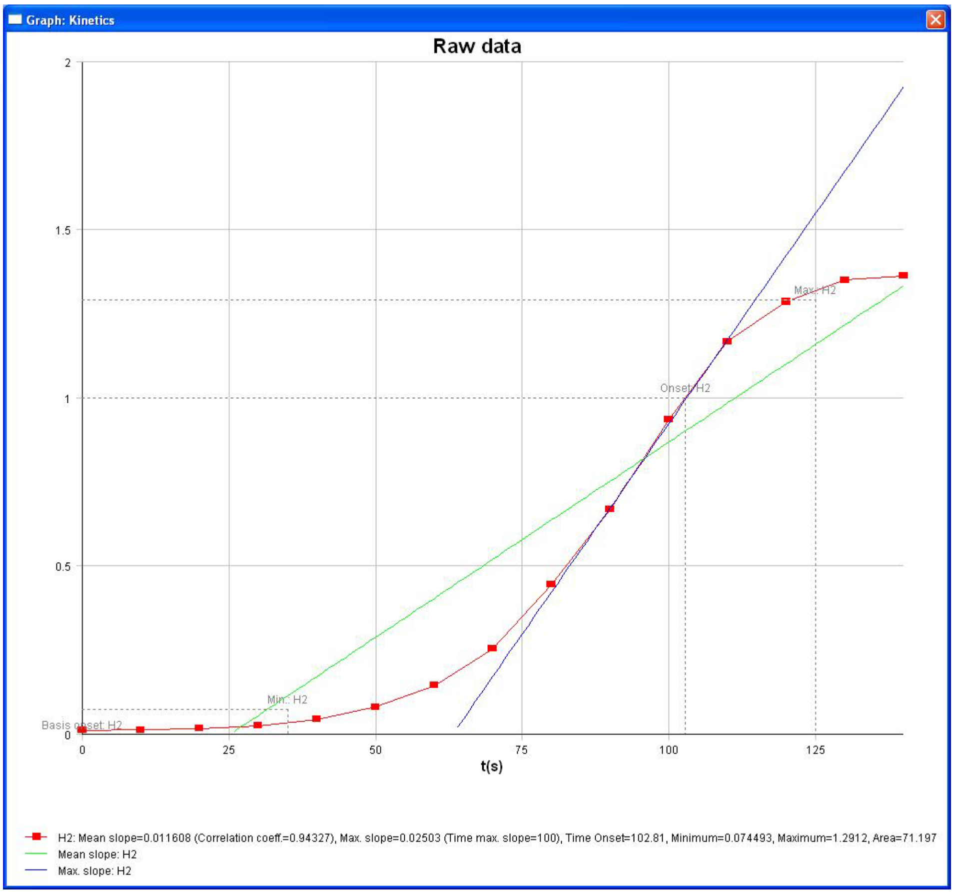
The **Graph: Kinetics** dialog box displays the graphs of kinetic measurements of one or more selected wells. The legend contains the calculated kinetic parameters.

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.



H2: Mean slope=0.011608 (Correlation coeff.=0.94327), Max. slope=0.02503 (Time max. slope=100), Time Onset=102.81, Minimum=0.074493, Maximum=1.2912, Area=71.197

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

Context-Sensitive Menu of 3D Spectra Graph

By right-clicking on the upper dialog frame, a context-sensitive menu is displayed.

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.
Data as Table	Opens a dialog box showing the spectrum as table. This allows copying the data to Excel or exporting in ASCII format.
Save as Bitmap	Saves the graph as a bitmap.

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.***

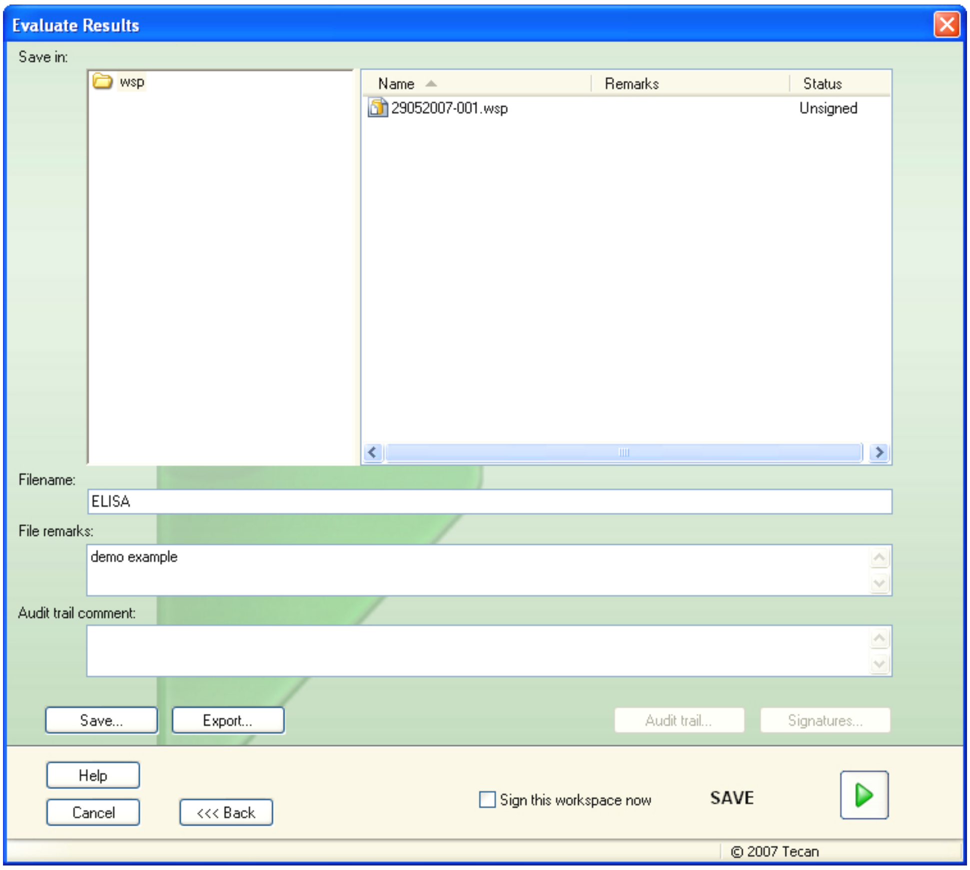
7.5 Edit Method Tab

Note
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

Note
The Edit method tab is displayed only if the currently working user has the appropriate rights
(cf. chapter 10.4.4 User Rights (magellan Tracker) and chapter 10.5.4 User Rights (magellan Standard).

7.6 Saving the Evaluated Results

Click **Next** on the **Results** dialog box to reach the **Save in** dialog box of the **Evaluate Results wizard**:



29052007-001.wsp Unsigned

Filename: ELISA

File remarks: demo example

Audit trail comment:

☐ Sign this workspace now

The **Evaluate Results** dialog box has the following elements:

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 as 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 using the name entered in the filename field.
Export…	Click this button to open the Export dialog (see chapter 4.3.14 Data Handling: Data Export).
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).

The **Evaluate Results** wizard **is** finished by pressing the **FINISH** button. In case of unsaved changes a message box appears asking the user to perform the saving.

An additional **Save** button is available for saving the data without closing the wizard.

8. Attach Signature Wizard

8.1 Introduction

Signatures are essential in assuring trustworthy records. Electronic signatures and electronic records have come to carry the same force and effect as handwritten signatures and records.

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.***

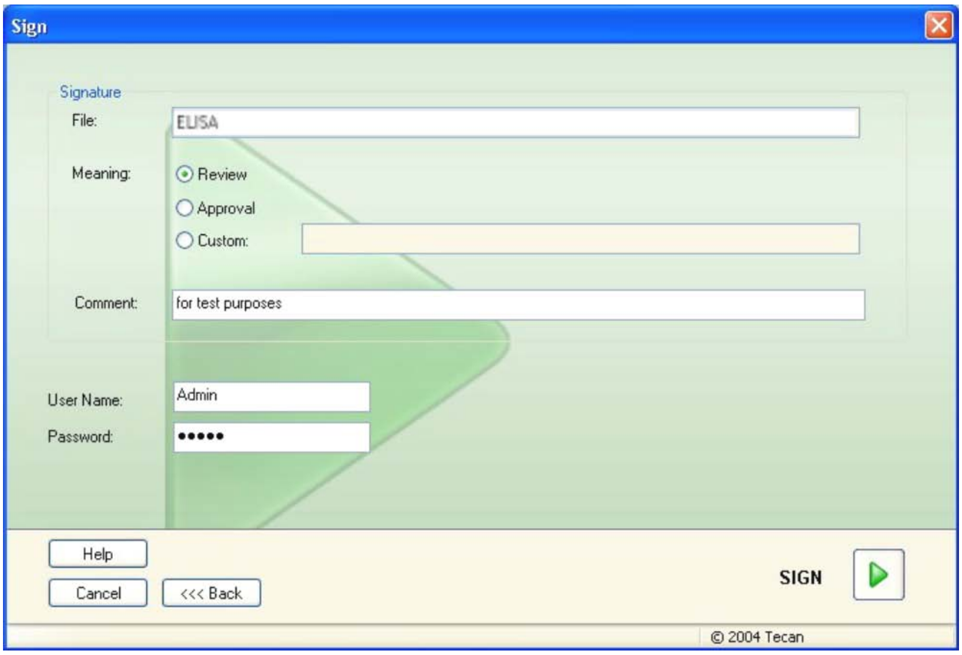
Click **Attach signature** to start the **Attach signature** wizard.

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:



Sign

Signature

File: ELISA

Meaning: ● Review ○ Approval ○ Custom:

Comment: for test purposes

User Name: Admin

Password: •••••

In the **Signature** group box, the following options are available:

Review	Can only be signed by a user with the appropriate rights.
Approval	Can only be applied by a user with the appropriate rights, if a review signature has already been applied to the record. 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. Batch Processing

9.1 Introduction

magellan supports batch processing with the Tecan **Connect** stacker and supported Tecan readers.

CAUTION
Do not use microplates with covers, when using the *Connect* stacker to perform batch processing.

9.2 Microplate Requirements for Batch Processing

The use of plate types is limited according to the specifications of the connected instrument. See the respective Instructions for Use for details.

Any common microplate ranging from 6 to 1536 well formats conforming to the ANSI/SBS standards (ANSI/SBS 1-2004; ANSI/SBS 2-2004, ANSI/SBS 3-2004 and ANSI/SBS 4-2004) may be used with the **Connect** stacker for batch processing.

Microplates with covers cannot be used with the **Connect**.

PARAMETERS	CHARACTERISTICS
Overall plate height	**From 7.3 mm to 20 mm**
Footprint	**Length = 127.76 mm ± 0.5 mm** **Width = 85.48 mm ± 0.5 mm**
Minimum difference between plate height and skirt height	**≥ 6 mm**

9.3 Hardware Connections

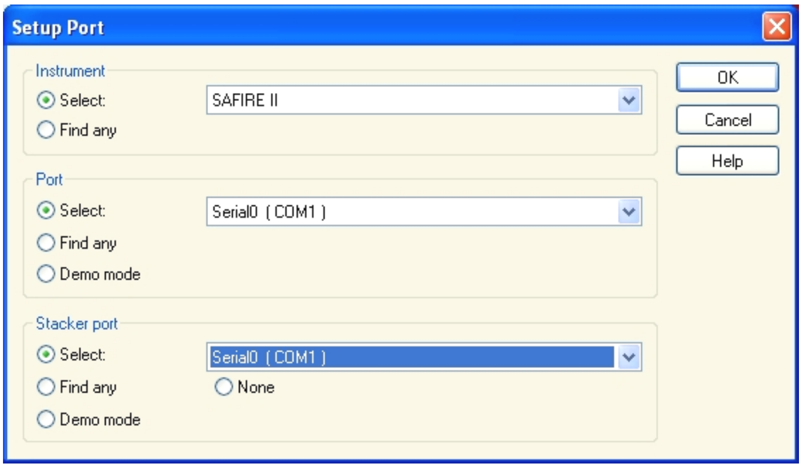
See chapter 3. Unpacking and Installation in the Instructions for Use for **Connect** for complete details about the hardware connections for the reader, stacker and computer.

9.4 Working with Tecan Readers

For **Infinite Series Readers**, see 9.5 Working with Infinite Series Readers.

9.4.1 *Software Connections*

If you want to use the **Connect** stacker with Tecan readers, select the **Stacker port** in the **Setup Port** dialog box to which the **Connect** stacker is connected. Or choose **Find any** to let the software search for a **Connect** stacker and click **OK** (refer to chapter 2.5.4 Connecting a Stacker).



Instrument
● Select: SAFIRE II
○ Find any

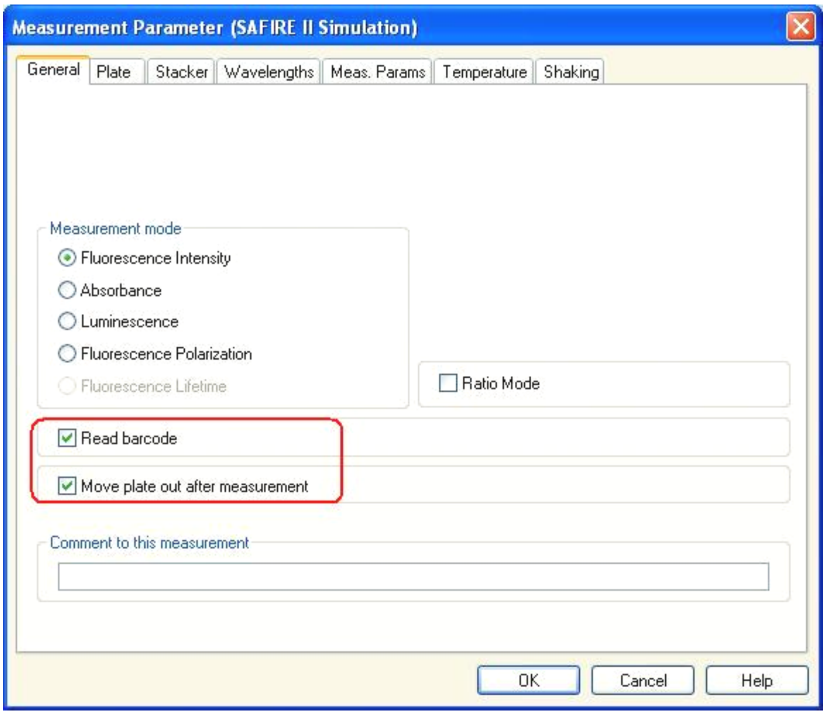
Port
● Select: Serial0 (COM1)
○ Find any
○ Demo mode

Stacker port
● Select: Serial0 (COM1)
○ Find any
○ None
○ Demo mode

9.4.2 *Prepare for Batch Processing*

Measurement Parameter - Read Barcode

In the **Create/Edit a Method** wizard (refer to chapter 4 Create/Edit a Method Wizard), tabs of the **Measurement Parameter** dialog box might contain different parameter settings, depending on the type of instrument connected.



Measurement mode
● Fluorescence Intensity
○ Absorbance
○ Luminescence
○ Fluorescence Polarization
○ Fluorescence Lifetime

☐ Ratio Mode

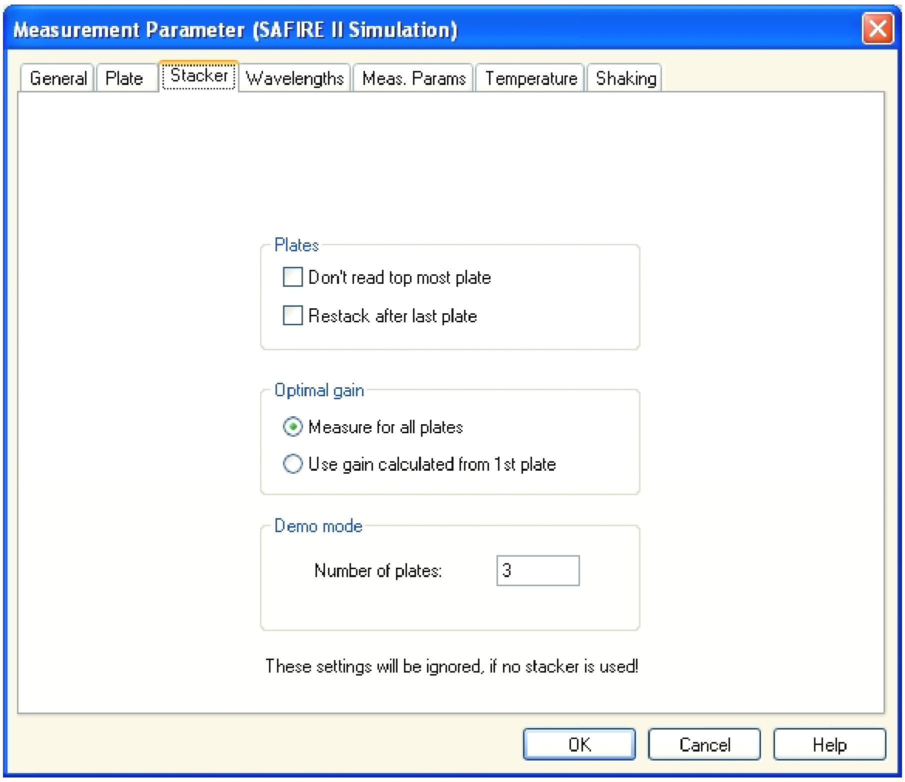
☑ Read barcode

☑ Move plate out after measurement

Comment to this measurement

Note
The option **Read barcode** *can be selected if either the reader or the* **Connect** *stacker has a barcode reader module.*

Measurement Parameter - Stacker Tab



Plates
☐ Don't read top most plate
☐ Restack after last plate

Optimal gain
● Measure for all plates
○ Use gain calculated from 1st plate

Demo mode
Number of plates: 3

These settings will be ignored, if no stacker is used!

The **Stacker** tab of **Measurement Parameter** window contains the following elements:

Plates group:

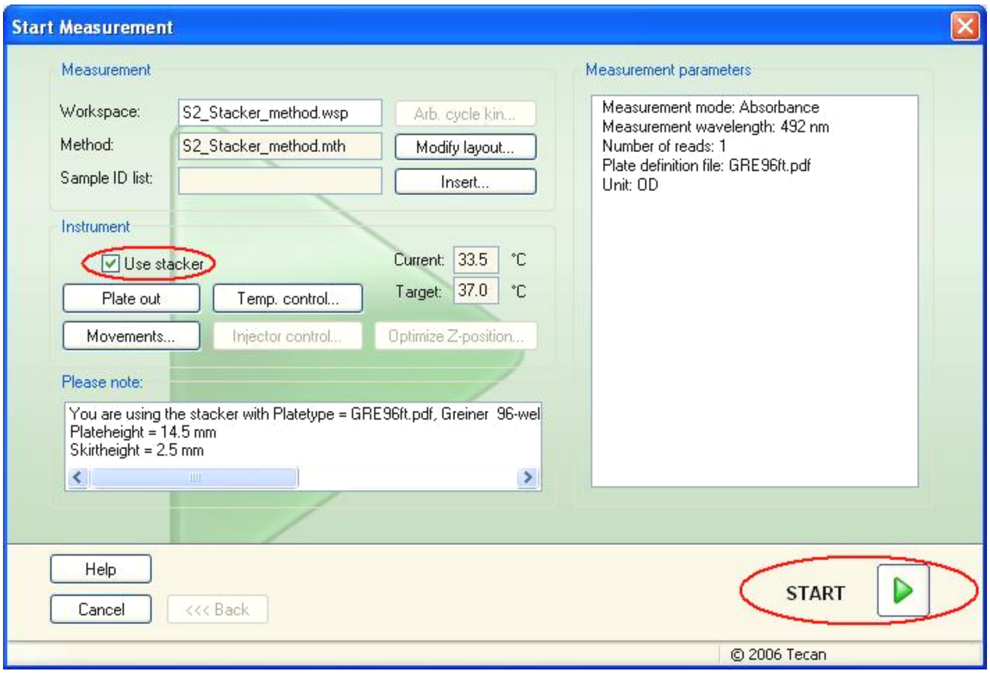
- **Don't read topmost plate**
  Select **Don't read topmost plate** if this plate has been used as a cover. The topmost plate will not be processed and will be moved to the output stack.
- **Restack after last plate**:
  Select **Restack after last plate** to return all plates to their original order in the input stack after all of the plates have been processed.

Optimal gain group:

- **Measure each plate**
  Measure the gain on each plate.
- **Use gain calculated from 1^{st} plate**
  Measure the gain only on the first plate and use this gain for all following plates.

9.4.3 Start Batch Processing

To run a measurement using the Tecan **Connect** stacker, click **Use stacker** in the **Start Measurement** dialog box of **Start Measurement** wizard (refer to chapter 6.6 Start Measurement) or **Create/Edit a Method** wizard (refer to chapter 4 Create/Edit a Method Wizard) and click **Start** to start a stacker run.



Workspace: S2_Stacker_method.wsp
Method: S2_Stacker_method.mth
Sample ID list:

☑ Use stacker

Current: 33.5 °C
Target: 37.0 °C

Please note:
You are using the stacker with Platetype = GRE96ft.pdf, Greiner 96-wel
Plateheight = 14.5 mm
Skirtheight = 2.5 mm

Measurement mode: Absorbance
Measurement wavelength: 492 nm
Number of reads: 1
Plate definition file: GRE96ft.pdf
Unit: OD

9.4.4 Control Stacker Movements

To control the movements of the **Connect** stacker, click the **Miscellaneous** icon in the **Wizard List** dialog box and select **Instrument control**. Click the **Movements…** button in the **Instrument control** dialog box. Depending on the type of instrument connected, **Movements…** dialog box may vary.

If a **Connect** stacker is connected, the **Movements** dialog box additionally contains a **Stacker** group:

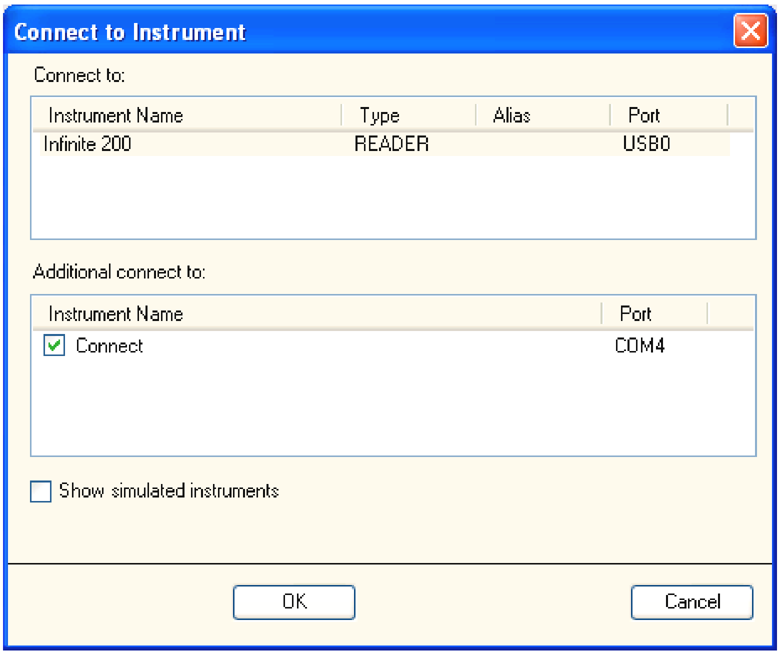
Park position button: The stacker moves the gripper into parking position.

Restack now button: The stacker moves all plates from the output stack into the input stack.

9.5 Working with Infinite Series Readers

9.5.1 Connecting Infinite Series Readers

If an Infinite series reader is selected in the **Port Setup** dialog box, the following dialog box appears when **OK** is clicked:



Instrument Name	Type	Alias	Port
Infinite 200	READER		USB0

Instrument Name	Port
☑ Connect	COM4

☐ Show simulated instruments

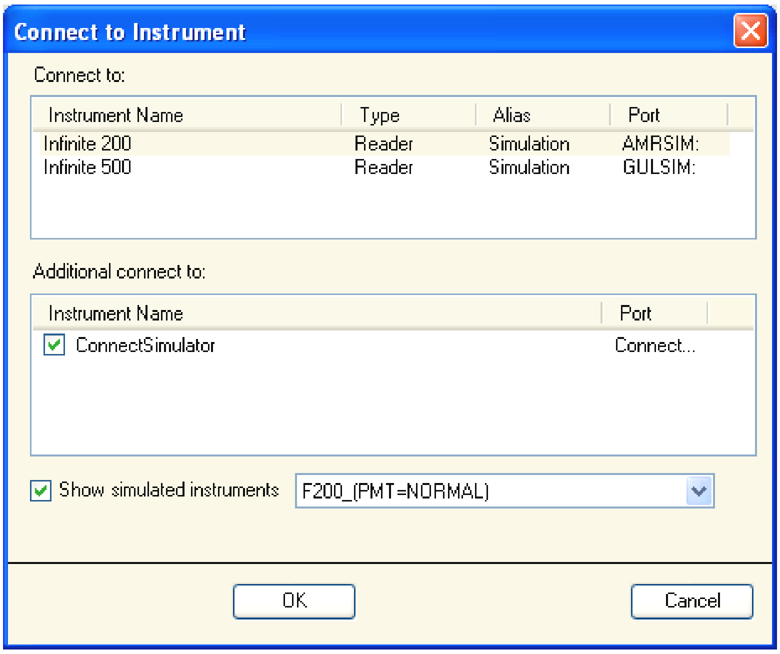
In the **Connect to Instrument** dialog box select the instrument name.

In the **Additionally connect to** field, select **Connect**, if a **Connect** stacker is connected for batch processing.

Click **OK** to confirm selections.

Simulated Instrument

To simulate the use of a **Connect** with an Infinite Series reader, select the **Show simulated instruments** check box and then select the instrument under **Connect to**.



Instrument Name	Type	Alias	Port
Infinite 200	Reader	Simulation	AMRSIM:
Infinite 500	Reader	Simulation	GULSIM:

Instrument Name	Port
☑ ConnectSimulator	Connect...

☑ Show simulated instruments F200_(PMT=NORMAL)

After selecting the simulated instrument, a drop-down list will appear offering several options, depending on the instrument selected above (see screenshot above).

For the Infinite 200, for example, these options are:

- Filter: F200 normal or F200 enhanced or F200 FP Option
- Monochromator: M200 normal or M200 enhanced

In the **Additionally connect to** field, select **ConnectSimulator**, to simulate the **Connect** stacker for batch processing.

Click **OK** to confirm selections.

For a more detailed description on defining parameters for the respective instrument, please refer to the instructions for use for the connected or simulated instrument.

9.5.2 *Prepare for Batch Processing for Infinite Series Readers*

Read Barcode

Plate definition: [GRE384st] - Greiner 384 Flat Transparent

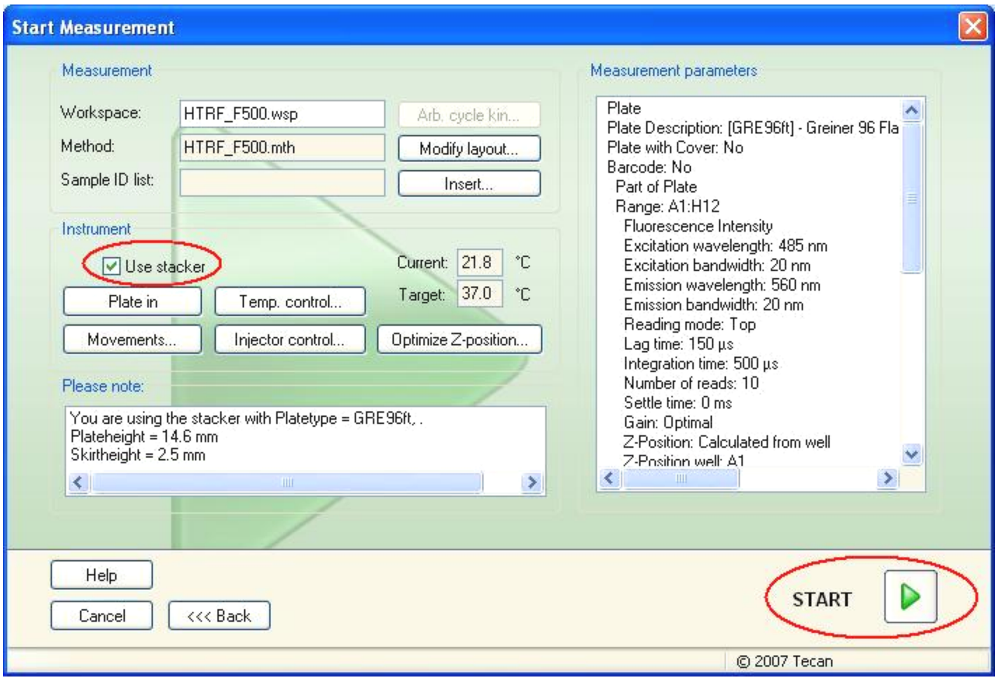
☐ Plate with cover ☑ Read Barcode

The **Read Barcode** checkbox appears in the Plate program element of the magellan software, if the Infinite Series reader has a barcode reader or if a **Connect** stacker is connected and has a barcode reader.

For more information about the Barcode Scanner option for the Infinite Series reader, refer to the Instructions for Use of the corresponding instrument.

9.5.3 Start Batch Processing for Infinite Series Readers

To run a measurement using the Tecan **Connect** Stacker, click **Use stacker** in the **Start Measurement** dialog box of **Start Measurement** wizard (refer to chapter 6.6 Start Measurement) or **Create/Edit a Method** wizard (refer to chapter 4 Create/Edit a Method Wizard).



Workspace: HTRF_F500.wsp
Method: HTRF_F500.mth
Sample ID list:

☑ Use stacker
Current: 21.8 °C
Target: 37.0 °C

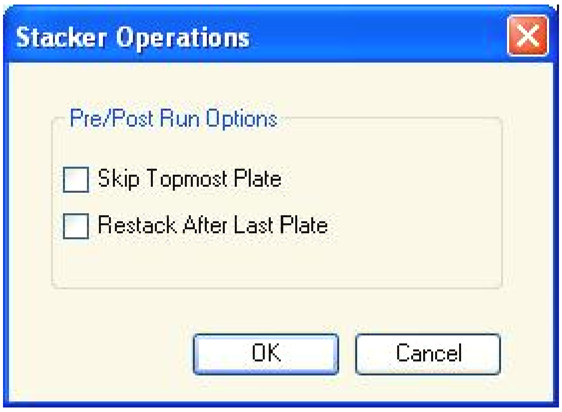
You are using the stacker with Platetype = GRE96ft, .
Plateheight = 14.6 mm
Skirtheight = 2.5 mm

Plate
Plate Description: [GRE96ft] - Greiner 96 Fla
Plate with Cover: No
Barcode: No
Part of Plate
Range: A1:H12
Fluorescence Intensity
Excitation wavelength: 485 nm
Excitation bandwidth: 20 nm
Emission wavelength: 560 nm
Emission bandwidth: 20 nm
Reading mode: Top
Lag time: 150 µs
Integration time: 500 µs
Number of reads: 10
Settle time: 0 ms
Gain: Optimal
Z-Position: Calculated from well
Z-Position well: A1

Click **Start** and the **Stacker Operations** dialog box appears.

Note
The defined script will be performed on each of the available plates in the input stack. It is not possible to run the entire stack more than once per script.

In the **Stacker Operations** dialog box the **Connect** options have to be set.



- Select **Skip topmost plate** if this plate has been used as a cover. The topmost plate will not be processed and will be moved to the output stack.
- Select **Restack after last plate** to return all plates to their original order in the input stack after all of the plates have been processed.

Click **OK** to confirm the settings and start batch processing of all microplates in the input stack.

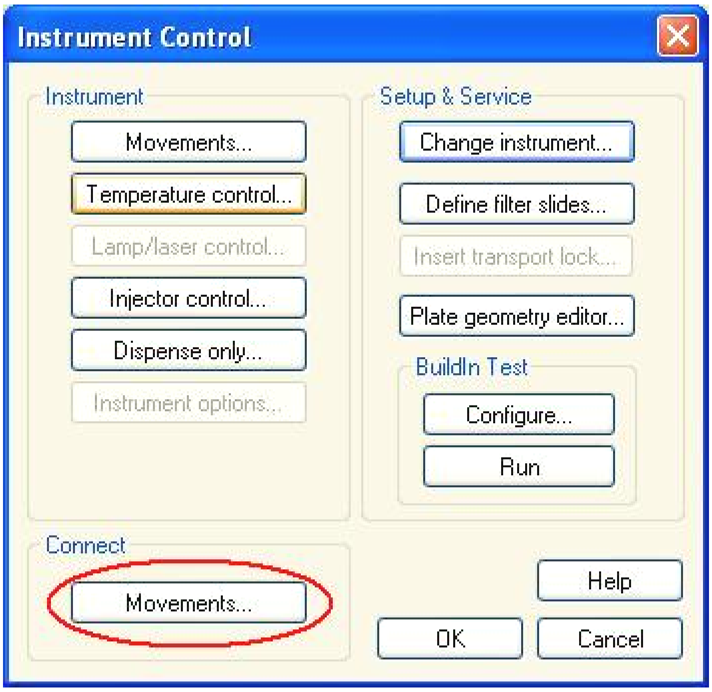
After finishing a batch run the **Evaluate Results Wizard** opens with the first measured workspace (.wsp) opened. If **Read barcode** has been selected in the **Plate** program element, the workspaces will be named according to the corresponding barcode number, otherwise they will be named as defined in the **Workspace Name** dialog box (see chapter 4.3.16 Data Handling: Automated Data Handling / More – Workspace Name).

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

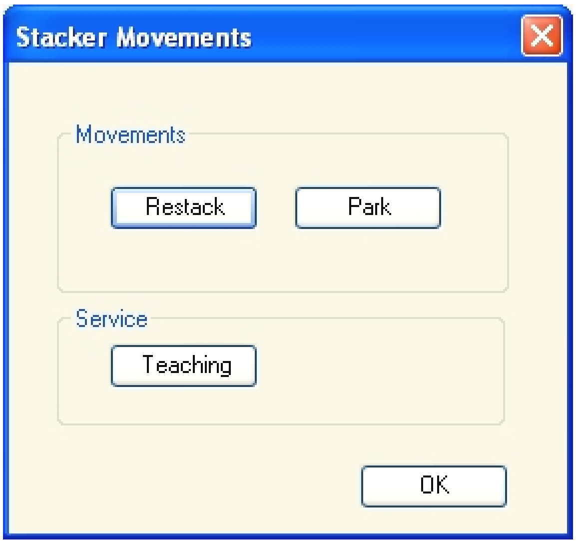
CAUTION
If the reader is operated while positioned within the *Connect* but without using the *Connect*, make sure that the gripper is in the park position and does not hinder any of the reader's moveable parts (e.g. plate carrier, cuvette carrier, filter slide, etc.).

9.5.4 Control Stacker Movements for Infinite Series Readers

To control the movements of the **Connect** stacker, click the **Miscellaneous** icon in the **Wizard List** dialog box and select **Instrument control**. If a **Connect** stacker is connected, the **Movements…** button in the **Connect** group box is now available.



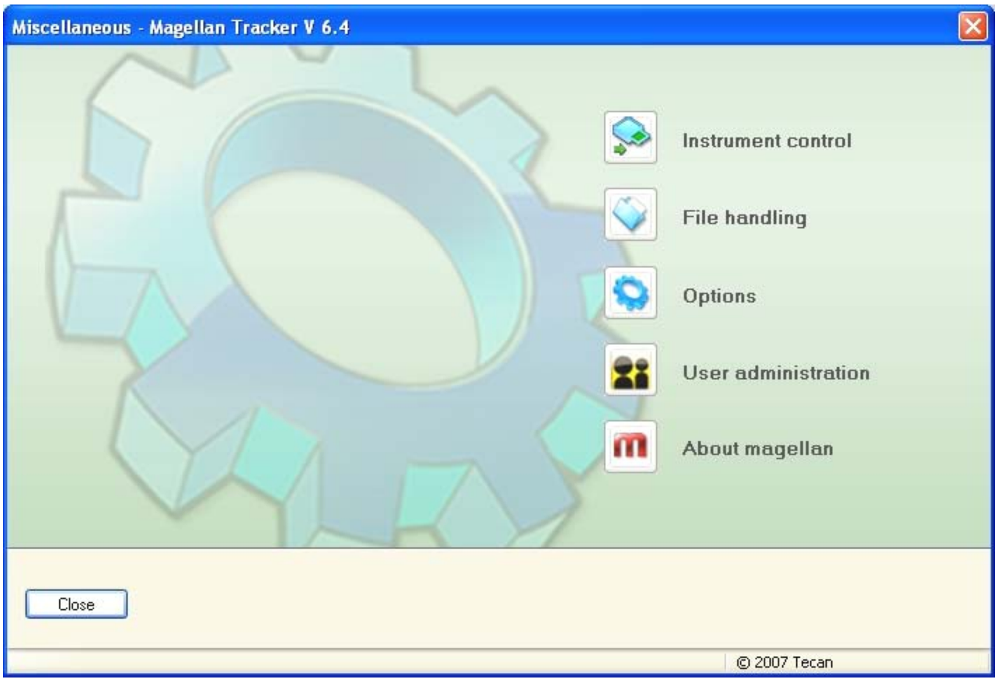
Click the **Movements…** button in the **Connect** group box to open the **Stacker Movements** dialog box.



- Select **Restack** to return the processed plates from the output stack to the input stack in their original order. After Restack is selected, a dialog box appears in which the plate type must be selected and confirmed with **OK**, before the restacking procedure is performed.
- Select **Park** to move the gripper into the park position.
- Select **Teaching** to start the Positioning wizard. For details, see the Instructions for Use for **Connect**, chapter **5. Positioning Wizard in** i-control **and** magellan.

10. Miscellaneous Icon

Click the **miscellaneous** icon in the wizard window and select between the following actions/ definitions:



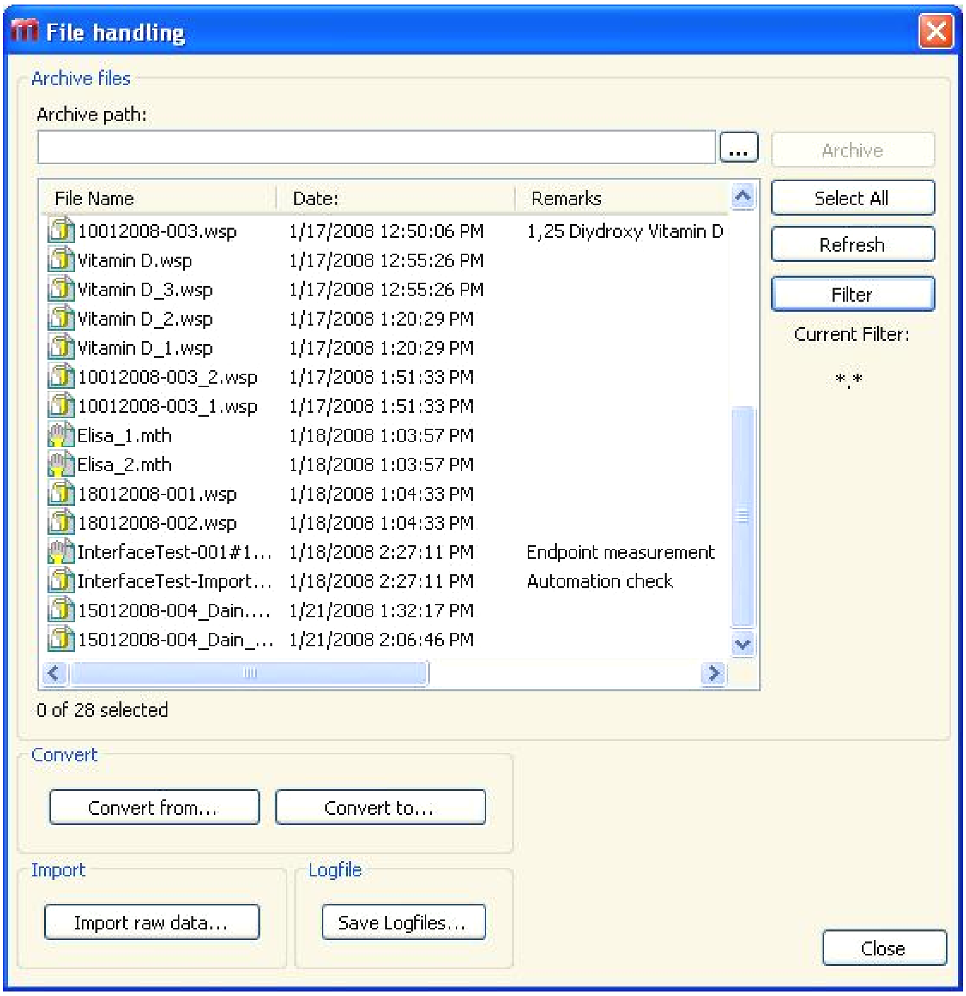
10.1 Instrument Control

See chapter 3 Instrument Control & Settings.

10.2 File Handling

10.2.1 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.



File Name	Date:	Remarks
10012008-003.wsp	1/17/2008 12:50:06 PM	1,25 Diydroxy Vitamin D
Vitamin D.wsp	1/17/2008 12:55:26 PM	
Vitamin D_3.wsp	1/17/2008 12:55:26 PM	
Vitamin D_2.wsp	1/17/2008 1:20:29 PM	
Vitamin D_1.wsp	1/17/2008 1:20:29 PM	
10012008-003_2.wsp	1/17/2008 1:51:33 PM	
10012008-003_1.wsp	1/17/2008 1:51:33 PM	
Elisa_1.mth	1/18/2008 1:03:57 PM	
Elisa_2.mth	1/18/2008 1:03:57 PM	
18012008-001.wsp	1/18/2008 1:04:33 PM	
18012008-002.wsp	1/18/2008 1:04:33 PM	
InterfaceTest-001#1...	1/18/2008 2:27:11 PM	Endpoint measurement
InterfaceTest-Import...	1/18/2008 2:27:11 PM	Automation check
15012008-004_Dain....	1/21/2008 1:32:17 PM	
15012008-004_Dain_...	1/21/2008 2:06:46 PM	

0 of 28 selected

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:

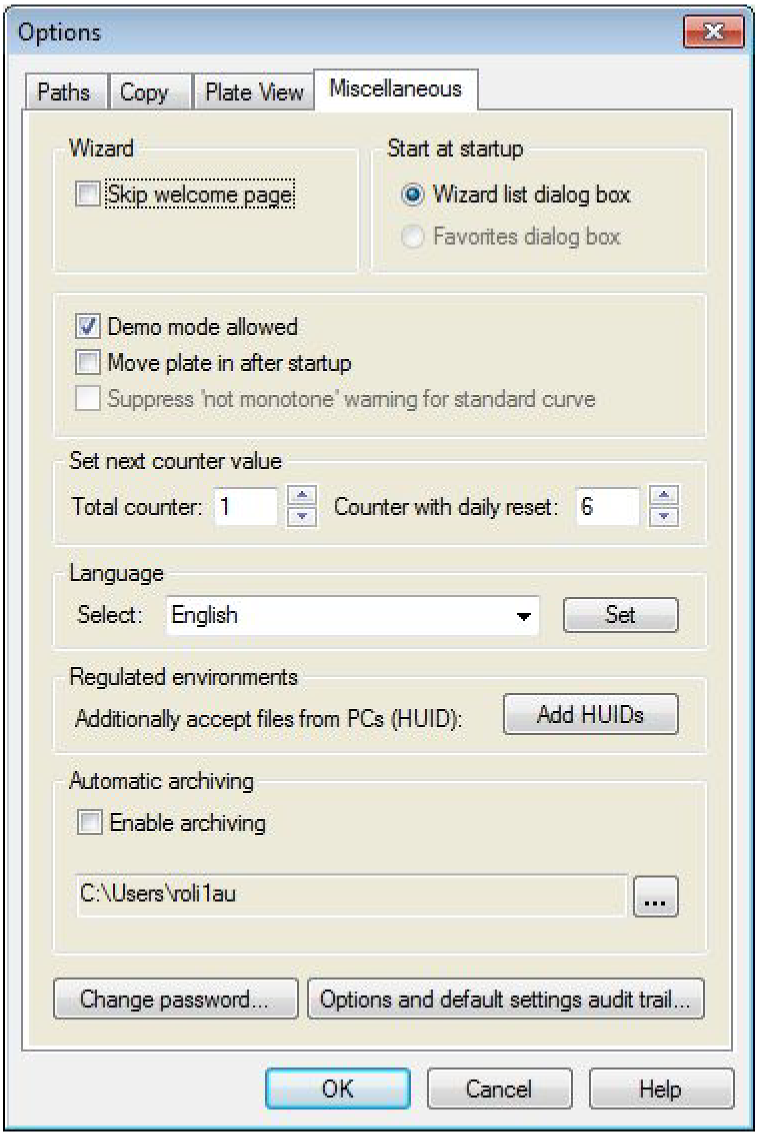
Archive path	The Archive path contains the path where the files shall be stored. Click the browse ... button to change the path.
File Name list	Lists all files saved by magellan filtered by the options entered via the **Filter** button. It consists of three columns: • **File Name** The file names of the workspaces, methods or sample ID lists saved by magellan. • **Date** The date and time a file was saved last. • **Remarks** The remarks entered when saving the file.
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	This button is used to display only specific files, or files, that contain a certain string in their file names. Click the button **Filter** and the Apply Filter dialog box appears: Enter the filter characters for the filter: • 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.

10.2.2 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.



☐ Skip welcome page

● Wizard list dialog box

○ Favorites dialog box

☑ Demo mode allowed

☐ Move plate in after startup

☐ Suppress 'not monotone' warning for standard curve

Total counter: 1

Counter with daily reset: 6

Select: English

Additionally accept files from PCs (HUID):

☐ Enable archiving

C:\Users\roli1au

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.

10.2.3 Import Raw Data

In the **File handling** dialog box, click **Import raw data….** to import measurement data in ASCII (.asc) format. A number of ASCII options make sure that the corresponding files can be opened and that the data is converted correctly.

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. Finally the file appears and the data is retrieved 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	The **Format** option button defines the expected data format: • **Table** (well data in rows) option button • **Table** (well data in columns) option button • **Matrix** (nested) option button • **Matrix** (separated) option button
Separator group box	The **Separator** defines which character is used for the separation of the data fields of the list or matrix: • If **Tabulator** is selected, the separator will be a tabulator. • If **Tabulator** is not selected, the separator will be any character entered in the **Other** text-field.
Orientation option button	The **Orientation** option button allows a definition of the data in either **horizontal** or **vertical** direction.
Measurement Parameters	
Info	The box shows the following parameters: • Plate format • Data unit • Number of measurements • Measurement interval
Measurement Parameters button	Select the measurement type, the plate type, kinetic cycle number and interval.

10.2.4 Convert To

Note
This option is available only when the current user has local administrator rights for the Windows system.

In the **File handling** dialog box, click **Convert To…** to open the *Convert Documents* dialog box.

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.

Important
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: • Sample ID list • Method • Workspace
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.

10.2.5 Convert From

In the **File handling** dialog box, click **Convert From…** to open the *Convert Documents* dialog box.

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.***

> **Important**
> **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: • Sample ID list • Method • Workspace • Test • Plate definition
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 this options correctly in the method and workspace files, use one of the following buttons: • Export to ASCII file… button • Export Options… button • Export to Excel… button • 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.

10.2.6 Save LogFiles

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 Expertline-at@tecan.com for support request.

10.3 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 can not 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.
- Use stacker
- 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:

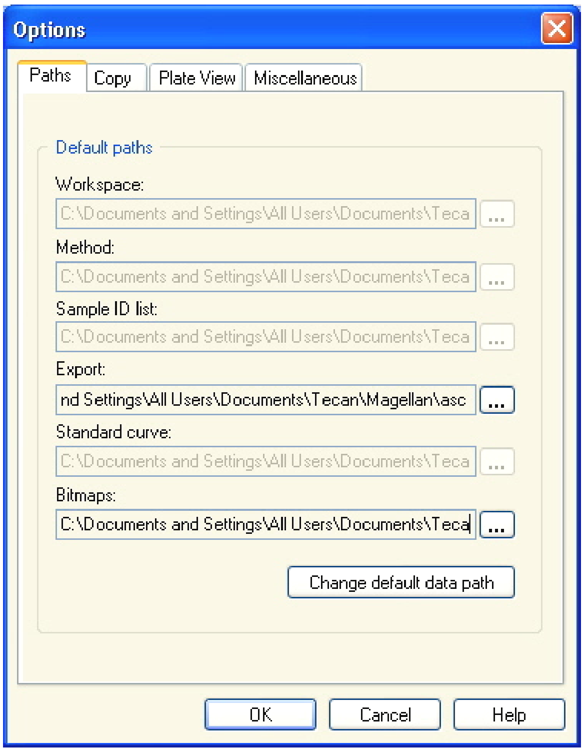
- Language
- Demo mode allowed
- Suppress ‘not monotone’ warning for standard curve
- Favorites
- Accepted HUIDs

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.***

10.3.1 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.



Workspace: C:\Documents and Settings\All Users\Documents\Teca

Method: C:\Documents and Settings\All Users\Documents\Teca

Sample ID list: C:\Documents and Settings\All Users\Documents\Teca

Export: nd Settings\All Users\Documents\Tecan\Magellan\asc

Standard curve: C:\Documents and Settings\All Users\Documents\Teca

Bitmaps: C:\Documents and Settings\All Users\Documents\Teca

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

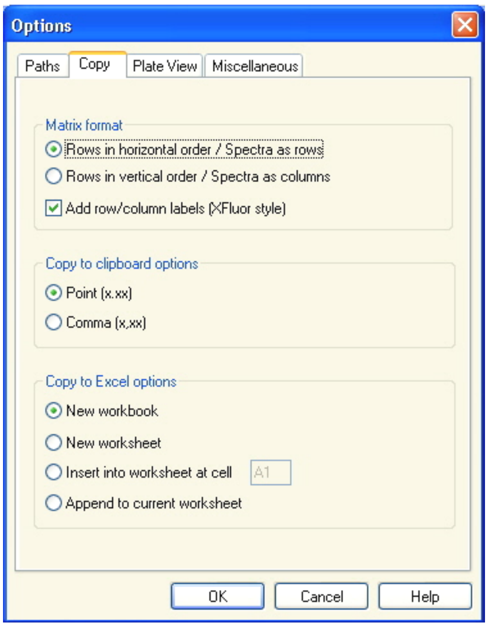
Default paths text fields	A text field for each of the following file types is displayed, containing the corresponding default paths: • **Workspace** • **Method** • **Sample ID list** • **Export:** for measurement data exported to ASCII files. • **Standard curve:** The path for standard curves is always 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.

10.3.2 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.



Matrix format
● Rows in horizontal order / Spectra as rows
○ Rows in vertical order / Spectra as columns
☑ Add row/column labels (XFluor style)

Copy to clipboard options
● Point (x.xx)
○ Comma (x,xx)

Copy to Excel options
● New workbook
○ New worksheet
○ Insert into worksheet at cell A1
○ Append to current worksheet

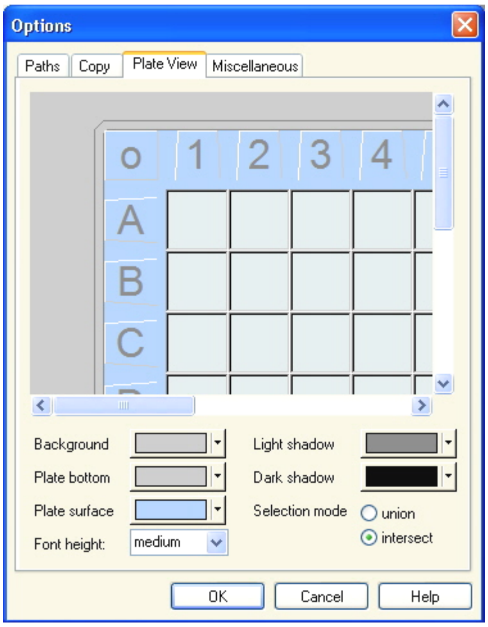
The **Copy** tab contains the following elements:

Matrix format group box	The user also has the following opportunities to define how he would like the data to be displayed. • **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	A format for the decimal point of numbers must be selected for the transferred data: - **Point (x.xxx)** option button Example: 7.893 - **Comma (x,xxx)** option button Example: 7,893
Copy to Excel options group box	The option buttons enable to define where to position the transferred data within Excel. - **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.

10.3.3 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.



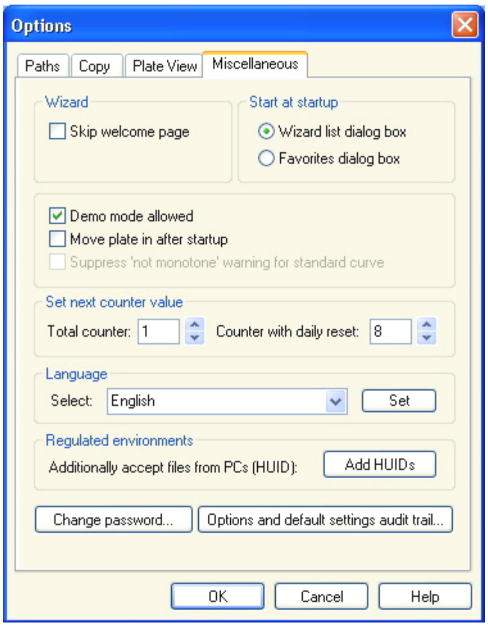
Font height: medium

Selection mode ○ union ● intersect

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

Background button	The background color of the *Pate view* window can be selected.
Plate bottom button	The frame color of the displayed plate can be selected.
Plate surface button	The surface color of the displayed plate can be selected.
Font height drop down list	The font height for the text within the wells can be selected: • Small • Medium • Large
Light shadow button	The light-shadow color of the plate frame can be selected.
Dark shadow button	The dark-shadow color of the plate frame can be selected.
Selection mode option buttons	Here the selection mode for marking wells with the mouse is established: • **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.

10.3.4 Miscellaneous



Wizard
☐ Skip welcome page

Start at startup
● Wizard list dialog box
○ Favorites dialog box

☑ Demo mode allowed
☐ Move plate in after startup
☐ Suppress 'not monotone' warning for standard curve

Set next counter value
Total counter: 1
Counter with daily reset: 8

Language
Select: English

Regulated environments
Additionally accept files from PCs (HUID):

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 *Wizard List* the *Favorite dialog* will show up after the start of the magellan software.
Group box	• **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	Two options are offered: • **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 the course of one day.

Language group box	The text field displays the applied language. A different language can be selected from the drop down list. See **Set** below.
Set button	Select a different language and click the **Set** button to restart the program with the selected language
Change password button	Click this button to open a dialog box, where the user can change his password (only available with magellan User Administration activated).
Add HUIDs button	A list of additional HUIDs can be defined which allows the user to open files created on another computer (only available in magellan Tracker).
Options and default settings audit trail… button	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). 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.

10.4 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.

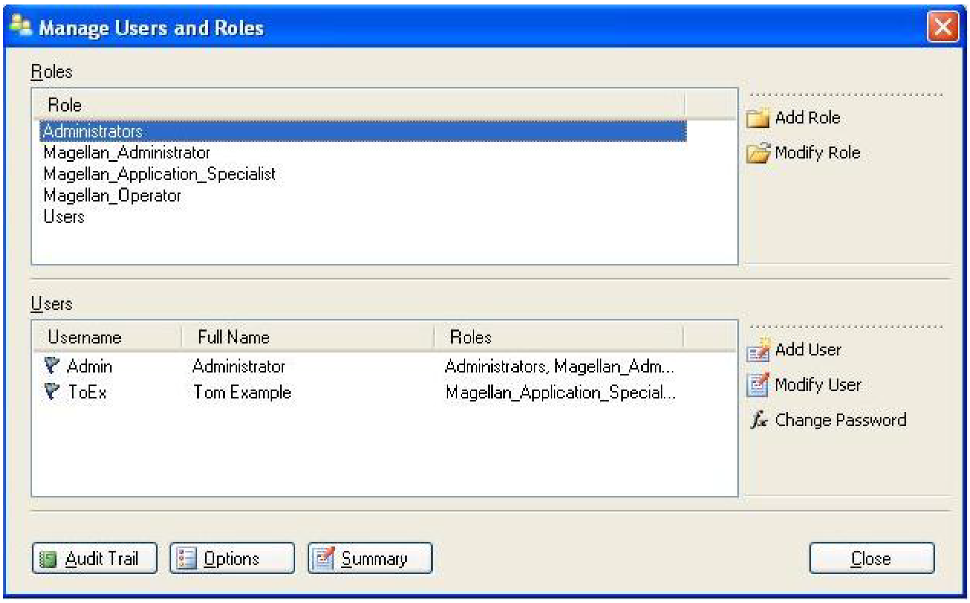
magellan offers password protection to prevent misuse of the software and to restrict access to parts of the software based on user rights.

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 Role** dialog box is displayed:



Manage Users and Roles

Roles

Role
Administrators
Magellan_Administrator
Magellan_Application_Specialist
Magellan_Operator
Users

Users

Username	Full Name	Roles
Admin	Administrator	Administrators, Magellan_Adm...
ToEx	Tom Example	Magellan_Application_Special...

Users and roles can be added and modified, user rights can be defined. Options for login, password, and email can be customized.

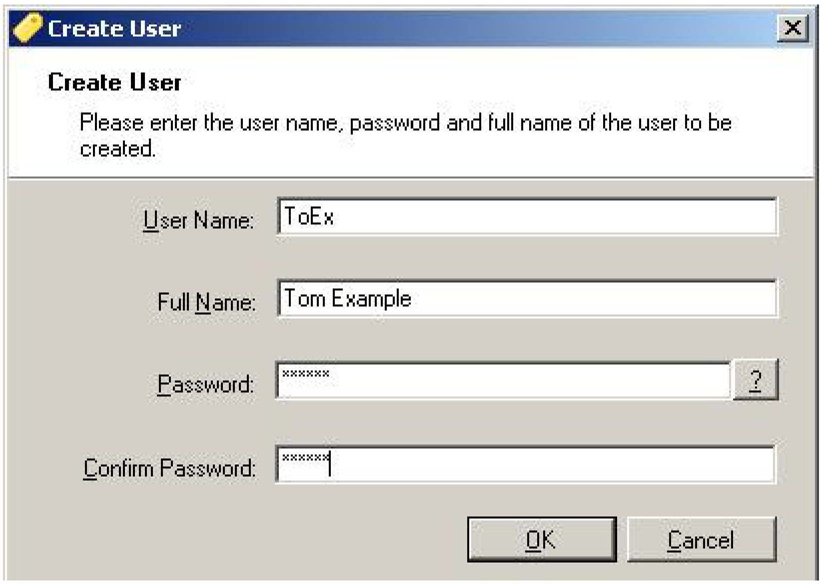
The **Manage Users and Role** dialog box contains the following elements:

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 username 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

10.4.1 *Add/Modify User (*magellan *Tracker)*

Click **Add User** in the *Manage Users and Roles* dialog box and the *Create User* dialog box appears:



Create User

Please enter the user name, password and full name of the user to be created.

User Name: ToEx

Full Name: Tom Example

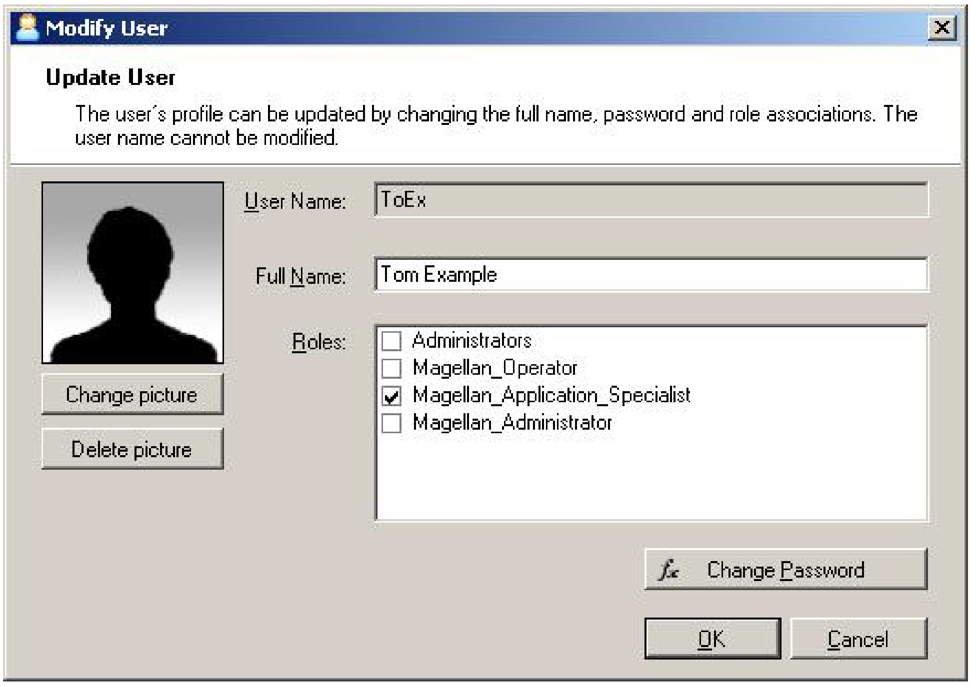
Password: ******

Confirm Password: ******

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.

Click OK and the *Modify User* dialog box appears:



Update User

The user's profile can be updated by changing the full name, password and role associations. The user name cannot be modified.

User Name: ToEx

Full Name: Tom Example

Roles:
- ☐ Administrators
- ☐ Magellan_Operator
- ☑ Magellan_Application_Specialist
- ☐ Magellan_Administrator

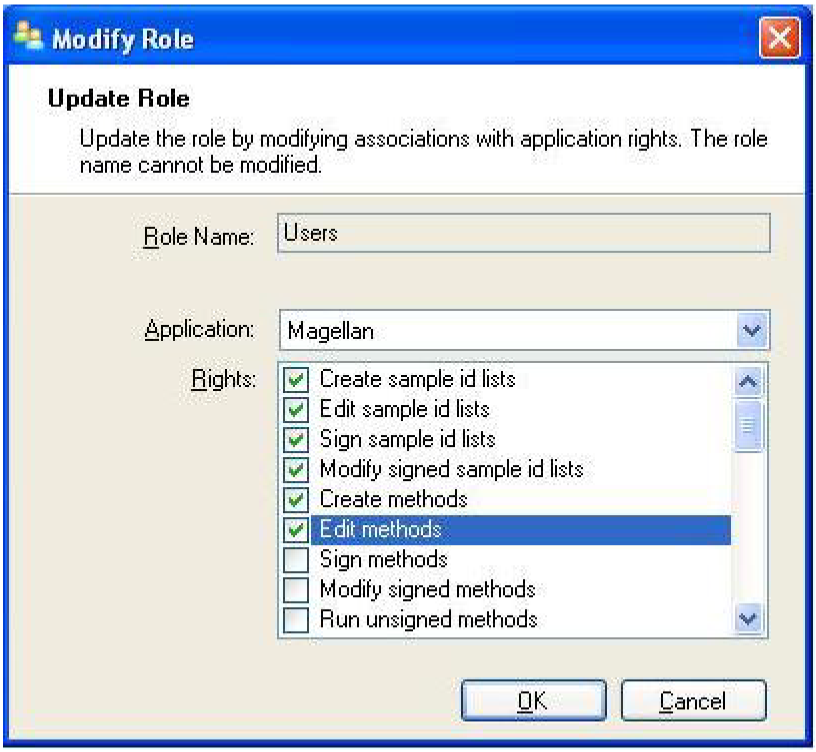
The *Modify User* dialog box contains the following elements:

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.

10.4.2 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:



Update Role

Update the role by modifying associations with application rights. The role name cannot be modified.

Role Name: Users

Application: Magellan

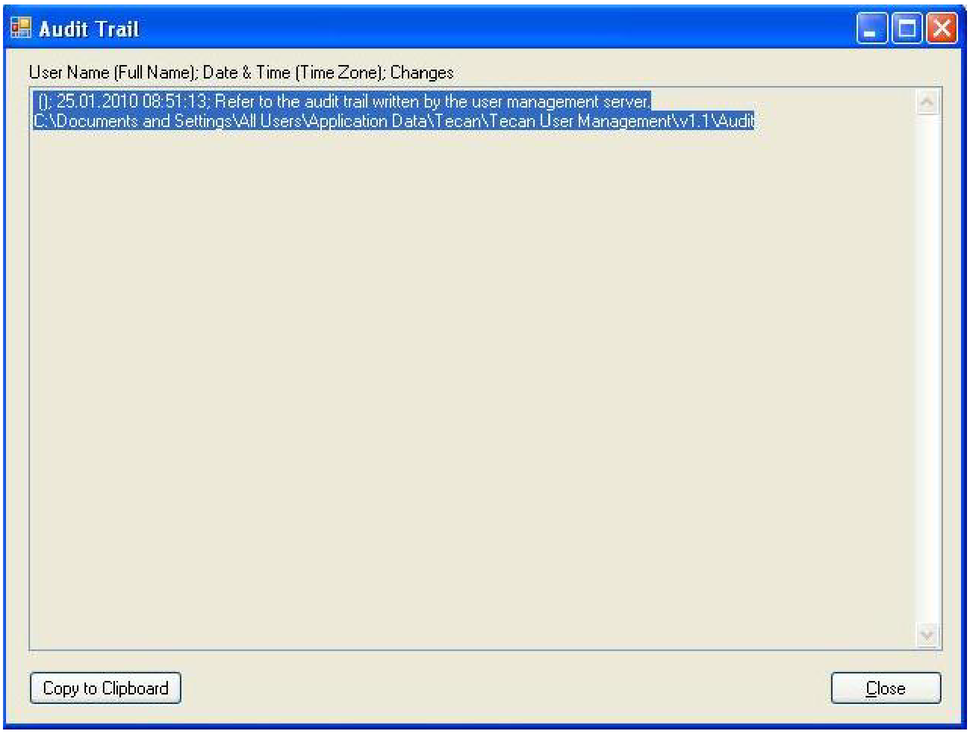
Rights:
- ☑ Create sample id lists
- ☑ Edit sample id lists
- ☑ Sign sample id lists
- ☑ Modify signed sample id lists
- ☑ Create methods
- ☑ Edit methods
- ☐ Sign methods
- ☐ Modify signed methods
- ☐ Run unsigned methods

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.

10.4.3 User Administration Audit Trail

Click **Audit Trail** in the *Manage Users and Roles* dialog box and the *Audit Trail* dialog box appears:



```
(); 25.01.2010 08:51:13; Refer to the audit trail written by the user management server.
C:\Documents and Settings\All Users\Application Data\Tecan\Tecan User Management\v1.1\Audit
```

All modifications of the user administration database are recorded in the user management audit trail written by the user management server.

10.4.4 User Rights (magellan Tracker)

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.

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
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.	Yes	No	No
Modify signed methods Edit a signed method and save it with the same name.	Yes	No	No
Run unsigned methods Run methods that haven't been signed. Note: Each signature (review, approval, custom) allows operators to run those 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

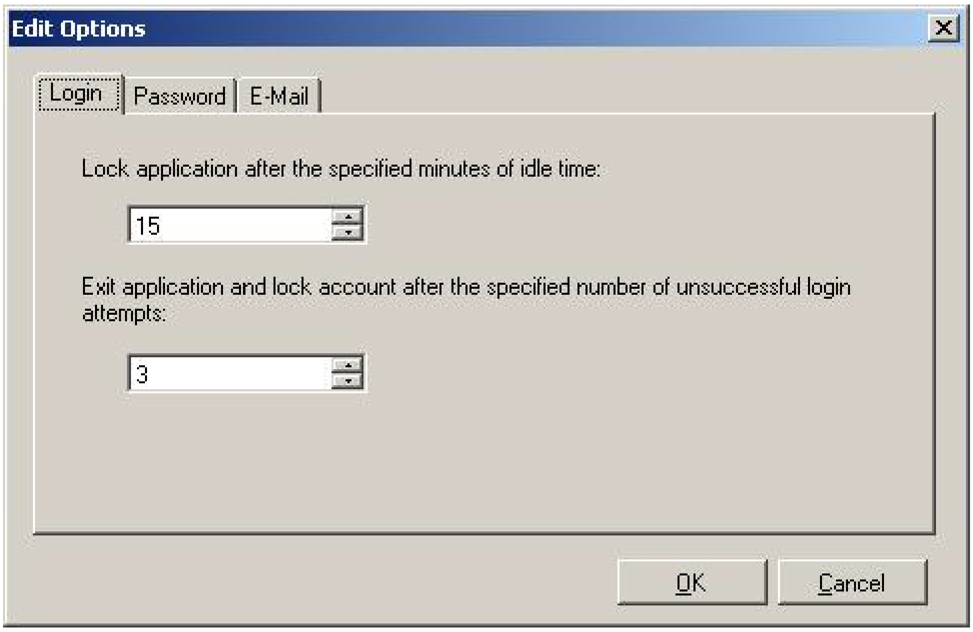
User Rights	magellan **Administrator**	magellan **Application Specialist**	magellan **Operator**
Workspace			
Create workspaces Perform a measurement and save the workspace with a new name – or – save an existing workspace with a new name.	Yes	Yes	Yes
Edit workspaces Edit an existing workspace and save it with the same name.	Yes	Yes	No
Sign workspaces Sign an existing workspace for review/approval.	Yes	No	No
Edit signed workspaces Edit a signed workspace and save it with the same name.	Yes	No	No
Continue evaluation when error Continue calculation after errors have occurred	Yes	Yes	No
Modify raw data (samples) Edit or mask measurement data of samples.	Yes	No	No
Modify raw data (standards) Edit or mask measurement data of standards, controls, blanks.	Yes	No	No
Import raw data Import raw data from ASCII file in an existing workspace.	Yes	No	No
Modify evaluation Change evaluation (method) settings in an existing workspace.	Yes	Yes	No
Reevaluate with another method Reevaluate an existing workspace with another method.	Yes	Yes	No
Modify layout Change measurement parameters, concentration and layout before starting a measurement.	Yes	Yes	No
Standard curve			
Create standard curve files Create a new standard curve and save it with a new name.	Yes	Yes	No
Edit standard curve files Edit an existing standard curve and save it with the same name	Yes	Yes	No
Sign standard curve files Sign an existing standard curve for review/approval.	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
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 Reviewed methods can be used for a measurement run. Note: This right can be used in combination with the right *Run unsigned methods* to allow the user to run already reviewed, but still not approved methods.	Yes	Yes	No
Reader Server			
Save plate definition files Create or edit plate definition files.	Yes	No	No
Save spin profile Create or edit spin profile files.	Yes	No	No

10.4.5 User Administration Options

Click **Options** in the *Manage Users and Roles* dialog box and the *Edit Options* dialog box appears.

Login Options



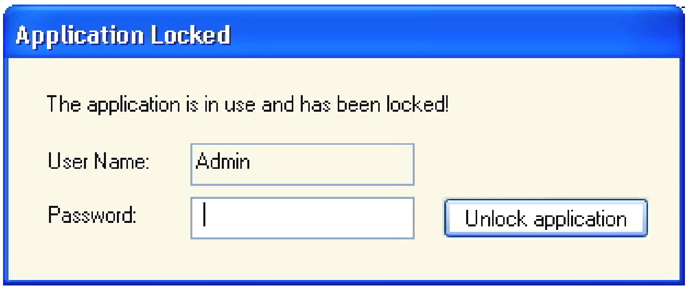
Lock application after the specified minutes of idle time:

15

Exit application and lock account after the specified number of unsuccessful login attempts:

3

Lock application...	If the user doesn't use the application for a specified time (1 min – 36500 hours), the application is automatically locked and 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.



The application is in use and has been locked!

User Name: Admin

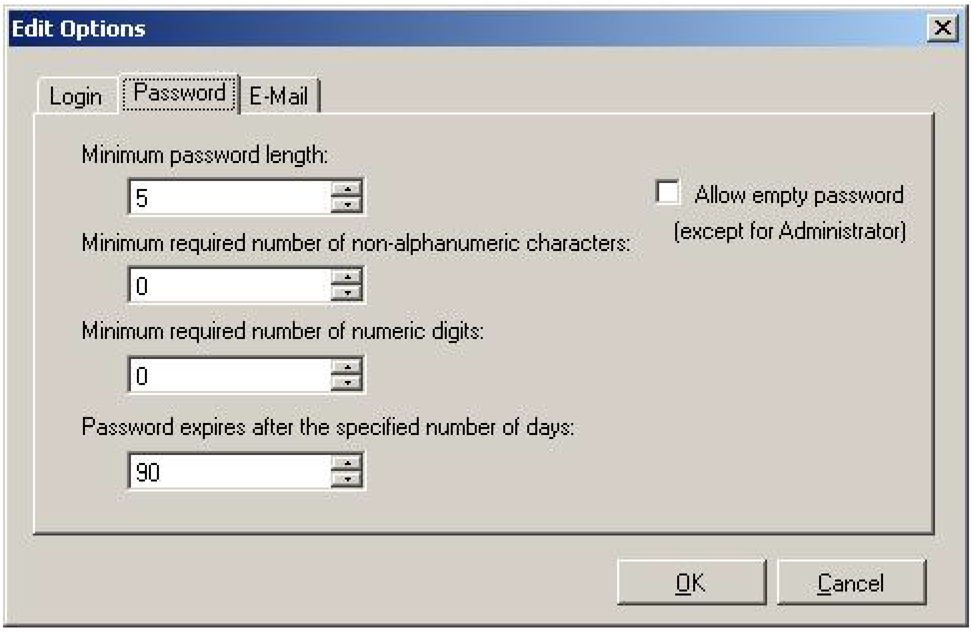
Password:

If the application has not been in use for the specified maximum time it will be locked. The password must be entered to unlock the application. See *Auto Lock* above.

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 1.4 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.

Password Options



Minimum password length: 5

Minimum required number of non-alphanumeric characters: 0

Minimum required number of numeric digits: 0

Password expires after the specified number of days: 90

☐ Allow empty password (except for Administrator)

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.

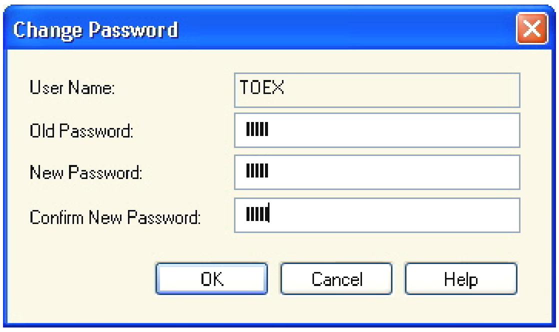
Password expires after the specified number if of days:

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 365 days).

Allow empty password:

Select this checkbox if it is allowed to have an empty password for a user except for the administrator.

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

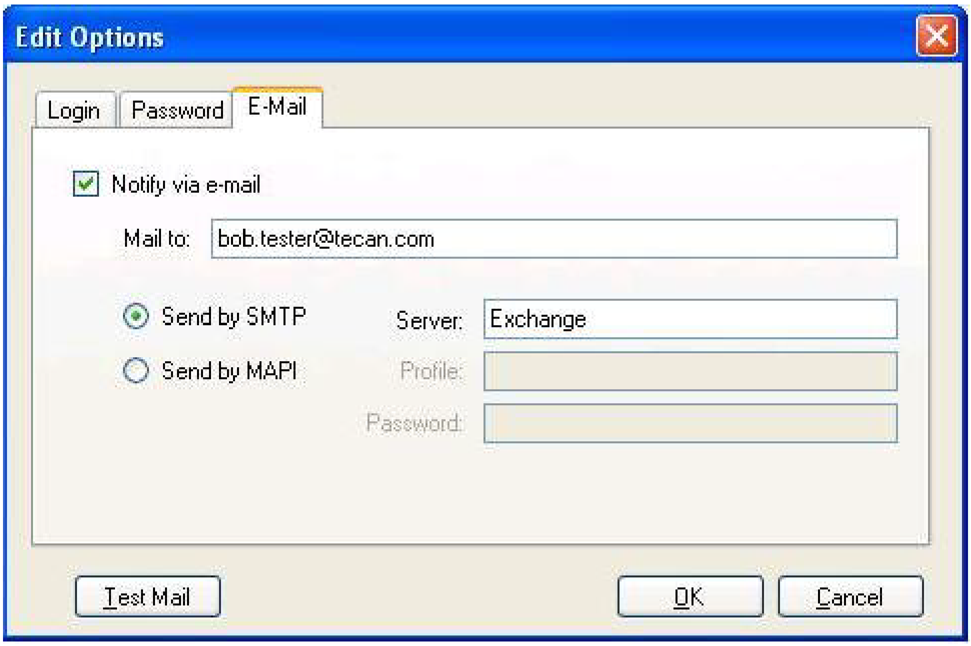


User Name: TOEX
Old Password: IIIII
New Password: IIIII
Confirm New Password: IIIII

The old password has to be entered.

The new password must comply with the specified password rules and has to be entered twice to prevent typing errors. The old passwords cannot be reused.

Email Options



☑ Notify via e-mail

Mail to: bob.tester@tecan.com

● Send by SMTP

○ Send by MAPI

Server: Exchange

An administrator can be notified in case of potential security attacks (a user account has been locked because a number of unsuccessful logins).

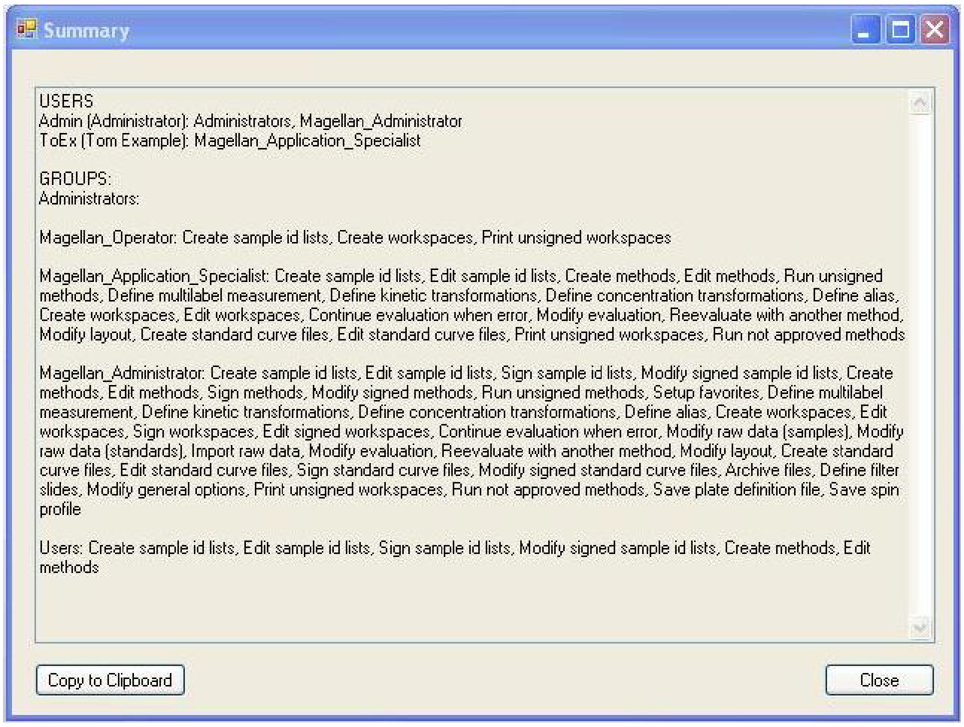
An email can be sent to the entered email address: Select one of the options:

- **SMTP server**: the IP address of the SMTP server has to be entered (f.e. SEUATEXCH01.eu.tecan.net)
- **MAPI**: the profile and password of the mail client has to be entered (f.e. Profile: MS Exchange Settings, Password: appropriate password)

Click **Test Mail** to send a test mail to verify that the settings are correct.

10.4.6 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.



USERS
Admin (Administrator): Administrators, Magellan_Administrator
ToEx (Tom Example): Magellan_Application_Specialist

GROUPS:
Administrators:

Magellan_Operator: Create sample id lists, Create workspaces, Print unsigned workspaces

Magellan_Application_Specialist: Create sample id lists, Edit sample id lists, Create methods, Edit methods, Run unsigned methods, Define multilabel measurement, Define kinetic transformations, Define concentration transformations, Define alias, Create workspaces, Edit workspaces, Continue evaluation when error, Modify evaluation, Reevaluate with another method, Modify layout, Create standard curve files, Edit standard curve files, Print unsigned workspaces, Run not approved methods

Magellan_Administrator: Create sample id lists, Edit sample id lists, Sign sample id lists, Modify signed sample id lists, Create methods, Edit methods, Sign methods, Modify signed methods, Run unsigned methods, Setup favorites, Define multilabel measurement, Define kinetic transformations, Define concentration transformations, Define alias, Create workspaces, Edit workspaces, Sign workspaces, Edit signed workspaces, Continue evaluation when error, Modify raw data (samples), Modify raw data (standards), Import raw data, Modify evaluation, Reevaluate with another method, Modify layout, Create standard curve files, Edit standard curve files, Sign standard curve files, Modify signed standard curve files, Archive files, Define filter slides, Modify general options, Print unsigned workspaces, Run not approved methods, Save plate definition file, Save spin profile

Users: Create sample id lists, Edit sample id lists, Sign sample id lists, Modify signed sample id lists, Create methods, Edit methods

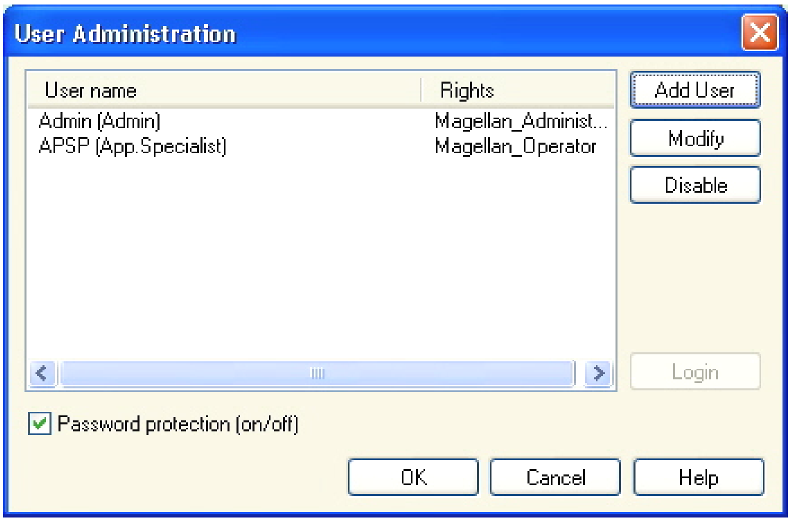
The text can be copied to a word processing program for printing.

10.5 User Administration (magellan Standard)

Click the **miscellaneous** icon in the wizard window and select **User administration** in the next window to open the user administration dialog box.

The magellan software offers protection against misuse of the software or access to the software from unauthorized users by providing a password protection facility.

Users can be added, edited, or deleted and their rights can be defined. Password protection can also be enabled.



User name	Rights
Admin (Admin)	Magellan_Administ...
APSP (App.Specialist)	Magellan_Operator

☑ Password protection (on/off)

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 list is maintained via the following three buttons: **Add User**, **Modify** and **Disable**. These buttons should be accessible only to personnel like department managers or data administrators.

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	All currently setup users are displayed within this list. There are two columns in the list: • **User name** The user names are displayed • **Rights** This column displays the rights of the corresponding user: Administrator, Application Specialist, or Operator. 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. (He can no more user the application).
Password protection (on/off) check box	This check box has to be selected to enable or disable the software's password protection facility. If enabled, the **Login** dialog box will be displayed upon starting magellan.

10.5.1 *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 10.5.4 User Rights (magellan Standard

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

User name text field	In this field, the full name of the user – as it shall be displayed – has to be entered.
UserID text field	Here, the user ID the user has to enter for login, has to be defined.
User rights option buttons	Here has to be determined which level of access to the software's facilities the user will be given: • **Operator** • **Application Specialist** • **Administrator**
Password text field	The password of the user has to be entered. It must consist of at least 5 characters.
Confirm password text field	The password will be required a second time as a precautionary measure. For security concerns, in this field, the password is not shown during entering. Every character is displayed as symbol.

Click the **OK** button to close the dialog box and the entered settings are saved.

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 2.4 Starting*** magellan***/ Login).***

10.5.2 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. The **Login** dialog box (see chapter 2.4.2 Starting Tracker Version / Login) will be displayed.

10.5.3 Change User

To change the active user, click the **Change user** icon in the wizard window. The **Login** dialog box is displayed (see chapter 2.4 Starting magellan/ Login).

10.5.4 *User Rights (*magellan *Standard)*

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
Method			
Create methods Create a new method or save an existing one with a new name.	Yes	Yes	No
Edit methods Edit an existing method and save it with the same name.	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

User Rights	magellan **Administrator**	magellan **Application Specialist**	magellan **Operator**
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
Continue evaluation when error Continue calculation after errors have occurred	Yes	Yes	Yes
Modify raw data (samples) Edit or mask measurement data of samples.	Yes	No	No
Modify raw data (standards) Edit or mask measurement data of standards, controls, blanks.	Yes	No	No
Import raw data Import raw data from ASCII file in an existing workspace.	Yes	No	No
Modify evaluation Change evaluation (method) settings in an existing workspace.	Yes	Yes	No
Reevaluate with another method Reevaluate an existing workspace with another method.	Yes	Yes	No
Modify layout Change measurement parameters, concentration and layout before starting a measurement.	Yes	Yes	No
Standard curve			
Create standard curve files Create a new standard curve and save it with a new name.	Yes	Yes	No
Edit standard curve files Edit an existing standard curve and save it with the same name	Yes	Yes	No
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

User Rights	magellan **Administrator**	magellan **Application Specialist**	magellan **Operator**
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
Reader Server			
Save plate definition files Create or edit plate definition files.	Yes	Yes	No
Save spin profile Create or edit spin profile files.	Yes	No	No

10.6 About magellan

Click the **miscellaneous** icon in the wizard window and select

About magellan .

Copyright information and software disclaimer are displayed.

A window showing copyright information and software disclaimer is displayed.

In the **About** magellan dialog box, information about the currently installed version of the magellan software, the version numbers of the components (tab **components**), and the program license of the user are displayed (tab **license**).

Register Wizard

For further details on the **Register** magellan **Wizard** see chapter 2.6.1 Registration Wizard.

11. Additional Features for magellan **Tracker**

11.1 User Administration

In magellan Tracker a user administration is obligatory. Refer to chapter 10.4 User Administration (magellan Tracker) for further details.

11.1.1 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 4.3.10 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.

11.2 File Handling

The measured data is always saved directly after the measurement.

11.2.1 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

11.2.2 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.

11.2.3 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.

11.2.4 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 **Id**entification Number) and
- License number (refer to chapter 2.6 Licensing magellan).

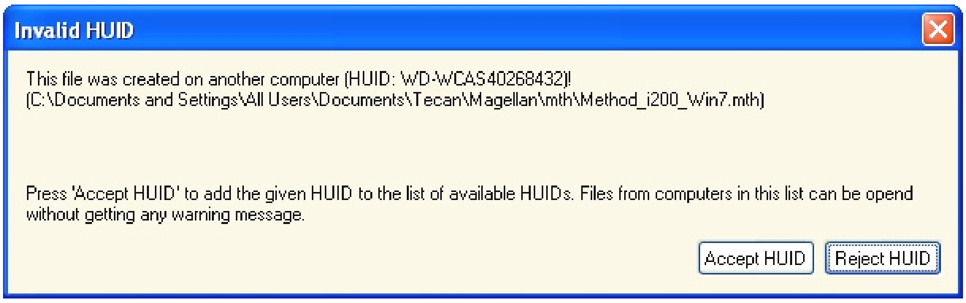
The HUID of a Personal Computer is configured during magellan registration and all files created and saved on this PC are linked to this special HUID.

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.



This file was created on another computer (HUID: WD-WCAS40268432)!
(C:\Documents and Settings\All Users\Documents\Tecan\Magellan\mth\Method_i200_Win7.mth)

Press 'Accept HUID' to add the given HUID to the list of available HUIDs. Files from computers in this list can be opend without getting any warning message.

11.3 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 XP:

C:\Documents and Settings\All Users\Documents\Tecan\LogFiles\SystemAuditTrail

Windows Vista and Windows 7:
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.

Magellan Events to be Tracked

Event	**Event Type**	**Description**
Magellan Start	StartUp	Magellan was started.
Magellan Exit	Exit	Magellan was closed.
Successful User LogOn	Login	A user logged in successfully.
Failed User LogOn	FailedLogin	Login failed, due to wrong username or password.
User LogOff	Logout	A user logged out.
New Workspace	New	A new workspace was created.
Load Workspace	Load	An existing workspace file was loaded into Magellan.
Save Workspace	Save	A workspace was saved.
New Method	New	A new method was created.
Load Method	Load	An existing method file was loaded into Magellan.
Save Method	Save	A method was saved.
New Sample ID List	New	A new sample ID list was created.
Load Sample ID List	Load	An existing sample ID list was loaded.
Save Sample ID List	Save	A sample ID list was saved.
Start Measurement	Measure	A new measurement was started.
Attach Signature	Signature	A workspace or method file was signed.

Export Results	ExportASCII ExportExcel ExportASTM ExportSampleTracking	Results were exported.
Prints Results	Print	Results were printed.
Automatic Archive	ArchiveFailed	The archiving of a workspace, method or sample ID list file failed.
CRC Failure	CRCFailed	Checksum of the previous log file was invalid.

12. Calculations

12.1 Evaluate Results – Calculation Procedure

Depending on the settings the calculation follows the procedure below:

1. Precalculation
    1.1 G-Factor calculation, polarization calculation (blank reduction, intensity, total intensity and anisotropy calculation)
    1.2 Cuvette data reduction
    1.3 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.

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.

12.1.1 Statistics

If a statistical value is calculated over e.g. the n replicates with values $x_1 \ldots x_n$ of a sample following formulas are used:

Name	**Formula**
mean value, average value	$\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$
standard deviation	$s = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \overline{x})^2}$ and s=0 for n=1
variation coefficient in percent	$v = 100\frac{s}{\overline{x}}$

For more information refer to chapter 12.4.5 Statistical Functions.

12.2 Polarization Data Reduction

12.2.1 Introduction

Fluorescence polarization measurements consist of two fluorescence intensity measurements, one with polarizers in parallel, and one with polarizers in perpendicular position. The G-factor compensates for differences in optical components between parallel and perpendicular measurement. A valid calibration of the instrument resulting in a G-factor is an important requirement for each fluorescence polarization measurement.

12.2.2 Determination of the G-Factor

First, the reader specific G-factor is determined. This occurs by fluorescence intensity measurements of the reference and the reference-blank solution with polarizers in parallel and in perpendicular position. The polarization P_{ref} [P] for the reference values is known:

$$G = \frac{(1 + P_{ref})(\overline{RFU}_{ref}^{per} - \overline{RFU}_{rbl}^{per})}{(1 - P_{ref})(\overline{RFU}_{ref}^{par} - \overline{RFU}_{rbl}^{par})}$$

P_{ref} … reference polarization value

$\overline{RFU}_{ref}$ … average of the relative reference fluorescence value

$\overline{RFU}_{rbl}$ … average of the relative reference blank fluorescence value

12.2.3 Blank Correction

If the method contains sample-blanks, a blank reduction process is run, whereby the average of the respective sample-blank is deducted from each sample value.

$$\Delta RFU^{par} = \begin{cases} RFU_{ref}^{par} - \overline{RFU}_{rbl}^{par} \\ RFU_{rbl}^{par} - \overline{RFU}_{rbl}^{par} \\ RFU_{smp}^{par} - \overline{RFU}_{sbl}^{par} \\ RFU_{sbl}^{par} - \overline{RFU}_{sbl}^{par} \end{cases} \quad for\,each\,well$$

$$\Delta RFU^{per} = \begin{cases} RFU_{ref}^{per} - \overline{RFU}_{rbl}^{per} \\ RFU_{rbl}^{per} - \overline{RFU}_{rbl}^{per} \\ RFU_{smp}^{per} - \overline{RFU}_{sbl}^{per} \\ RFU_{sbl}^{per} - \overline{RFU}_{sbl}^{per} \end{cases} \quad for\,each\,well$$

RFU_{smp} … relative sample fluorescence value

RFU_{sbl} … relative sample blank fluorescence value

12.2.4 Intensity Calculation

The vertical and horizontal intensities of the raw data, or the result of the blank reduction are then determined using the G-factor.

$$I^{par} = G * \Delta RFU^{par}$$

$$I^{per} = \Delta RFU^{per}$$

12.2.5 Calculation of the Polarization / Anisotropy / Total Intensity

The following data is calculated using the intensities:

Polarization

$$P = \frac{I^{par} - I^{per}}{I^{par} + I^{per}}$$

Anisotropy

$$A = \frac{I^{par} - I^{per}}{I^{par} + 2 * I^{per}}$$

Total Intensity

$$I_{tot} = I^{par} + 2 * I^{per}$$

Note
Polarization and Anisotropy are displayed in units of mP; Total Intensity is displayed in units of RFU.

12.3 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.

12.3.1 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:

$$g_i = \sum_{n=-n_L}^{n_R} c_n f_{i+n}$$ where n_R-n_L+1=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 12.4.8 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!

12.4 How to Write a Formula

12.4.1 Introduction

A variety of formulas are necessary for the calculations, the cutoff requirements and the validation. These formulas resemble the syntax of BASIC commands. Therefore, the calculations are relatively easy to define.

All values are calculated in double precision although they are displayed depending on the desired number format.

12.4.2 Formula Variables

All of the previously defined abbreviations for the identifiers contained within the analysis plate can be employed as variables in calculations.

For example:

PC1, SM1_1, BL1…Average values

PC1_1, SM1_1_1, BL1_1…Individual values, individual replicates

> ***Note***
> ***The program differentiates between lower and upper case letters when dealing with these labels.***

It is also possible to work with the well coordinates.

For example: A2, B3, H12

> ***Note***
> ***Well coordinates must always be written using upper case letters.***

> ***Note***
> ***The symbol** x **refers to the current value within a well. For example: x-BL1…subtracts the empty value (blank) from the current value.***

> ***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 4.3.7 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
^	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)

12.4.3 Formula Functions

The expressions “and” and “or” can be incorporated into the same equation through the use of 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:

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)

12.4.4 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:

abs(-1) = 1

abs(1) = 1

exp(argument)

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

Example: exp(1) = e^1 = 2.718

frac(argument)

This function separates out the fraction section of argument.

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

Example: frac(1.7) = 0.7

int(argument)

This function separates out the integer sections of argument.

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

Example: int (1.7) = 1

Log(argument)

log(arg1;arg2)

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

Example:

The well holds a value of 100.

log(x;10)

The result here will be 0.5.

ln(argument)

This function takes the natural logarithm of argument.

Example: *ln(10) = 2,303*

lg(argument)

This function takes the logarithm to base 10 of argument.

Example: *lg(10) = 1*

round(argument)

This function rounds argument to an integer value.

Example:

To round 12.579 to two decimal places use the following formula:

round(12.579*100)/100

The result is 12.58.

sqr(argument)

This function raises argument to the power of 2

Example: *sqr(3) = 9*

sqrt(argument)

This function takes the square root of argument

Example: *sqrt(9) = 3*

12.4.5 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:

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:

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:

Median (NC1)

Assume NC1_1=0.1, NC1_2=0.05, NC1_3=0.04

The median value of these negative controls will be determined as follows.

The order of the values gives:

0.04 0.05 0.1

The median is therefore 0.05.

medianPlate()

The median of the whole plate can be determined using this function. The individual values are ordered in terms of size and the median determined by taking the middle value in the order. If the number of values is an even number, the average of the two middle values will be determined.

Example:

medianPlate()

Assume BL1=1, NC1=2, PC1=3, SM1_1=4, SM1_2=5 and no other wells defined.

The median of the whole plate is 3.

max(argument) and min(argument)

This function calculates the minimum/maximum of argument. The argument must be an identifier.

Example:

max(SM1)

The maximum of all the samples in the first experimental group will be formed.

min(ST1_1)

Determines the minimum of the individual replicates of the first standard.

maxAvg(argument) and minAvg(argument)

This function gives the maximum/minimum average value of argument. The argument must be an identifier.

Example:

minAvg(SM1)

If a number of results are found for SM1, only the minimum average will be given.

PointwiseCV(argument)

The average point wise coefficient of variation (CV) is determined. The result can be used to validate the standard curve. The argument must be an identifier.

Example:

PointwiseCV(ST1)

Assume

ST1_1_1=0.54 ST1_1_2=0.52 cv=2.668
ST1_2_1=0.72 ST1_2_2=0.77 cv=4.746
ST1_3_1=1.08 ST1_3_2=0.99 cv=6.148

The result of pointwiseCV is the average of the CV of ST1_1, ST1_2 and ST1_3 and is 4.5209.

Sum(argument)

This function calculates the sum of argument.

Example:

sum(SM1)

The sum of all the samples in the first experimental group will be formed.

sum(ST1_1)

Determines the sum of the replicates of the first standard.

stddev(argument)

This function calculates the standard deviation of argument. The argument must be an identifier.

Example:

stddev(NC1)

The standard deviation of the negative control in the first experimental group will be formed.

12.4.6 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)

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**

***NC1_2* = 0.439** $\overline{NC1} = 0.288$

***NC1_3* = 0.208**

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

$\mid NC1\_1 - \overline{NC1} \mid$	**|0.217-0.288|**	**0.071**		**NC1_2 (0.439)**
$\mid NC1\_2 - \overline{NC1} \mid$	**|0.439-0.288|**	**0.151**	→	**NC1_3 (0.208)**
$\mid NC1\_3 - \overline{NC1} \mid$	**|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 <= 0.3625 → valid
0.217 <= 0.3625 → 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.

12.4.7 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 – concX gives the difference between the calculated and the original concentration of the well.

12.4.8 Spectra Functions

smooth(numPts)

Smoothes 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;wlStart;wlEnd;peakIndex:percLimit)

Delivers the peak as data set (intensity, wavelength, width, area). Peaks lower than the threshold will not be found.
Peak search is done in the given wavelength range.

peakIndex = -1 → returns max. peak

peakIndex = -2 → returns min. peak

peakIndex = 0, 1, 2, … → returns peak at the given index

percLimit is a percentage used for calculating width and area.

numPeaks(threshold;wlStart;wlEnd)

Delivers the number of peaks found in the given wavelength range. Peaks lower than the threshold will not be found.

derive(degree)

Calculates the derivate of the given degree. Valid degrees are 1 and 2; e.g. derive(2).

intensity(function)

Delivers the intensity of either a data pair or a peak; e.g. intensity(minimum()).

wavelength(function)

Delivers the wavelength of either a data pair or a peak; e.g. wavelength(maximum())

width(function)

Delivers the width of a peak; e.g. width(peak0.5;450;650;-1;50)).

area(function)

Delivers the area of a peak; e.g. area(peak0.5;450;650;-1;50)).

12.4.9 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 deduced 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.

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.

12.5 Standard Curve Analysis Types

12.5.1 Definitions

Given n base points (x_1, y_1), …, (x_n, y_n), $x_1 < \ldots < x_n$

Name	Formula
correlation coefficient	$r = \dfrac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}}$
average square deviation	$d = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2}$
goodness of fit	$goodness = 1 - d$

12.5.2 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”.

12.5.3 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.

12.5.4 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:

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

$$x\mapsto y_i+\frac{y_{i+1}-y_i}{x_{i+1}-x_i}\cdot(x-x_i)\qquad if\ x\in[x_i,x_{i+1}]$$

12.5.5 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:

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

$$x\mapsto A\cdot x+B$$

where A and B are determined by minimizing the error function

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

The solution is unique if

$$rank\begin{pmatrix}x_1 & 1\\ \vdots & \vdots\\ x_n & 1\end{pmatrix}=n$$

, which is true if $x_i\neq x_j\forall i,j=1,\ldots,n$ (see general condition)

12.5.6 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 EFFECT HUGE DEVIATIONS BETWEEN THE GIVEN BASE POINTS AND CALCULATED POINTS!

Mathematical Description

Approximation function:

$$f : [x_1, x_n] - \{-b\} \to R$$

$$x \mapsto \frac{A \cdot x}{B + x}$$

where A and B are determined by solving the linear regression problem for the transformed base points

$$(x_1, \frac{x_1}{y_1}), \ldots, (x_n, \frac{x_n}{y_n})$$

Linear regression:

$$g : [x_1, x_n] \to R$$

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

$A = \frac{1}{k}$ and $B = \frac{d}{k}$

This function f is not continuous at –B.

12.5.7 Polynomial

2^{nd} order: parabolic or quadratic

3^{rd} 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:

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

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

(n>order)

where $a_{order},\ldots,a_0$ are determined by minimizing the error function

$$err(a_{\text{order}},\ldots,a_0)=\sum_{i=1}^{n}(f(x_i)-y_i)^2$$

The solution is unique if

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

12.5.8 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.

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

12.5.9 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,…,n

$$m_i = \frac{q_i \,|\, q_{i+2} - q_{i+1} \,|\, + q_{i+1} \,|\, q_i - q_{i-1} \,|}{|\, q_{i+2} - q_{i+1} \,|\, + \,|\, q_i - q_{i-1} \,|}$$, i=3,…,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} □ q_{i+2} , so is $y'_i = q_i$ (analog for $q_{i+1} = q_{i+2}$).

Is $q_{i-1} = q_i$ and $q_{i+1} = q_{i+2}$, set $$m_i = \frac{q_i + q_{i+1}}{2}$$.

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, …, 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.

12.5.10 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

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

$$x\mapsto D+\frac{A-D}{1+\left(\frac{x}{C}\right)^B}$$

for the description of sigmoid correlation of data.

The parameter can be interpreted as:

$$A=\lim_{x\to 0} f(x)$$

$$D=\lim_{x\to\infty} f(x)$$

$$f(C)=\frac{A+D}{2}$$

A, D are determined as the minimum respectively maximum (or vice versa if the function is decreasing).

Then the linear regression problem is solved for transformed base points.

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

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

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

$x\mapsto k\cdot x+d$, 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).

12.5.11 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 12.5 Standard Curve Analysis Types – LogitLog for further information.

Mathematical Description

Approximation function:

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

$$x \mapsto D + \frac{A - D}{1 + \left(\frac{x}{C}\right)^B}$$

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

12.5.12 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 12.5 Standard Curve Analysis Types – LogitLog for further information.

Mathematical Description

Approximation function:

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

$$x \mapsto D + \frac{A - D}{1 + \left(\frac{x}{C}\right)^B}$$

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.

12.5.13 Five Parameters – Marquardt

The five-parameter approximation basically needs to fulfill the same base point requirements as LogitLog. The sigmoid curve may however be non-symmetric.

The resulting curve will be produced using the Levenberg-Marquardt method. This method produces an increasingly more accurate approximation of the result throughout the interval. The five-parameter method requires considerably more time to be processed. As with LogitLog, an S-shaped curve is produced.

A minimum of five base points is required for this calculation.

If necessary, extrapolation can also be implemented in this process. The parameters A, B, C, D, and E can be employed as parameters in the transformations. The approximation is always applied to the unscaled base point values.

In the Standard Curve dialog box following additional information is displayed:

- Coefficient values A, B, C, D, and E
- Average square deviation d
- Absolute value of the correlation coefficient r (correlation of data and fit)

Restrictions for the Process Application

Refer to chapter 12.5 Standard Curve Analysis Types – LogitLog for further information.

Mathematical Description

Approximation function:

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

$$x \mapsto D + \frac{A - D}{(1 + (\frac{x}{C})^B)^E}$$

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.

12.5.14 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

$$d = \sqrt{\frac{1}{\sum_{i=1}^{n} k_i} \sum_{i=1}^{n} k_i \left(y_i - f(x_i)\right)^2}$$

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.

12.6 Calculation of Dilution Series

12.6.1 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.

12.6.2 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 12.5 Standard Curve Analysis Types for more detailed information about the algorithms mentioned above.

12.6.3 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.

$$dilution = C * \left(\frac{A - I_{IC}}{I_{IC} - D}\right)^{\frac{1}{B}}$$

13. Application Example

13.1 Introduction

The magellan ***example files*** package provide magellan workspaces and the corresponding Instructions for Use (IFU) to introduce the software and to ease the user's work with it. The files can be installed separately and include examples for different measurement modes; they are based on commercial available applications. For further information please refer to the IFU for the example files.

13.2 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.

13.2.1 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

The calculated IgM concentration of both negative controls must be under 8 UA/mL.

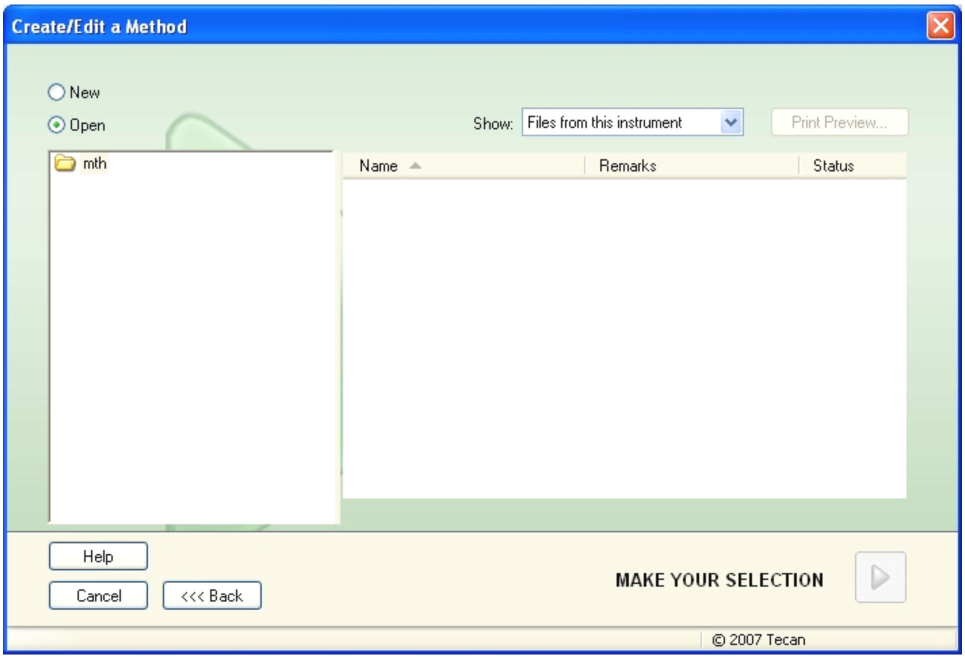
Data Handling

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.

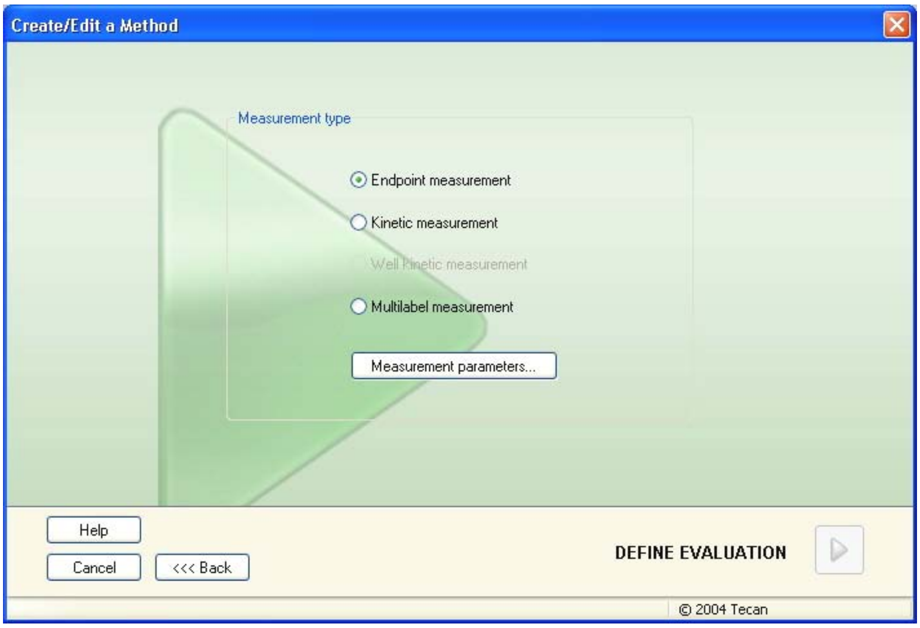
13.2.2 Create a Method

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**.

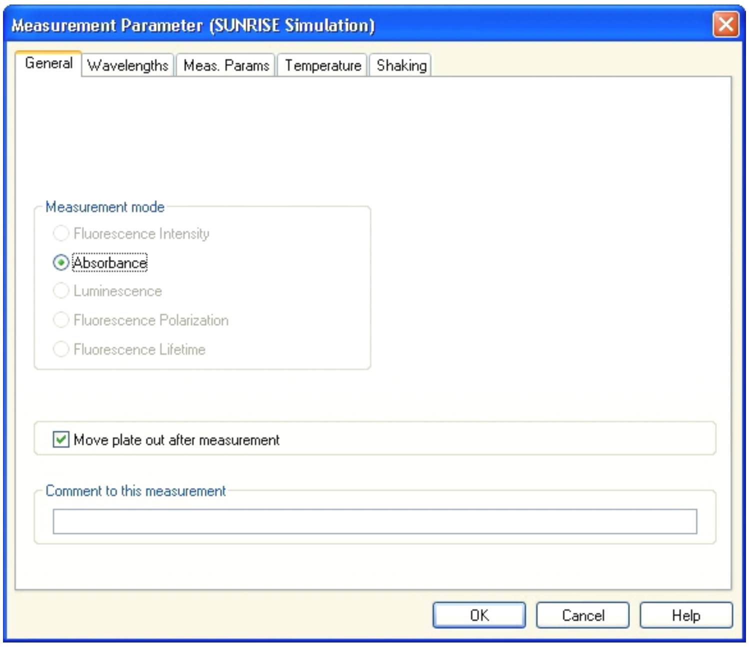


Measurement Parameters

Click **Next** and the **Measurement parameter** dialog box appears.



Select **Endpoint measurement** and click the **Measurement parameters** button. The following dialog box appears:



Measurement mode
○ Fluorescence Intensity
● Absorbance
○ Luminescence
○ Fluorescence Polarization
○ Fluorescence Lifetime

☑ Move plate out after measurement

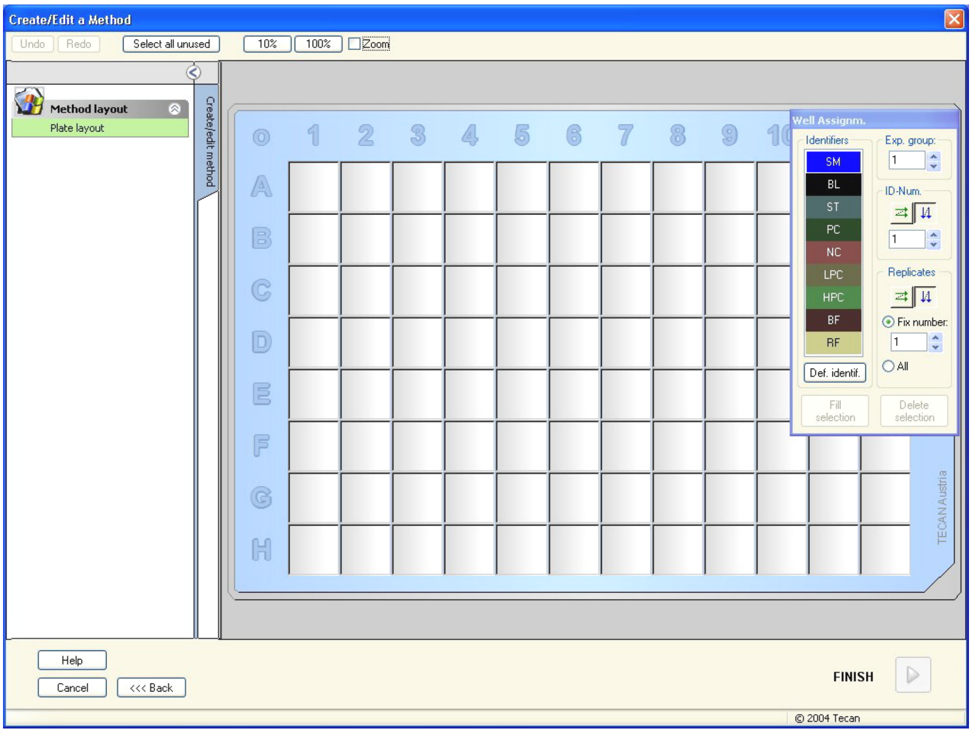
Comment to this measurement

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.



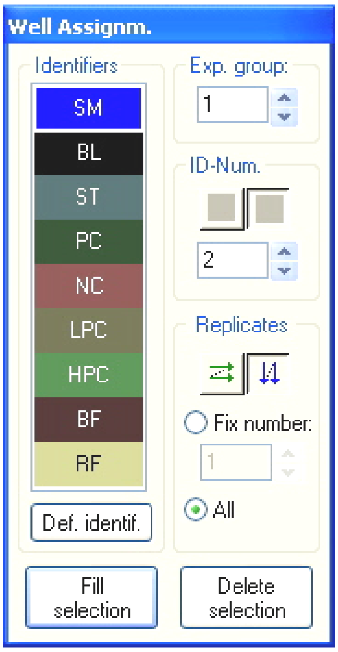
Design Layout

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**.



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).

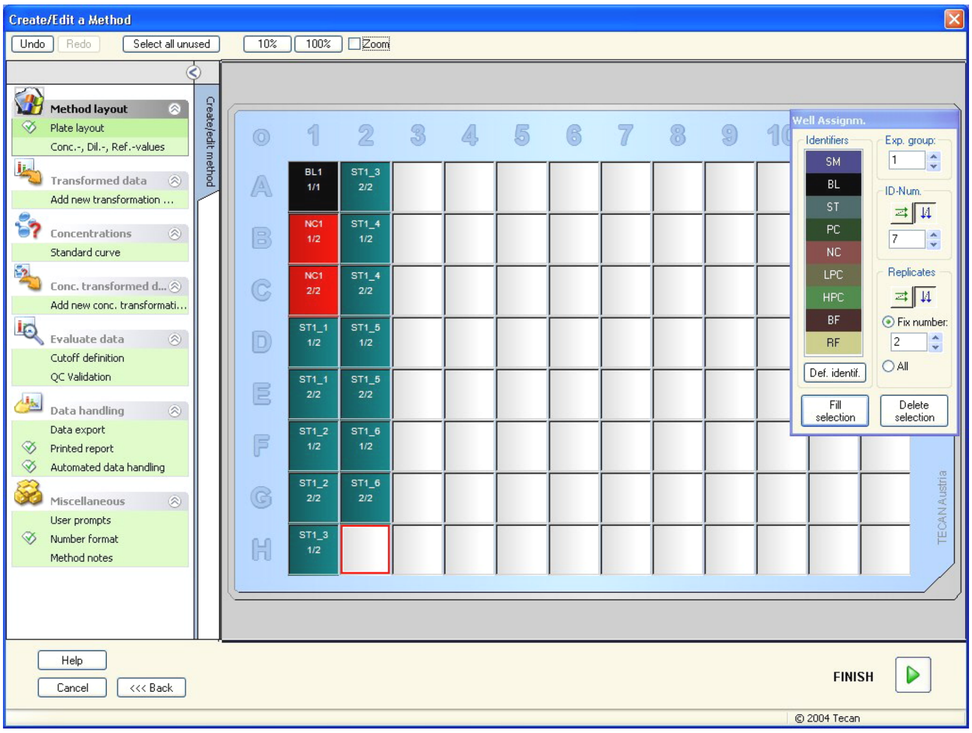
In this example select **Fix Number** and **2**.

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*.

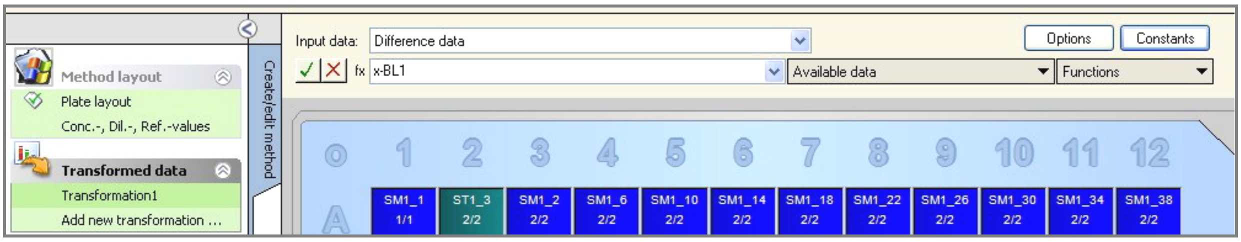
In the **Experimental** group box the number **1** remains.

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.



Input data: Difference data

fx x-BL1

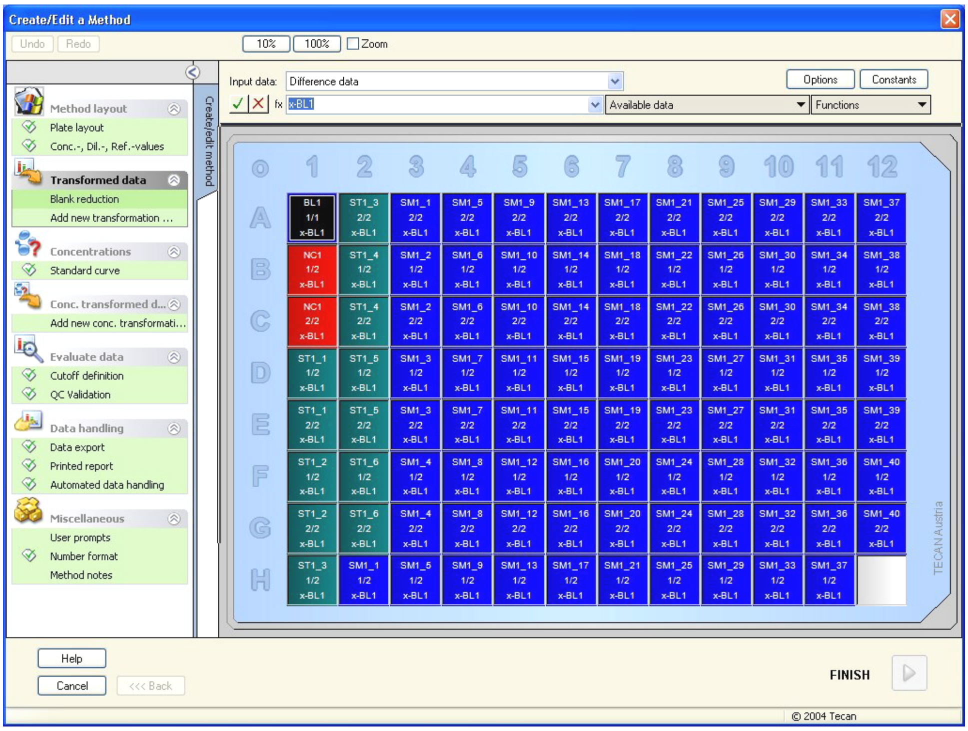
o	1	2	3	4	5	6	7	8	9	10	11	12
A	SM1_1 1/1	ST1_3 2/2	SM1_2 2/2	SM1_6 2/2	SM1_10 2/2	SM1_14 2/2	SM1_18 2/2	SM1_22 2/2	SM1_26 2/2	SM1_30 2/2	SM1_34 2/2	SM1_38 2/2

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

Select **Difference Data** in the **Input data** box. By default the transformation is named Transformation1 (see control bar). If you have confirmed the definition of a blank reduction before, the software automatically names it **Blank reduction**.

In the **Formula** box automatically appears **x-BL1** for this blank reduction, where x refers to the current input data value in a well and BL1 is the mean value of the blank wells of experimental group 1.

Now select the whole plate by clicking the O 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. Fur further details and explanations concerning the definition and assignment of transformations, refer to chapter 4.3.7 Transformed Data: Add New Transformation. The following window appears:



Input data: Difference data

fx x-BL1

o	1	2	3	4	5	6	7	8	9	10	11	12
A	BL1 1/1 x-BL1	ST1_3 2/2 x-BL1	SM1_1 2/2 x-BL1	SM1_5 2/2 x-BL1	SM1_9 2/2 x-BL1	SM1_13 2/2 x-BL1	SM1_17 2/2 x-BL1	SM1_21 2/2 x-BL1	SM1_25 2/2 x-BL1	SM1_29 2/2 x-BL1	SM1_33 2/2 x-BL1	SM1_37 2/2 x-BL1
B	NC1 1/2 x-BL1	ST1_4 1/2 x-BL1	SM1_2 1/2 x-BL1	SM1_6 1/2 x-BL1	SM1_10 1/2 x-BL1	SM1_14 1/2 x-BL1	SM1_18 1/2 x-BL1	SM1_22 1/2 x-BL1	SM1_26 1/2 x-BL1	SM1_30 1/2 x-BL1	SM1_34 1/2 x-BL1	SM1_38 1/2 x-BL1
C	NC1 2/2 x-BL1	ST1_4 2/2 x-BL1	SM1_2 2/2 x-BL1	SM1_6 2/2 x-BL1	SM1_10 2/2 x-BL1	SM1_14 2/2 x-BL1	SM1_18 2/2 x-BL1	SM1_22 2/2 x-BL1	SM1_26 2/2 x-BL1	SM1_30 2/2 x-BL1	SM1_34 2/2 x-BL1	SM1_38 2/2 x-BL1
D	ST1_1 1/2 x-BL1	ST1_5 1/2 x-BL1	SM1_3 1/2 x-BL1	SM1_7 1/2 x-BL1	SM1_11 1/2 x-BL1	SM1_15 1/2 x-BL1	SM1_19 1/2 x-BL1	SM1_23 1/2 x-BL1	SM1_27 1/2 x-BL1	SM1_31 1/2 x-BL1	SM1_35 1/2 x-BL1	SM1_39 1/2 x-BL1
E	ST1_1 2/2 x-BL1	ST1_5 2/2 x-BL1	SM1_3 2/2 x-BL1	SM1_7 2/2 x-BL1	SM1_11 2/2 x-BL1	SM1_15 2/2 x-BL1	SM1_19 2/2 x-BL1	SM1_23 2/2 x-BL1	SM1_27 2/2 x-BL1	SM1_31 2/2 x-BL1	SM1_35 2/2 x-BL1	SM1_39 2/2 x-BL1
F	ST1_2 1/2 x-BL1	ST1_6 1/2 x-BL1	SM1_4 1/2 x-BL1	SM1_8 1/2 x-BL1	SM1_12 1/2 x-BL1	SM1_16 1/2 x-BL1	SM1_20 1/2 x-BL1	SM1_24 1/2 x-BL1	SM1_28 1/2 x-BL1	SM1_32 1/2 x-BL1	SM1_36 1/2 x-BL1	SM1_40 1/2 x-BL1
G	ST1_2 2/2 x-BL1	ST1_6 2/2 x-BL1	SM1_4 2/2 x-BL1	SM1_8 2/2 x-BL1	SM1_12 2/2 x-BL1	SM1_16 2/2 x-BL1	SM1_20 2/2 x-BL1	SM1_24 2/2 x-BL1	SM1_28 2/2 x-BL1	SM1_32 2/2 x-BL1	SM1_36 2/2 x-BL1	SM1_40 2/2 x-BL1
H	ST1_3 1/2 x-BL1	SM1_1 1/2 x-BL1	SM1_5 1/2 x-BL1	SM1_9 1/2 x-BL1	SM1_13 1/2 x-BL1	SM1_17 1/2 x-BL1	SM1_21 1/2 x-BL1	SM1_25 1/2 x-BL1	SM1_29 1/2 x-BL1	SM1_33 1/2 x-BL1	SM1_37 1/2 x-BL1	

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

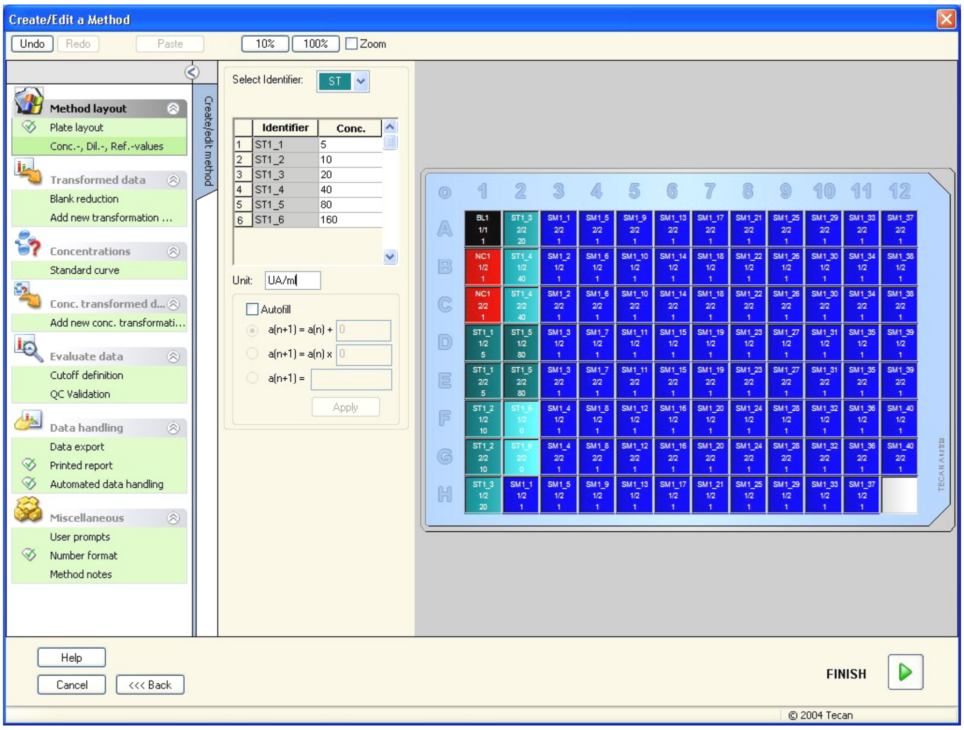
In the control bar select **Conc., Dil., Ref.-value**s from the **Method layout** item to define the respective values as described in the test kit.

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:



Select Identifier: ST

	Identifier	Conc.
1	ST1_1	5
2	ST1_2	10
3	ST1_3	20
4	ST1_4	40
5	ST1_5	80
6	ST1_6	160

Unit: UA/ml

o	1	2	3	4	5	6	7	8	9	10	11	12
A	BL1 1/1 1	ST1_3 2/2 20	SM1_1 2/2 1	SM1_5 2/2 1	SM1_9 2/2 1	SM1_13 2/2 1	SM1_17 2/2 1	SM1_21 2/2 1	SM1_25 2/2 1	SM1_29 2/2 1	SM1_33 2/2 1	SM1_37 2/2 1
B	NC1 1/2 1	ST1_4 1/2 40	SM1_2 1/2 1	SM1_6 1/2 1	SM1_10 1/2 1	SM1_14 1/2 1	SM1_18 1/2 1	SM1_22 1/2 1	SM1_26 1/2 1	SM1_30 1/2 1	SM1_34 1/2 1	SM1_38 1/2 1
C	NC1 2/2 1	ST1_4 2/2 40	SM1_2 2/2 1	SM1_6 2/2 1	SM1_10 2/2 1	SM1_14 2/2 1	SM1_18 2/2 1	SM1_22 2/2 1	SM1_26 2/2 1	SM1_30 2/2 1	SM1_34 2/2 1	SM1_38 2/2 1
D	ST1_1 1/2 5	ST1_5 1/2 80	SM1_3 1/2 1	SM1_7 1/2 1	SM1_11 1/2 1	SM1_15 1/2 1	SM1_19 1/2 1	SM1_23 1/2 1	SM1_27 1/2 1	SM1_31 1/2 1	SM1_35 1/2 1	SM1_39 1/2 1
E	ST1_1 2/2 5	ST1_5 2/2 80	SM1_3 2/2 1	SM1_7 2/2 1	SM1_11 2/2 1	SM1_15 2/2 1	SM1_19 2/2 1	SM1_23 2/2 1	SM1_27 2/2 1	SM1_31 2/2 1	SM1_35 2/2 1	SM1_39 2/2 1
F	ST1_2 1/2 10	ST1_6 1/2 0	SM1_4 1/2 1	SM1_8 1/2 1	SM1_12 1/2 1	SM1_16 1/2 1	SM1_20 1/2 1	SM1_24 1/2 1	SM1_28 1/2 1	SM1_32 1/2 1	SM1_36 1/2 1	SM1_40 1/2 1
G	ST1_2 2/2 10	ST1_6 2/2 0	SM1_4 2/2 1	SM1_8 2/2 1	SM1_12 2/2 1	SM1_16 2/2 1	SM1_20 2/2 1	SM1_24 2/2 1	SM1_28 2/2 1	SM1_32 2/2 1	SM1_36 2/2 1	SM1_40 2/2 1
H	ST1_3 1/2 20	SM1_1 1/2 1	SM1_5 1/2 1	SM1_9 1/2 1	SM1_13 1/2 1	SM1_17 1/2 1	SM1_21 1/2 1	SM1_25 1/2 1	SM1_29 1/2 1	SM1_33 1/2 1	SM1_37 1/2 1	

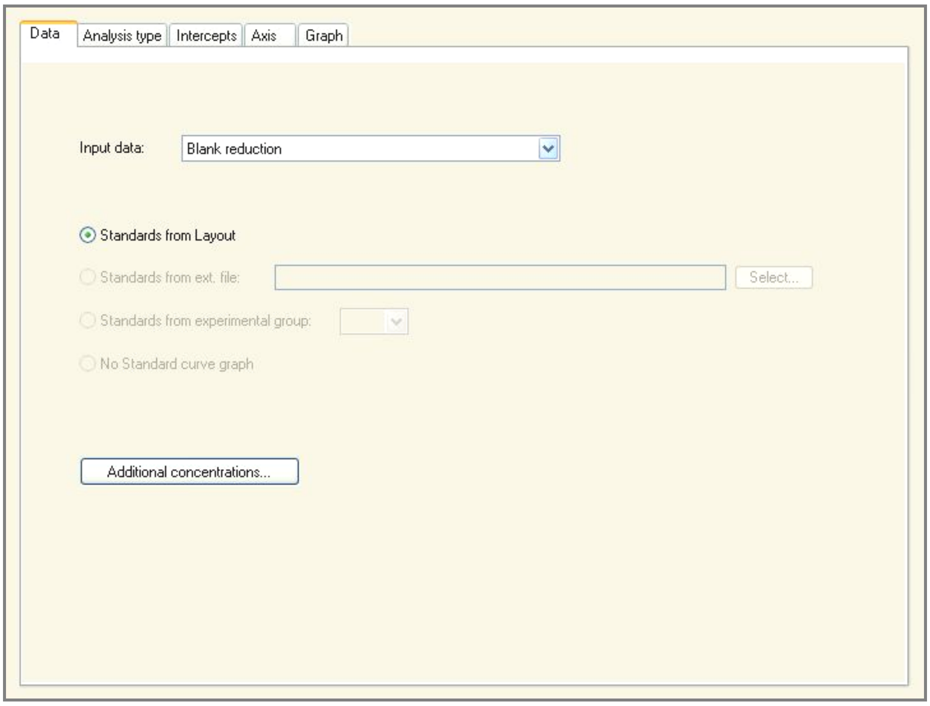
Standard Curve

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.



Input data: Blank reduction

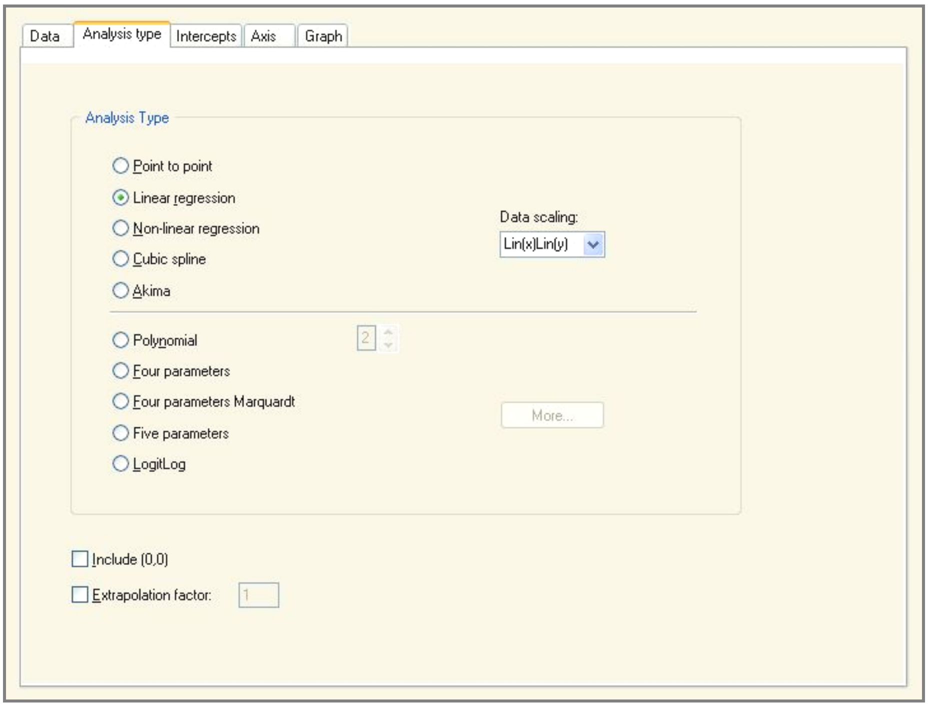
● Standards from Layout

○ Standards from ext. file:

○ Standards from experimental group:

○ No Standard curve graph

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



○ Point to point

● Linear regression

○ Non-linear regression

○ Cubic spline

○ Akima

○ Polynomial 2

○ Four parameters

○ Four parameters Marquardt

○ Five parameters

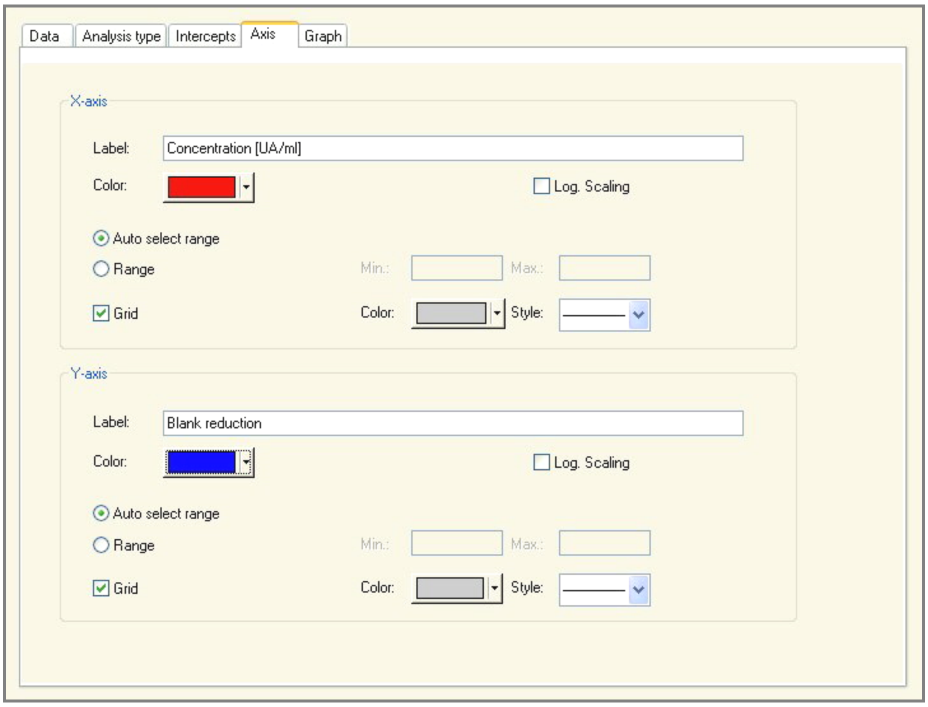
○ LogitLog

Data scaling: Lin(x)Lin(y)

☐ Include (0,0)

☐ Extrapolation factor: 1

On the **Axis tab,** define the labeling and the scaling of the axis as shown below:



X-axis

Label: Concentration [UA/ml]

Color: 🟥

☐ Log. Scaling

● Auto select range

○ Range Min.: Max.:

☑ Grid Color: Style:

Y-axis

Label: Blank reduction

Color: 🟦

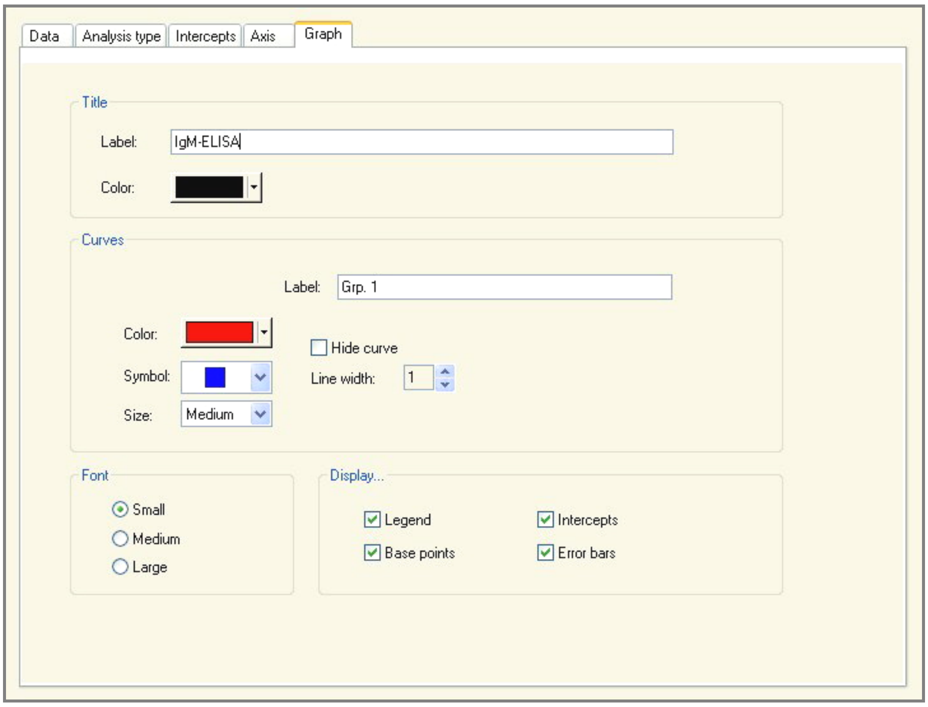
☐ Log. Scaling

● Auto select range

○ Range Min.: Max.:

☑ Grid Color: Style:

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



Title

Label: IgM-ELISA

Color: ⬛

Curves

Label: Grp. 1

Color: 🟥

☐ Hide curve

Symbol: 🟦

Line width: 1

Size: Medium

Font

● Small

○ Medium

○ Large

Display...

☑ Legend

☑ Intercepts

☑ Base points

☑ Error bars

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.

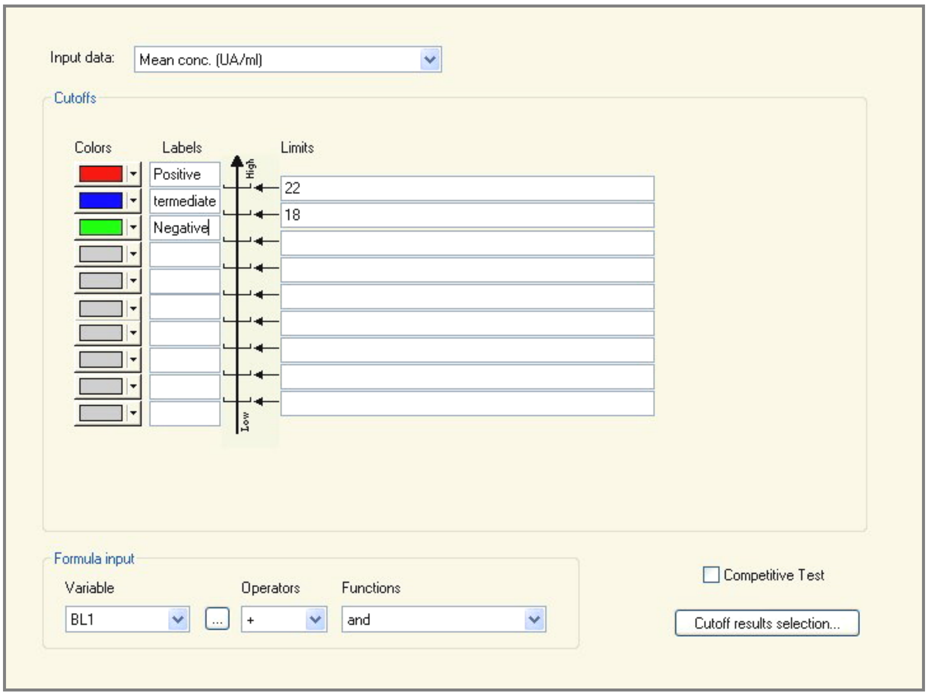
In **Labels**, enter the test interpretation (**Positive**, **Intermediate** and **Negative**) into the individual boxes. Use the drop down color palette to assign a color:

Positive – Red

Intermediate – Blue

Negative – Green

The screen contains the following:



Input data: Mean conc. (UA/ml)

Colors	Labels	Limits
🟥	Positive	22
🟦	termediate	18
🟩	Negative	

Variable: BL1

Operators: +

Functions: and

☐ Competitive Test

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)**.

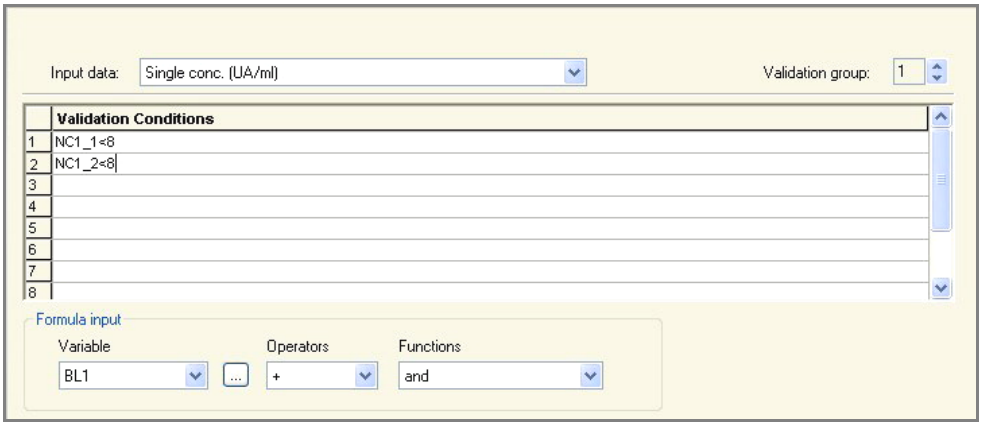
In the first row, type **NC1_1<8**, or enter the formula using the available **variables**, **operators** and **functions**.

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:



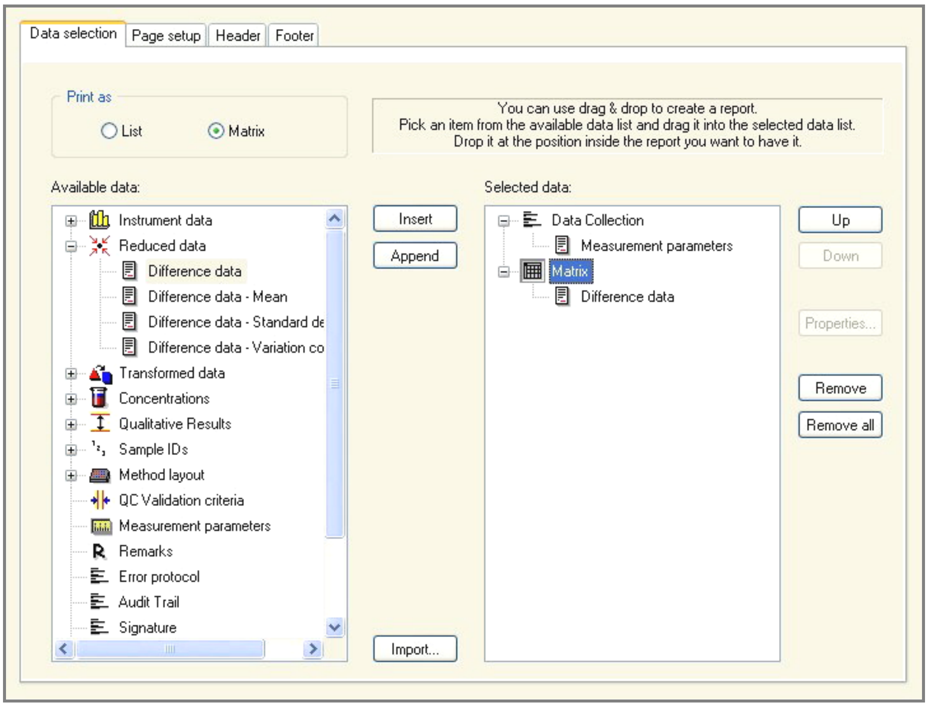
Input data: Single conc. (UA/ml)

Validation group: 1

	Validation Conditions
1	NC1_1<8
2	NC1_2<8
3	
4	
5	
6	
7	
8	

Organize Printed Report

In the control bar, click **Printed report** from the **Data handling** item. The following screen is displayed:



Print as: ○ List ● Matrix

You can use drag & drop to create a report.
Pick an item from the available data list and drag it into the selected data list.
Drop it at the position inside the report you want to have it.

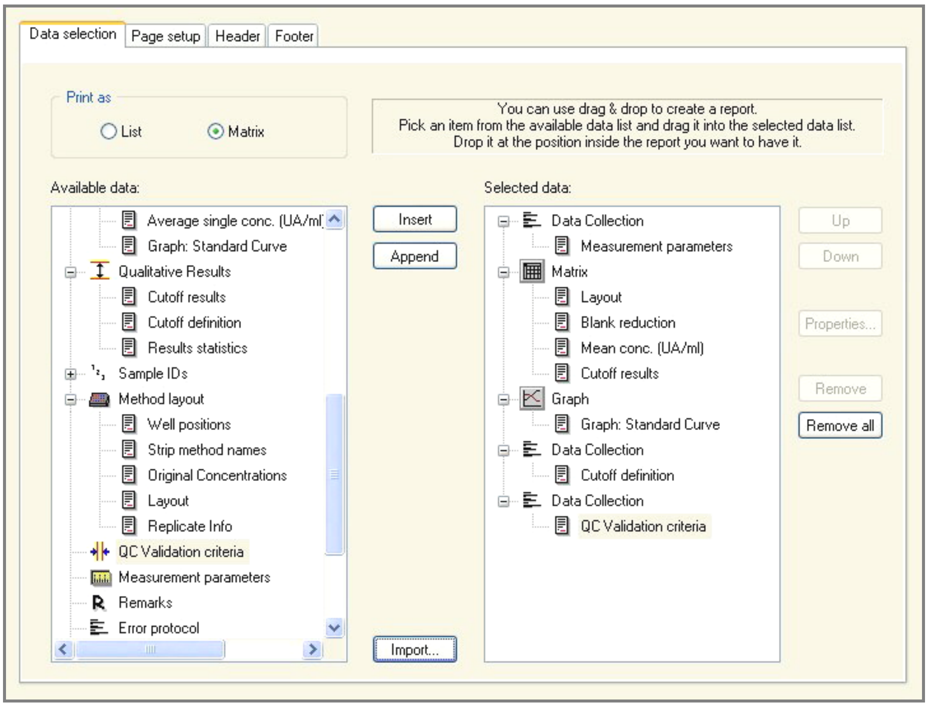
On the **Data selection** tab, all available report data is contained in the **Available data** box. Using the **Insert and Append** buttons, data can be transferred into the **Selected data** box. Data can also be transferred using drag-and-drop.
In the **Print as** box, choose between printing the data as a matrix or as a list with a special orientation.

In this example a report containing the measurement parameters, plate layout, blanked values, standard curve, IgM-concentrations, cutoff definition, qualitative results of the samples and validations should be created.

Before creating the report, the default **Matrix Difference data** must be removed from the **Selected data** box. So only **Measurement parameters** remain in the **Selected data** box.

Select **Method layout**/**Layout** in the **Available data** box and attach it as a matrix to the report by clicking **Append**. Then insert **Blank reduction**, **Mean conc. (UA/mL)** and **Cutoff results** into the matrix by selecting the corresponding items and clicking **Insert**.

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



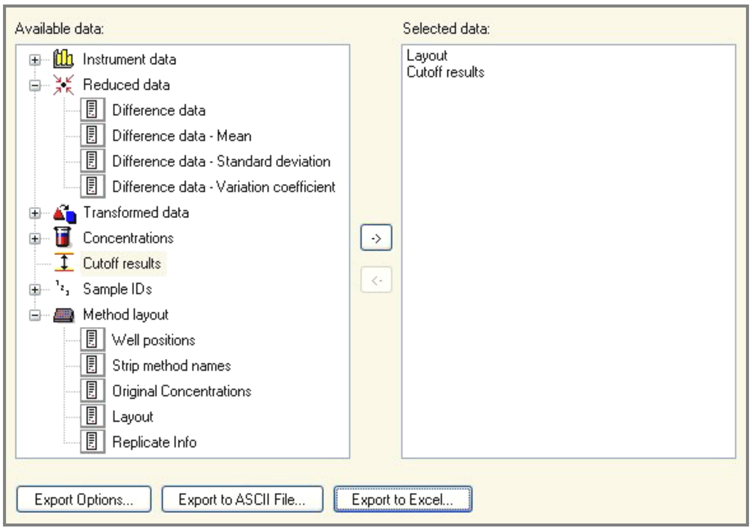
You can use drag & drop to create a report.
Pick an item from the available data list and drag it into the selected data list.
Drop it at the position inside the report you want to have it.

Print as: ○ List ● Matrix

On the **Header** and **Footer** tabs, define the layout of the header and the footer of the report (see chapter 4.3.15 Data Handling: Printed Report for further details).

Data Export

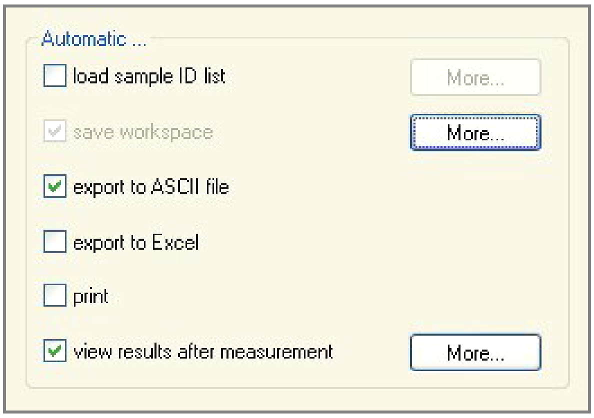
In the control bar, select **Data export** from the **Data handling** item. In this example, the layout and cutoff results should be stored as ASCII file. Select **Layout** and **Cutoff** results from the **Available data** window; click the → arrow to insert them into the **Selected data** window. The 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.


Automatic ...

☐ load sample ID list

☑ save workspace

☑ export to ASCII file

☐ export to Excel

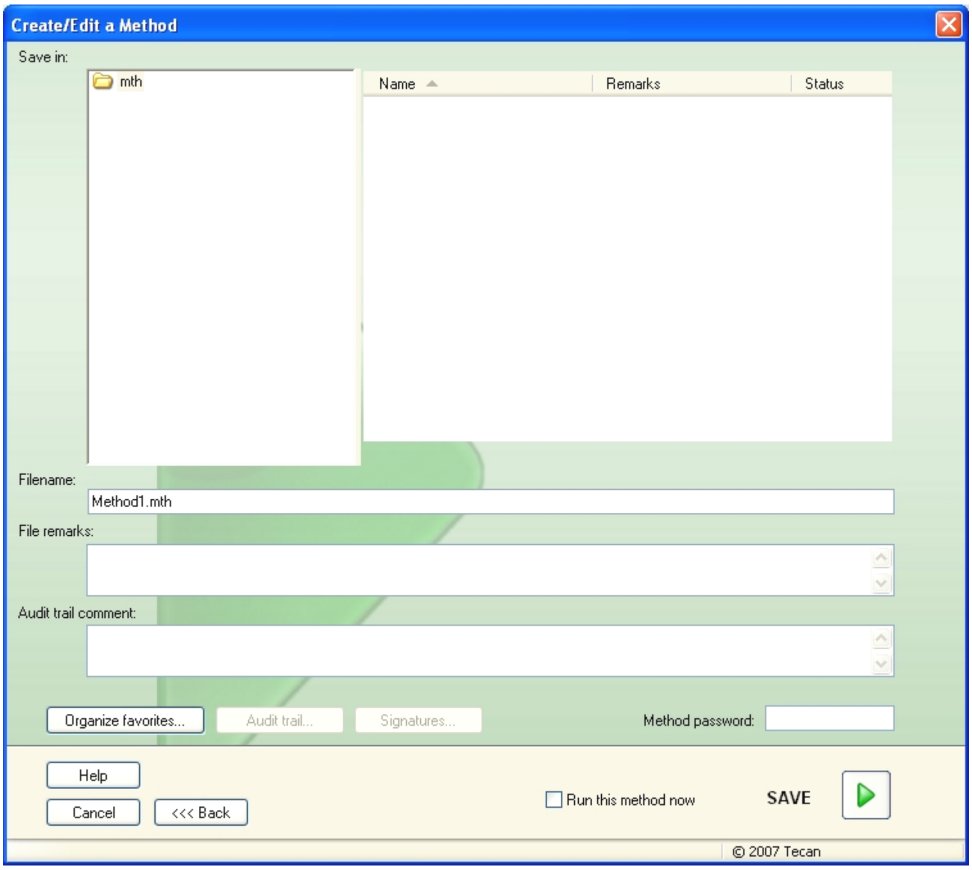
☐ print

☑ view results after measurement

Select **export to ASCII file**, and **view results after measurements**. In magellan **Tracker, save workspace** is selected by default and cannot be modified.

Save the Method

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


Create/Edit a Method

Save in: mth

Filename: Method1.mth

File remarks:

Audit trail comment:

Method password:

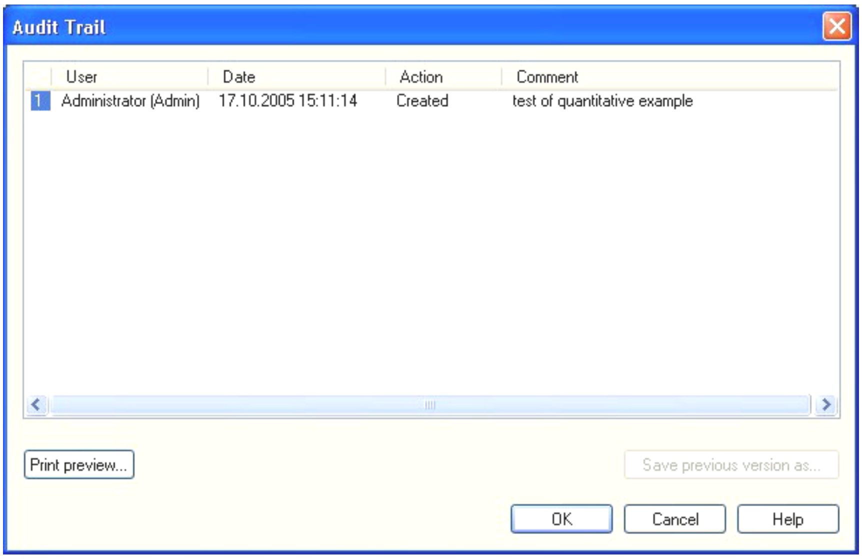
☐ Run this method now

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. *This option is only available with* magellan **Tracker***.*
Audit trail… button	The **Audit Trail** dialog box appears. *This option is only available with* magellan **Tracker***.*
Organize Favorites… button	The **Organize Favorites** dialog box appears. (See chapter 6.5 Start Favorite – Organize Favorites).
Signatures… button	The **Signature** dialog box appears. *This option is only available with* magellan **Tracker***.*
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:



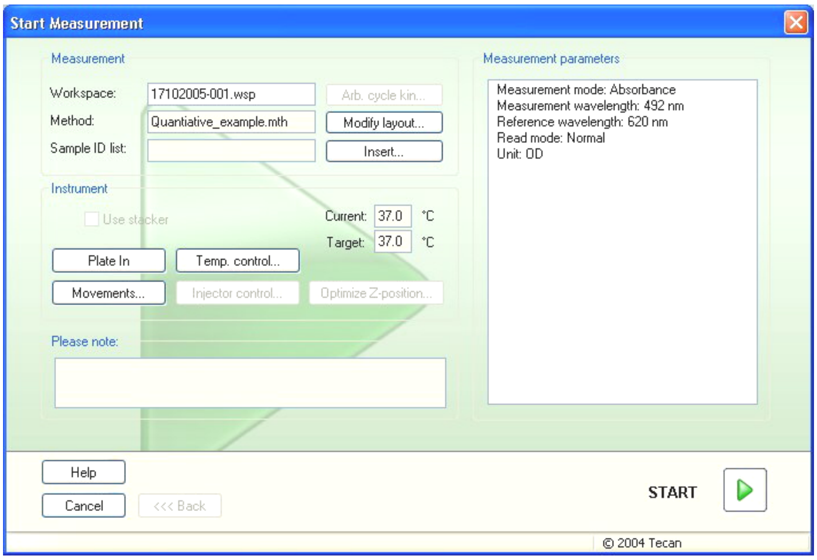
	User	Date	Action	Comment
1	Administrator (Admin)	17.10.2005 15:11:14	Created	test of quantitative example

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.

13.2.3 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:



Start Measurement

Measurement

Workspace: 17102005-001.wsp

Method: Quantiative_example.mth

Sample ID list:

Instrument

☐ Use stacker

Current: 37.0 °C

Target: 37.0 °C

Please note:

Measurement parameters

Measurement mode: Absorbance
Measurement wavelength: 492 nm
Reference wavelength: 620 nm
Read mode: Normal
Unit: OD

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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.

13.2.4 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.

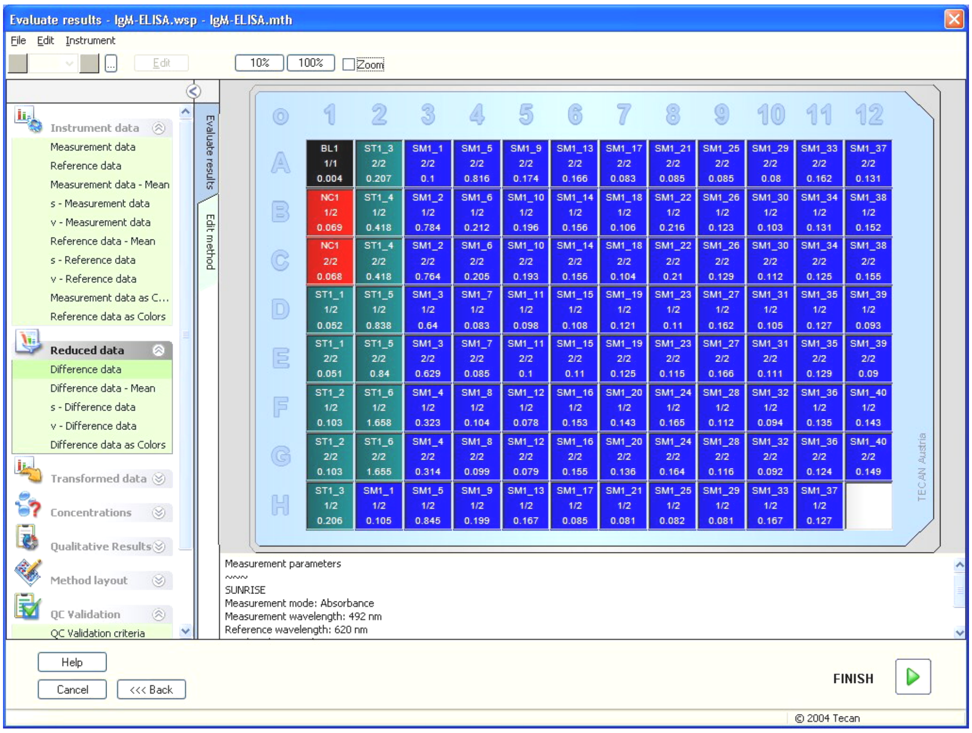
Note

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:

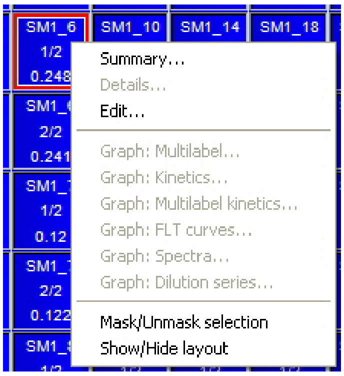


o	1	2	3	4	5	6	7	8	9	10	11	12
A	BL1 1/1 0.004	ST1_3 2/2 0.207	SM1_1 2/2 0.1	SM1_5 2/2 0.816	SM1_9 2/2 0.174	SM1_13 2/2 0.166	SM1_17 2/2 0.083	SM1_21 2/2 0.085	SM1_25 2/2 0.085	SM1_29 2/2 0.08	SM1_33 2/2 0.162	SM1_37 2/2 0.131
B	NC1 1/2 0.069	ST1_4 1/2 0.418	SM1_2 1/2 0.784	SM1_6 1/2 0.212	SM1_10 1/2 0.196	SM1_14 1/2 0.156	SM1_18 1/2 0.106	SM1_22 1/2 0.216	SM1_26 1/2 0.123	SM1_30 1/2 0.103	SM1_34 1/2 0.131	SM1_38 1/2 0.152
C	NC1 2/2 0.068	ST1_4 2/2 0.418	SM1_2 2/2 0.764	SM1_6 2/2 0.205	SM1_10 2/2 0.193	SM1_14 2/2 0.155	SM1_18 2/2 0.104	SM1_22 2/2 0.21	SM1_26 2/2 0.129	SM1_30 2/2 0.112	SM1_34 2/2 0.125	SM1_38 2/2 0.155
D	ST1_1 1/2 0.052	ST1_5 1/2 0.838	SM1_3 1/2 0.64	SM1_7 1/2 0.083	SM1_11 1/2 0.098	SM1_15 1/2 0.108	SM1_19 1/2 0.121	SM1_23 1/2 0.11	SM1_27 1/2 0.162	SM1_31 1/2 0.105	SM1_35 1/2 0.127	SM1_39 1/2 0.093
E	ST1_1 2/2 0.051	ST1_5 2/2 0.84	SM1_3 2/2 0.629	SM1_7 2/2 0.085	SM1_11 2/2 0.1	SM1_15 2/2 0.11	SM1_19 2/2 0.125	SM1_23 2/2 0.115	SM1_27 2/2 0.166	SM1_31 2/2 0.111	SM1_35 2/2 0.129	SM1_39 2/2 0.09
F	ST1_2 1/2 0.103	ST1_6 1/2 1.658	SM1_4 1/2 0.323	SM1_8 1/2 0.104	SM1_12 1/2 0.078	SM1_16 1/2 0.153	SM1_20 1/2 0.143	SM1_24 1/2 0.165	SM1_28 1/2 0.112	SM1_32 1/2 0.094	SM1_36 1/2 0.135	SM1_40 1/2 0.143
G	ST1_2 2/2 0.103	ST1_6 2/2 1.655	SM1_4 2/2 0.314	SM1_8 2/2 0.099	SM1_12 2/2 0.079	SM1_16 2/2 0.155	SM1_20 2/2 0.136	SM1_24 2/2 0.164	SM1_28 2/2 0.116	SM1_32 2/2 0.092	SM1_36 2/2 0.124	SM1_40 2/2 0.149
H	ST1_3 1/2 0.206	SM1_1 1/2 0.105	SM1_5 1/2 0.845	SM1_9 1/2 0.199	SM1_13 1/2 0.167	SM1_17 1/2 0.085	SM1_21 1/2 0.081	SM1_25 1/2 0.082	SM1_29 1/2 0.081	SM1_33 1/2 0.167	SM1_37 1/2 0.127	

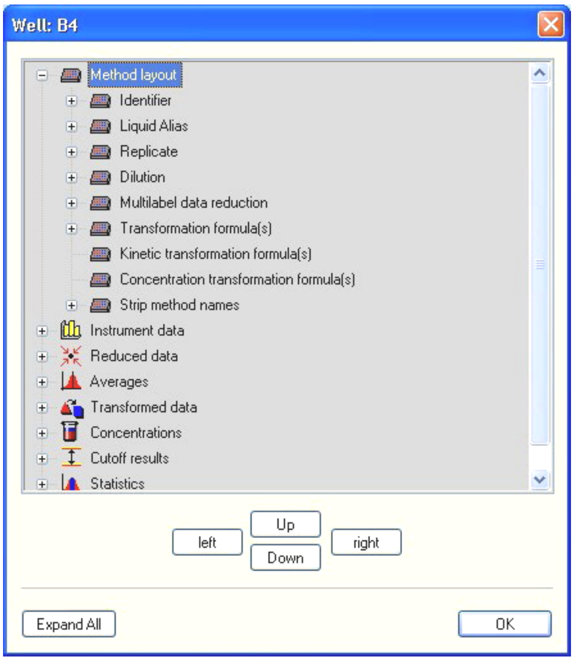
```
Measurement parameters
~~~~
SUNRISE
Measurement mode: Absorbance
Measurement wavelength: 492 nm
Reference wavelength: 620 nm
```

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.

13.2.5 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

14. Glossary of Terms

Term	Definition
Anisotropy	Data calculated with polarization measurements
Average single conc. (???)	Concentration calculated by averaging the single concentrations
Basis ???	Kinetic Parameter: Basis OD/RFU/RLU value of the onset calculation
Basis ??? %	Kinetic Parameter: Basis value of the onset calculation in %
Blank Reduction – parallel	Reduced data calculated with polarization measurements
Blank Reduction – perpendicular	Reduced data calculated with polarization measurements
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.
G-Factor	The G-factor is a instrument constant used in calculations of polarization measurements. In order to determine the G-factor a calibration measurement has to be performed.
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.

14. Glossary of Terms

Term	Definition
Hidden	Displayed if well data is hidden when printing
HUID	**H**ardware **U**nit **Id**entification Number
IC 50	The dilution/concentration which results in 50% of the maximum response
Intensity – parallel	Reduced data calculated with polarization measurements
Intensity – perpendicular	Reduced data calculated with polarization measurements
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 ???/hr	Kinetic Parameter: Maximum slopes of the kinetic curves per hour
Max. slope ???/min	Kinetic Parameter: Maximum slopes of the kinetic curves per minute
Max. slope ???/sec	Kinetic Parameter: Maximum slopes of the kinetic curves per second
Maximum ???	Kinetic Parameter: Maximum value of the kinetic curves
Mean slope ???/hr	Kinetic Parameter: Average slopes of the kinetics curves per hour
Mean slope ???/min	Kinetic Parameter: Average slopes of the kinetics curves per minute
Mean slope ???/sec	Kinetic Parameter: Average slopes of the kinetics curves per second
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 ???	Kinetic Parameter: Minimum value of the kinetic curves

Term	Definition
Multiple Reads per Well Measurement	A variety of readers have the ability to run a number of measurements within the same well. The average of the individual values will be determined for use in the evaluation and, if required, chosen values can be masked from the calculations of the mean value.
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.
Overflow	Overflow occurred during measurement in this well
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.
Strip Method Names	File names of the strip methods (useful for export of strip method results)
Polarization	Data calculated with polarization measurements
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
RFU – parallel	Data measured with polarization measurements
RFU – perpendicular	Data measured with polarization measurements
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

Term	Definition
Test	In previous versions a test contained the evaluation settings but not the measurement parameters. Tests are not longer supported in magellan and are replaced by the more powerful methods.
Time Basis ???	Kinetic Parameter: Time until the basis value is reached
Time Basis ??? %	Kinetic Parameter: Time until the basis value % is reached
Time Basis to Onset ???	Kinetic Parameter: Time between basis value and onset value
Time Basis to Onset ??? %	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 ???	Kinetic Parameter: Time until the maximum is reached
Time minimum ???	Kinetic Parameter: Time until the minimum is reached
Time Onset ???	Kinetic Parameter: Time until the defined onset value is reached
Time Onset ??? %	Kinetic Parameter: Time until the defined onset in % is reached
Time points	Time stamps of the single measurements of a kinetic measurement
Total Intensity	Data calculated with polarization measurements
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

Term	Definition
*****	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

Numbers refer to pages.

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