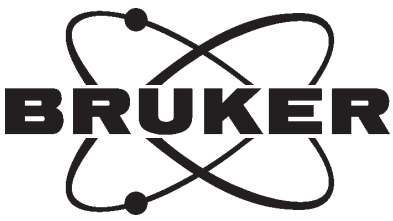
OPUS

Spectroscopy Software

Version 8

User Manual

LAB



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The description given in this manual is based on the technical specifications and the technical design valid at the time of publication. Technical specifications and technical design may be subject to change.

This manual is the original documentation for the OPUS/LAB spectroscopy software.

Table of Contents

1 Introduction

OPUS LAB is a software program designed for routine quality control. This program allows to measure product-specific IR spectra, perform qualitative and/ or quantitative analyses, and log evaluation results.

A product is defined by its membership in a specific product group, and its user-defined analysis parameters. These parameters are defined by the *Product Setup* command.

In detail, a product is described by a certain measurement experiment, QUANT, INTEGRATION, NeuroDeveloper classification and/or IDENT methods to be used, as well as additional parameters defined for data storage.

The evaluation results are displayed on the screen and can be saved or printed in a log file.

1.1 User rights

OPUS LAB distinguishes between two types of users:

1) **Administrator/LabManager**: users defined as *Administrator* or *LAB-Manager* in OPUS have access to the entire program functionality (including the OPUS LAB setup which requires signed XPM files and methods) and create and modify products.
2) **Operator**: users defined as *Operator* in OPUS perform pre-defined measurements and analyses in OPUS LAB.

The user rights are defined on the OPUS *Setup* menu by the *User settings* command. The *Administrator* has to ensure that the OPUS LAB *Operator* has only access to special commands (e.g. signature of spectra) within the OPUS workspace assigned to the *Operator*.

OPUS LAB user	OPUS user group
Administrator	Administrator
LABManager	LABManager
Operator	Operator

1.2 GMP mode

For each individual product the GMP (**G**ood **M**anufacturing **P**ractice) mode can be activated. In this mode relevant analysis information is automatically printed after each measurement.

1.3 21 CFR Part 11 compatibility

If OPUS LAB is to be run in a 21 CFR Part 11 compatible mode (setup via the OPUS workspace), the administrator must ensure that the operator has no right to modify the OPUS LAB configuration files. This can be done by refusing the operator any write access to the following directory:

Applicationpath\Data

In this case *Applicationpath* is the directory in which OPUS LAB has been installed.

1.4 Providing experiment, QUANT and IDENT method files

The OPUS LAB program requires experiment method files as well as QUANT 1, QUANT 2, INTEGRATION, NeuroDeveloper (ANN) classification, IDENT or Multi Evaluation methods.

To use these files within OPUS LAB they have to be stored in certain folders.

Structure of OPUS LAB folders

Folder	To store...
Data	• experiment (*Experiment.txt*) • product group (*ProductGroups.txt*) • product data
ECSpec	background spectra
IDENT	IDENT method files (**.faa*)
Log	log files (**.log*)
ME	Multi Evaluation method files (**.me*)
QT	quality test method files (**.qt*)
QUANT	QUANT method files (**.int, *.q2, *.q1*)

Folder	To store...
Spec	spectra measured
SpecExportConfig	configuration files (*.*ini*)
XPM	experiment files (*.*xpm*)

Where to copy the experiment files?

Experiment file	Copy into ...
all required experiment files	*Applicationpath\Xpm* directory (this is the directory in which OPUS LAB has been installed
QUANT method files (QUANT 1, QUANT 2, INTEGRATION)	*Applicationpath\Quant* directory
IDENT method files (NeuroDeveloper, IDENT)	*Applicationpath\Ident* directory
Multi Evaluation method files	*Applicationpath\ME* directory

Note: Make sure that the measurement experiment file is compatible with QUANT, INTEGRATION, IDENT and Multi Evaluation methods. Otherwise, OPUS LAB will be aborted.

Note that in case of a QUANT method, which always consists of several components, only the first component will be evaluated. Details on how to create Multi Evaluation methods are described in the OPUS Reference Manual .

1.5 Using a sample changer

When performing analyses using a sample changer you have to inform OPUS about the installed sample changer. In case of previous spectrometer series (e.g. VECTOR) you have to specify this kind of data by means of the *General Setup* in OPUS LAB. The new spectrometer generation (e.g. MATRIX, TENSOR, MPA, VERTEX) provides this kind of information automatically. Two different cases are described in the following:

Case 1: Sample changer for NIR spectrometers

To configure the sample wheel you have to perform the following steps:

1) On the OPUS LAB interface, click the *General Setup* button .
2) To define the maximum number of sample wheel positions click the *Sample wheel* tab.
3) Select the *mot60* option from the *Command for turning the wheel* drop-down list.

4) Define the number of sample positions by means of the *Number of sample wheel positions* drop-down list displayed.

Case 2: Sample changer for MIR spectrometers

To configure the sample wheel you have to perform the following steps:

1) On the OPUS *Measure* menu, select the *Optic Setup and Service* command.
2) Click the *Devices/Options* tab.
3) Select the *Sample Changer* check box and click the *Setup* button next to it. A new dialog pops up which displays a list of sample changer positions. Use the *Sample Changer* drop-down list to define the correct number of positions suitable to your sample changer.

When working with OPUS LAB you have to specify the type of command to be used to rotate the sample wheel. Perform the following steps:

1) Click the *General Setup* button.
2) Click the *Sample wheel* tab (see also chapter 2.4).
3) Use the *Command for turning the wheel* drop-down list to select the correct command to be able to rotate the wheel.

Two types of turning commands are available:

- SNR (Sample Number): for MIR sample wheels
- motXX: for NIR sample wheels, with XX being the motor number of the sample wheel. In case of NIR sample wheels the motor number is mostly 60.

The *Use mos60 command for zero point setting* check box is only relevant for VECTOR series spectrometers. It distinguishes the sample wheel control of a VECTOR 22/N-T and VECTOR 22/N-I. These spectrometers use the *MOS60* command to define the zero point of the sample wheel (transmission or reflection measurement).

1.6 Test Channel Status

The lower right OPUS status light on the OPUS interface indicates the spectrometer status based on the currently active channel or measurement experiment loaded. This status is stored on the instrument, not on the PC.

The color of the status light can be as follows:

- **Green:** The *active test channel* is active, the tests have passed and not expired.
- **Yellow:** The time interval for one or all the tests for the *active test channel* has expired.
- **Red:** One or all the tests for the *active test channel* have failed.

Each time the user loads an experiment file, the corresponding channel is set as active channel. The status of this new active channel is checked and indicated by the status light.

The active test channel refers to one of the IT channel positions defined in the *OVP Setup* dialog (see also chapter 13 in the OPUS Reference Manual).

1.7 Multiple measurements

There are two possibilities to perform standard multiple measurements (see chapter 4.3):

- By using a probe, in this case the measurement is controlled by the control button on the probe.
- By any measurement channel (e.g. integrating sphere) of the MPA spectrometer. In this case the measurement is controlled by the *Start* button on the display at the MPA front side.

In the latter case you require the following OPUS configuration:

1) On the *Measure* menu, select the *Optic Setup and Service* command.
2) Click the *Devices/Options* tab.
3) Activate the *Ext. Synchronisation* check box.
4) Additionally, you also have to activate the *External Synchronisation* option for the experiment. In this case select the *Setup Measurement Parameters* command on the *Measure* menu. Click the *Optic* tab and select *ON* from the *External Synchronisation* drop-down list.

Note: If the *External Synchronisation* option has been activated, a window pops up which you can alternatively use to start the measurement. If you want to skip this window, it is recommended to start OPUS using the */HIDEEXTSYNC=ON* command line option. To enter the command line right click the OPUS icon in the Windows *Start* menu and select the *Properties* command.

2 General Setup

Before starting sample measurements using OPUS LAB, you first have to setup general parameters which require Administrator or LabManager user rights.

2.1 Starting OPUS LAB

1) On the *Measure* menu, click the *OPUS LAB* command. Alternatively, click  on the toolbar.

Note: If you have OPUS LAB Administrator or LABManager rights, the OPUS LAB starting dialog (see figure 1) opens. Otherwise, the measurement dialog (see figure 36 on page 54) is shown on the screen.

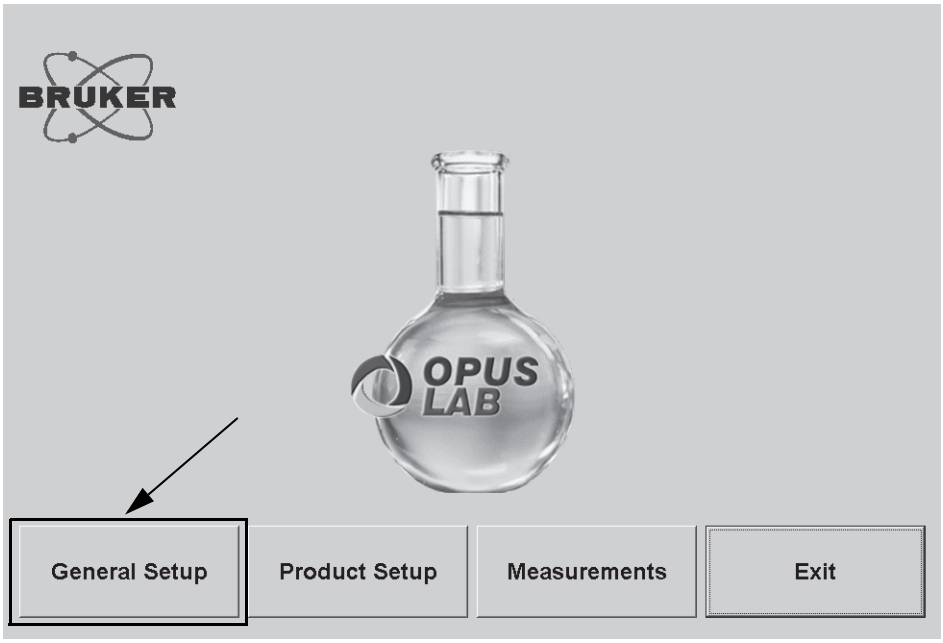


Figure 1: OPUS LAB starting dialog

2) Click the *General Setup* button.

2.2 General

If you position the cursor on one of the check boxes on the *General* tab, the command is briefly described in the selection field on the right (see A in figure 2).

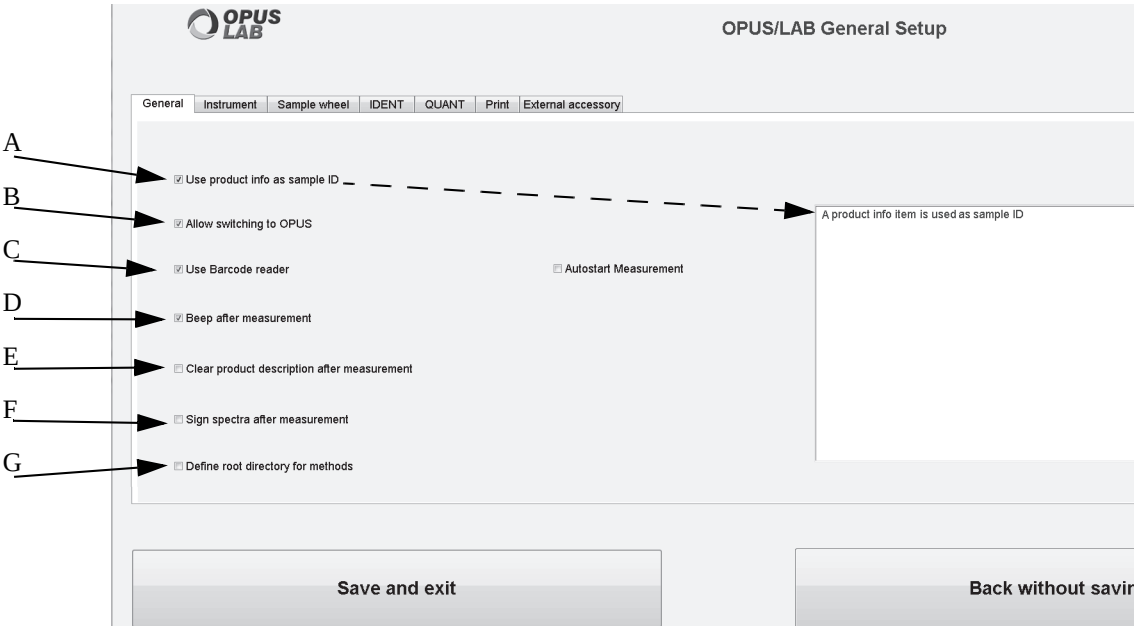


Figure 2: OPUS LAB General Setup - General

A) The details given on product information can be used to identify the sample. Activating or deactivating the option effects all products available in OPUS/LAB.

A message box informs that an info field (chapter 3.7) for the sample ID will either be added or deleted for each product when activating or deactivating the option. If all 5 info fields have already been used in case of existing products, the fifth info field will be overwritten by the sample ID information. Confirm the message box and click the *Start* button. An overview table contains the results of the changes made. The results can be indicated as follows:

- : result ok
- : result not ok
- : far-reaching changes have been made, e.g. info field has been overwritten
- : special information on result

Note: This option cannot be used in case of container measurements. If OPUS LAB is connected to a database, the information on the sample ID are written into the database.

B) This option allows switching between the OPUS and OPUS LAB user interface and vice versa. On top of the screen a button (Switch To Opus / Switch To OpusLAB) is displayed which you can use to switch to the respective interface.

C) Barcodes can be scanned by using a barcode reader. The barcode reader needs to have an RS232 interface and must be connected to the COM Port 1. If you activate the check box, a second checkbox is displayed. If you activate the second checkbox, the measurement automatically starts after scanning the barcode has been finished.

D) An acoustic signal indicates the end of measurement.

E) All product information entries will be deleted from the dialog box after the measurement has been finished.

F) Spectra can be signed from within OPUS LAB. If spectra are not signed when measuring in GMP mode, an error message pops up. Single reports include information on who has signed which spectra.

When working with a sample changer, the first run will be measured and at the end of the measurement all spectra have to be signed by means of the *Add Signature* command from the *Validation* menu in OPUS. For further details on signing spectra refer to the OPUS VALIDATION manual.

G) OPUS LAB method files[1] for products which are directly evaluated by an IDENT, QUANT or conformity test method can be saved in any directory, a file server. Make sure that the directory selected has the following sub-structure:
...\Data
...\Ident
...\QT (Quality Test)
...\Quant
...\Xpm
As soon as you change the path of the OPUS LAB basic directory you also have to store the respective method files into this new path, according to the structure described.

Note: If the new OPUS LAB basic directory and OPUS LAB are both located on the same computer, OPUS LAB retrieves the method files from this new directory. If the new OPUS LAB basic directory and OPUS LAB are located on different computers (e.g. file server), OPUS LAB copies a local copy of the method file required from the new OPUS LAB basic directory to a local, temporary directory. The local copy is deleted as soon as measurement and evaluation have been completed. In this case, the HISTORY data block of the OPUS spectrum file contains the path of this local copy. The OPUS LAB analysis report contains the path defined in the OPUS LAB *General Setup*.

1. In case of OPUS LAB methods which are evaluated by multi evaluation (ME), you have to define the ME base path separately for the file server, by selecting the OPUS *User Settings* command and clicking the *General* tab. Details on the base path are described in the OPUS Reference Manual.

2.3 Instrument

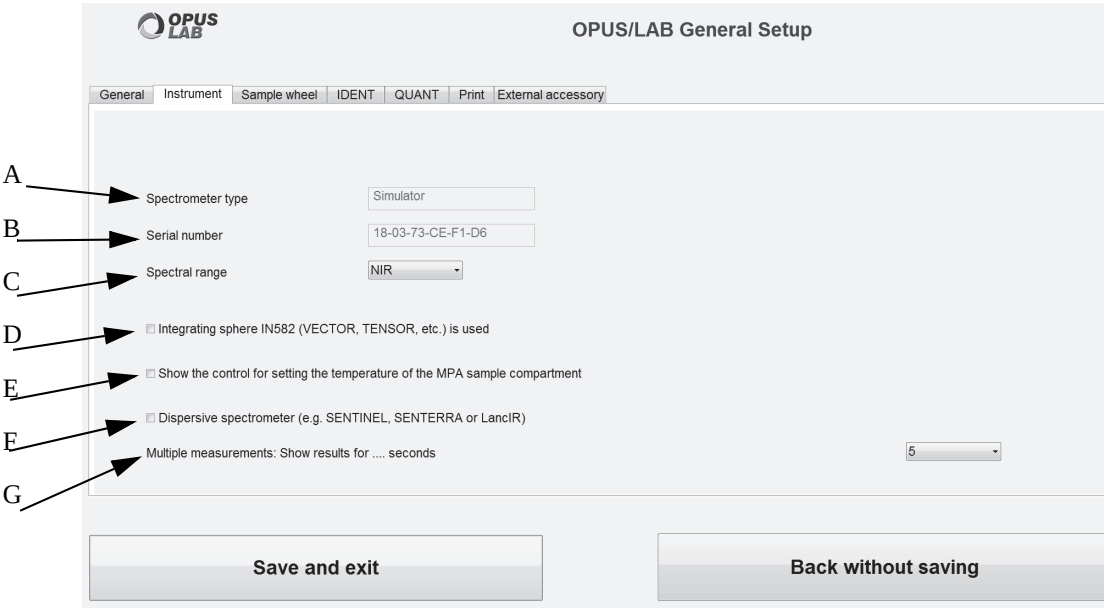


Figure 3: OPUS LAB General Setup - Instrument

A) The type of spectrometer is indicated in the selection field on the right.

B) The serial number of the spectrometer is indicated in the selection field on the right.

C) Define the spectral range, i.e. MIR or NIR, by means of the drop-down list.

D) In case of spectrometers using a conventional integration sphere (IN582) you have to activate this check box. For further information on this subject refer to chapter 3.1.

E) Activate this check box if you want to set the temperature in the MPA sample compartment. Consequently, during measurement the *Set sample temperature* button is displayed in the upper left corner of the screen. Click this button and set the temperature accordingly.

F) If you work with dispersive spectrometers, you have to activate this check box. To be able to use dispersive spectrometers a special basic script has to be created first. For further information on how to create such a script refer to the Bruker Service.

G) In case of multiple measurements you can have the results displayed. Define the display time (in seconds) by means of the drop-down list on the right. When entering "-1" the result is permanently displayed on the screen.

2.4 Sample Wheel

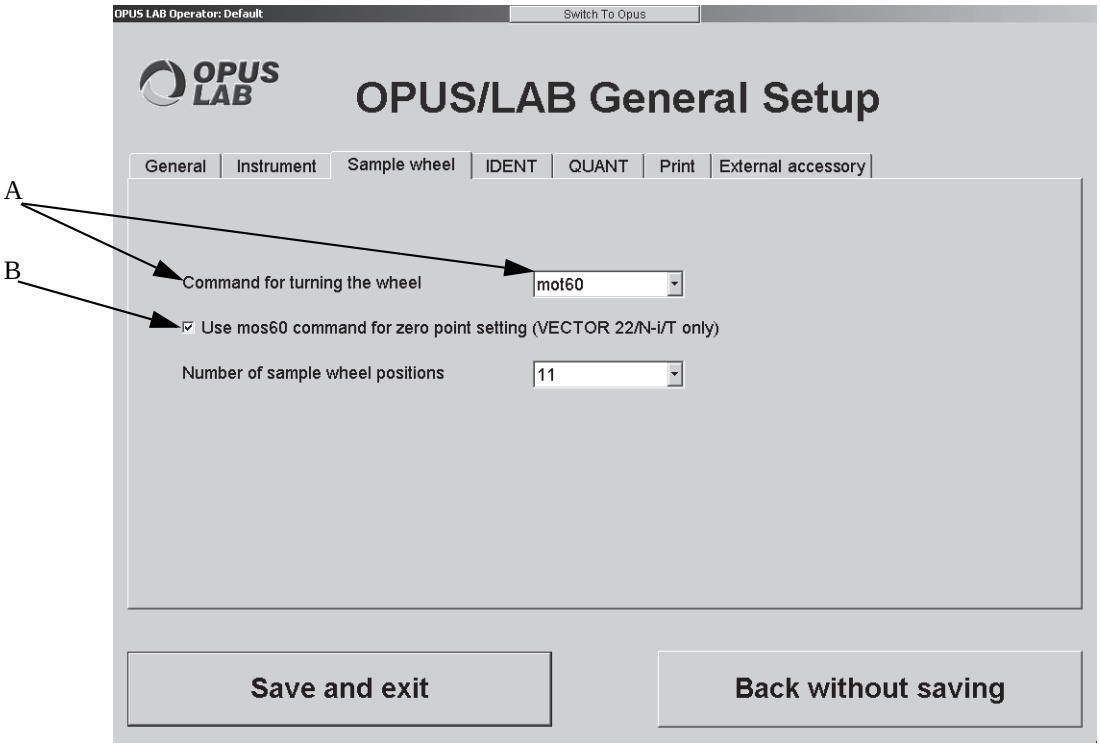


Figure 4: OPUS LAB General Setup - Sample wheel

A) Select the turning wheel command from the drop-down list. For further details refer to chapter 1.5 and 4.4.3.

B) If you activate the check box, the zero position of the sample wheel will be defined. This applies to spectrometer series VECTOR 22/N-I/T only. For further details refer to chapter 1.5 and 4.4.3. Define the number of sample wheel positions by means of the drop-down list on the right.

2.5 IDENT

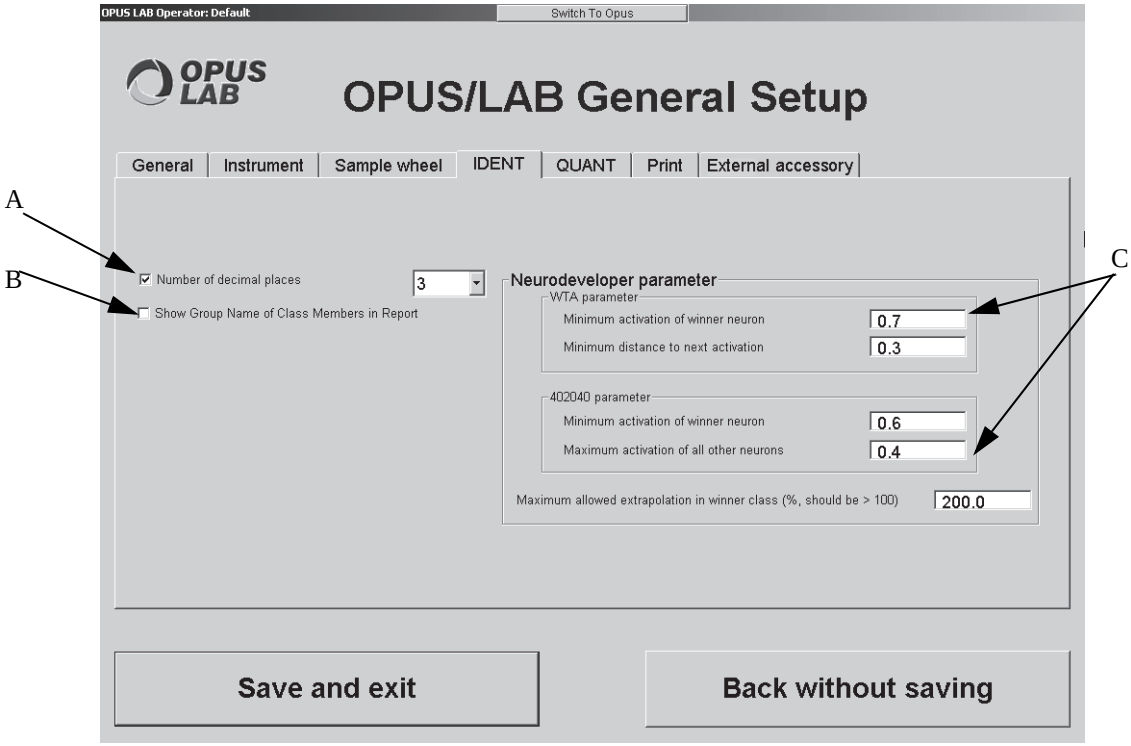


Figure 5: OPUS LAB General Setup - IDENT

A) If you activate the check box, an appropriate drop-down list will be displayed. Use this drop-down list to define the number of decimal places to be included in the IDENT analysis report.

B) If you activate the check box, the IDENT analysis report includes the group names of the particular class member.

C) Use the entry fields to set the different NeuroDeveloper parameters. For further details on this subject refer to the corresponding NeuroDeveloper documentation.

2.6 QUANT

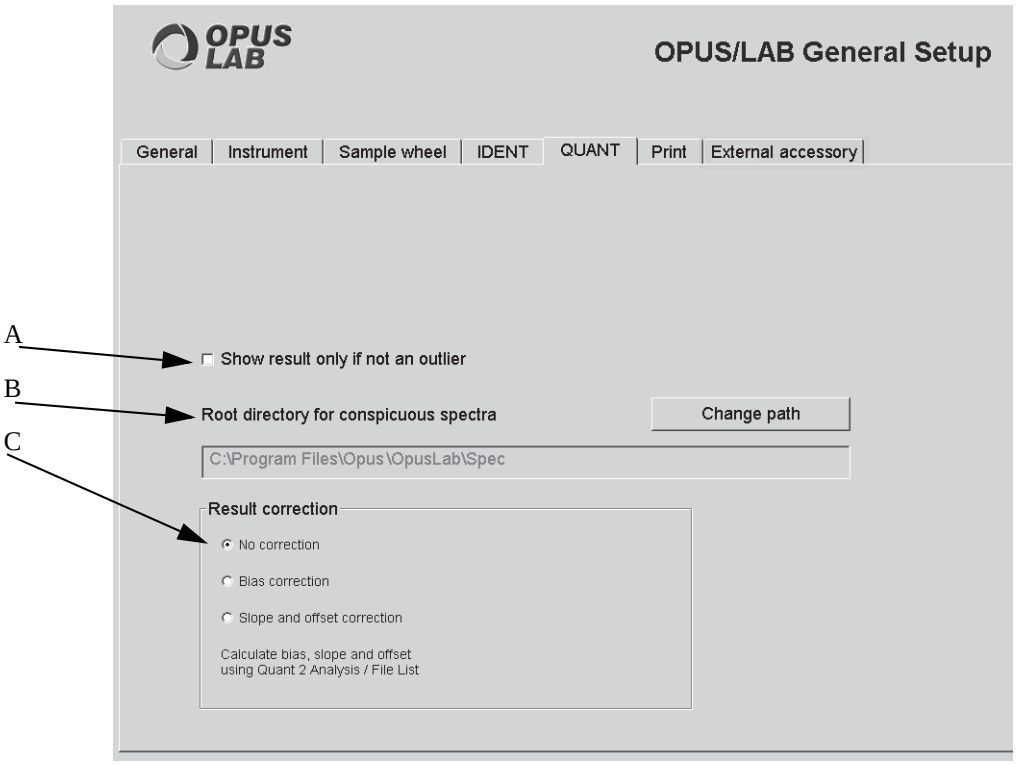


Figure 6: OPUS LAB General Setup - QUANT

A) If you activate this check box, the QUANT result will only be shown if there are no outliers. In case of outliers in the QUANT analysis, the report indicates that there are outliers but does not show any value.

B) It is possible to create a root directory for conspicuous spectra, i.e. spectra which include e.g. outliers. Click the *Change path* button to specify the path for this kind of directory. The kind of conspicuous features to be considered in spectra can be clearly defined by means of *Product Setup*. See also chapter 3.4.

C) The QUANT evaluation result can be corrected. If you activate one of these option buttons a correction of either bias, slope or offset is performed during runtime. The *No correction* option button is activated by default. This correction option applies to QUANT 2 analysis/File list, only. For details on how to define the values for bias, slope or offset refer to chapter 3.4.

D) **Note:** A correction cannot be performed when working in validated mode, even if you have selected a respective option button in the dialog.

2.7 Print

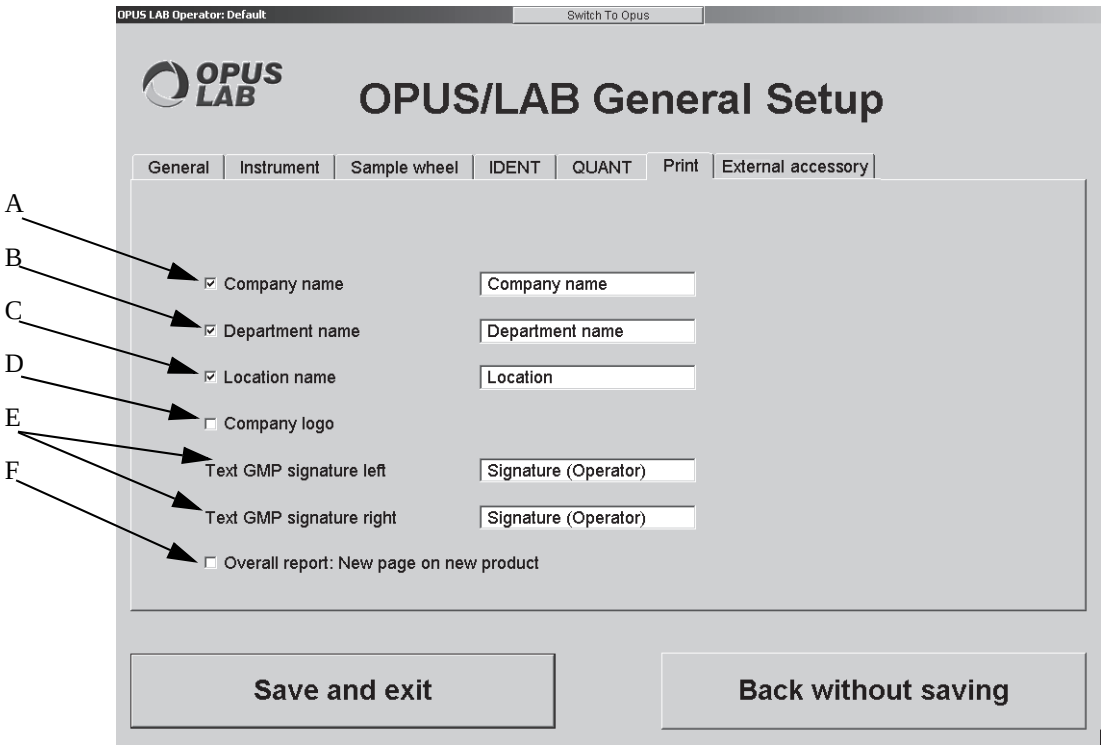


Figure 7: OPUS LAB General Setup - Print

A) The print-out of the OPUS LAB measurement result may also include the company name. If you activate the check box, an additional entry field will be displayed. Enter the corresponding company name into this entry field.

B) The print-out of the OPUS LAB measurement result may also include the department name. If you activate the check box, an additional entry field will be displayed. Enter the corresponding department name into this entry field.

C) The print-out of the OPUS LAB measurement result may also include the location name. If you activate the check box, an additional entry field will be displayed. Enter the corresponding location name into this entry field.

D) The print-out of the OPUS LAB measurement result may also include the company logo. Make sure that you use a bitmap file in this case. To properly fit the print-out you have to resize the logo bitmap file. Width: 180 pixels, height: up to 360 pixels (recommended).

E) The two entry fields will only be displayed, if you work in GMP mode. The terms used by default can be changed.

F) In case of measurements with different products you will get an overall report, with each product being printed on a separate page.

2.8 External accessory

If external accessory is connected to the spectrometer, the appropriate instrument configuration must be activated.

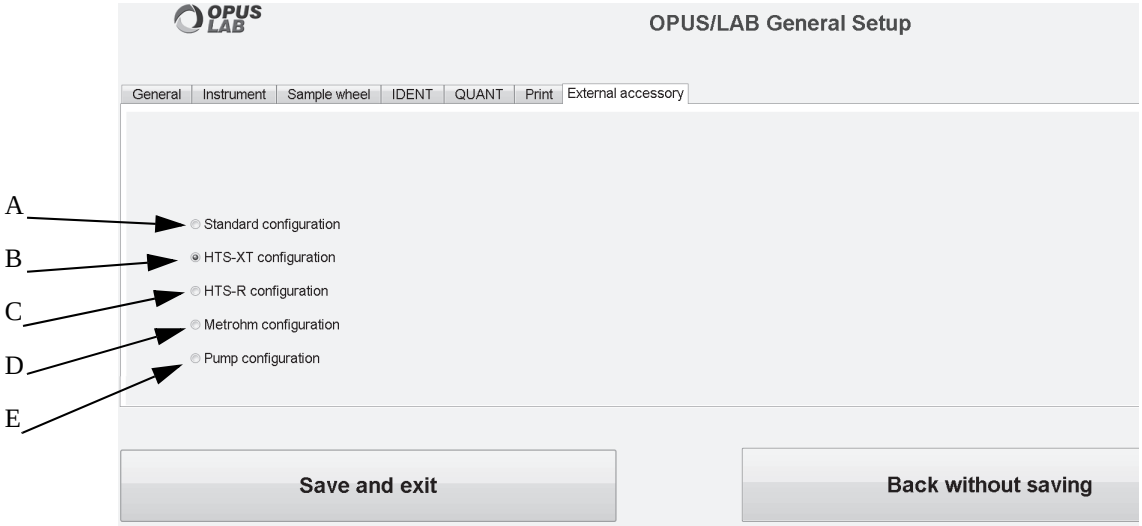


Figure 8: OPUS LAB General setup - External accessory

A) The option button may only be activated if no accessory is connected to the spectrometer.

B) The option button must be activated if the HTS-XT module is connected to the spectrometer.

C) The option button must be activated if the HTS-R module for Raman measurements is connected to the spectrometer.

D) The option button must be activated if the Metrohm 838 Autosampler for automated measurements of liquids is connected to the spectrometer.

E) The option button must be activated if the ISMATEC Reglo Digital pump for automated measurements of liquids is connected to the spectrometer.

2.9 Storing general setup

Click the *Save and exit* button. The *OPUS LAB* user interface will be completely closed and the settings made will be stored into the *OPUS LAB.ini* file.

2.10 Modifying general setup

On the *Measure* menu click the *OPUS LAB* command again and make the necessary changes. Alternatively, click  on the toolbar.

3 Product Setup

The *Product Setup* allows to define parameters of a new product or product group, to change previously defined products and to delete existing entries.

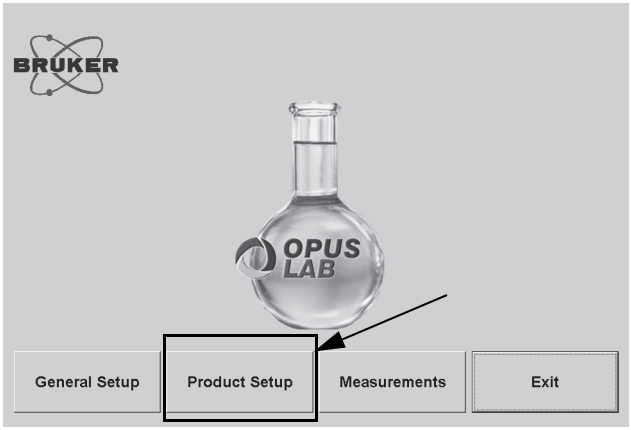


Figure 9: OPUS LAB Product Setup

A product is always defined by the following parameters:

- Experiment
- Background
- QUANT (quantitative analysis parameters)
- IDENT (identity test parameters, NeuroDeveloper)
- Storing options
- Product info
- Log/report parameters

Each product belongs to a product group. If you select a certain product group, the *Product* drop-down list includes all products specified for the respective product group. Those five products which have been used most frequently are displayed as favorites.

Note: OPUS LAB allows to use the name of the product or product group as path name. Therefore, the name of the product or product group must not contain any of the following symbols:

\ / : * ? " < > |

It is possible to assign several products or evaluation methods to one experiment.

Note: In general, all modifications made with regard to the settings of existing products have to be saved before you continue to select a new product.

3.1 Experiment

The *Experiment* tab (figure 10) contain setting options concerning parameters which relate to the respective experiment. These parameters are related to the **OPUS measurement experiment** and not to the product.

If you change these parameters for one product, they will automatically be changed for all the other products, provided these products are based on the same OPUS experiment file (*.xpm).

First Steps

1. Creating new product group:

- Click the *New product group* button.
- Enter a name for the product group into the entry field displayed.

2. Creating new product

- Click the *New product* button.
- Enter a name for the product into the entry field displayed.

3. Deleting existing product group:

- Click the *Delete product group* button.
- Click *Yes* to confirm.

4. Deleting existing product:

- Click the *Delete product* button.
- Click *Yes* to confirm.

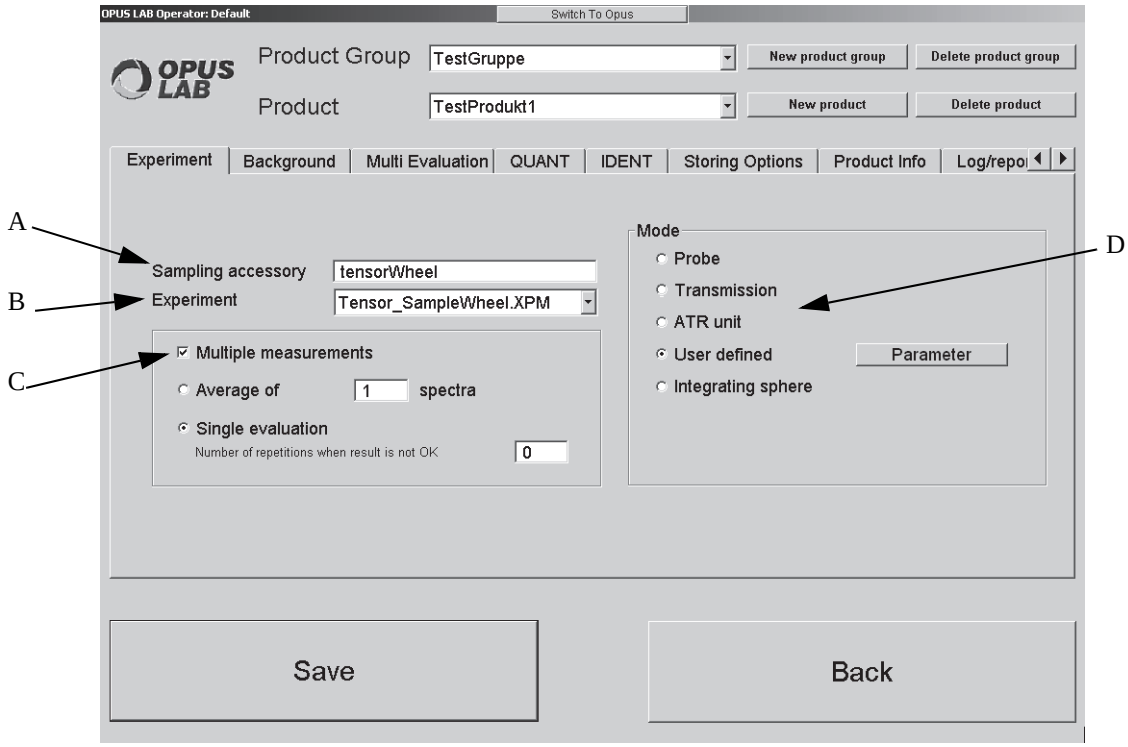


Figure 10: OPUS LAB Product Setup - Experiment

A) The name of the sampling accessory is used in OPUS LAB in case of user instructions and user information (e.g. on background measurements). You can individually specify the name of the sampling accessory. Enter the respective name into the entry field.

B) You can select the OPUS experiment file (*.xpm) from the *Experiment* drop-down list. Note that this drop-down list only includes experiment methods which are stored in the *Applicationpath\Xpm* directory. *Applicationpath* is the path in which OPUS LAB has been installed.

C) There are two types of multiple measurements. First, the evaluation of an average spectrum and second the single evaluation. If you activate the *Average of N spectra* option button, *N* spectra will be measured and averaged. *N* represents the number of averaged spectra. Afterwards the averaged result spectrum will be evaluated[1].

If you activate the *Single evaluation* option button, you can measure single container measurements. Enter the number of repetitive measurements into the entry field. This number defines how many times a sample, which has not been correctly identified during the first measurement, has to be successfully identified before the total result reads: *Identified*. If a repetitive measurement gets the result *Not identified,* the total result will automatically read: *Not identified*. In this case no further repetitive measurements have to be performed. For further details on recommended settings in OPUS LAB to identify raw materials, refer to chapter 3.5.1.1.

1. If a product with the *Average of N spectra* (N >1) option is used in connection with *Sample changer* (chapter 4.4), the *N* is automatically set to *1*. This means that only one spectrum is measured on each sample changer position.

D) In the *Mode* group field you define the type of accessory to be used for product measurement. This group field is not available if you use external measuring accessory (i.e. non-Bruker accessory). In this case, the OPUS LAB ini file contains the *[EXTERNAL_ACC] ACTIVE = YES* entry. This means for example, when adding *=HTS-XT* or *=HTS-R* to the *ITYPE* ini file entry, the group field remains non-available.

This definition is only used for operator instructions within OPUS LAB (e.g. on background measurements). The following options are available:

- Probe
- Transmission (e.g. cuvette or vial)
- ATR unit: can only be selected for measurements in the mid-infrared range (set the spectral range to MIR in the OPUS LAB *General Setup*, see chapter 2.3).
- User-defined: if you check the *User-defined* option button, the *Parameters* button will be displayed. When using user-defined accessory you can define special instructions which are displayed before starting the background and/or sample measurement. If you click the *Parameter* button, the following view opens:

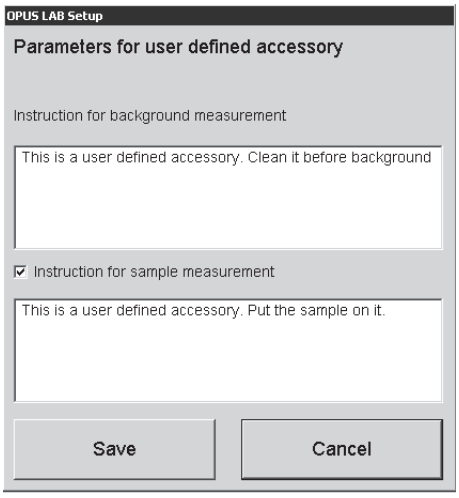


Figure 11: Parameters for user-defined accessories

Write the instructions into the entry fields and click the *Save* button to confirm.

- Integrating sphere: if you check the *Integrating sphere* option button, the *Internal reference* check box will be displayed. Activate this check box to automatically perform a background measurement prior to each sample measurement. As the user does not have to perform any background measurement, no respective button is displayed.

Note: The *Internal reference* distinguishes between two different spectrometer types. Spectrometers, e.g. VECTOR 22, which use the IN582 integrating sphere, and spectrometers which use a less-conventional version, e.g. MPA-R or MATRIX-I.

While the IN582 integrating sphere is controlled by so-called *mot* commands, the modernized version can be directly controlled by the

experiment settings. On the OPUS *Measure* menu, select the *Setup Measurement Parameters* command. Click the *Optic* tab. If you can select *Sphere Background* from the *Background Meas. Channel* drop-down list, the less-conventional integrating sphere will be available. Depending on the kind of integrating sphere used, you first have to activate the respective check box by means of the *General Setup* (see chapter 2.3).

3.2 Background

The *Background* tab contains setting options concerning background and cleanness test as well as spectra quality test. The settings made are stored with the measuring experiment, except for those regarding the spectra quality test.

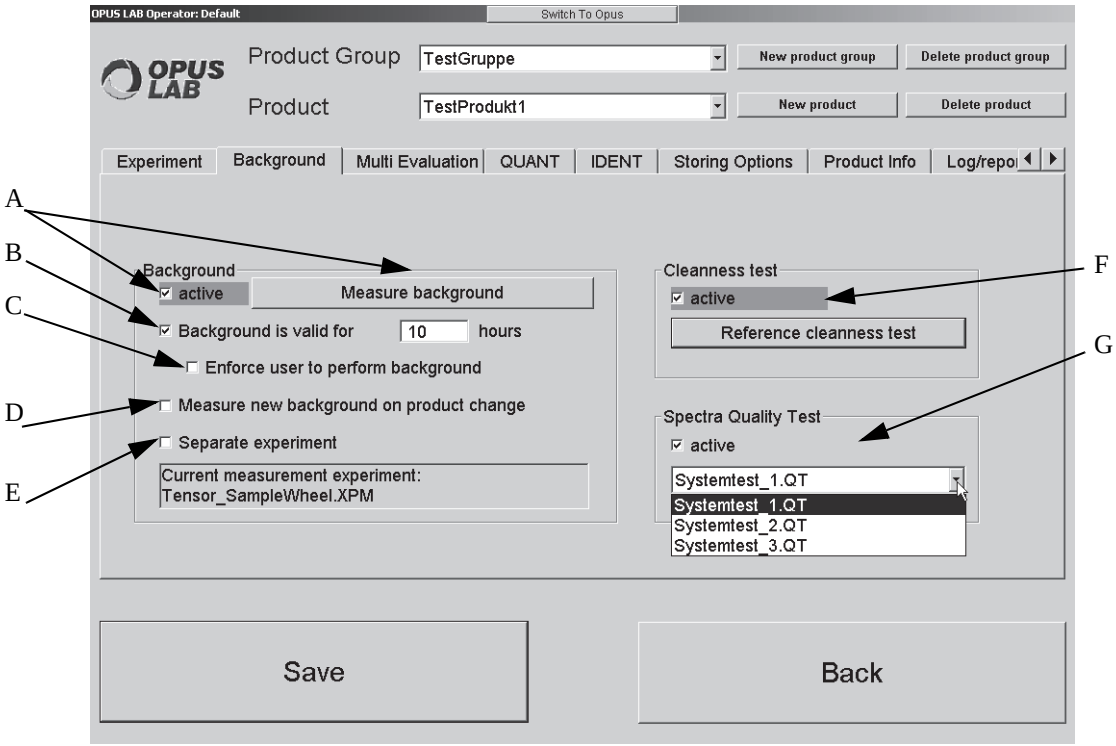


Figure 12: OPUS LAB Product Setup - Background

A) If the *Active* check box is activated, background measurements can be performed at any time. When clicking the *Start* button (see chapter 4.1), another dialog opens with the *Measure background* button displayed. Click this button. If the *Active* check box (figure 12) is deactivated, the *Measure background* button will be grayed out.

Note: The other options designed for background measurement do not depend on whether the *Active* check box is activated or not. If you click the *Measure background* button, the *Background measurements* dialog will open (see chapter 4.1.1).

B) By means of regular background measurements you can deduct any instrument-specific features from the sample spectrum. You can define a validity period (in hours) for the current background spectrum.

Note: It is also possible to enter floating point numbers, e.g. the *1.5 hours* entry corresponds to 90 minutes.

C) The check box is only available if the *Background is valid for n hours* check box has been activated. If the *Force user to perform background* check box is activated, you have to measure a new background spectrum, e.g. if the validity period of a background spectrum has expired. If the check box is deactivated, you will only be informed that the validity period of the background spectrum has expired.

D) If the *Measure new background on product change* check box is activated, you will be requested to measure a new background spectrum as soon as the product to be analyzed has changed.

Note: This feature is only available for single-sample measurements.

E) Certain applications require different experiment files for sample and background measurements. However, the most essential parameters, e.g. optical resolution, of these files have to be identical. This e.g. also applies to measurements of an *internal reference* on integrating spheres within the new spectrometer generation (MAP, MATRIX), or to background measurements of the *External Transmission* measurement channel on the MPA. In this case an internal SPECTRALON reference can be used.

If you activate the *Separate experiment* check box, a drop-down list will be displayed. Use this list to select a separate experiment method file for the background measurement.

Note: This drop-down list only includes experiment methods which have been defined in the *Applicationpath\Xpm\Ref* directory. *Applicationpath* is the path in which OPUS LAB has been installed.

F) If you activate the check box, a cleanness test will be performed during the background spectra measurement, and the *Reference cleanness test* button is enabled. Click this button to open another dialog used for a new background spectrum. This dialog allows to measure the reference spectra and set the threshold value required for the test. For details of the cleanness test refer to chapter 4.5.

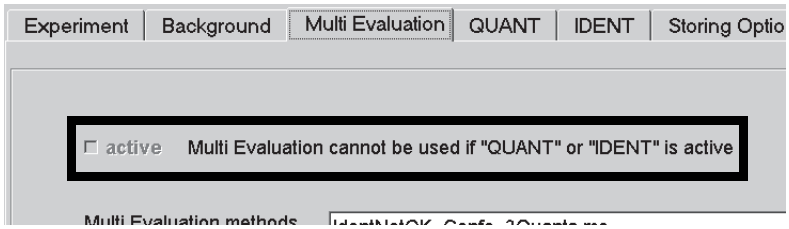
G) If you activate the check box, the quality of each spectrum measured will be tested. A method file will be created in OPUS. To perform a quality test select a method file (*.*QT*) from the drop-down list. This file has to be stored in the *Applicationpath* data path.

3.3 Multi Evaluation

The *Multi Evaluation* tab contains setting options for Multi Evaluation parameters, which can, however, only be used in connection with an appropriate *Multi Evaluation* method previously created. Detailed information on how to create a Multi Evaluation method are provided in the OPUS Reference manual.

In OUPS LAB, the Multi Evaluation cannot be simultaneously performed together with a separate QUANT or IDENT analyses.

If the *Active* check box on the *QUANT* or *IDENT* tab has already been activated, the *Active* check box on the *Multi Evaluation* tab will be disabled and a corresponding message displayed.



The Multi Evaluation result is based on the Multi Evaluation method previously defined. This means that the IDENT results will be indicated in the IDENT Report, QUANT results in the QUANT report. The methods used and the structure path are included in the ME (ME) data block, to be seen in the OPUS browser.

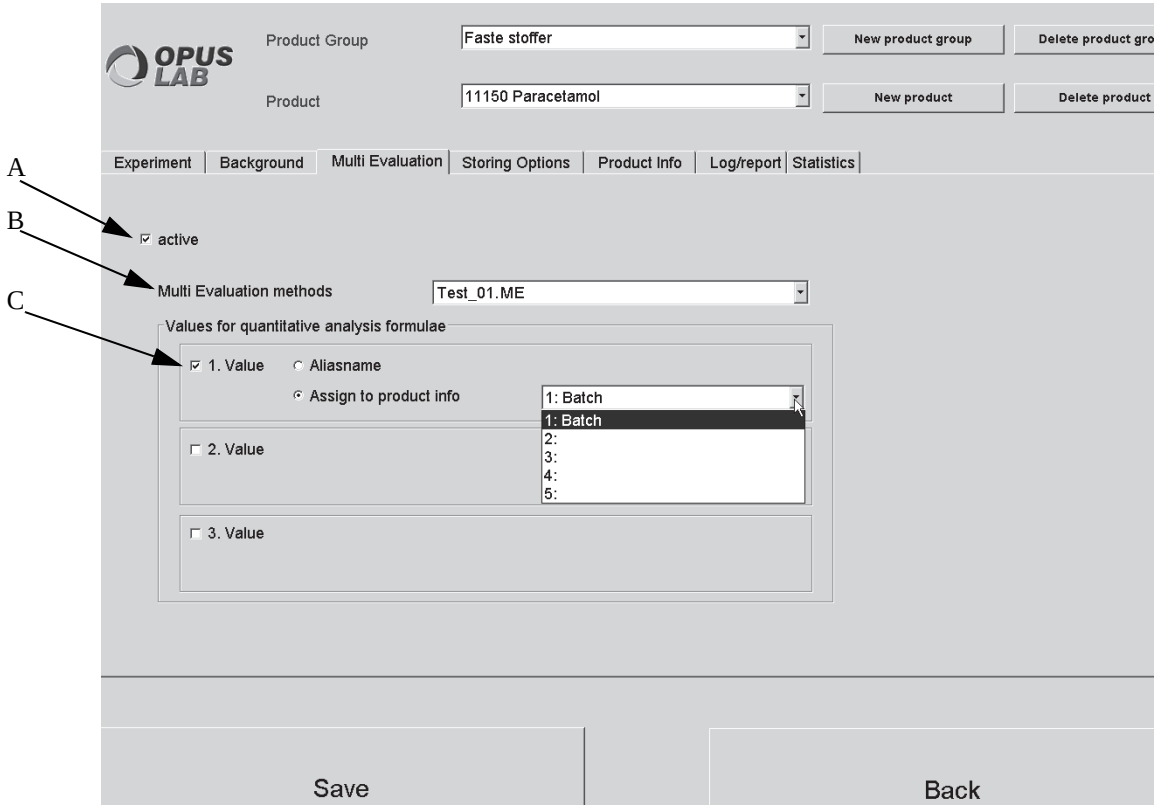


Figure 13: OPUS LAB Product Setup - Multi Evaluation

A) Activate the check box if a Multi Evaluation has to be performed. In this case no QUANT or IDENT analysis is possible.

B) Use the drop-down list to select a Multi Evaluation method which has been previously created in OPUS. For further details on how to create a Multi Evaluation method refer to the OPUS Reference Manual.

C) Defining values for a quantitative analysis only makes sense if the Multi Evaluation method includes a formula with appropriate input parameters. Activate the check box and specify the entry field to be used for the input parameter during measurement.

If you check the *Aliasname in OPUS LAB* option button, a new entry field will be displayed. Enter the appropriate parameter into this entry field. If you later click the *Measure* button in the dialog for single sample measurements, a new window can be opened before measurement, which allows to modify the parameters, if required.

A drop-down list is displayed if the *Assign to Product Info* option button is activated. Select the appropriate info field from this list, which is used to enter the input parameter. Make sure that you have previously defined the info field on the *Product Info* tab (see chapter 3.7). During measurement the value for the quantitative analysis will be entered into the info field defined.

Note: Do not select the *Sample ID* info field for the value of quantitative analysis.

3.4 QUANT

The *QUANT* tab contains setting options for QUANT parameters, which can, however, only be used in connection with an appropriate QUANT method previously created. Detailed information on how to create a QUANT method refer to the OPUS QUANT manual.

In OUPS LAB, the QUANT analysis cannot simultaneously be performed with a Multi Evaluation. Therefore, if the *Active* check box on the *Multi Evaluation* tab has already been activated, the *QUANT* tab will no longer be available.

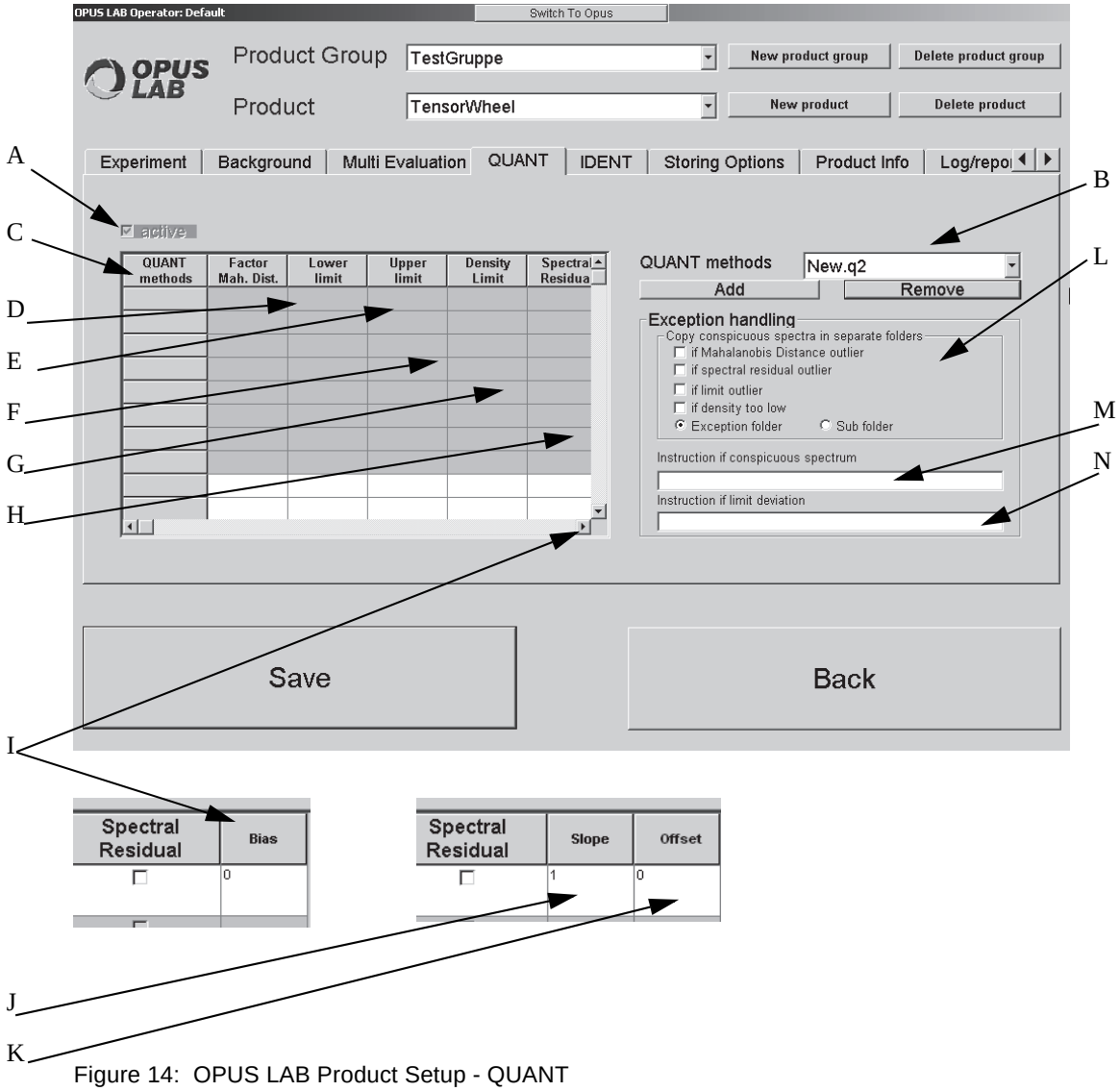


Figure 14: OPUS LAB Product Setup - QUANT

A) Activate the check box if a QUANT analysis has to be performed.

B) Select the corresponding QUANT method from the *QUANT methods* drop-down list. This drop-down list only includes those methods which have been stored in the *Applicationpath\Quant* directory. *Applicationpath* is the path in which OPUS LAB has been installed.

Note: You can use QUANT 1 as well as QUANT 2 analysis and integration methods. However, the *Factor M.-distance* is of no importance to QUANT 1 and integration methods.

Having selected a QUANT method, click the *Add* button. The QUANT method selected will be displayed in the *QUANT method* column. If you want to delete a QUANT method, select the respective method and click the *Remove* button.

C) The components to be analyzed are defined in the table. The first column includes the name of the QUANT method which allows the evaluation of a single component. If more than one product component has to be analyzed, appropriate individual QUANT methods have to be created and assigned in OPUS LAB.

D) The scaling factor for the maximum Mahalanobis distance scales the sensitivity for outlier detection. The Mahalanobis distance is a statistical parameter calculated on the basis of a QUANT 2 analysis. This distance allows conclusions to be drawn from the similarity between the measured and calibrated spectra.

The report contains the Mahalanobis distance determined for each component, and the maximum Mahalanobis distance. A relatively low numerical value of this constant indicates a satisfactory measurement result, while a relatively high numerical value indicates insufficient calibration conformity. The status value of a component analysis is set as *outlier* if the Mahalanobis distance determined is higher than the product from the scaling factor multiplied by the maximum Mahalanobis distance. The default value is 1.

E) This is the possible lower concentration limit (optional) of the component being analyzed.

F) This is the possible upper concentration limit of the component being analyzed.

The values displayed in the *Factor M-distance*, *Lower limit* and *Upper limit* columns can be changed manually. If you have not specified any lower and upper limit, no concentration range test will be performed. This also applies for the *Density Limit*.

G) This limit indicates the so-called *Component Value Density* and informs about the number of calibration samples existing within the calibration model at the predicted concentration value (for further details also see the OPUS QUANT manual). If the QUANT analysis results in a value < than the limit defined, the spectra concerned will be marked. This requires the QUANT 2 method to include a certain number of spectra (at least 30). For further details on this subject refer to the QUANT manual.

H) This column can only be activated or deactivated. As soon as the spectral residuals are activated, a green check mark will be displayed. To be able to consider this value during analysis make sure that the *Spectral residuals* check box has been activated when creating a QUANT 2 method in OPUS. This check box is included on the *Store Method* tab. For further details on this subject refer to the OPUS QUANT manual.

I) This column is only available if you have activated the appropriate option button on the *QUANT* tab in the *General Setup* (chapter 3.4). In this

column you can define the value for a bias (additive factor) correction of a QUANT evaluation result. The bias is a systematic deviation of the predicted value from the true value, due to a particular measurement method. In practice, it is intended to avoid such systematic errors. A bias correction may be helpful. This kind of correction changes the values of a regression straight line into the values of an origin straight line. In this case the bias (ordinate) of these lines is deducted from the respective points, i.e.:

$Result_{corr} = Result_{QUANT} - Bias$

For further details refer to the OPUS QUANT manual.

J) This column is only available if you have activated the appropriate option button on the *QUANT* tab in the *General Setup* (chapter 3.4). In this column you can define the value for a slope (multiplicative factor) correction of a QUANT evaluation result. Compared to bias correction, the slope of the straight lines is set to 1.

K) This column is only available if you have activated the appropriate option button on the *QUANT* tab in the *General Setup* (chapter 3.4). In this column you can define the value for an offset (additive factor) correction of a QUANT evaluation result. The offset is the y-value of a regression straight line if x = 0. The result correction of J) and K) is calculated as follows:

$Result_{korr} = (Result_{QUANT} - Offset)/Slope$

L) Spectra distinguished by some kind of conspicuous features can be stored into a separate folder. There are two options: product-specific errors only will be stored in the *Sub-folder*. The sub-folder includes the following standard directories: *Density, Limit, Mhd, SpecRes*, which cannot be changed. All errors detected, except for product-specific errors, will be stored in the *Exception folder*. By means of the different check boxes you can further specify the conspicuous features.

M) As soon as an outlier is detected for at least one component (i.e. an error occurred during the analysis), a corresponding error message will be displayed on the screen. The message text displayed can be changed by the administrator.

N) If the predicted value is beyond the range defined by the lower and upper limit, an error message relating to this circumstance will be displayed on the screen. The message text displayed can be changed by the administrator.

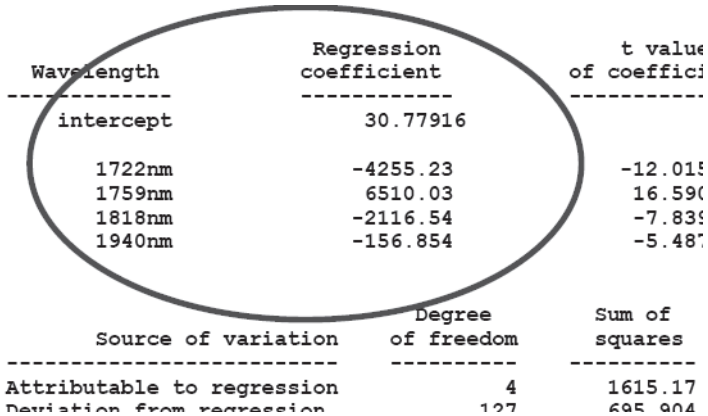
3.4.1 Filter Calibration

OPUS allows to transfer calibrations which are based on former filter systems. Select a macro previously created, with the **.mtx* extension, from the *QUANT methods* drop-down list.

To create macros you can use the OPUS macro editor. For detailed information on the macro editor refer to the OPUS Programming manual. Store the macro into the *Quant* sub-directory of the *OpusLab* folder.

General

A filter calibration consists of *B* or *F* values. For prediction, the *B* value will be multiplied with the absorbance of the wavelength. Then, all values will be added. The *B0* or *F0* value is the intercept and can be used to perform a bias correction. Generally, the calibration protocols contain all these values.



Wavelength	Regression coefficient	t value of coeffici
intercept	30.77916	
1722nm	-4255.23	-12.015
1759nm	6510.03	16.590
1818nm	-2116.54	-7.839
1940nm	-156.854	-5.487

Source of variation	Degree of freedom	Sum of squares
Attributable to regression	4	1615.17
Deviation from regression	127	695.904

Figure 15: Calibration protocol excerpt

Transfer in OPUS

- Store the filter calibration file into the *Quant\MacroInput* sub-directory of the *OpusLab* folder.
- Enter the coefficients by using the macro editor. Change the component name and unit (%), as well as the decimal places (2) for the new parameters.
- Change the intercept (this is 30.78 in the example of figure 15) and the *B* value for each wavelength of this component. In case of filters which have not been used for this parameter, use *0.0* for the wavelength.
- Store the modified file with the extension **.mtx* into the *OpusLab\Quant* sub-directory, by using a new file name.

In many cases a bias correction has to be performed. Therefore, measure 10 different samples by using both OPUS LAB and a former filter system.

Calculate the average from the OPUS LAB measurements and from the former filter system. If the OPUS LAB average is lower than the one calculated by means of the former filter system, add the difference to the intercept. If the OPUS LAB average is greater, subtract the difference from the intercept.

3.5 IDENT

The IDENT tab contains setting options for IDENT parameters, which, however, can only be used in connection with an appropriate IDENT method previously created. Detailed information on how to create an IDENT method are provided in the OPUS IDENT manual.

Note: In addition to the quantitative analysis (QUANT) of individual components it is also possible to perform a qualitative analaysis (IDENT). The IDENT analysis is always performed before a QUANT analysis.

The IDENT analysis cannot be simultaneously performed with Multi Evaluation in OUPS LAB. If the *Active* check box on the *Multi Evaluation* tab has already been activated, the *IDENT* tab will no longer be available.

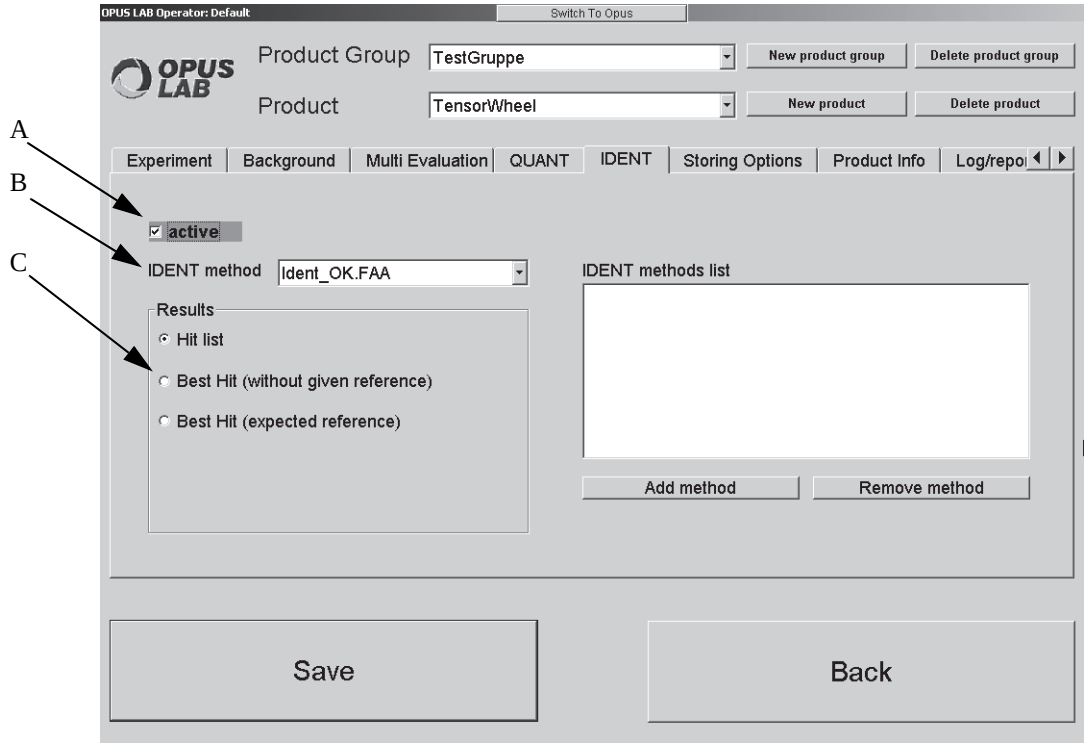


Figure 16: OPUS LAB Product Setup - IDENT

A) Activate the check box if an IDENT analysis has to be performed.

B) Select the identity test method from the *IDENT method* drop-down list.

Note: This list only includes methods which are stored in the *Applicationpath\Ident* directory. *Applicationpath* is the path in which OPUS LAB has been installed. For details on how to create an IDENT method refer to the OPUS IDENT manual.

C) Define the kind of results by means of the option buttons. The exact meaning of the three options are described in the OPUS IDENT manual. If you check the *Hit list* option button, the *IDENT methods list* selection

field will be displayed. You can add several IDENT methods to this list. Select the respective method from the *IDENT method* drop-down list and click the *Add method* button. To delete methods from the list, click the *Remove method* button. All analysis results are completely written into the analysis report.

If you activate the *Best Hit (expected reference)* option button, a selection field is displayed on the right which includes group names of the reference spectra defined in the IDENT method. Select the respective reference from the field.

Below the selection field an entry field is displayed. You can enter text into this field, which will be displayed in the result dialog if the substance has been identified.

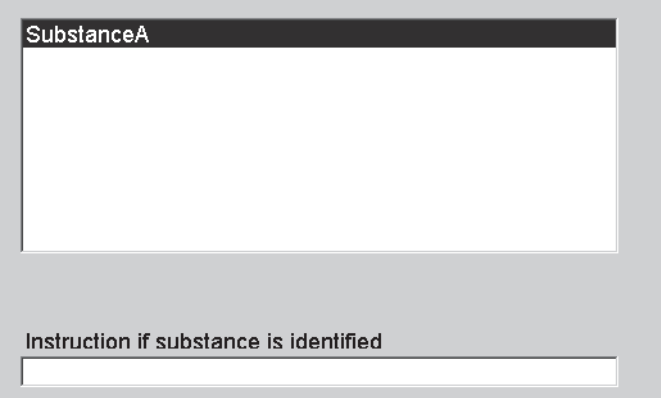


Figure 17: Selection field with reference spectra group name

Note: In OPUS LAB the IDENT evaluation is based on the group names defined in the IDENT method (on the OPUS *Evaluate* menu see *Reference Spectra* tab in the *Setup Identity Test Method* dialog). Therefore, previous identity test methods which do not include this option will not be supported by OPUS LAB. However, they can easily be converted into the new format. On the OPUS *Evaluate* menu, load the methods by clicking the *Setup Identity Test Method* command and save them again.

3.5.1.1 Notes on how to use OPUS LAB to identify raw materials

It is recommended to create an IDENT main library (IP1) for both *Solids* and *Liquids*. If the internal validation of a library indicates that there are some raw materials which cannot be uniquely identified, you have to assign these confusable substances to a sub-library (IP2).

Due to modified evaluation conditions (spectral range, data preprocessing, evaluation algorithm) these substances can then partially be distinguished from each other in this sub-library. If, however, internal validation still indicates that there are additional raw materials which cannot be uniquely identified, try to distinguish the substances in question by using an IP3, IP4,...., IPn library.

Individual pieces of raw material have to be gradually separated due to the identity test result: *uniquely identified.* Generally, an IP1 library can be assigned to many IP2 libraries.

Previously created IDENT methods can also be used in OPUS LAB. IDENT methods which have been created using a previous OPUS version (< OPUS 4.0) have to be loaded into the IDENT *Setup Identity Test Method* command of the current OPUS version, validated and stored in the new format.

When using OPUS LAB at least one validated and, if required, signed IDENT method has to be stored in the *\\OPUSLab\Ident* directory. Additionally, you have to store the measurement experiment (possibly signed) in the *\\OPUSLab\XPM* directory. This measurement experiment is used to measure the reference spectra of the IDENT libraries.

Note that some raw materials are defined as *Products* (in plain text, e.g. o-acetylsalicylic acid or as article number, e.g. 47B11YX0815) within one product group (e.g. *Raw Material*). This ensures that raw materials are compared with an *Expected Reference* regardless of whether the material is stored in different IDENT libraries (e.g. *solids* and *liquids*).

Individual short SOP texts[1] are displayed and include possible sample pre-processing or post-measurement cleaning notes. To locate previous spectra (or batches) you can create product-specific log files and paths to store spectra.

It would be advisable to successively assign the raw material of an IDENT library to the corresponding OPUS LAB products as most of the settings remain unchanged. You only have to change the *Expected References* as well as specific SOPs.

After storing one product the settings will also be available for the next *New Product*. Therefore, it is recommended to initially assign products to 2 or 3 raw materials only and perform a test. This test allows to find out whether the settings made are really practical for your operating procedures.

It is less complex to change the settings (e.g. *Storing Options, Product Info, GMP Mode* or *Overall Report)* in this initial phase as they always have to be changed for each product separately. Later, the changes will be more extensive.

The settings in the OPUS LAB *Configuration* dialog can be as follows:

- **Experiment**

  The measurement experiment is the same for all products which have been assigned to the raw materials of an IDENT library. Set the experiment to *Ext. Synchronisation=ON*.

  Activate the *Multiple measurements* check box and select the *Single evaluation* option. Enter the number of repetitions into the corresponding box.

1. SOP: Standard Operating Procedure

Measurements have to be repeated if the first measurement result turns out to be *NOT OK*, e.g. 3 or 5. If one of the repeated measurements is *NOT OK*, the measurement series will be stopped and the overall result will read out *NOT OK*.

- **Background**

  Generally, you should measure a new background spectrum when changing to a different product. You can set the validity period of a background measurement, e.g. to 2 hours.

  If you want to perform a *Cleanness test* of the measurement accessory prior to a new container measurement, you can set the validity period to the minimum value of 0.01 hours. This yields to a background measurement prior to each sample measurement. In this case, do not activate the *Active* check box in the *Cleanness test* group field.

  A separate background experiment is required when using the MPA spectrometer, e.g. for *External transmission measurements.* To perform their background measurements you have to insert a SPECTRALON filter into the optical path.

  This filter attenuates the signal and cannot be defined as measurement channel. In case of other measurement accessories (fibre-optic probe, integrating sphere) it is advisable to use a separate background measurement if an extended measurement time has been set for the background measurement (with unchanged parameters) to enhance the signal-to-noise ratio of the overall measurement.

- **QUANT**

  Do not activate the *Active* check box.

- **IDENT**

  Activate the *Active* check box.

  Select the IDENT method which includes the raw material just defined as product.

  Activate the *Best Hit (expected reference)* option and select the corresponding raw material from the list box of references.

  Enter a corresponding text into the *Instruction if substance is identified* field.

- **Storing options**

  Activate the two check boxes *Active* and *Current date in data path*. Select the *Default path* option and define the basic path on C:\ or D:\. Check the *Product info* option in the *Spectra name* group field.

- **Product Info**

  Activate the *Container measurement* check box. If you have defined the product as article number, you have to enter the raw material name into the *Field 1 Name* entry field. This text will be the first part of the file name and should be unchangeable.

  The second *Field 2 Name* entry field has to enforce the entry of the goods receiving number. This number will be the second part of the file name.

The third *Field 3 Name* entry field has to enforce the entry of the delivery date. This date will be the third part of the file name, which can be extremely long.

The fourth *Field 4 Name* entry field has to allow the entry of the supplier's name or batch number.

In the fifth *Field 5 Name* entry field you can pre-define an SOP as unchangeable text about sample pretreatment or measurement.

The measurement does not need to have been performed according to a definite sequence. Therefore, activate the *Force user to enter text* check box. If you then click the *Measure* button in the dialog for *Single samples* (chapter 4.2), a message pops up, indicating e.g. that you have to enter text for the sample description.

- **Log/Report**

  Activate the *Active* check box both in the *General logfile* and *Product-specific logfile* group field. The product-specific log file is stored in the *OpusLab\Log\Produktgruppe\Produkt_MM_YYYY.log* directory. This enables spectra to be located at a later date (e.g. after complaints) due to its measurement date.

  Activate the *GMP Mode* check box in the *Print* group field.

  Store the settings and define the next product from the same IDENT library. If you define the products of the next IDENT library (e.g. liquids) and select a different measurement experiment (e.g. with a different measurement channel), you have to verify all the remaining settings in the entire *Configuration* dialog.

The explanations mentioned before outline possible settings to be defined when using OPUS LAB to identify raw materials.

Other settings may also be possible, e.g. if you connect one IDENT library (including its raw materials) to one (OPUS LAB) product.

In this case the IDENT search has to be performed on the basis of *Best Hit (expected reference)*. However, you will not be able to predefine product-specific SOPs in the entry fields (see *Product Info*). This also applies to data storage which will be based on different criteria.

3.6 Storing Options

The *Storing Options* tab contains setting options concerning spectra path and spectra name.

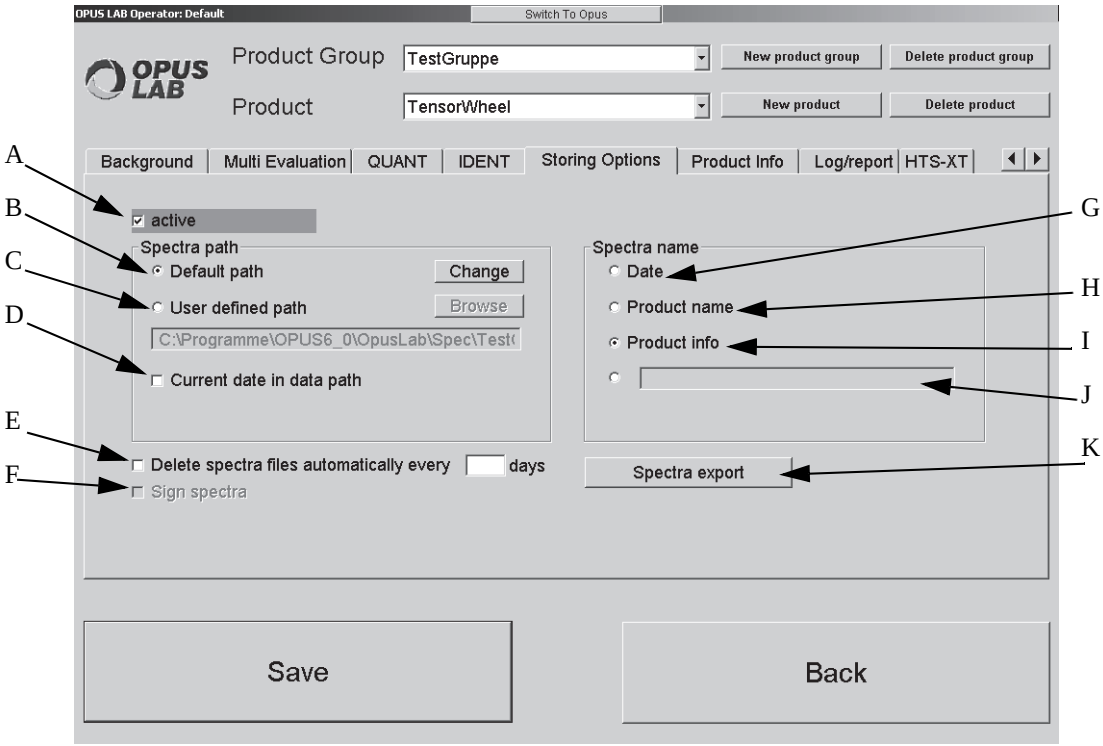


Figure 18: OPUS LAB Product Setup - Storing Options

A) Activate the check box if the measured spectra have to be stored automatically.

B) If you check the *Default path* option button, the spectra will be stored in the following path:

BasePath\Productgroupname\Productname

With:

BasePath: Directory of the base path.

Productgroupname: Name of the product group

Productname: Name of the product

Click the *Change* button to change the default path. Define the path accordingly.

C) Check the option button if you want to individually select the spectra storage path. Click the *Browse* button to define the path.

D) In case of this option a separate directory using the format YYYY_MM_DD is created for each day:

YYYY: Year (e.g. 2010)

MM: Month (e.g. 11)

DD: Day (e.g. 14)

Note: If the *Delete spectra files automatically every n days* check box is activated, a sub-directory of the *YYYY_MM_DD* structure will be created. In this case the *Current date in data path* check box will be disabled.

E) Activate the check box if you want to delete spectra which have exceeded a certain validity period. In this case the program controls the sub-paths of the *\YYYY_MM_DD* structure in the spectra path and deletes all spectra if that exceed the validity period defined in days. The sub-paths are automatically created if the *Delete spectra files automatically every n days* check box is activated.

F) The check box is only enabled, if you have activated the *Sign spectra after measurement* check box in the OPUS LAB *General Setup* (see chapter 2.2). For further details on signing spectra refer to the OPUS VALIDATION manual.

If the measurement has been finished, the OPUS *Login for Signature* dialog opens. Enter the User ID and the password.

Note: In case of single measurements the operator has no access to other OPUS commands, except for the login for signature. In case of multiple measurements the operator has to add the spectra files to be signed into the *Files to be signed* selection field in the OPUS *Add Signature* dialog. This enables the operator to have complete access to all OPUS commands. If the OPUS access is supposed to be limited, the Administrator has to create and assign an operator-specific workspace.

G) Check the option button if you want to include the date into the spectra file name. The following format is valid: *YYYYMMDD.**

With:

YYYY: Year (e.g. 2003)

MM: Month (e.g. 01)

DD: Day (e.g. 31)

*: OPUS spectra file extension (e.g. 0)

H) If you check the option button, the product name is used as spectra file name.

I) Check the option button if the product info has to be used as file name. For more details on *Product Info* refer to chapter 3.7.

J) You can also specify a user-defined spectra name. Activate the option button and enter the name into the entry field.

K) When exporting spectra spectra files are stored as copy into different formats other than the OPUS format. Thus, it is possible to automatically store one measured spectrum in different formats.

The *Spectra export* button is only enabled if a configuration file has been created before and stored in the *SpecExportConfig* sub-directory of the *OpusLab* folder. Use a text editor to create a configuration file which always has the file extension **.ini*. Make sure that the following parameters are defined in the configuration file:

- Data format: JCAMP-DX, SPC (GRAMS), ASCII XY (Data point table; corresponds to the formats used in the *Save As* command in OPUS)

- Storing path: either enter *Default* to store the spectra in the path as defined in B), or any different path

- Converting options for nm scale

Note: When converting a particular frequency range into *nm* (wavelength) you first have to select the range into cm^{-1} (wavenumbers) in OPUS. The parameters correspond to the settings made in the *1/cm <-> nm* OPUS command. Thus, you can first try out the correct parameters in OPUS, and later assign them accordingly by means of the macro editor (see figure 19, of example 3). The *Method (LME)* parameter controls the conversion direction: *Method 4 = cm-1 -> nm* (see figure 19).

When exporting spectra the file names are automatically converted into new file names with pre-defined standard file extensions. It is, however, possible to have the OPUS extension still included in the file name as the following example shows:

test.0 (OPUS format) → *test_0.dx* (JCAMP format) → *test_0.spc* (GRAMS format) → *test_0.xy* (data point table format)

1st example of a configuration file for exporting spectra:

```
//Data Format (0=OPUS, 1=JCAMP-DX, 2=GRAMS, 3=XY-Format)
[FORMAT]
DataFormat=1

//Storing path (Default or path)
[PATH]
Path=C:\Daten\JCAMPDX

//Include OPUS extension in new file name
[EXTENSION]
IncludeOPUSExt=YES

//Converting wavenumber -> nanometer
[CONVERTING]
ConvertToNM=NO
```

2nd example of a configuration file for exporting spectra:

```
//Data Format (0=OPUS, 1=JCAMP-DX, 2=GRAMS, 3=XY-Format)
[FORMAT]
DataFormat=3

//Storing path (Default or path)
[PATH]
Path=C:\Daten\ASCII_XY

//Include OPUS extension in new file name
[EXTENSION]
IncludeOPUSExt=YES

//Converting wavenumber -> nanometer
[CONVERTING]
ConvertToNM=NO
```

3rd example of a configuration file for exporting spectra:

```
//Data Format (0=OPUS, 1=JCAMP-DX, 2=GRAMS, 3=XY-Format)
```

```
[FORMAT]
DataFormat=2
//Storing path (Default or path)
[PATH]
Path=C:\Daten\Grams
//Include OPUS extension in new file name
[EXTENSION]
IncludeOPUSExt=YES
//Converting wavenumber -> nanometer
[CONVERTING]
ConvertToNM=YES
QL1=4003.202560
Ql2=9090.909090
Ql3=700
%LCF=2.000000
%LME=4
%LYS=0
%QL0=0
```

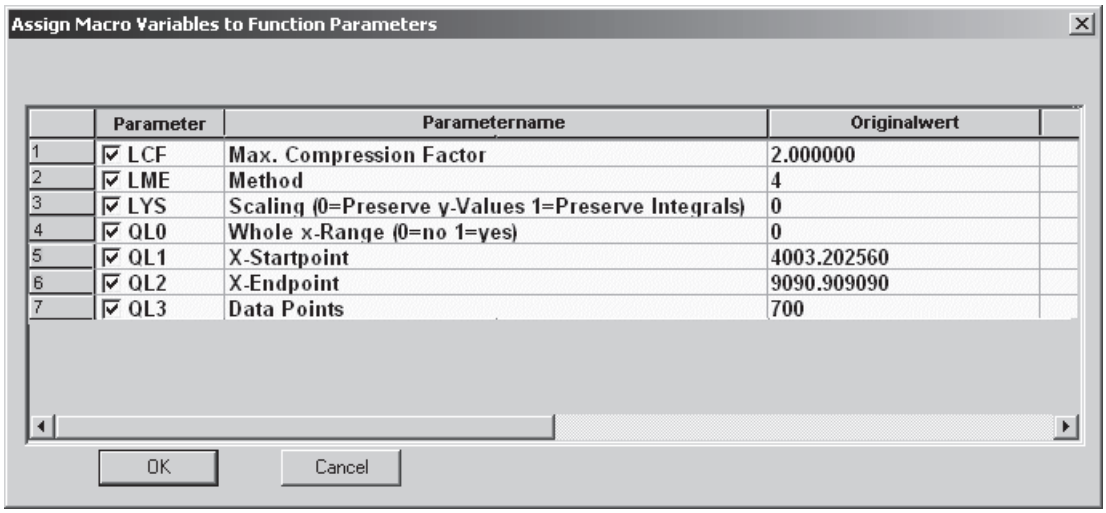


Figure 19: Macro editor - Assigning parameters

3.7 Product Info

The *Product Info* tab contains setting options concerning product information.

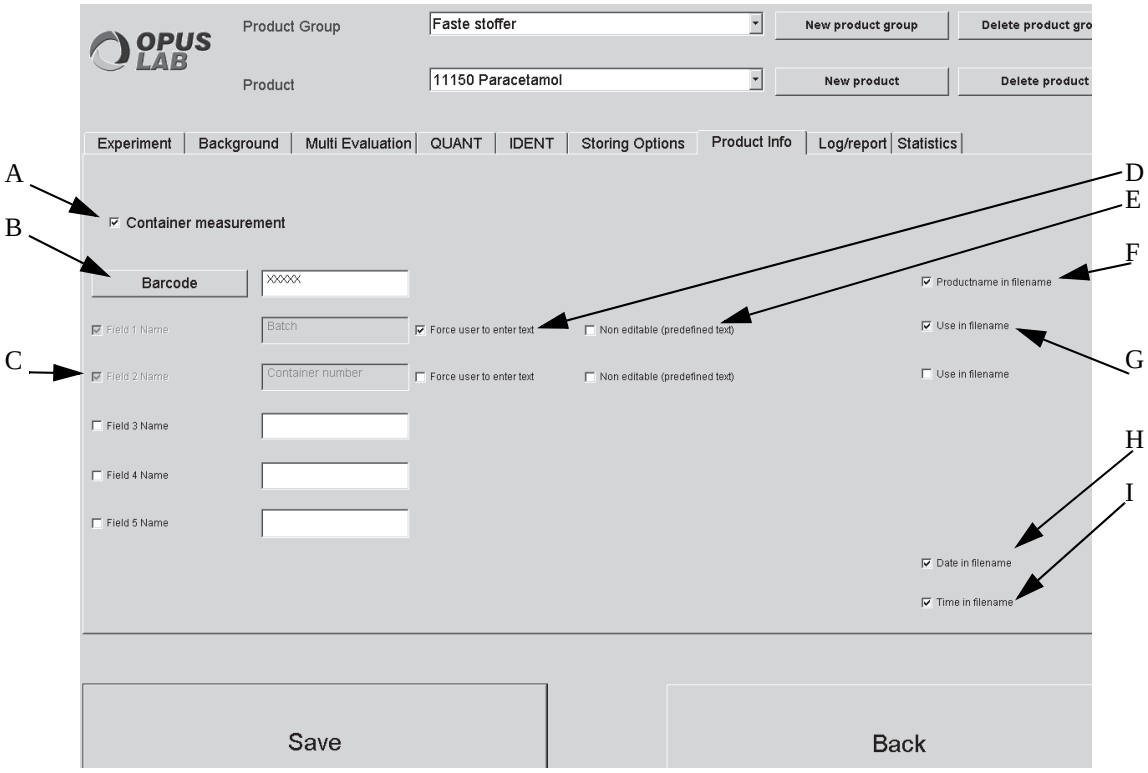


Figure 20: OPUS LAB Product Setup - Product Info

A) Activate the check box if you want to perform a container measurement. **Note:** If you have set up the option to use product information as sample ID in the *General Setup* (chapter 2.2), a warning message pops up as soon as the *Container measurement* checkbox is activated. In connection with container measurement, product information cannot be used as sample ID.

B) For further information on this subject refer to chapter 3.7.1.

C) You can define up to 5 info fields for product information. If the product information is to be used as sample ID (chapter 2.2), the info field is disabled by default.

You can define specific product features within each product information entry field, e.g.:

D) If you activate the *Force user to enter text* check box, you have to enter text before the measurement starts.

E) If you activate the *Non-editable (pre-defined text)* check box, you can enter text during the measurement setup. This text cannot be changed during measurement. Enter the text into the entry field on the right.

F) The *Product name in file name* check box is displayed and activated by default, if you have activated the *Product info* option button on the *Storing Options* tab.

G) The *Use in file name* check box is displayed and activated by default, if you have selected the *Product Info* option button on the *Storing Options* tab. Then, the file name includes the respective product info.

H) The *Date in file name* check box is displayed and activated by default, if you have selected the *Product Info* option button on the *Storing Options* tab. Then, the file name also includes the date.

Format of date:
YYYYMMDD
With:
YYYY: Current year
MM: Current month
DD: Current day

I) The *Time in file name* check box is displayed and activated by default, if you have selected the *Product Info* option button on the *Storing Options* tab. Then, the file name also includes the time.

Format of time:
HHMMSS
With:
HH: Current hour
MM: Current minute
SS: Current second

Note: If the file name is assembled by different components, these components are separated by an underscore. Example:

ProductInfo1_ProductInfo2_YYYYMMDD_HHMMSS.0

3.7.1 Barcode

To select the correct product in OPUS LAB you can also use a barcode. To be able to scan the barcode a barcode reader[1] is required which you have to connect to the COM Port 1 of your computer[2]. Activate the *Use barcode reader* check box by means of the *General Setup* (see chapter 2.2). The *Barcode* button will be displayed on the *Product Info* tab of the *Product Setup*.

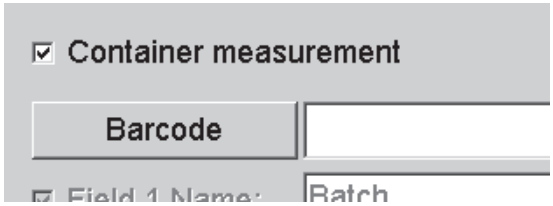


Figure 21: Product Info with *Barcode* button

Clicking the *Barcode* button opens the following dialog:

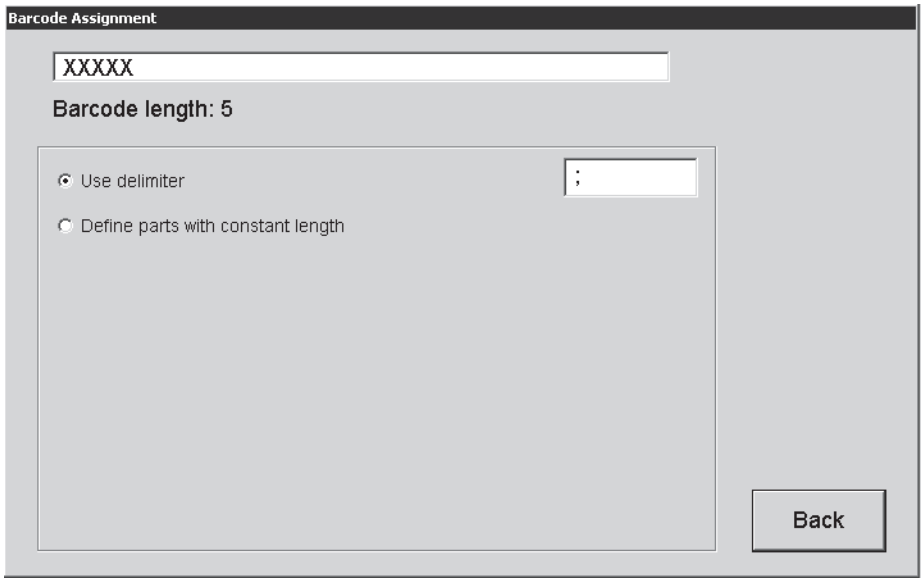


Figure 22: Product Info - Barcode assignment

Scan the barcode to have it displayed in the entry field on top. You can also enter the barcode manually. There are different possibilities to distinguish between the single barcode elements:

1. Barcode readers with USB interface must be able to simulate the RS232 protocol. The protocol must end with a carriage return command.
2. COM 1 settings required:
   - 9600 baud
   - 8 data bits
   - Parity none
   - 1 stop bit

- Delimiter
- Constant barcode length

In the first case delimiters will be added to the barcode at certain parts. If you check the *Use delimiter option* button, an entry field will be displayed. Enter the delimiter into this entry field, e.g. a semicolon.

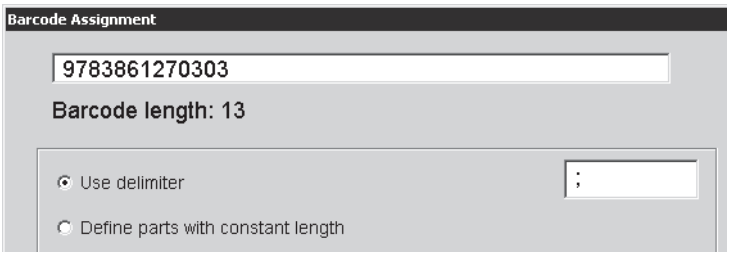


Figure 23: Barcode - Delimiter option

To define constant barcode lengths check the *Define parts with constant length* option button. Additional entry fields are displayed. Enter into these fields the respective numerical value *from/to*, e.g. 1-11, for the product identifier (mandatory) and for up to 5 product info fields (optionally).

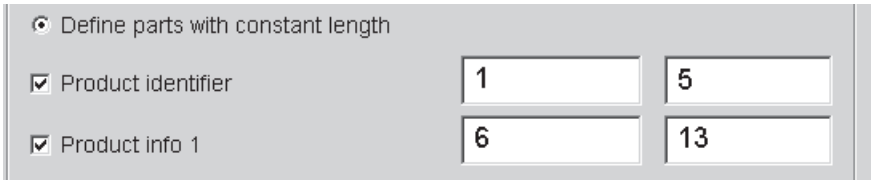


Figure 24: Barcode - Defining parts

If you perform single measurements in OPUS LAB, the product will be selected by reading in the barcode with each piece of product information being filled in according to the definition specified.

3.7.1.1 Barcode option - interface for other product data entry systems

Product data can also be imported to OPUS LAB from other types of entry systems (e.g. SAP, LIMS) via the barcode option. In this case, a PC with stored product data is connected to the RS232 interface instead of the barcode reader.

To avoid entering the product data manually when performing measurements in OPUS LAB, use the barcode option. On the *Barcode Assignment* dialog (figure 22), set the type of data to be read. Activate the *Product identifier* checkbox (figure 24) and specify the data.

As soon as you connect the PC to the RS232 interface the product data, previously written from the entry system (e.g. SAP, LIMS) to the RS232 interface, are imported to OPUS LAB.

3.8 Log/Report

The *Log/Report* tab contains setting options concerning the general and product-specific log file, and printing options.

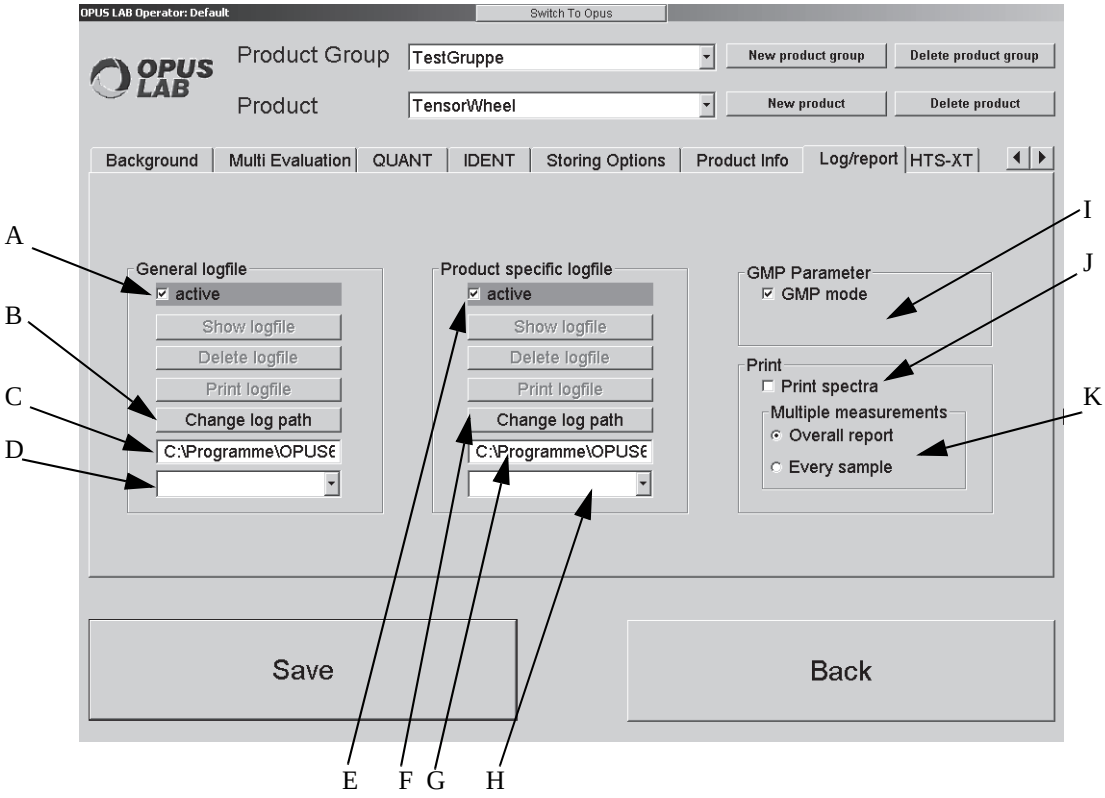


Figure 25: OPUS LAB Product Setup - Log/Report

A) If you activate the *Active* check box, the analysis results will be written into a general log file. This applies to all products and gives an overview of the analyses which have been performed within a certain period of time. For information on how to assemble the log file name, refer to chapter 6.1.2.

B) Click the button if you want to change the log path of the general log file.

C) The selected log path of the general log file is displayed.

D) This drop-down list includes the names of already existing general log files.

E) If you activate the *Active* check box, the analysis results of the product selected will be written into a product-specific log file. For information on how to assemble the log file name, refer to chapter 6.1.3.

F) Click the button if you want to change the log path of the product-specific log file.

G) The selected log path of the product-specific log file is displayed.

H) This drop-down list includes the names of already existing product-specific log files.

I) If you activate the *GMP Mode* check box, the analyses will be performed in the GMP (**G**ood **M**anufacturing **P**ractice) mode. The differences between the normal mode and the GMP mode are:

- After each analysis the results are automatically printed, i.e. the *Print* button is deactivated.
- The print-outs include two signature fields, e.g. one defined for the operator and the other for the person who releases the product.
- Spectra can be signed from OPUS LAB. If they are not signed when measuring in GMP mode, an error message pops up.
- If the instrument status indicates a warning, measuring is not possible. OVP starts automatically.

J) If you activate the *Print spectra* check box, the spectra measured will be printed. In case of an IDENT analysis the print-out will also include the reference spectra. If you have activated the *Store Average Spectra* check box on the *Store Method* tab when creating an IDENT method, the average spectra with the file extension *.*AV* will be stored in a corresponding sub-folder. The name of this sub-folder is the same as of the IDENT method.

K) This group field is only available if you have activated the GMP mode. Check the *Overall report* option button if an overall GMP report has to be printed. A separate page will be printed for each sample if you check the *Every sample* option button.

Note: Multi-sample measurements comprise measurements using either a sample changer, microtiter plate or Metrohm auto sampler, or container measurements.

3.9 Statistics

The *Statistics* tab contains setting options for the statistical evaluation of spectra. These spectra are either included in a spectra file list or in a connected database.

To be able to perform a statistical evaluation a QUANT, IDENT or MultiEvaluation method has to be previously created. Based on certain method components (QUANT) or method reference values (IDENT, conformity test) you define control limits for the statistical evaluation on the *Statistics* tab.

Note: When using QUANT method components for statistical evaluation, make sure that these components have a unique name. If you use more than one QUANT method for statistical evaluation, the respective component name must only be used once in one particular method. Otherwise, it is not possible to distinguish between the single components during statistical evaluation.

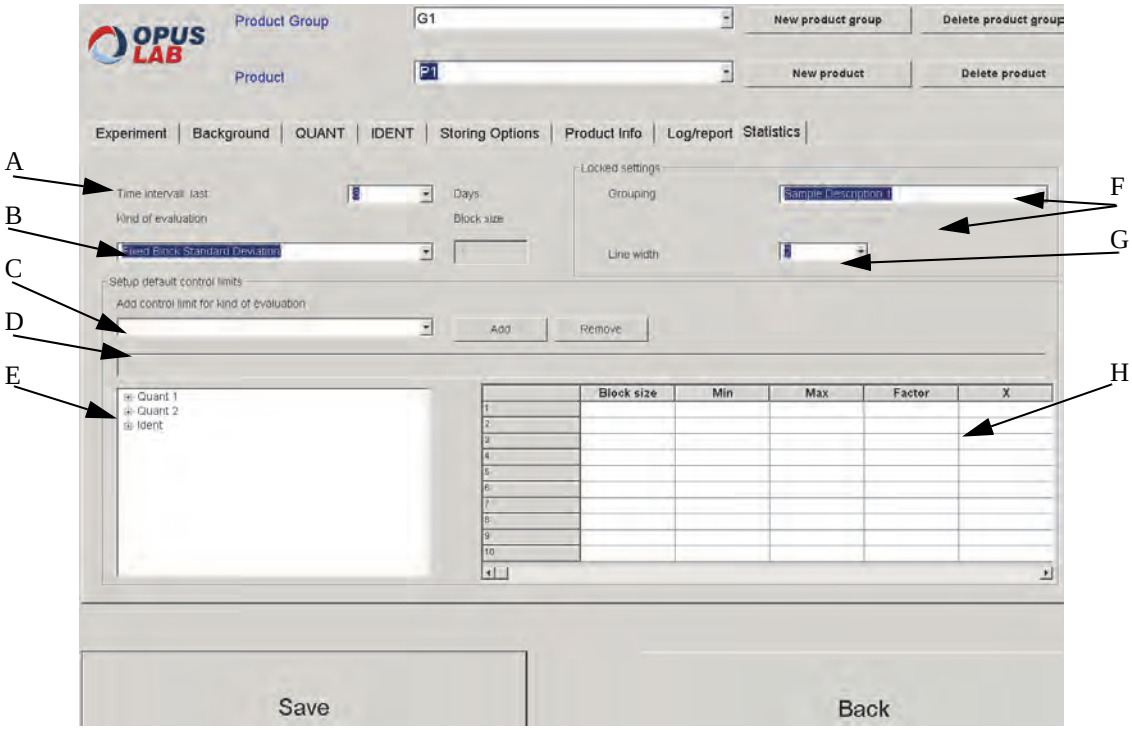


Figure 26: OPUS LAB Product Setup - Statistics

A) This setting option allows to define the time interval for statistical evaluation. Starting from the current date, select the number of days to be considered for statistical evaluation from the drop-down list.

B) The drop-down list is used to predefine a special type of statistical evaluation. This means, if an evaluation dialog with a *Statistics* button is displayed after a measurement has finished and you click this *Statistics* button, the subsequent evaluation is based on the evaluation type selected in (B).

In case of some of these evaluation types you can define the block size, i.e. the number of batch numbers summed up to one block. Example: if you enter 5, each block consists of 5 batch numbers.

The following evaluation types (chapter 3.9.2) are available:

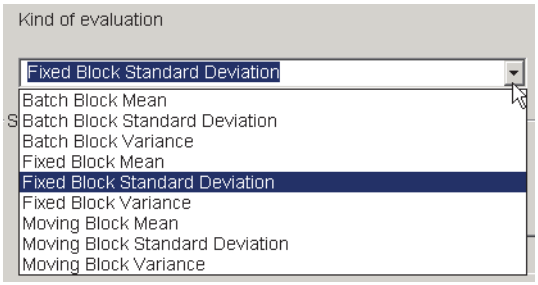


Figure 27: Statistical evaluation types

C) You define a control limit (chapter 3.9.3) for the evaluation result of the method component or method reference value by selecting the appropriate option from the drop-down list, and clicking the *Add* button. In case of statistical evaluation do not substantially exceed or undercut the control limit.

D) If you have selected *Standard Deviation Factor* in (C), a spectra file list is required for the method component to be statistically evaluated. In this case you have created a file list for the respective method component. This file list must contain spectra which are characteristic for the measurement. During statistical evaluation, the standard deviation is calculated of the spectra from this file list. This calculated value can be added by a factor from table (H), which forms the limit for the respective method component.

If you have selected *Standard Deviation Factor* in (C) and clicked the method component, the field (D) shows the path and file name of the list valid for the method component (chapter 3.9.4). If no spectra file list has yet been defined for the method component, click the *Add* button. The *Setup Filelist* dialog opens and allows to create or load a file list. After saving or loading the file list, the path and file name is displayed in field (D).

E) The tree shows the structure of the evaluation method selected.

F) This kind of setting option refers to the trend chart depiction. The statistical evaluation is displayed in a trend chart. You select the type of product information from the drop-down list. This kind of information has to be defined on the *Product Info* tab (chapter 3.7) first.

The drop-down list only contains the kind of product information defined on the *Product Info* tab. Example:

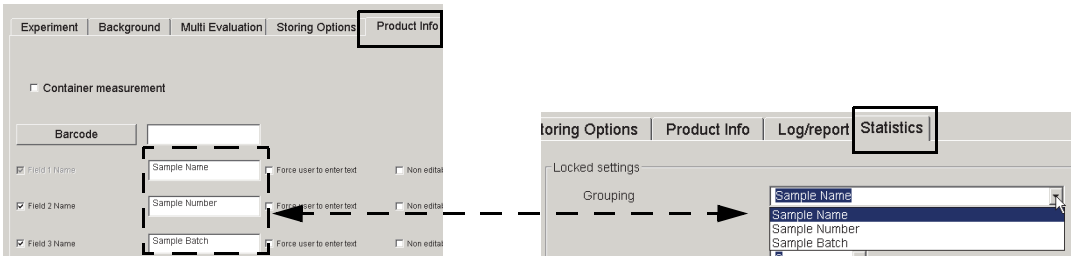


Figure 28: Product information

The *Grouping* standard setting is obligatory if you have selected an option in (B) which uses batch blocks for evaluation, as this standard setting uniquely defines the batch.

G) The drop-down list contains line width options to be used for the line depiction in the trend chart. You can select a line width between 1 and 4.

H) The table shows the control limits defined for the kind of evaluation function selected. The control limits refer to a particular method component or method reference value. Example:

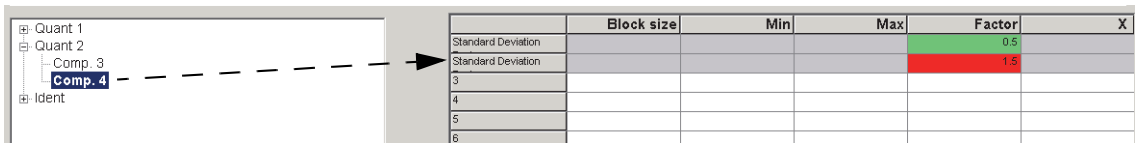
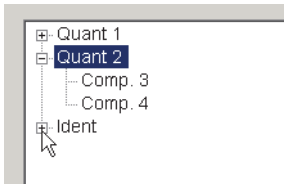
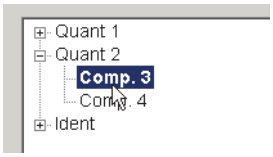


Figure 29: Example of control limits defined

3.9.1 Order to be observed when making the settings

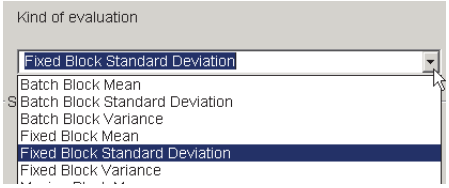


Step 1:
Set the tree structure in such a way that you can see all parts of the method. Click ⊞ to open the sub-levels.

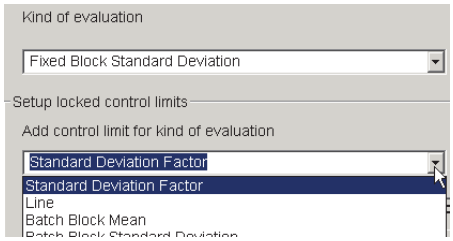


Step 2:
Click e.g. a method component.

Note: A selected component is displayed in bold in the tree structure.



Step 3:
Select the kind of statistical evaluation.



Step 4:
Optionally, select the control limit definition for the respective component of the evaluation method.

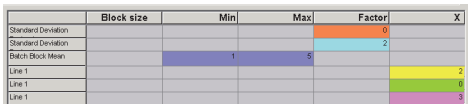
Step 5:
Click the *Add* button.

The table shows the control limit definition.

Note: Selecting standard deviation requires a spectra file list. Therefore, another dialog opens and prompts you to load or create a spectra file list (see chapter 3.9.4).

Step 6:
Enter the control limit.

Note: Depending on the control limit definition selected, you can only enter the value into the respective table cell provided. It is only possible to enter values into white table cells.



Step 8:
- Right click into a defined table cell. A color palette is displayed.
- Select a color. The table cell with the defined control limit is colorized.

Note: The color defined for the particular control limit is depicted in the trend chart if statistical evaluation has been performed.

Step 9:
Click the *Save* button.

If required, repeat the steps 1 to 9 for further method components or method reference values.

3.9.2 Evaluation options

Possible trend chart depiction	Example
fixed block	xxx|xxx|xxx
batch block	A1A1A1|A2A2A2|A3A3A3
moving block	xxx|x|xxx|xx|xxx|

With all types of evaluation options (standard deviation, mean and variance) the result is depicted in blocks in the trend chart. In case of *moving*, always the oldest measurement is discarded and the last 3 results are evaluated. The *moving block* is useful with standard deviation, if no or minor signal changes are expected. In case of *batch block*, the blocks depicted in the trend chart refer to the respective batch name defined.

3.9.3 Defining control limit for statistical evaluation

Based on method components or method reference values, certain control limits are defined for statistical evaluation. Depending on the kind of evaluation selected, the control limits can be factors, minimum or maximum values or block sizes.

The tree structure for the method shows the single parts of a method, i.e. name of method, components as well as reference values.

Figure 30 exemplifies a structure of a multi evaluation method.

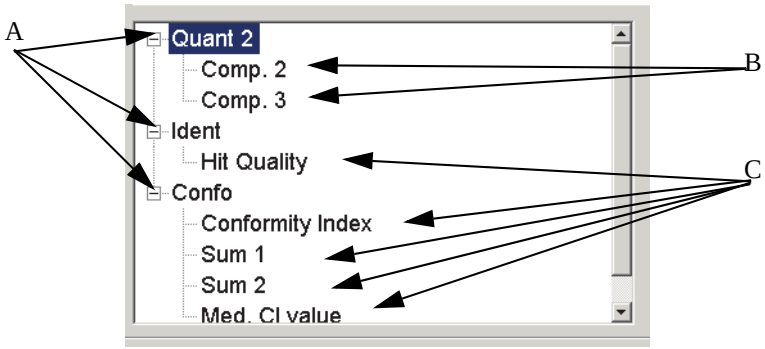


Figure 30: Structur of a multi evaluation method

A) Method name

B) Component name

C) Names of reference values

3.9.4 Setting up file list

There are only two cases which require a spectra file list to statistically evaluate spectra:

- to calculate the limit for standard deviation
- to statistically evaluate spectra which are not included in the database

The set-up procedure is the same for both cases. However, to be able to statistically evaluate spectra which are not included in the database, you have to define a separat column for the batch number.

1) On the *Edit* menu, click the *Setup File List* command.

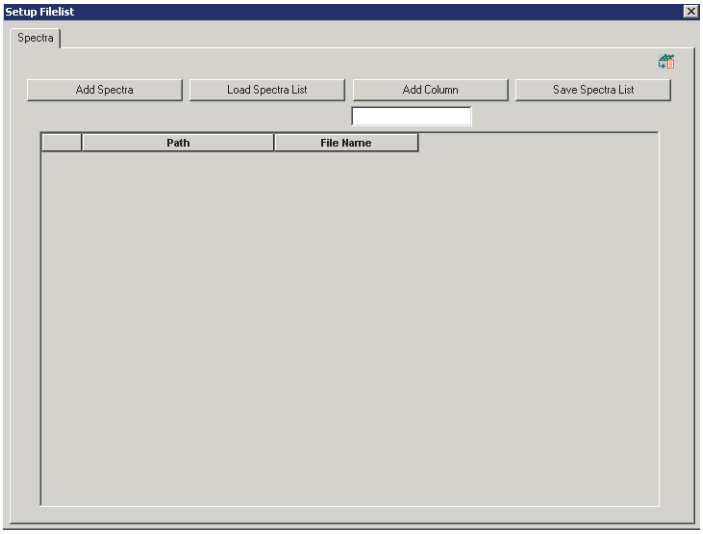


Figure 31: Setup Filelist

2) Click the *Add Spectra* button to load the spectra from the particular directory. If you use the spectra file list to calcuate the limit for the standard deviation factor, ideally select those spectra which you have been used when creating the method.

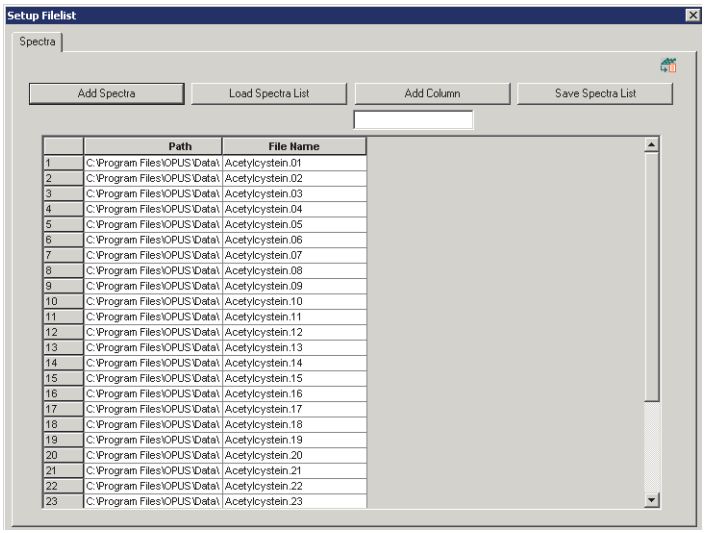


Figure 32: Loaded spectra

The path and file name of each spectrum is displayed in a table. This table can be customized, i.e. enlarged by as many columns as you like. Enter the name of the column into the entry field below the *Add Column* button. If you click the *Add Column* button, the new column will be added to the table.

Note: If you use the spectra file list to statistically evaluate spectra which are not included in the database, it is mandatory to add a separate table column. Define the name of this column as *Batch Number*.

3) Click the *Save Spectra List* button. Define a specific name for the list.

Note: Spectra file lists are stored as reports in the OPUS format. The file extension of the list may be incremented, i.e. automatically increased by 1. This is especially helpful if you want to use the same name for different spectra file lists.

For further details on the file list refer to the OPUS Reference manual.

3.10 Pump

The functions available on the *Pump* tab can be applied in connection with spectrometers which use a pump for the automatic measurement of liquids. The functions allow to control the sequence of the sample measurement and cleaning cycles.

3.10.1 Defining sequence for measurement and cleaning

1) From the *Tube* drop-down list, select the desired control option.
   ➢*Details on the setting options are described in chapter 3.10.2.*
2) In the table, click the desired line number to select the complete line.
3) Click the *Add* button.
   ➢*The control option must be displayed in the table.*
4) Enter the time manually.
   ➢*The time is measured in minutes.*
5) If required, enter a comment.
6) Click the *Save* button.

3.10.2 Setting options

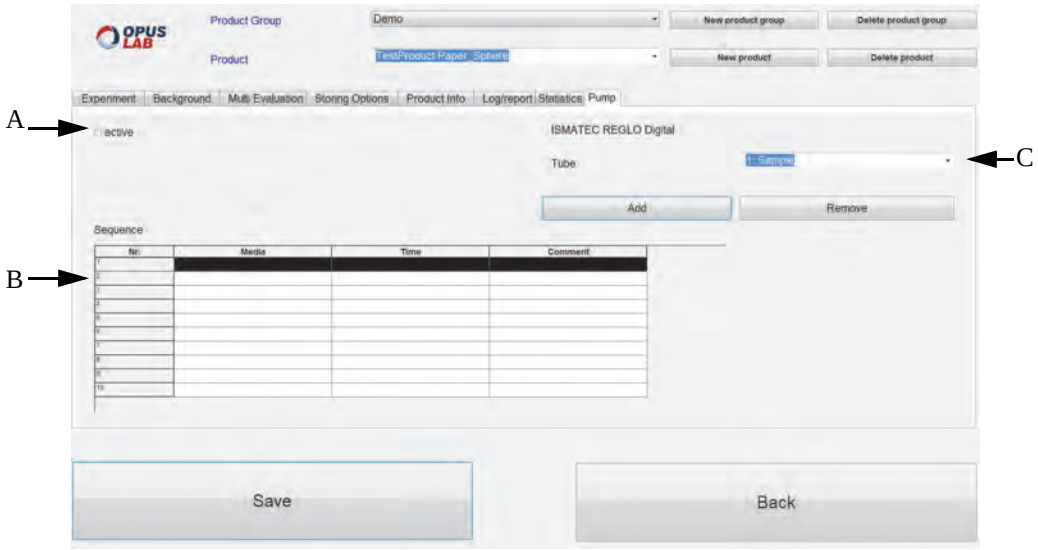


Figure 33: OPUS LAB Product Configuration - Pump

A) The checkbox must be activated to enable the control of the cycles.

B) Depending on the control option selected, the table contains the single cycles in a certain sequence. The lines of the *Time* and *Comment* columns can be edited. The time is measured in minutes. Entering a comment is optional.

C) The following control options are available:

- **Sample:** cycle of sample measurement
- **Standard cleaning:** the standard cleaning is an intermediate cleaning which comprises 1 cleaning cycle.
- **Final cleaning:** the final cleaning comprises 3 cleaning cycles.

3.10.3 Deleting a line from the sequence

1) From the *Tube* drop-down list, select the correct control option.
2) Select the particular table line you want to delete.

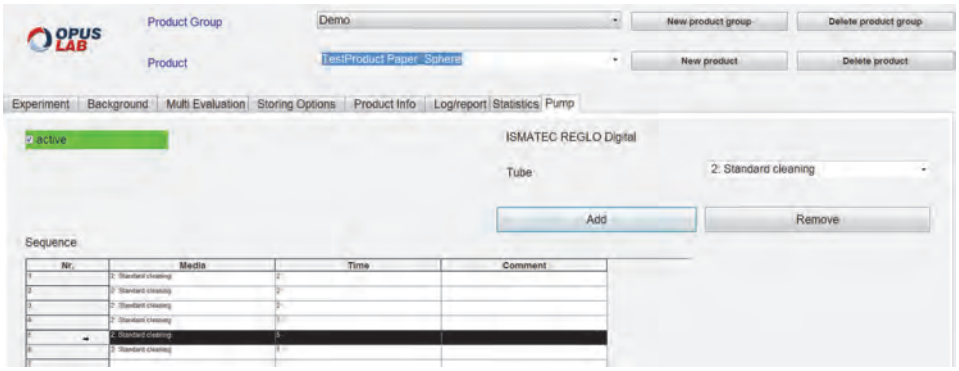


Figure 34: Deleting a line from the sequence

3) Click the *Remove* button.
4) Click the *Save* button.

4 Measurements

To perform sample measurements and a statistical evaluation click the *Measurements* button.

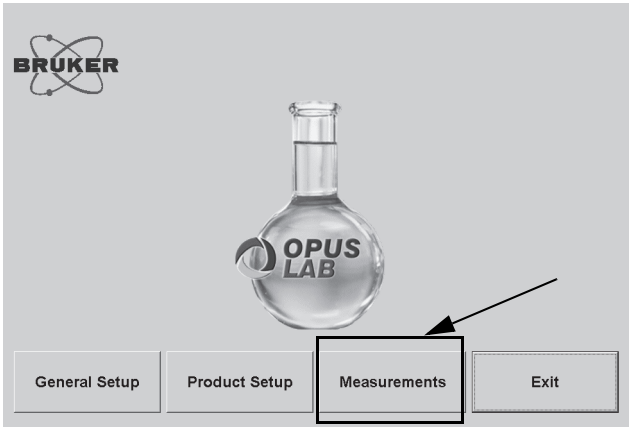
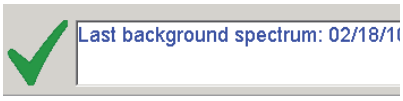


Figure 35: OPUS LAB Measurements

4.1 Performing background measurement

Before measuring a new sample you have to perform a background measurement. The status of the last background measurement is indicated by date and time.

The status of a background measurement is displayed in OPUS as follows:

Display in OPUS LAB	Definition
	A green checkmark indicates that a current background spectrum is available for the sample.
	A red cross indicates that no current background spectrum is available for the sample.

Additionally, the validity period of the of the respective background spectrum can be read as well. The validity period is set up in the *Product Setup* on the *Background* tab (chapter 3.2).

If the validity has expired, a new background spectrum has to be measured. You are automatically prompted to do so.

Note: The quality of the background spectrum measurement is a crucial factor with regard to the quality of the analysis. Therefore, the *Measure background* button can be locked during the setup to prevent the operator from accidentally acquiring a background spectrum of inferior quality.

4.1.1 Measuring Procedure

1) Click the *Measurements* button (figure 35 on page 53). The following dialog opens:

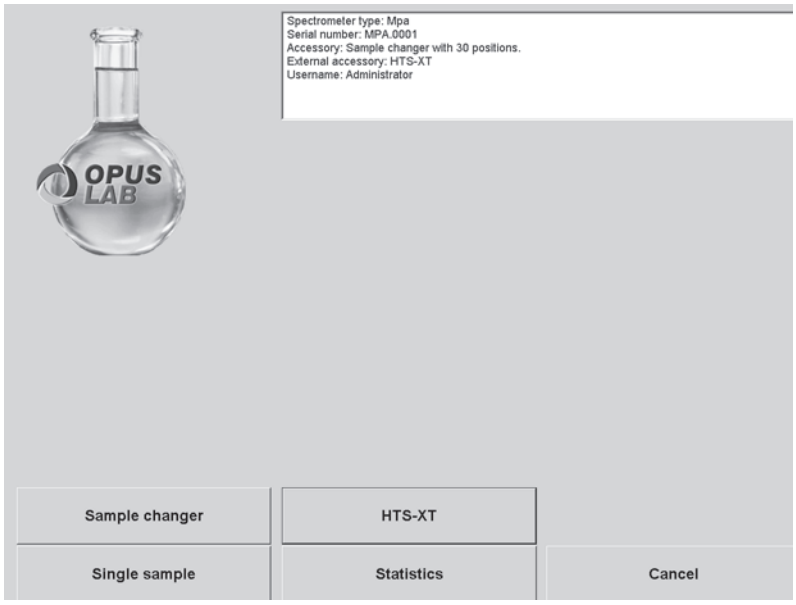


Figure 36: OPUS LAB measurement dialog

2) The background spectrum can be acquired for single samples or measurements using a sample changer. Click the respective button. Another dialog opens:

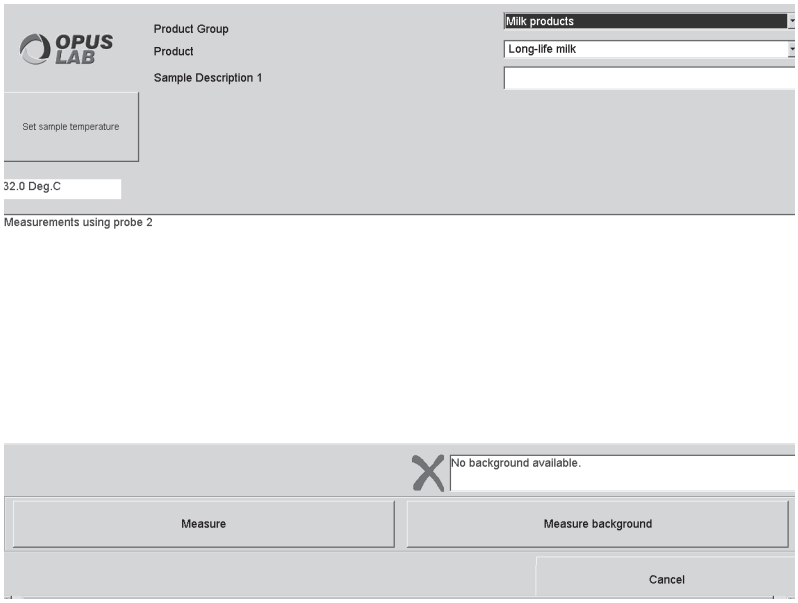


Figure 37: OPUS LAB Measurements - Single sample

3) Select the product group and the product. Specify the sample description.

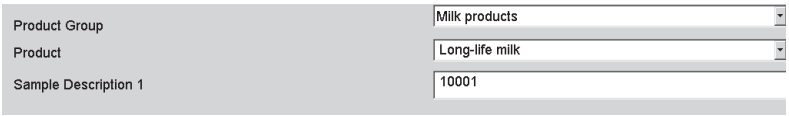


Figure 38: Selecting product group and specifying sample description

4) Click the *Measure background* button.

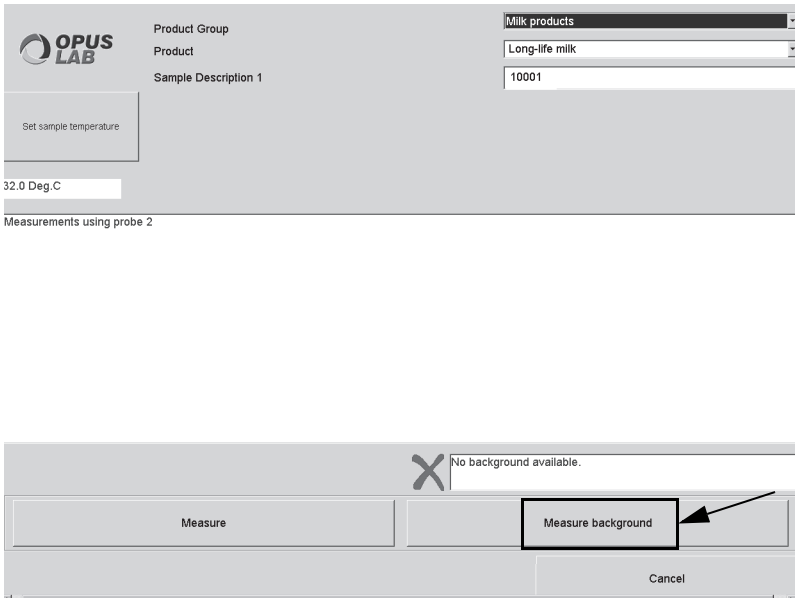


Figure 39: Starting background measurement

Another dialog opens.

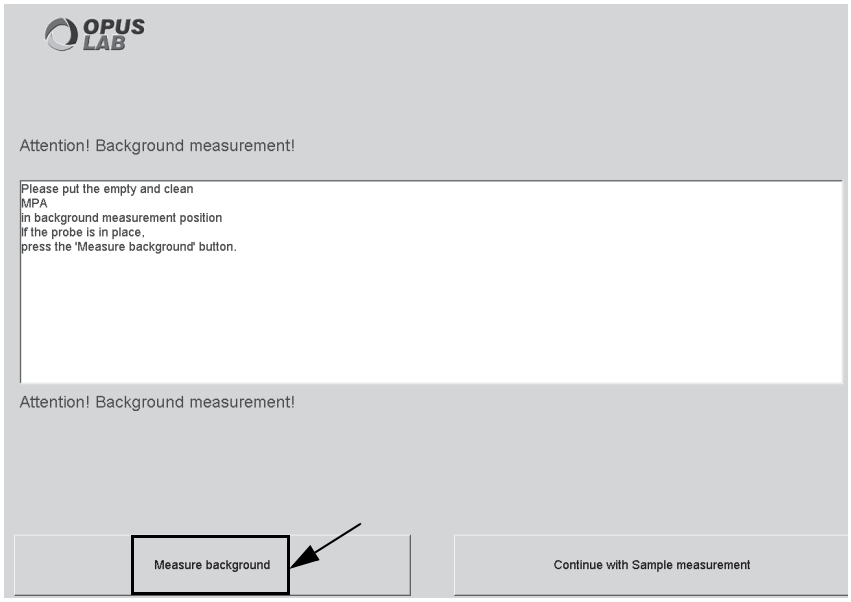


Figure 40: OPUS LAB - Background measurement

5) Click the *Measure* background button (figure 40). A new background spectrum is measured which replaces the old one. The new background spectrum has been acquired as soon as the *Measurement finished* message is displayed in the white list box.

4.2 Measuring single samples

1) Click the *Measurements* button (figure 35 on page 53). The following dialog is displayed:

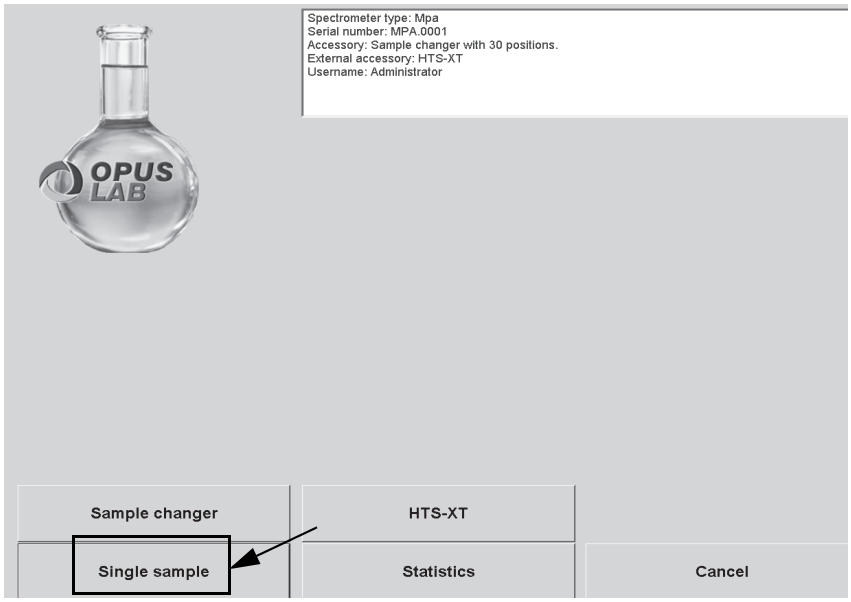


Figure 41: OPUS LAB - Measuring single sample

2) Click the *Single sample* button to open the following dialog:

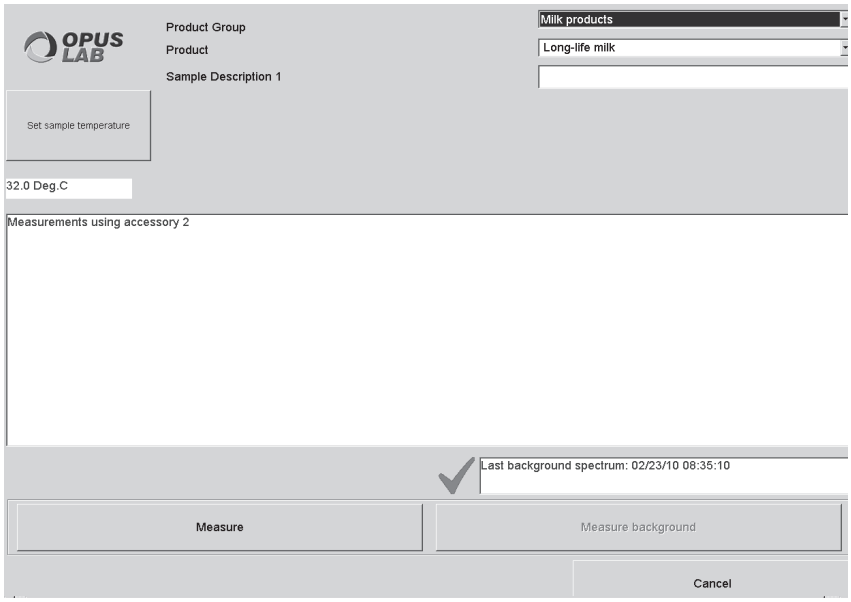


Figure 42: OPUS LAB - Measuring dialog for single samples

3) Select the product group and the product. Specify the sample description.

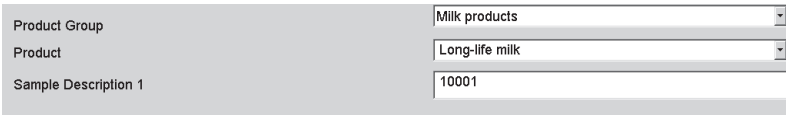


Figure 43: Selecting product group and specifying sample description

4) Click the *Measure background* button if no background spectrum has been measured yet (see chapter 4.1).
5) Click the *Continue with sample measurement* button after background measurement has been finished.
6) Click the *Measure* button (figure 44). Now, you start the single sample measurement.

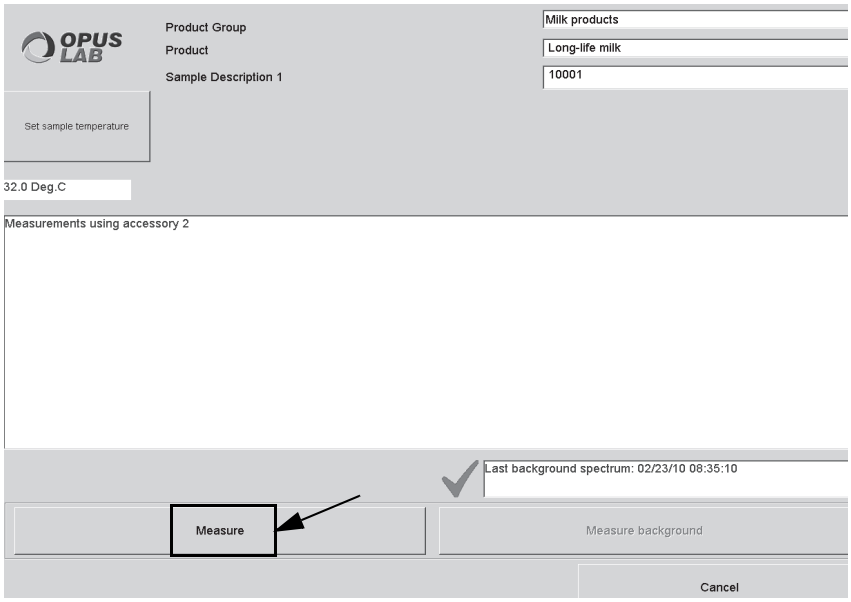


Figure 44: OPUS LAB - Starting single sample measurements

As soon as the measurement has finished, the file name, date and time of the measurement is indicated in the white list box.

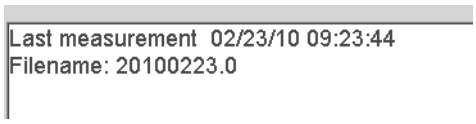


Figure 45: The last sample measurement

4.2.1 General information on sample measurement

Instrument Status

The instrument status is indicated below the large white list box.

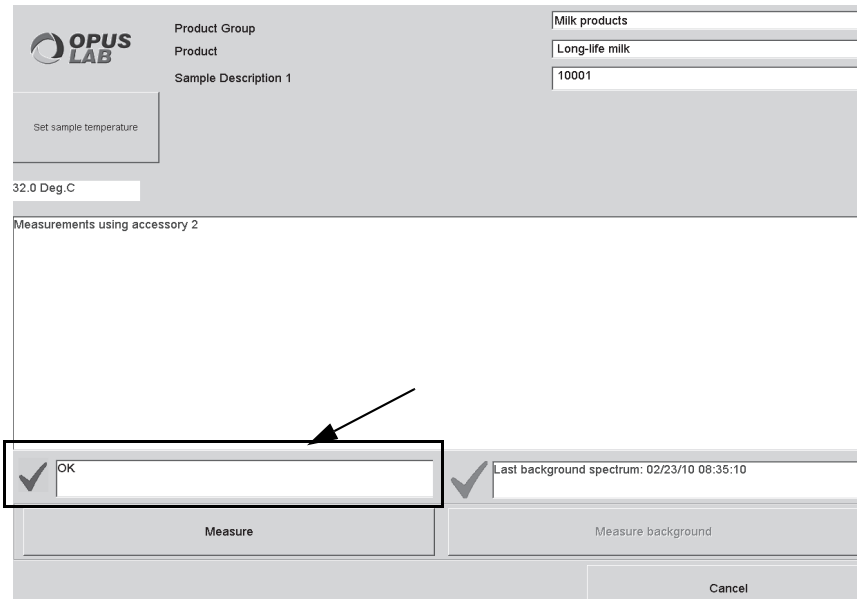


Figure 46: Instrument status

The instrument status is only displayed if an instrument test has been assigned to the current experiment (see chapter 1.6). If the instrument test is NOT OK, e.g. if the validity has expired, you will be requested to perform a new instrument test.

Deleting Spectra

If spectra have to be deleted automatically after a defined number of days, OPUS LAB verifies all the spectra measured and deletes only those evaluated to have exceeded the storage period.

This option has to been set up first, using the *Storing Options* tab in the *Product Setup* (chapter 3.6).

Measuring by using integrating sphere or probe

When performing measurements, using either the integrating sphere or a probe, multiple measurements are also possible. In case of probe measurements, single measurements are triggered by pressing the button on the probe.

The chronological measuring procedure, in case of the integrating sphere, is defined by mouse clicks. After each sample measurement a window is displayed. Clicking the *OK* button triggers the next measurement.

4.2.2 Setting sample temperature

In case of measurements in connection with a heatable vial/cuvette holder integrated in, e.g. the MPA spectrometer, you can set the sample temperature in OPUS LAB.

Note: This kind of global setting has to be defined first with the *General Setup* on the *Instrument* tab (chapter 2.3).

1) Click the *Set sample temperature* button.

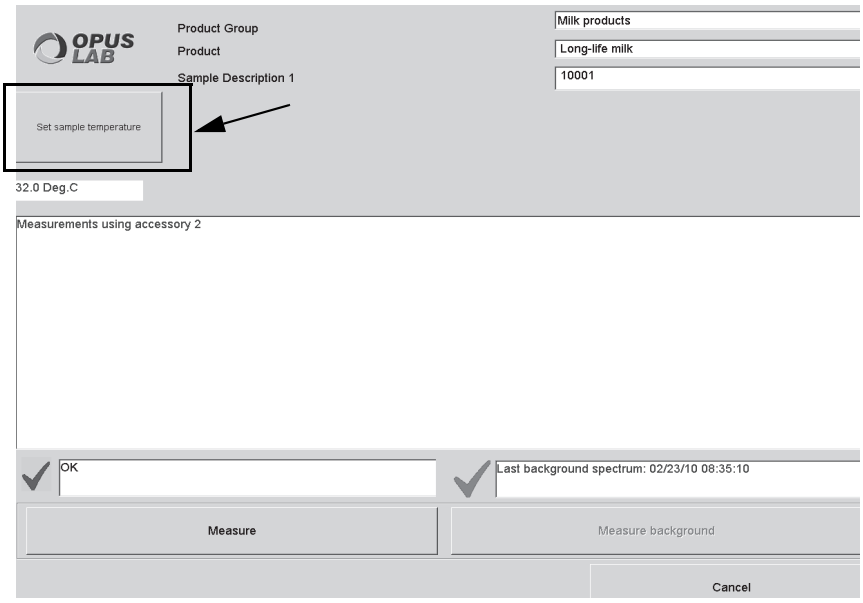


Figure 47: Setting sample temperature

2) Enter a number between 20 and 120 for the temperature.

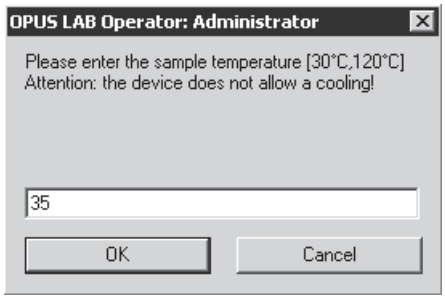


Figure 48: Specifying sample temperature

3) Click the *OK* button to confirm.

If the temperature has been set by means of an xpm-file in OPUS, this kind of setting will be accepted by OPUS LAB.

4.3 Multiple measurements

This option enables measurements of single containers to analyze the corresponding raw material. If multiple measurements are performed by using e.g. a probe, you can control these measurements by clicking the button located on the probe. For details, refer to chapter 1.7.

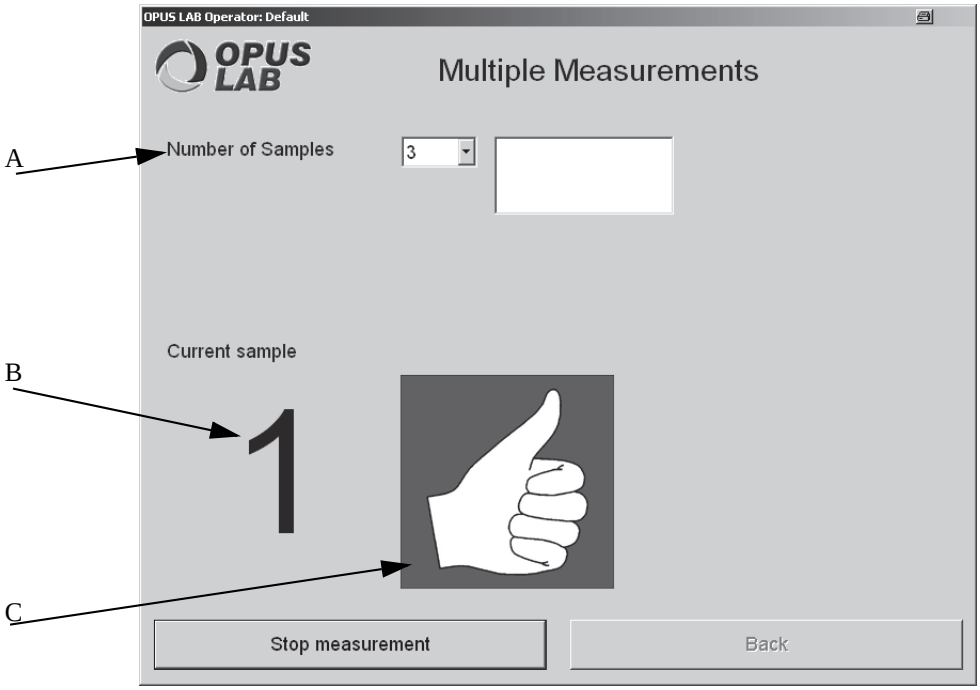


Figure 49: OPUS LAB multiple measurements dialog

A) The *Number of Samples* drop-down list allows to define the number of samples to be measured (e.g. as container for a specific product).

If you have defined the number of repetitive measurements in case of single container measurements (see chapter 3.1), the result of the single measurements performed will be indicated by means of a small traffic lights indicator.

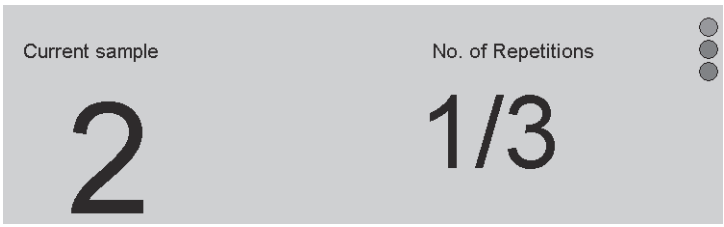


Figure 50: Number of repetitions to be done for sample 2

B) The number of the current sample measured is displayed.

C) The status of the sample measurement is displayed. A green thumb up means: status ok.

4.3.1 Container Measurement

If you have activated the *Container measurement* check box on the *Product Info* tab (see chapter 3.7), the multiple measurement dialog looks slightly different:

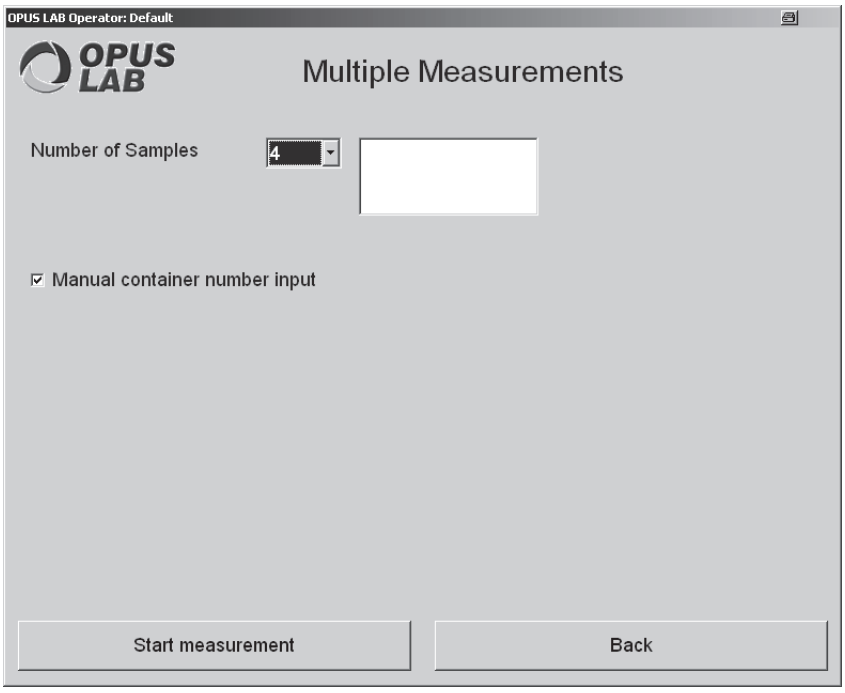


Figure 51: OPUS LAB multiple container measurements

Specify the number of samples by means of the drop down-list. If you have activated the *Manual container number input* check box, the following dialog pops up for each measurement:

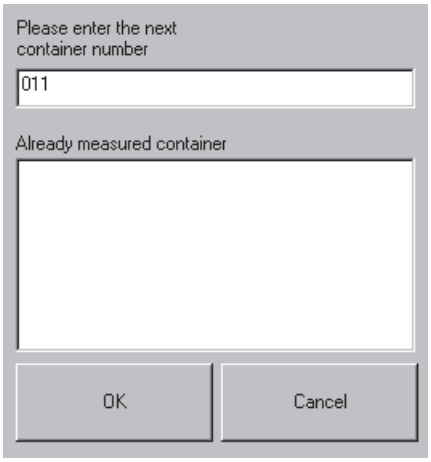


Figure 52: OPUS LAB - manual input of container number

Enter the next container number manually and confirm the entry by the *OK* button. Container numbers have at least 3, and at most 19 digits. In case of missing digits zeros are added, i.e. if you enter *1* as container number, *001* will be displayed in the dialog.

4.3.1.1 Starting measurement

Click the *Start measurement* button.

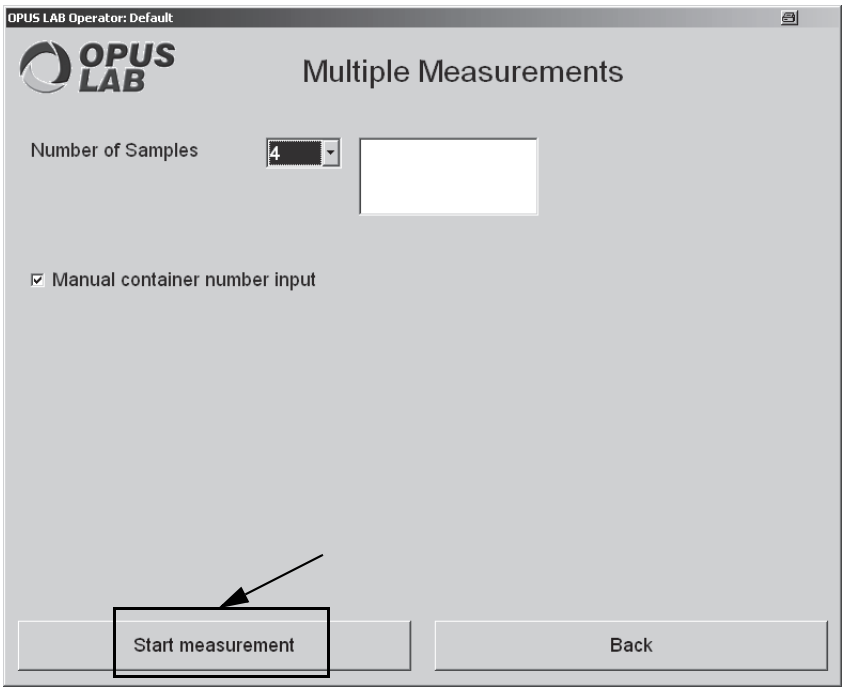


Figure 53: OPUS LAB - Starting container measurements

A defined measurements series starts and the button label changes to *Stop measurement*. Clicking the *Stop measurement* button will interrupt the measurement series as soon as the analysis for the current measurement has been completed.

4.3.2 Measuring procedure for spectrometers with AQP

This measuring procedure refers to spectrometers like VECTOR, EQUINOX and other spectrometer types using AQP.

The green LED on the probe signalizes that the spectrometer is ready for measurement.

Press the button on the probe.

The red LED on the probe signalizes that the spectrometer is measuring.

After the measurement has been finished the LED indicates the evaluation result:

- Green blinking - measurement OK
- Green and red blinking - measurement NOT OK; repeat the measurement for this sample (if defined in the setup)
- Red blinking - measurement definitely NOT OK; continue with next sample

Besides, the measurement result is displayed on the screen:

- Green thumb up and green spectrum: measurement OK
- Red thumb down and red spectrum: measurement not OK
- No thumb at all: additional measurements are required

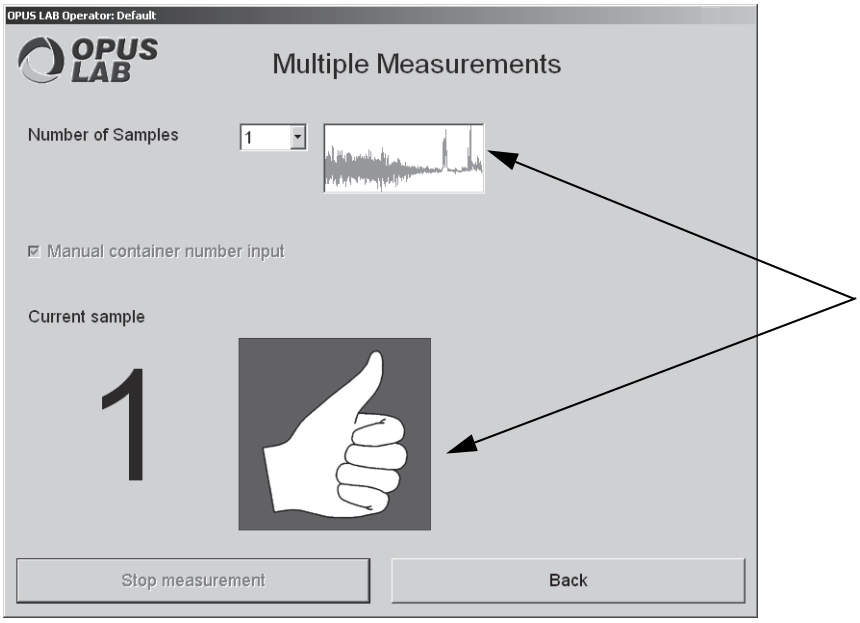


Figure 54: Multiple measurement result - OK

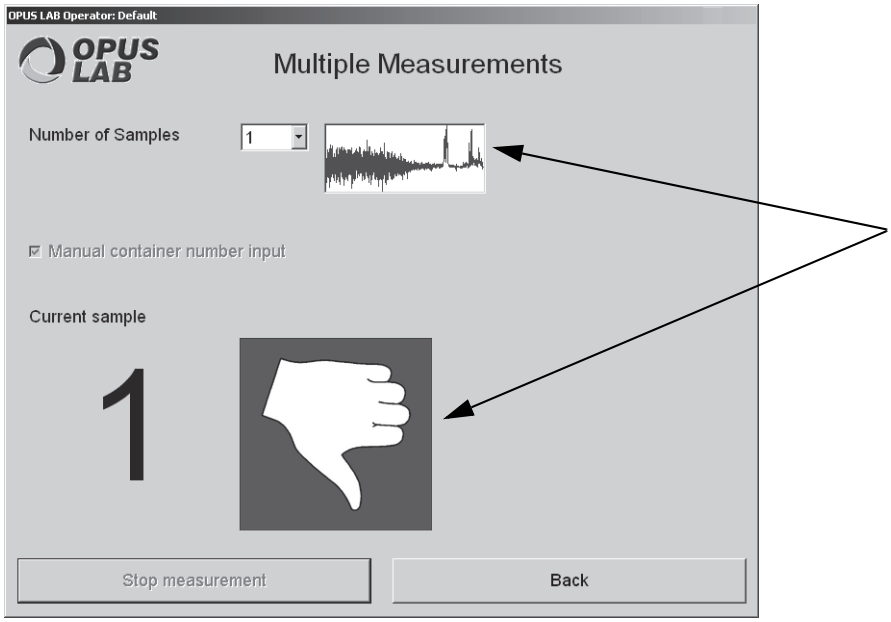


Figure 55: Multiple measurement result - Not OK

Press the button on the probe.

If additional measurements are necessary, the program repeats the first measurement step, otherwise it stops.

4.3.3 Measuring procedure for spectrometers without AQP

The green blinking LED on the probe indicates that the spectrometer is ready for measurement.

Press the button on the probe.

The red LED on the probe indicates that the spectrometer is measuring.

After the measurement has been finished the green LED is switched on. The evaluation result is not shown on the probe LED. It is only displayed on the screen:

- Green thumb up: measurement OK
- Red thumb down: measurement not OK
- No thumb at all: additional measurements are required

The program continues depending on the setting made on the *Instrument* tab in the *General Setup* (see chapter 2.3).

If the entry is lower than 0, a message box opens. Confirm the message to continue. If the entry is higher than 0, the program waits as many seconds as being selected in the drop-down list and continues with the next step.

If additional measurements are necessary, the program repeats the first measurement step, otherwise it stops.

4.4 Sample Changer

Using a sample changer also allows to perform single sample or multiple measurements. In case of multiple measurements activate the *Container measurement* check box (see chapter 4.3.1) and define a batch and numerical container number.

Make sure that you use different container numbers for the single products. The measurement result will be indicated in the analysis report. The report is sorted according to the container number.

4.4.1 Measuring Procedure

1) Click the *Sample changer* button.

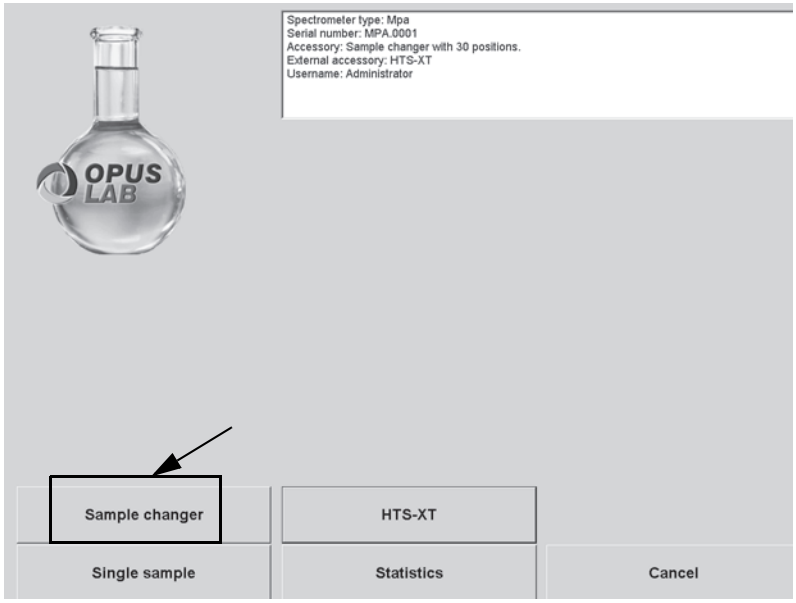


Figure 56: OPUS LAB measurements with sample changer

The following dialog opens:

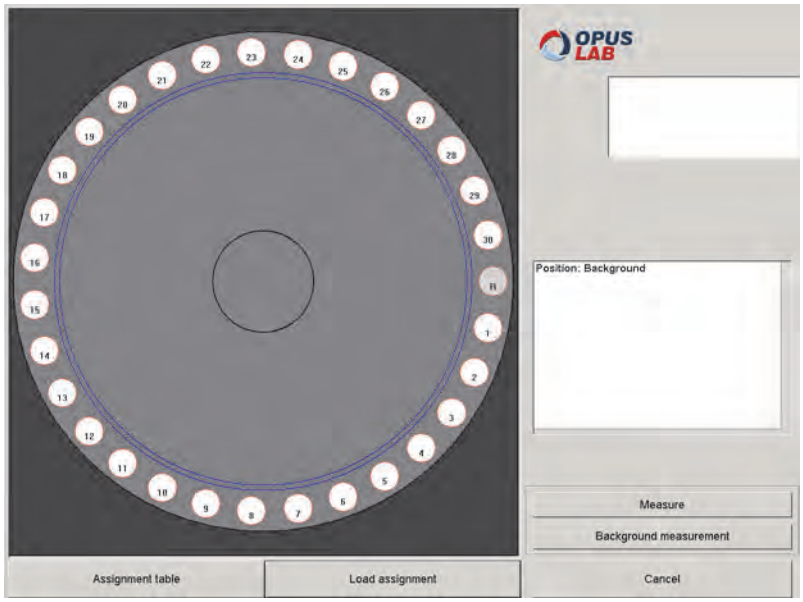


Figure 57: Sample changer - Measuring dialog

2) Select the positions desired by left clicking. To select several positions simultaneously press the *Ctrl* key. The positions must now be yellow.

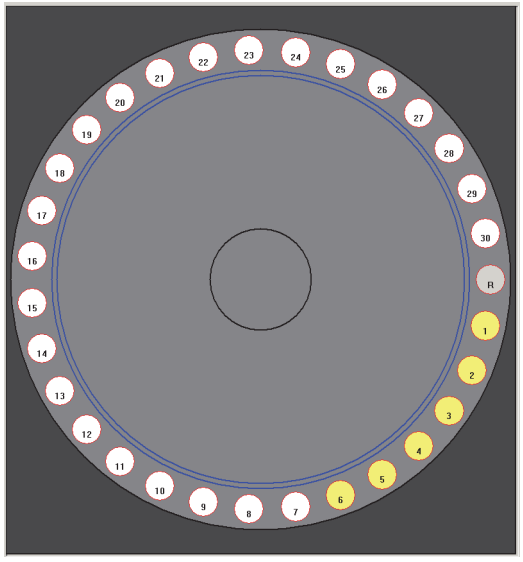


Figure 58: Sample changer - Selected positions

When selecting the single positions the following color code applies:

- White: free
- Yellow: marked
- Orange: assigned
- Dark orange: occupied
- Red: error

Red-colored positions may be attributed to an IDENT analysis failed, or to the fact that there have been outliers with regard to a QUANT analysis.

3) Click the *Assignment table* button (also see chapter 4.4.2).

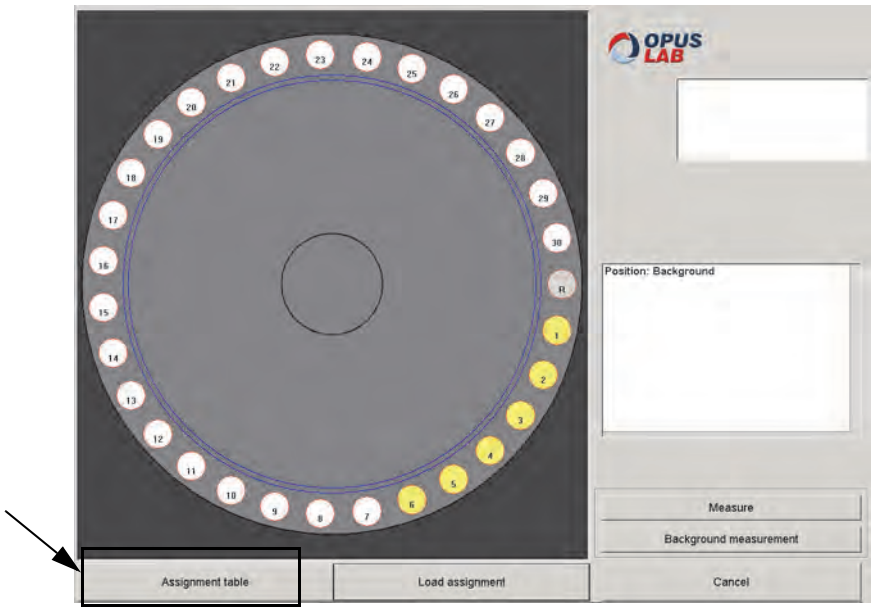


Figure 59: Sample changer - Opening assignment table

4) Select the product group and the product in the dialog that opens. Specify the sample description.
5) Mark the position(s) which are to be assigned to this product. Left click the table row. To mark several sample positions simultaneously press the *Ctrl* key.

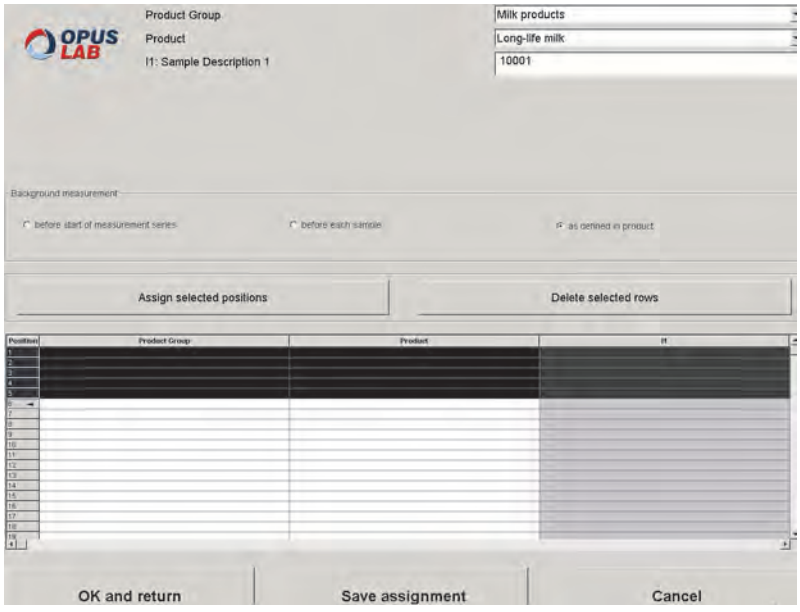


Figure 60: Sample changer - Assignment table

6) Click the *Assign selected* positions button. The table rows now contain the name of the product group and the product as well as the sample description.

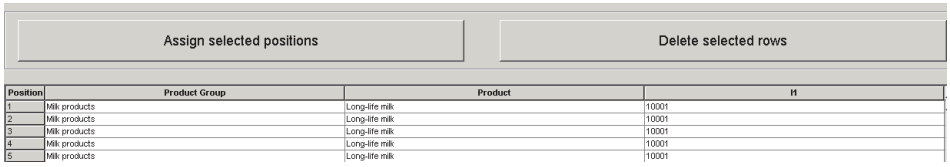


Figure 61: Sample changer - Assignment table with marked positions

7) Click the *Save assignment* button and specify a name for the assignment table. Then, click the *OK and return* button. The assigned positions must now be orange.

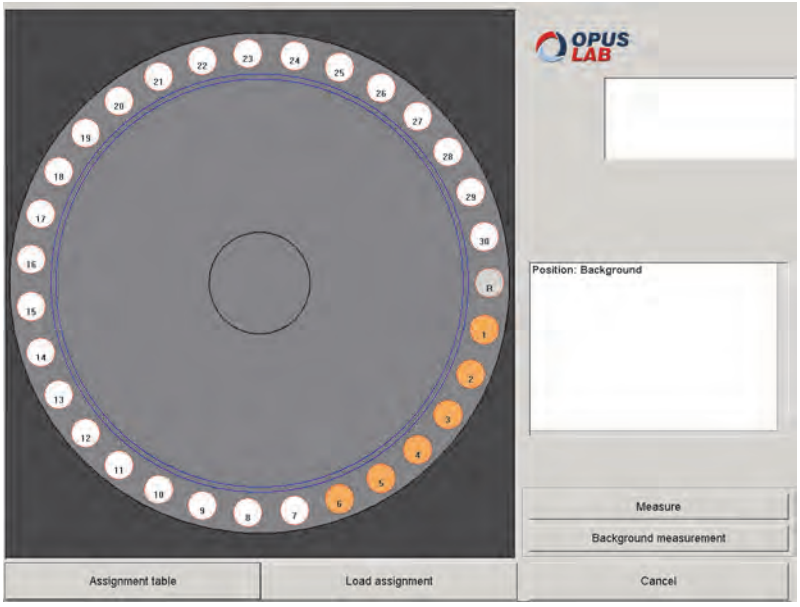


Figure 62: Sample changer - Assigned positions

8) Click e.g. position 1. The position now gets dark orange. The list box on the right shows the position data.

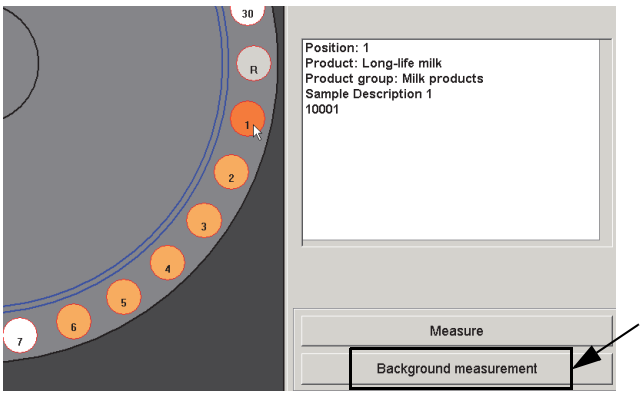


Figure 63: Sample changer - Occupied position 1

9) Click the *Background measurement* button (figure 63).

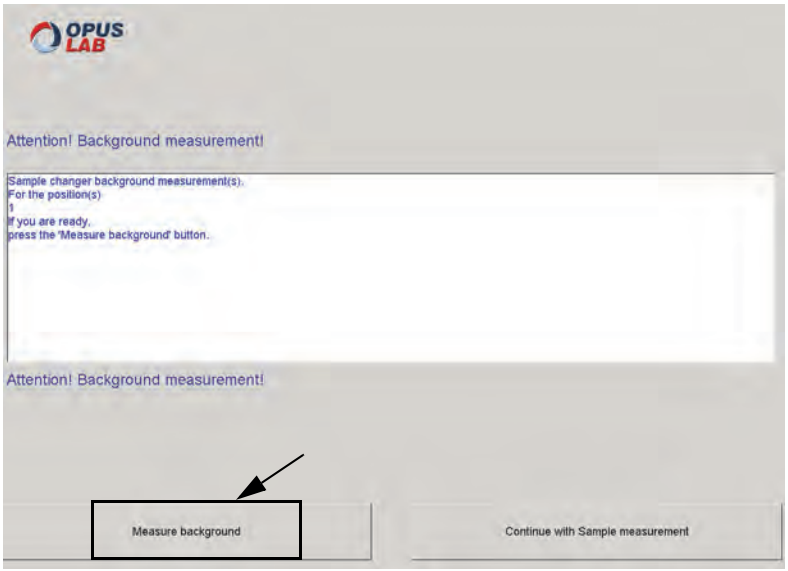


Figure 64: Sample changer - Background measurement

10) Click the *Measure background* button (figure 64). As soon as the background measurement has been finished, the white list box shows the measurement status.

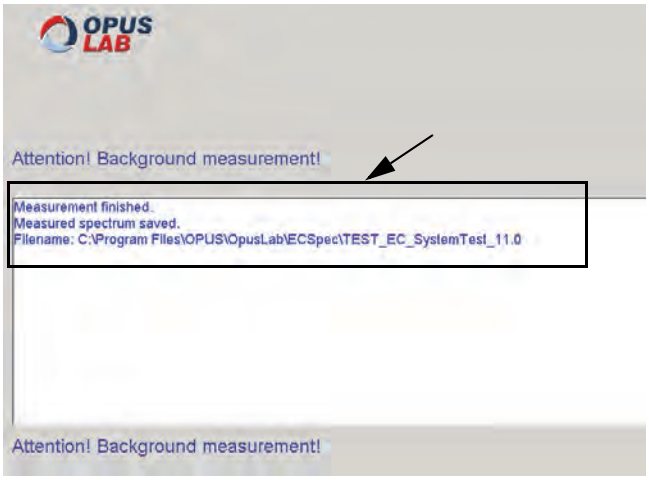


Figure 65: Sample changer - Background measurement status

11) Click the *Continue with sample measurement* button. Then, click the *Measure* button.

After sample measurement the positions are green. The spectrum last measured is displayed above the position data.

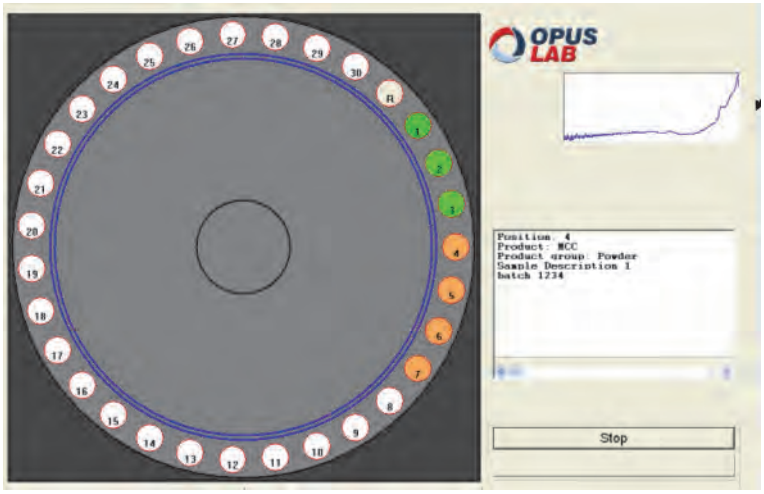


Figure 66: Sample changer - Measured positions

4.4.2 Assignment Table

Before starting any measurement using the sample changer, you have to assign the products to the corresponding sample positions. Click the *Assignment table* button.

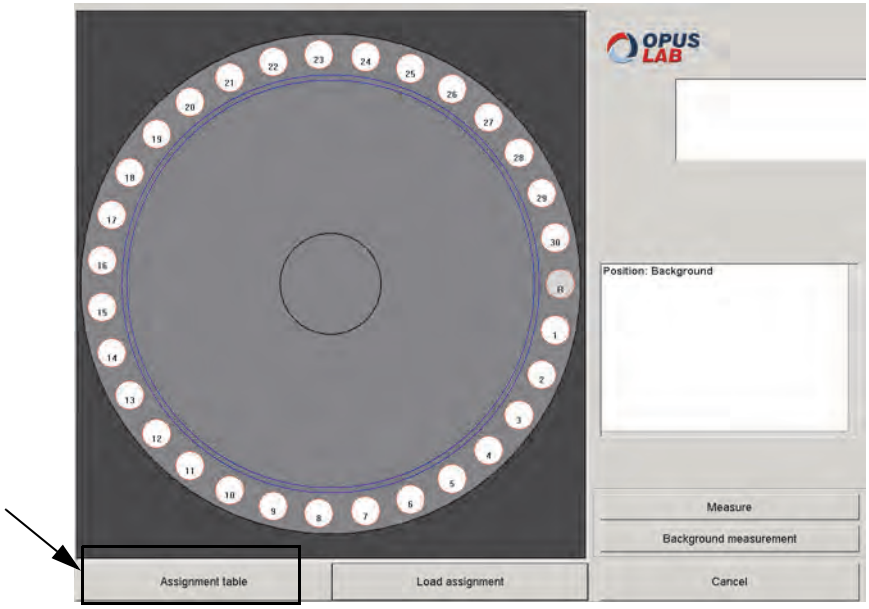


Figure 67: Sample changer - Opening assignment table

The assignment table opens.

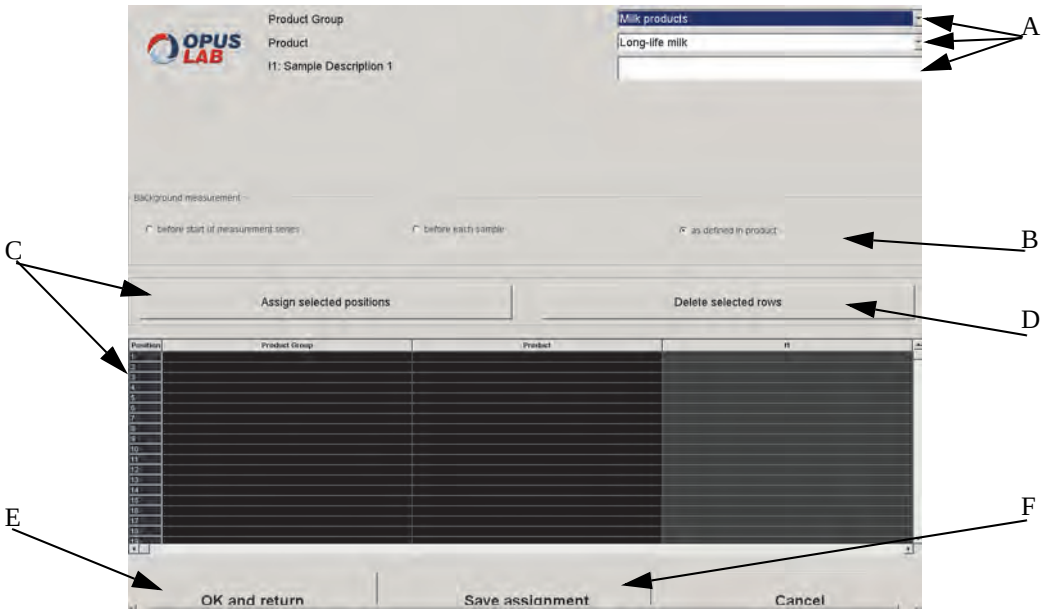


Figure 68: Sample changer - Assignment table

A) The drop-down lists contain the names of the product group and products defined. The sample description has to be written into the entry field.

B) The group field is only displayed if you have OPUS LAB administrator rights. You can select between three different options. If you have defined a validity period for the background measurement (*Product Setup*, chapter 3.2) and activated the respective option button (figure 68), it is checked whether all background measurements to be used are still valid. If they are not valid any more, a new background measurement starts for the respective positions.

C) The table rows represent the single measuring positions. To mark a row click the first table cell. In case of measurement series which consist of identical samples, you can select several sample positions simultaneously by pressing the *Ctrl* key. This allows to select all lines and columns simultaneously. The sample description can later be changed, if required.

Clicking the *Assign selected positions* button writes the product data into the table cells.

D) To delete certain positions, first select the positions which are to be deleted and then click the *Delete selected rows* button.

E) Clicking this button opens the measuring dialog for the sample changer again. The measuring positions must now be orange.

F) It is recommended to save the assignment table to be able to use it later. Define a name for the table.

4.4.3 VECTOR 22/N-T, VECTOR 22/N-I: specific notes

- The sample changer of these two spectrometers can have two different zero points. One zero point is used for external transmission measurement and the other for integrating sphere measurements. The zero position used is determined by the measurement mode settings in the *General Setup* (see chapter 2.4). The *mos60* command allows to switch between these two zero positions.
- VECTOR 22/N-T or VECTOR 22/N-I uses the *mot60* command to control the sample changer. You have to define this command in the *General Setup* (see chapter 2.4).
- The VECTOR 22/N firmware does not support the *Sample changer* functionality provided by OPUS. Therefore, you have to deactivate the *Sample changer* in OPUS. On the *Measure* menu, select the *Optic Setup and Service* command.

  Click the *Devices/Options* tab and deactivate the *Sample Changer* check box. In this case you have to specify the number of sample changer positions in the *General Setup* (see chapter 2.4).

4.5 Cleanness Test

When performing measurements using probes a cleanness test is required. Based on reference spectra, this test checks the cleanness of the probe. It determines the deviation between the spectrum of the S_{test} probe and the reference spectrum of the clean S_{ref} probe. The deviation is calculated as follows:

$$\text{deviation} = \Delta k\left(\sum_{i=1}^{N}(S_{ref,i} - S_{test,i})^2\right)$$

- with Δk = distance of the wavenumber lattice points
- N = number of the points in the spectrum
- $S_{ref,i}$ = spectral value of the reference spectrum at the lattice point i
- $S_{test,i}$ = spectral value of the spectrum at the lattice point i which has to be tested

If the deviation exceeds the user-defined threshold, the probe is identified as being contaminated.

4.5.1 Measuring reference spectrum

1) Make sure that you use a clean probe when measuring a reference spectrum.
2) On the *Product Setup*, click the *Background* tab.
3) Activate the *Active* checkbox in the *Cleanness test* group field.

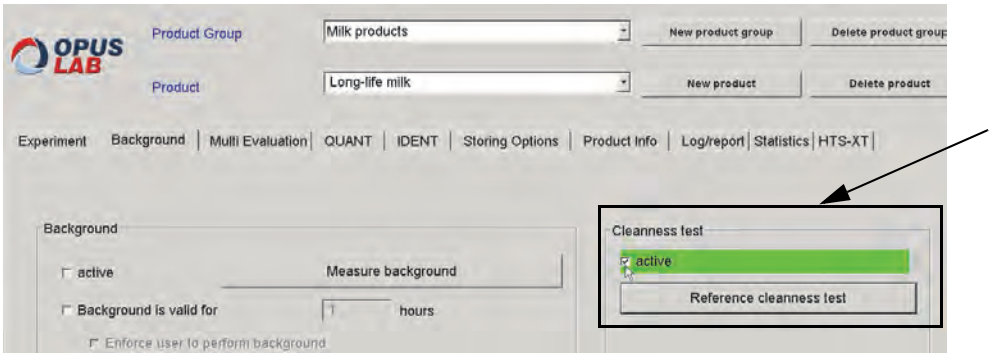


Figure 69: Background - Cleanness Test

4) Click the *Reference cleanness test* button. The following dialog opens:

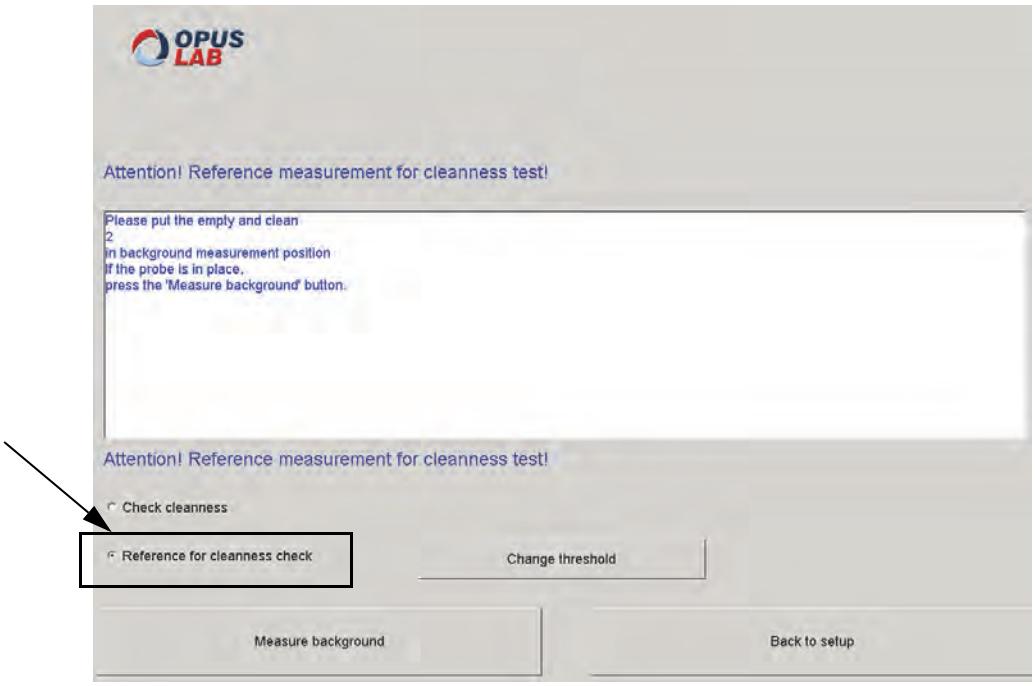


Figure 70: Reference measurement for cleanness test

5) Activate the *Reference for cleanness check* option button in this dialog (figure 70).
6) Click the *Measure background* button. As soon as the reference measurement has been finished the status is displayed in the white list box.

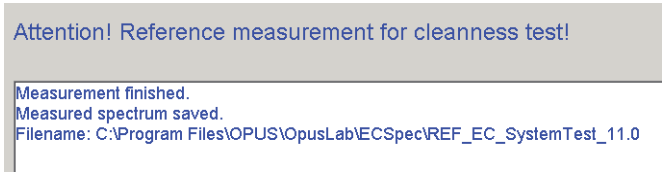


Figure 71: Status of reference measurement

4.5.2 Performing probe cleanness test

1) Activate the *Check cleanness* button.

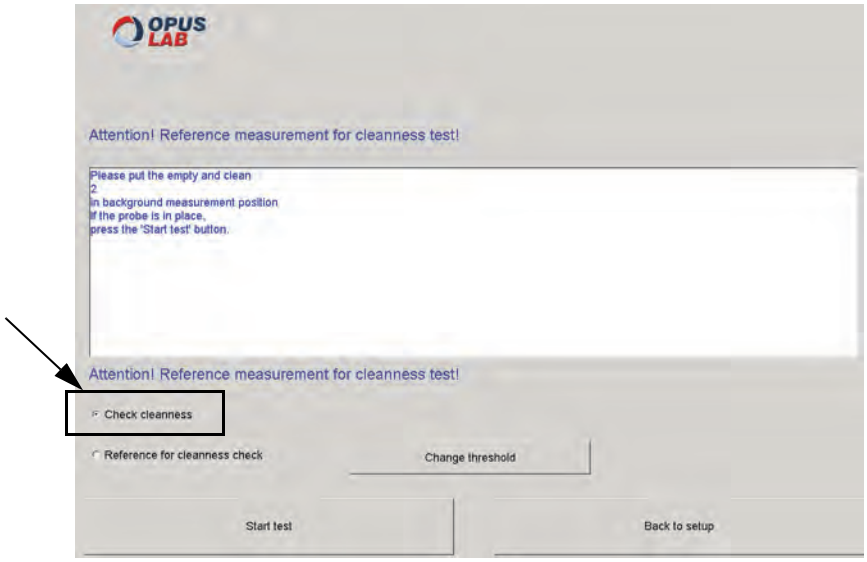


Figure 72: Cleanness test of probe

2) Click the *Change threshold* button and define a threshold.
3) Click the Start test button. The test result is displayed, for example:

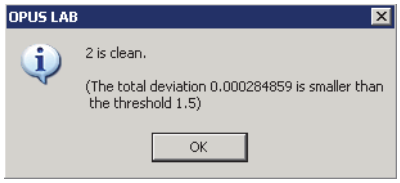


Figure 73: Cleanness test result

5 Evaluation

5.1 Multi Evaluation

The multi evaluation (ME) results are based on the ME method and evaluation options selected in the *Product Setup*. Further details are described in chapter 3.3.

Figure 76 exemplifies a product setup for a multi evaluation.

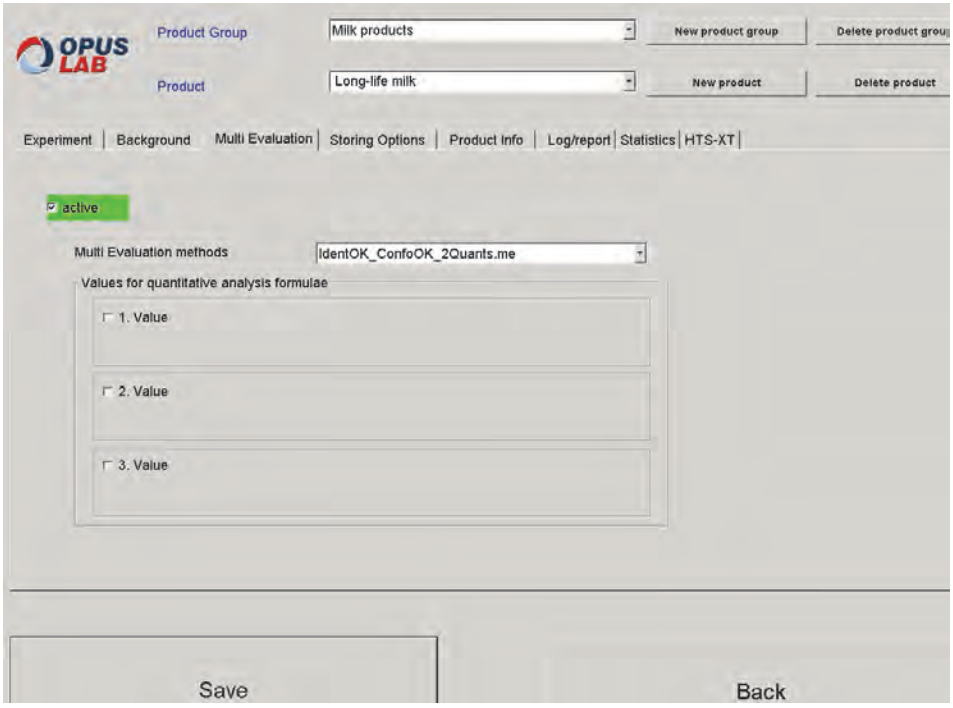


Figure 74: Exemplified product configuration for a multi evaluation

To be able to perform a multi evaluation you first have to define the *OPUSLab\Me* path in OPUS. On the *Setup* menu, select the *User Settings* command from and specify the path (figure 75).

Note: Use the *Multi evaluation path (old)* if you use multi evaluation methods which have been created with OPUS versions <7.0. Use the *ME base path* if you use multi evaluation methods which have been created with OPUS versions >7.0.

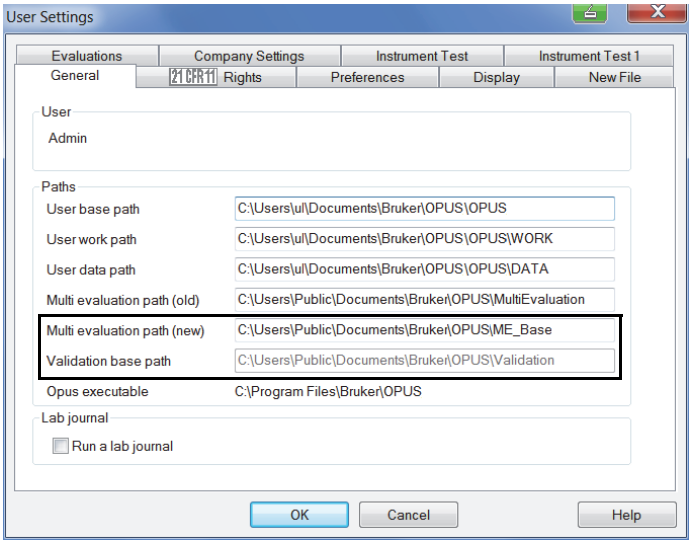


Figure 75: OPUS User Settings - Multi Evaluation path

Depending on the single methods used to build a multi evaluation method, the results of the evaluation are displayed separately for QUANT (chapter 5.2) or IDENT (chapter 5.3).

5.2 QUANT

The QUANT evaluation (quantitative analysis) results are based on the QUANT method and evaluation options selected in the *Product Setup*. Further details are described in chapter 3.4.

Figure 76 exemplifies a product setup for a QUANT evaluation.

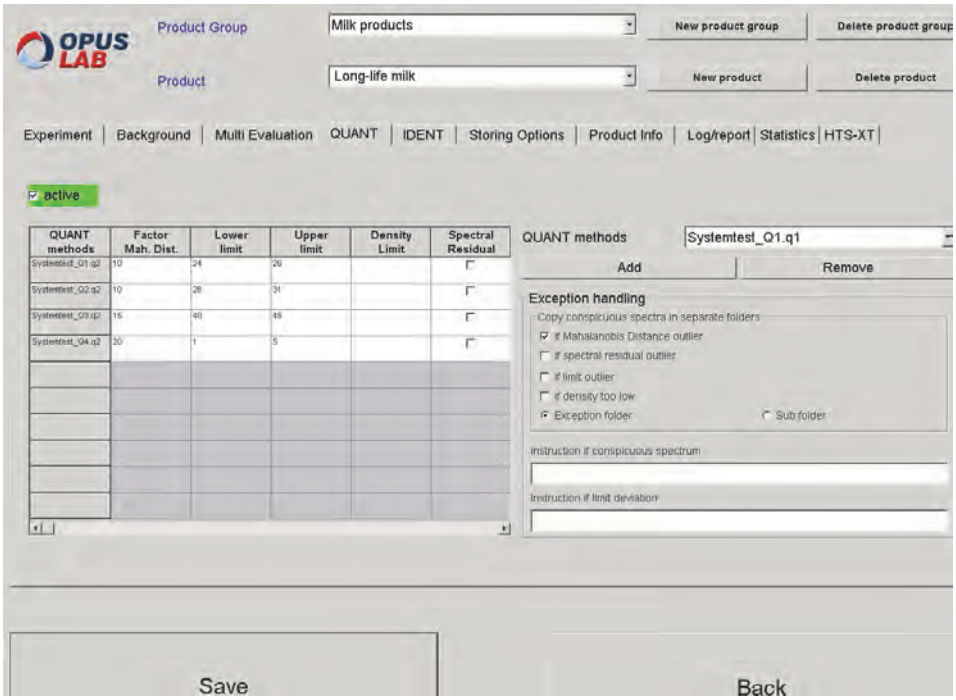


Figure 76: Exemplified product configuration for a QUANT evaluation

5.2.1 Displaying QUANT results

After the measurement has finished, click the *Show last QUANT results* button.

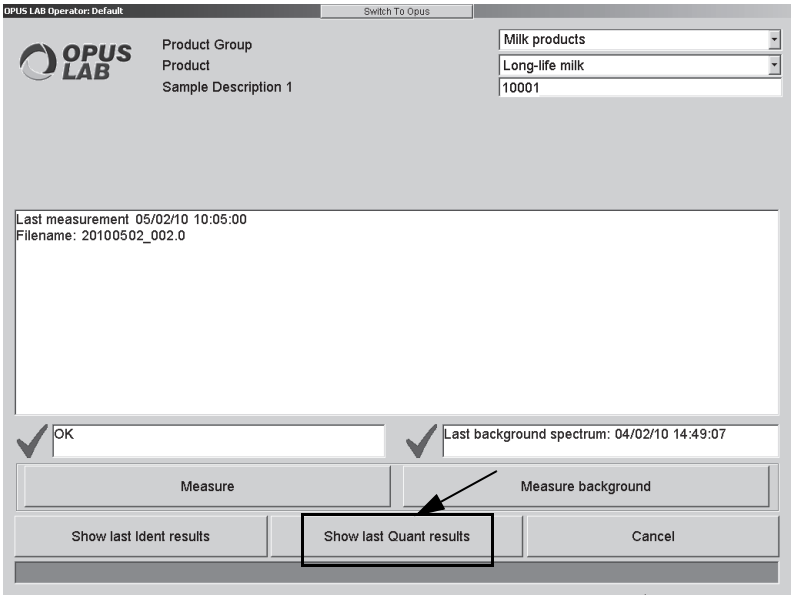


Figure 77: OPUS LAB - Show last QUANT results

The overall result is displayed in the result field above the table.

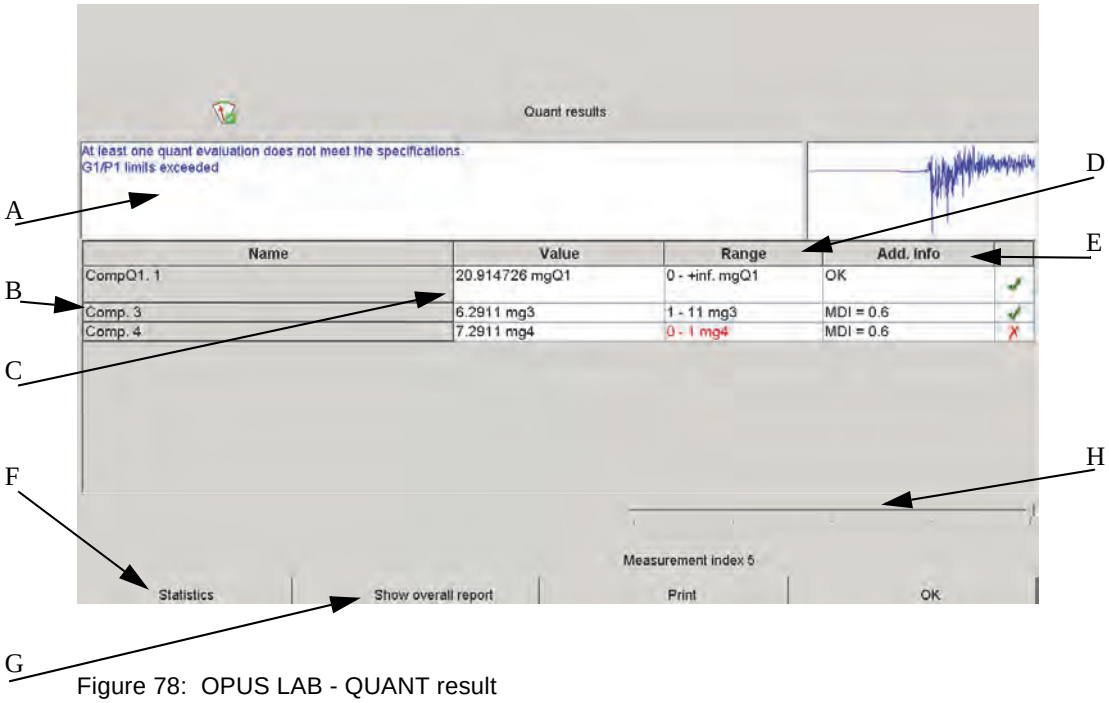


Figure 78: OPUS LAB - QUANT result

A) Overall result of QUANT evaluation

B) Component names as defined in QUANT 2 method

C) Quantitative analysis result specified by the corresponding unit.

D) This column indicates whether the values are within or beyond the specified range limits. The lower and upper range limits are defined in the *Product Setup* (see chapter 3.9). The result can be indicated as follows:

- OK: the value is within the range limits.
- < lower limit: the value is below the lower range limit.
- > upper limit: the value exceeds the upper range limit.

There will be a new table column for density outlier, as this feature is not an error but some kind of information. The spectrum might be considered for a calibration method expansion.

E) Additional information is provided:

- Green check mark: analysis is O.K
- Red cross: the maximum Mahalanobis distance value has been higher during the analysis. If you position the cursor on the column, you get further information on troubleshooting. The Mahalanobis distance index (MDI) is specified as quantitative measure for the deviation and is calculated as follows:

$$MDI = \frac{MHD}{MHDLIMIT \times MHDFACTOR}$$

with MHD = Mahalanobis distance

MHDLIMIT = Mahalanobis distance threshold

MHDFACTOR = Factor as defined in configuration form

F) To statistically evaluate the QUANT result click the *Statistics* button. The statistics view opens and shows the result in a trend chart:

)

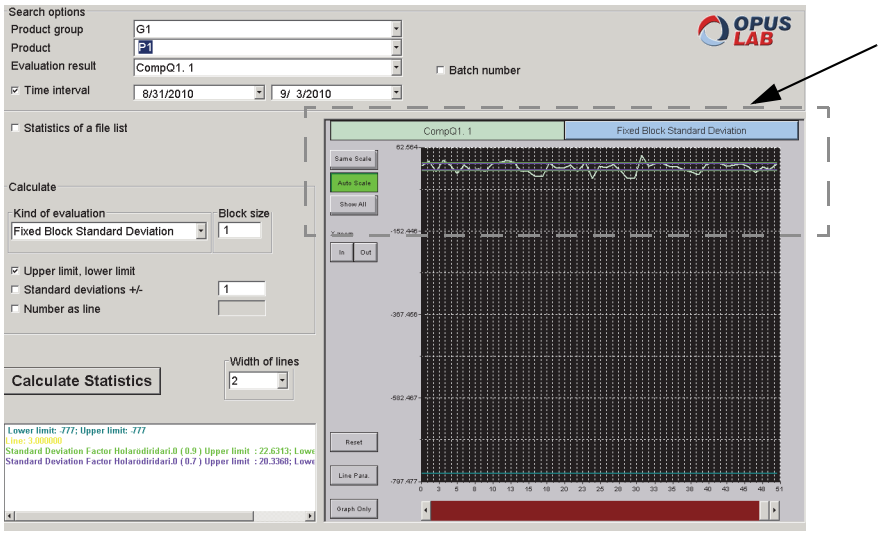


Figure 79: Trend chart of QUANT result

G) The *Show overall report* button is only displayed if you have performed multiple measurements. Clicking this button shows the overall report of all QUANT evaluations (see chapter 5.4). In case of single measurements the *Comment* button is displayed instead of the *Show Overall report* button. If you click the *Comment* button, the following view opens:

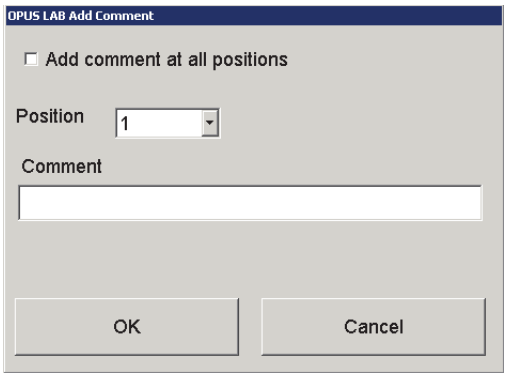


Figure 80: Add comment to measurement result

Enter a comment into the C*omment* entry field. The comment is stored in the HISTORY data block (HISTORY).

H) In case of multiple measurements a slider allows to have the QUANT evaluation results shown of each single measurement. Move the slider to the respective position to see the evaluation result. The *Measurement index 5* annotation below the slider in figure 81 means that the fifth evaluation result of a series of 10 measurements is shown in the table.

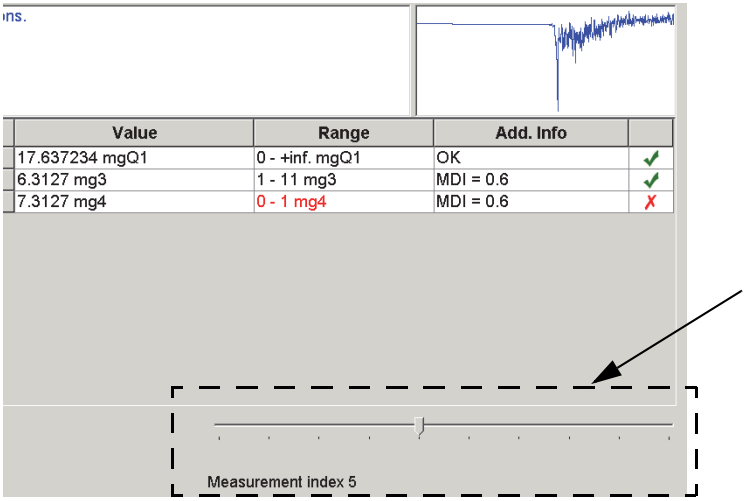


Figure 81: Slider to show single evaluation results

5.3 IDENT

The IDENT evaluation (qualitative analysis or identity test) results are based on the IDENT method and evaluation options selected in the *Product Setup*. Further details are described in chapter 3.5.

Figure 82 exemplifies a product setup for an IDENT evaluation.

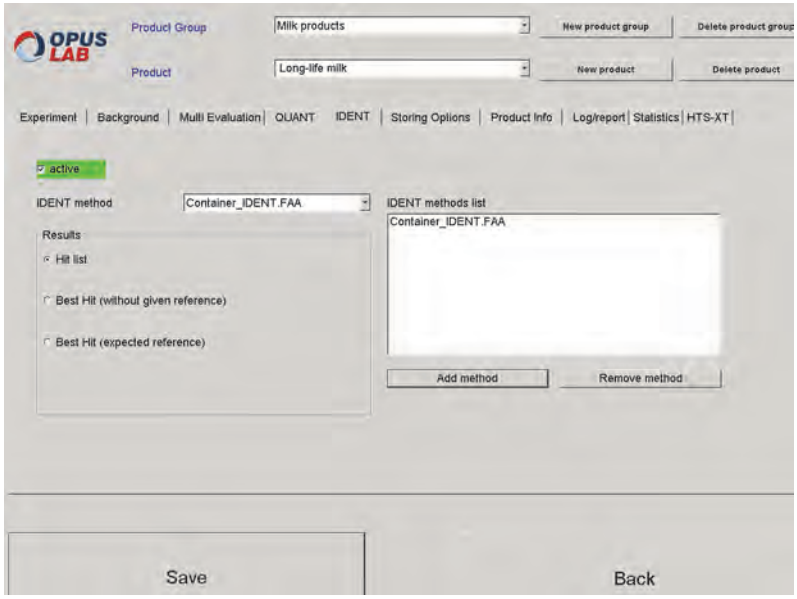


Figure 82: Exemplified product configuration for an IDENT evaluation

5.3.1 Evaluation Result

The *Product Setup* provides three different options on how to display the evaluation result of a qualitative analysis.

5.3.1.1 Hit List

A list with the best hits is displayed. The following evaluation results are possible:

- Identified as
- Not identified
- No unique identification possible

The result table shows the hit quality as well as the thresholds. In case of the *Identified as* result the hit quality of the first hit is less than the corresponding threshold. The hit quality of all the other hits has to be greater than the corresponding threshold.

The *Not identified* result indicates that the hit quality of all reference substances is greater than the corresponding threshold.

The *No unique identification possible* result indicates that the hit quality of more than one hit is less than the corresponding threshold.

5.3.1.2 Best hit (without given reference)

The list with the best hits is displayed. The following evaluation results are possible:

- Identified as
- Not identified
- No unique identification possible

The *Identified as* result indicates that the first hit in the result table is the best hit. A thumb points up, and the result field is green. The spectrum of the substance identified as well as of the reference are displayed.

In case of the *Not identified* result a thumb points down, and the result field is red.

The *No unique identification possible* result indicates that the hit quality of more than one hit is less than the corresponding threshold.

5.3.1.3 Best hit (expected reference)

In this case it is tested whether the substance is identical to the expected reference. For details on how to define the expected reference, refer to the OPUS IDENT manual.

The following evaluation results are possible:

- Identical to
- Not identical to
- Can be confused with

The *Identical to* result indicates that the first hit in the result table is the expected reference. The hit quality of the first hit is less than the threshold of the expected reference. A thumb points up, and the result field is green.

The *Not identical to* result indicates that the hit quality between the test spectrum and the expected reference is greater than the threshold. A thumb points down, and the result field is red. Additionally, the name of the expected reference specified in the pre-defined *List of references* is also displayed.

The *Can confused with* result indicates that the hit quality of the test spectrum is less compared to at least one other average spectrum, than the confidence region.

5.3.2 Displaying IDENT results

After the measurement has finished, click the *Show last IDENT results* button.

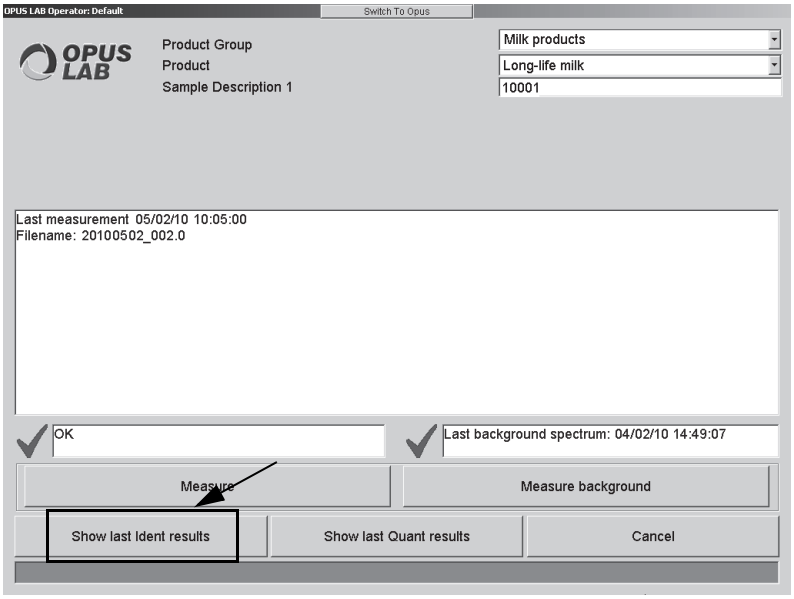


Figure 83: OPUS LAB - Show last IDENT results

Figure 84 shows a positive result of an IDENT evaluation.

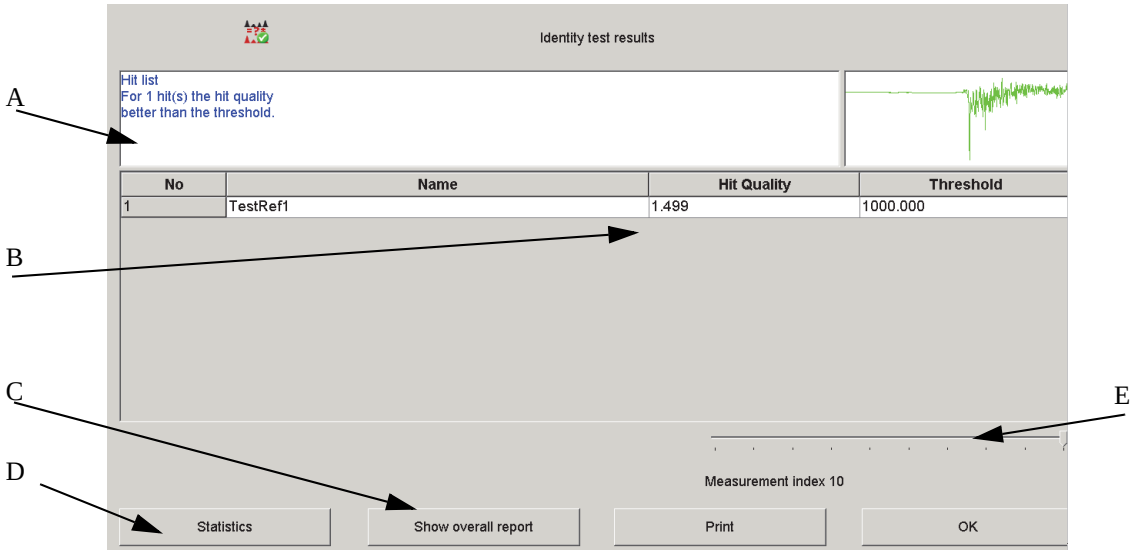


Figure 84: OPUS LAB - IDENT result

A) Overall result of IDENT evaluation

B) The best hit is shown.

C) The *Show Overall report* button is only displayed if you have performed multiple measurements. Clicking this button shows the overall report of all QUANT evaluations (see chapter 5.4). In case of single measurements the *Comment* button is displayed instead of the *Show Overall report* button. If you click the *Comment* button, the following view opens:

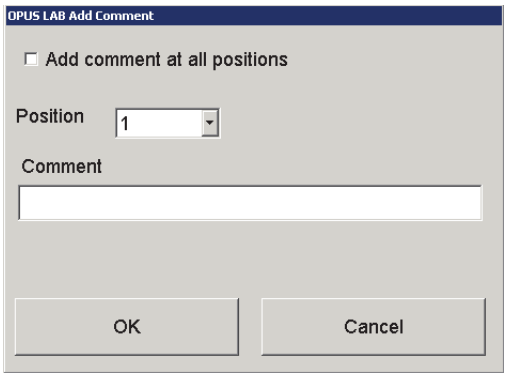


Figure 85: Add comment to measurement result

) Enter a comment into the C*omment* entry field. The comment is stored in the HISTORY data block (HISTORY).

D) To statistically evaluate the IDENT result click the *Statistics* button. The statistics view opens and shows the result in a trend chart.

E) In case of multiple measurements a slider allows to have the IDENT evaluation results shown of each single measurement. Move the slider to the respective position to see the evaluation result. The *Measurement index 10* annotation below the slider in figure 86 means that the tenth evaluation result of a series of 10 measurements is shown in the table.

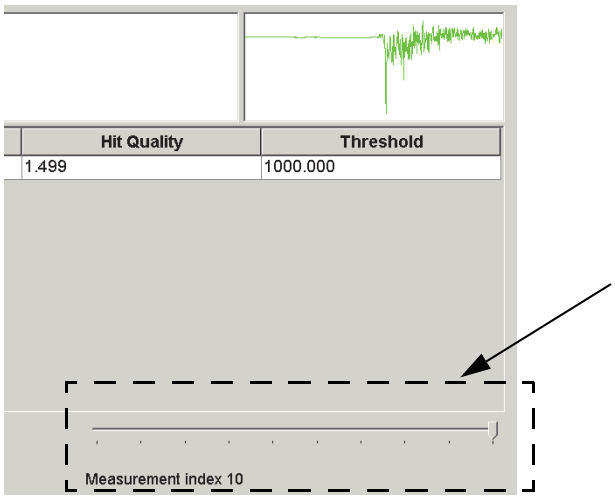


Figure 86: Slider to show single evaluation results

5.3.3 Notes on hierarchical IDENT and class tests

If the *Class test* option has been activated in the IDENT method and the result of the IDENT test is identical to the class, the OPUS LAB result will be OK. In this case the following information is displayed:

- **Sample is identical to *Groupname***
  if the sample is identified and identical to the class
  With:
  Groupname being a placeholder for the current group name.
- **Sample is member of *Classname* class**
  if the sample is not identified and identical to the class
  With:
  Classname being a placeholder for the current class name.
- **Sample is identical to *Groupname* (member of *Classname* class)**
  if the sample is not identified and identical to the class
  With:
  Groupname being a placeholder for the current group name.
  Classname being a placeholder for the current class name.

5.4 Multi-sample evaluation results

If you perform multi-sample evaluations (e.g. using a sample changer or performing multiple measurements), it is possible to display and print an overall report of the results.

In this case the *Show overall report* button is shown. Click this button to display the corresponding overall report dialog.

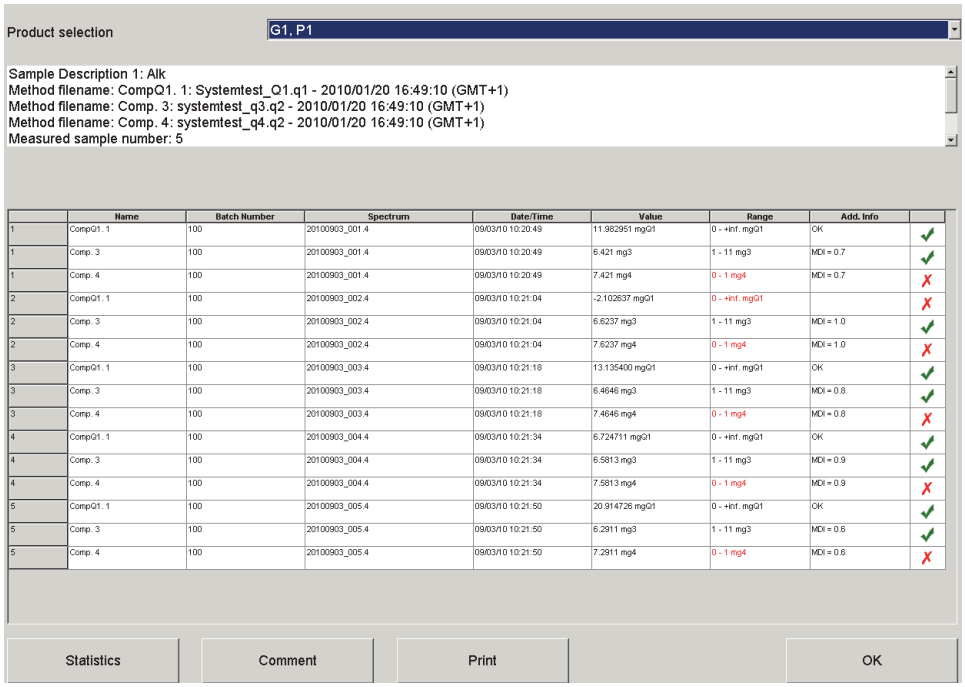


Figure 87: OPUS LAB overall report - QUANT evaluation

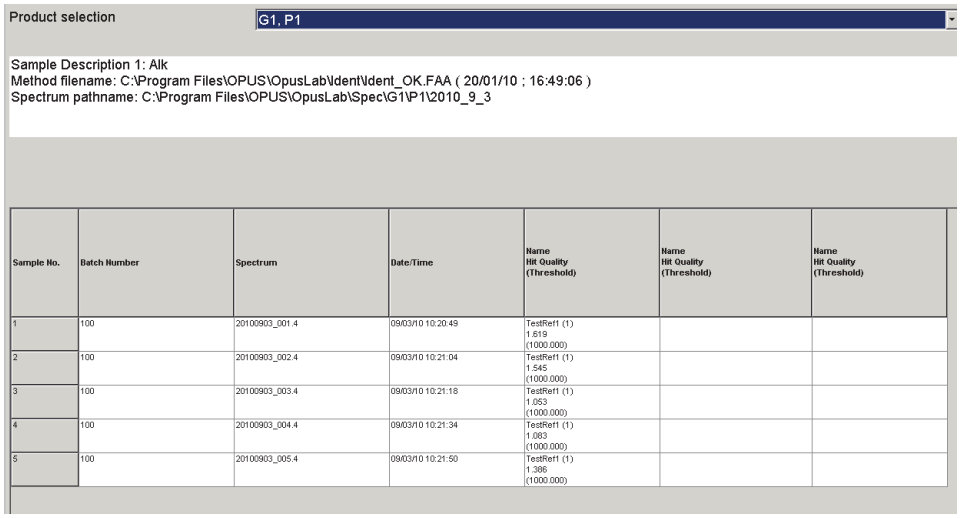


Figure 88: OPUS LAB overall report - IDENT evaluation

If you click the *Print* button, the evaluation results of the current product will be printed. Click the *Comment* button to add a comment to the results.

5.5 Statistics

OPUS LAB allows to statistically evaluate special kinds of results generated from evaluations such as QUANT, IDENT or Multi Evaluation. The statistical evaluation results are displayed in a trend chart.

The statistical evaluation uses spectra from a spectra file list or from a connected database.

The statistical evaluation results are based on the setup options selected in the *Product Setup*. Further details are described in chapter 3.9.

Figure 82 exemplifies a product setup for statistical evaluation.

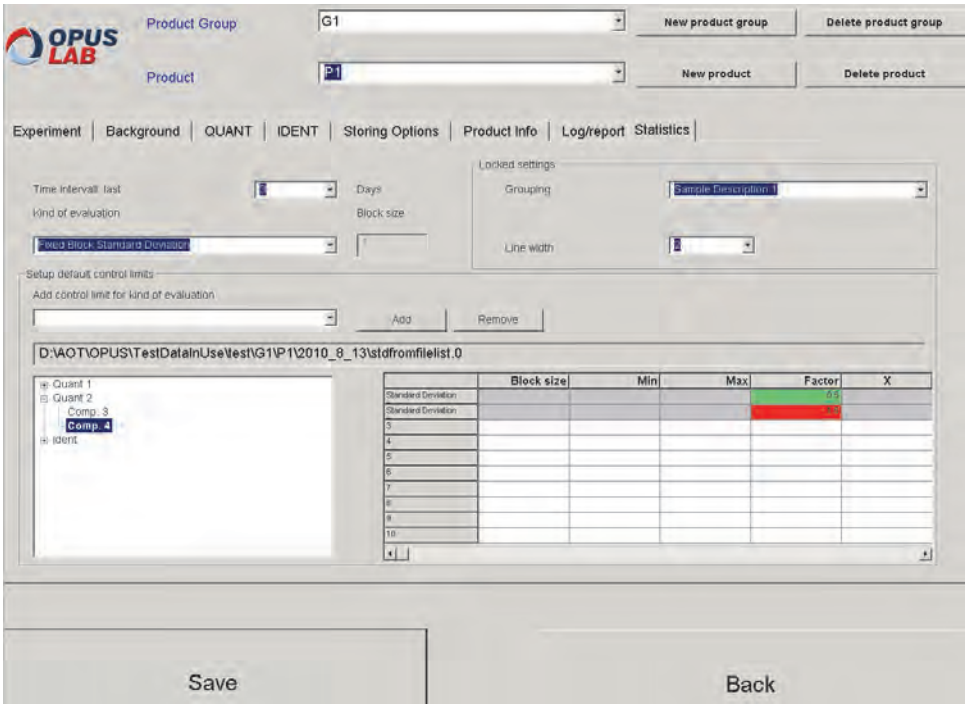


Figure 89: Exemplified product configuration for a statistical evaluation

5.5.1 Starting statistical evaluation

1) Click the *Statistics* button.

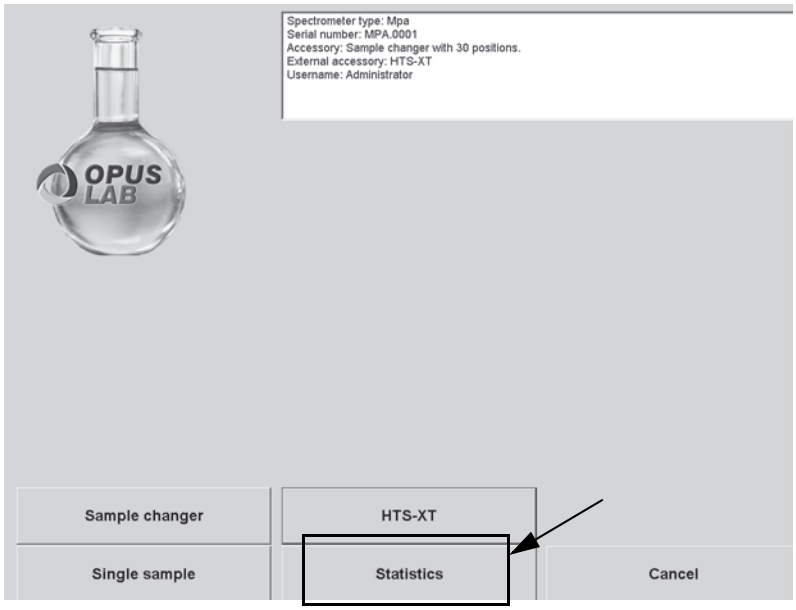


Figure 90: OPUS LAB measurement dialog

The statistics dialog is displayed. By default, the selection fields and selection lists contain the latest settings made in *Product Setup* (chapter 3.9).

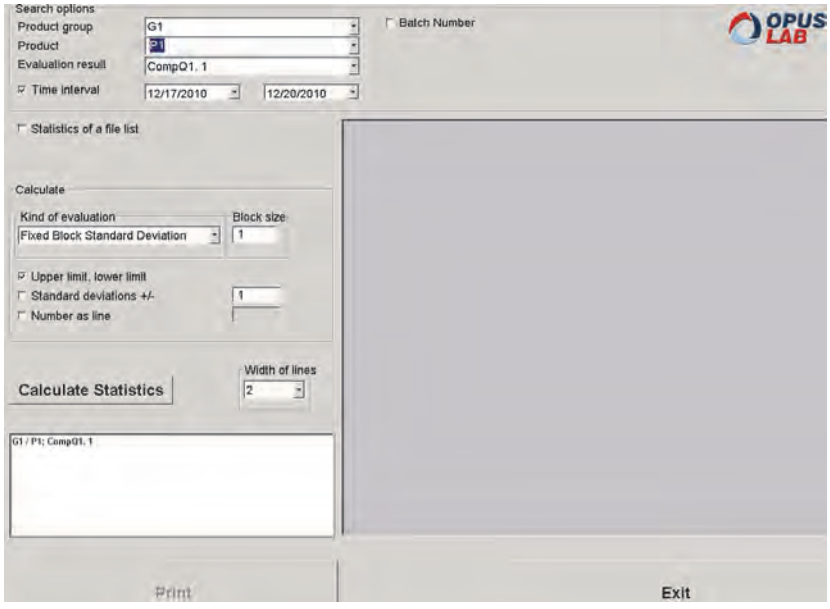


Figure 91: OPUS LAB - Statistics

2) Select the product group and the product from the drop-down list. This is only required if the statistical evaluation is to be performed with a product group or product other than displayed.

3) Select the method component for which the statistical evaluation is to be performed. The drop-down list only contains those method components for the product selected, which you have been defined before in *Product Setup* (chapter 3.9).
4) Define the time interval to be considered for statistical evaluation. If required, activate the *Time Interval* check box. By default, the right field shows current date, the left one the current date minus the number of days defined in *Product Setup* (chapter 3.9). If you click the arrow head, a calendar view pops up.
5) Activate the *Batch number* checkbox and select the numbers from the drop-down list. The list contains all the batch numbers found in the database for the time interval defined.

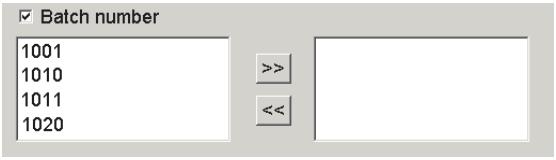


Figure 92: Selecting batch number

The user-specific description of the charge number has to be defined first, in the *Field 1* on the *Product Info* tab in the *Product Setup* (chapter 3.7). The actual batch number has to be entered into the corresponding entry field in the measuring dialog. The spectra get a batch number during measurement.

In case of statistical evaluation you select the batch numbers, for which statistical evaluation is to apply, from the list.

6) Select the kind of evaluation from the drop-down list. Details on how to evaluate in batch blocks are described in chapter 5.5.2.

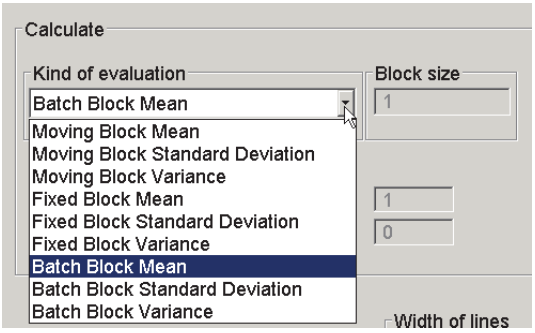


Figure 93: Kind of statistical evaluation

In case of some evaluation functions you can select the block size as well, i.e. the number of container number to be used for each block. To get reasonable results make sure that you define a meaningful block size. The larger the block size, the coarser the curve line in the trend chart.

7) Make further settings with regard to the depiction of statistical evaluation. The following options are available:

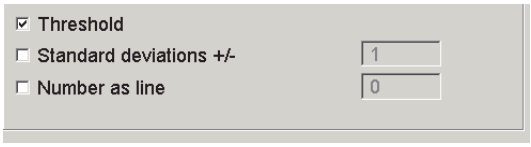


Figure 94: Setting options for depiction in trend chart

- **Threshold:** Based on the entire spectrum range, this option considers the limit in case of IDENT, the upper and lower limit in case of QUANT, the limit in case of conformity and the sum limit in case of sum 1/2. This option is not available for integration.
- **Standard deviation:** This option considers the standard deviation for the entire spectrum range, i.e. all data points in the trend chart.
- **Number as line:** If you activate this check box, the right entry field is enabled. Enter a value. In the trend chart, a line is displayed at a certain *y* section of the spectrum. The width of this line is defined using the drop-down list.

8) Define the width valid for all lines which are displayed in the trend chart.

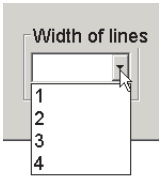


Figure 95: Setting options for depiction in trend chart

9) Click the *Calculate Statistics* button.

5.5.2 Evaluation in batch blocks

When evaluating in batch blocks the file list contains additional traces. This requires an additional table column when generating a spectra file list (chapter 3.9.4). The column has to contain the batch numbers.

The statistical evaluation in data blocks uses spectra which have the same batch number. Additionally, these spectra with the same batch numbers have to be located next to each other. Reasonable evaluation results are not possible in case of spectra with overlappings. The following methods are available in case of evaluating in batch blocks: mean, standard deviation, variance.

5.5.3 Trend chart depiction

The statistical evaluation is depicted in a trend chart.

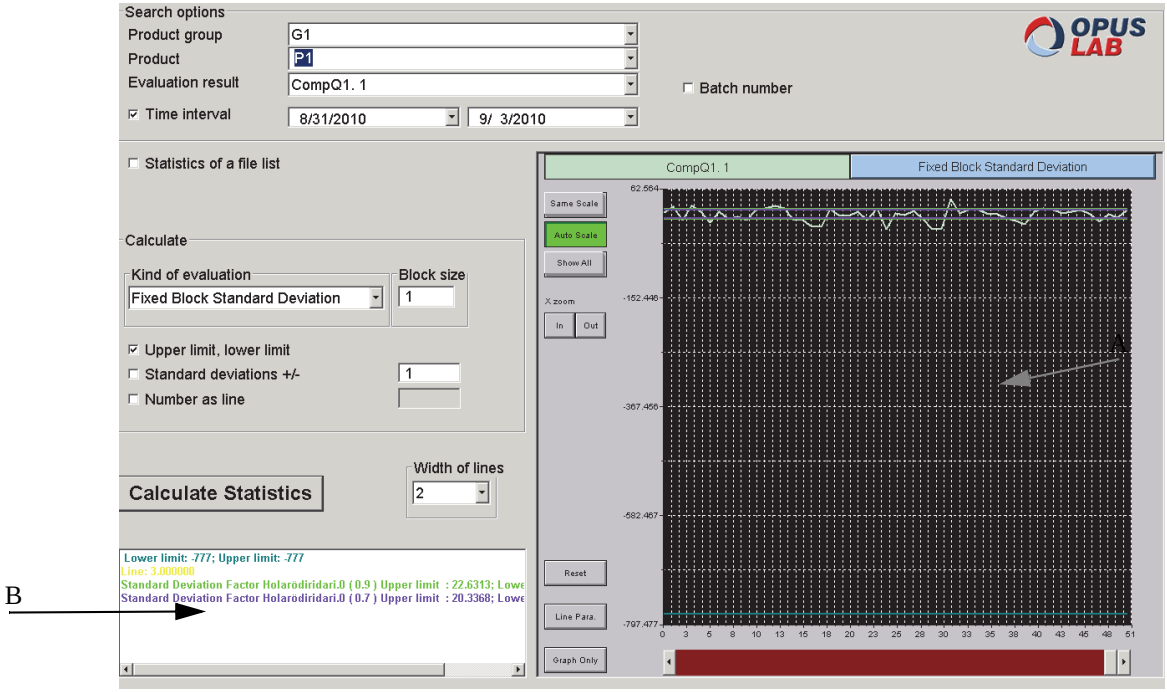


Figure 96: OPUS LAB - Trend chart

A) Trend chart

B) This list box shows the name of the product as well as the results of the average or limit values. The results have the same color as the corresponding lines displayed in the trend chart.

In case of standard deviation, the control limits indicated refer to reference spectra of the respective method used (IDENT, QUANT, Multi Evaluation etc.). These reference spectra are combined in a file list and have to contain the data block of the type of evaluation desired.

5.5.4 Printing trend chart

The trend chart can be printed. Click the *Print* button. The output format is a PDF.

5.5.5 Statistical evaluation of file list

Evaluation functions can be used for the complete file list, in the same way as being used for single spectrum files.

Loading file list

1) Activate the *Statistics of a file list* checkbox. The drop-down lists for the search options become disabled.

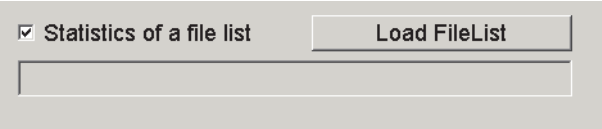


Figure 97: Activating statistics for file list

2) Click the *Load FileList* button.
3) Select the file list from the respective directory. If you have selected a file list, the path is displayed.

Statistically evaluate file list

1) Select the kind of evaluation (see chapter 5.5.1).
2) Click the *Calculate Statistics* button.

Evaluation result of file list

The evaluation result is displayed in the trend chart.

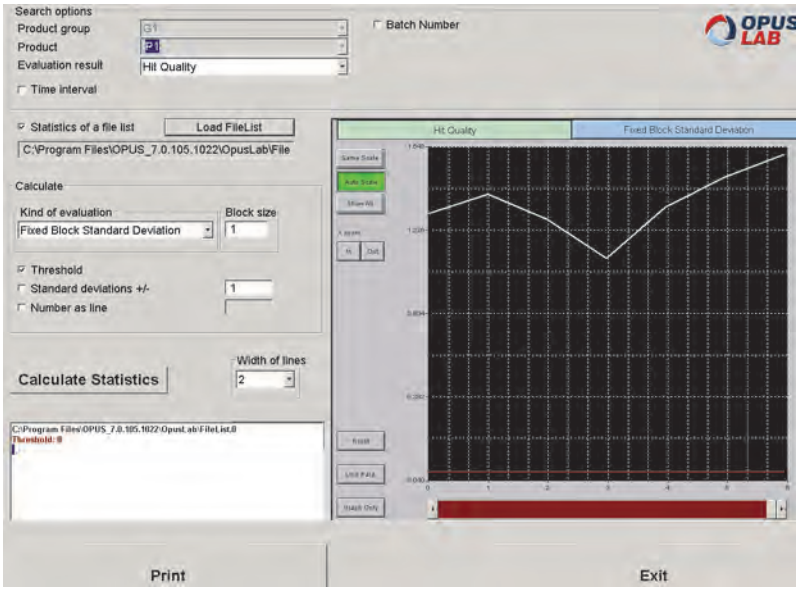
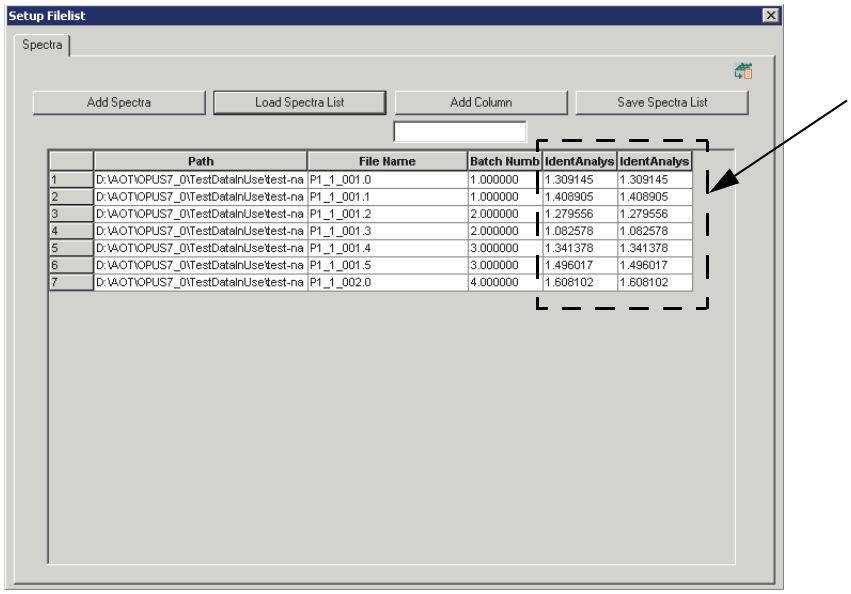


Figure 98: Example of spectra list evaluation result displayed in trend chart

Depending on the type of statistical evaluation, the spectra file list is enlarged by the respective number of columns. These columns contain the evaluation result (figure 99).



	Path	File Name	Batch Numb	IdentAnalys	IdentAnalys
1	D:\AOT\OPUS7_0\TestDataInUse\test-na	P1_1_001.0	1.000000	1.309145	1.309145
2	D:\AOT\OPUS7_0\TestDataInUse\test-na	P1_1_001.1	1.000000	1.408905	1.408905
3	D:\AOT\OPUS7_0\TestDataInUse\test-na	P1_1_001.2	2.000000	1.279556	1.279556
4	D:\AOT\OPUS7_0\TestDataInUse\test-na	P1_1_001.3	2.000000	1.082578	1.082578
5	D:\AOT\OPUS7_0\TestDataInUse\test-na	P1_1_001.4	3.000000	1.341378	1.341378
6	D:\AOT\OPUS7_0\TestDataInUse\test-na	P1_1_001.5	3.000000	1.496017	1.496017
7	D:\AOT\OPUS7_0\TestDataInUse\test-na	P1_1_002.0	4.000000	1.608102	1.608102

Figure 99: Example of spectra file list after statistical evaluation

6 File interface

6.1 OPUS LAB log files

6.1.1 Initialization file

Format

ASCII. Each line consists of a key word followed by an equal sign (=) and the value of the entry. The italicized values are placeholders, their content is explained in the following chapter.

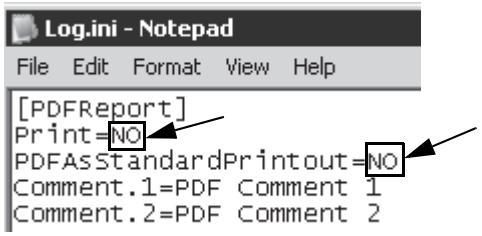
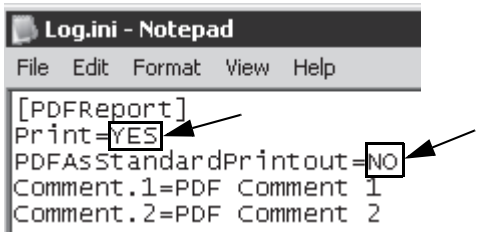
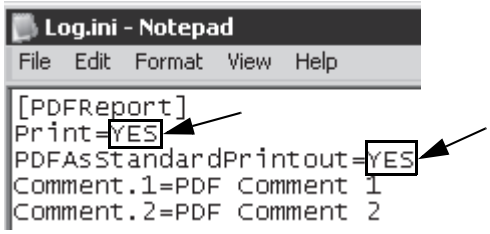
Path

Applicationpath\Log\Log.ini

Note: *Applicationpath* is the directory, in which OPUS LAB has been installed.

	Content	**Definition**
[GENERAL]	Separator=*SeparatorSign*	Sign which separates the individual entries in the log file. • Value range: Any • Format: Character string **Note:** If this entry is missing, a semicolon (;) is used as standard.
	CSVFile=*FlagCSVFile*	Flag, if log file is stored as *csv* file (*csv* = comma-separated file). A *csv* file has the extension **.csv* and can be directly loaded into Microsoft Excel. Values: YES = log file is stored as *csv* file **Note:** For all other values the log file extension is **.log*.

	Content	Definition
	DateFormat=*DateFormat*	The flag sets the date. • Format: %*Y-%m-%s*, i.e. Y = year, m = month, d = day. Example: *2019-05-24*. The order of the year/month/day can optionally be changed. You can either omit the minus signs or replace them by „__“. The latter case produces the following date format: *2019__05__24*. The following format specifiers can optionally be added, always beginning with a percentage (%) sign: • *%c*: date and time representation, e.g. *Thu May 23 14:55:02 2019* • *%h*: abbreviated month name, e.g. *Aug*
	TimeFormat=*TimeFormat*	The flag sets the time. • Format: %*H:%M:%S*, i.e. H = hour, M = minute, S = second. Example: *08:15:00*. The following format specifiers can optionally be added, always beginning with a percentage (%) sign: • *%p*: am or pm designation, e.g. *08:50:54 AM*, *08:50:54 PM* • *%c*: date and time representation, e.g. *Thu May 23 14:55:02 2019*
	UTC_Offset=*UTCOffset*	The flag sets the time difference (offset) of a time zone from the coordinated universal time (UTC), for a particular place and date. • Value YES: offset is displayed • Value NO: offset is not displayed The offset is shown in the following format: ±<*hh*><*mm*>, with *h* being hours, and *m* minutes. Example: *+0200* means that the time zone is 2 hours ahead of UTC time. *-0200* means that the time zone is 2 hours behind UTC time.
	UTC_OffsetSEPERATED=*UTCOffsetSeparator*	The flag has only an effect if the flag *UTC_Offset=YES*. The flag sets a separator between date/time specifications and the time difference of a time zone from the coordinated universal time (UTC). • Value YES: separator is set • Value NO: separator is not set Example: *2019-05-24;08:15:12;+0200* **Note:** By default, a semicolon is used as separator.

	Content	Definition
[PDFReport]	Print=*FlagPrintPDFReport*	This flag is set, if PDF print-out file is to be created. • Value range: YES = create a PDF file. For all other values no additional PDF file is created. • Format: Character string **Example:** Printed report only 
	PDFAsStandardPrintout=*FlagPDFAsStandardPrintout*	This flag is only set if *FlagPrintPDFReport = YES*. If *FlagPDFAsStandardPrintout* is true, only a PDF print-out is created. • Value range: YES = only one PDF file is created. For all other values both a printer output and a PDF file is created. • Format: Character string **Example:** Printed report and PDF file  **Example:** PDF file only 
	Comment.1-2 = *PDFComment1-2*	To distinguish a PDF print-out from a standard print-out you can add up to 2 comments into the PDF file.

	Content	Definition
[OverallReport]	PrintHitList=*FlagPrintHitList*	Flag is set if list of similar substances is to be printed. • Value range: YES = list of similar substances is printed. For all other values no list of similar substances is printed. • Format: Character string
	AddToHitListOnlyResultNotOK=*FlagAddToHitListOnlyResultNotOK*	This flag is set if the hit list has to contain only evaluation results of spectra which are not identified (not ok). • Value range: YES = report hit list includes only results of spectra which are not ok. For all other values the hit list does also contain other results. • Format: Character string
	IndexProductInfoLineInSummery=*FlagIndexProductInfoLineInSummery*	This flag is used if the header of a summary report is to summarize the entries of the product info description fields (1, 2, 3, 4 or 5). • Value range: -1 = no output. For all other values the header includes the definition of the respective entry field. • Format: Integer
	SingleReportIfResultNotOK=*FlagSingleReportIfResultNotOK*	Flag is set if single reports are to be printed, especially for evaluation results which are not ok. • Value range: YES = single reports are printed for evaluation result which are not ok. For all other values no single reports are printed. • Format: Character string

	Content	Definition
[GenericLog]	NrEntries=*NrEntries*	Number of component analyses recorded in the log file. • Value:1 up to 100 • Format: Integer
	Entry.i=*EntryKeyWord*	*i* Index of the *i*-th analysis date • Value range: 1 up to *NrEntries* • Format: Integer *EntryKeyWord* Key word which is assigned to the *i*-th analysis date. Format: Character string The following key words are supported: • !PRD: Sample description • !PRG: Product group • !PRN: Product • !DAT: Time of measurement • !SPP: Spectra path • !SPN: Spectra file name • !IDR: Identity test result Ident;ID_OK or Ident;ID_NOT_OK • !QAR: QUANT results ComponentName; QuantResultValue; QuantResultUnit; • !QAE: QUANT extended results ComponentName; QuantResultValue; QuantResultUnit; MahDistValue; MahDistThreshold MDIIndex • !QAO: QUANT outlier marker (chemometric alarm) Value=0 (no outlier) Value=1 (outlier) • !QAB: QUANT threshold value deviation marker (method range) Value=0 (OK) Value=-1 (below lower range limit) Value=1 (above upper range limit) • !XPM: Experiment file

	Content	Definition
	Entry.i=*EntryKeyWord*	**Note:** If these entries are not available, the following standard values will be used: NrEntries=6 Entry.1=!DAT Entry.2=!PRG Entry.3=!PRN Entry.4=!SPP Entry.5=!SPN Entry.6=!XPM

	Content	Definition
[ProductLog]	NrEntries=*NrEntries*	Number of component analyses recorded in the log file. • Value:1 up to 100 • Format: Integer
	Entry.i=*EntryKeyWord*	*i* Index of the *i*-th analysis date • Value range: 1 up to *NrEntries* • Format: Integer *EntryKeyWord* Key word which is assigned to the *i*-th analysis date. Format: Character string The following key words are supported: • !PRD: Sample description • !PRG: Product group • !PRN: Product • !DAT: Time of measurement • !SPP: Spectra path • !SPN: Spectra file name • !IDR: Identity test result Ident;ID_OK or Ident;ID_NOT_OK • !QAR: QUANT results ComponentName; QuantResultValue; QuantResultUnit; • !QAE: QUANT extended results ComponentName; QuantResultValue; QuantResultUnit; MahDistValue; MahDistThreshold MDIIndex • !QAO: QUANT outlier marker (chemometric alarm) Value=0 (no outlier) Value=1 (outlier) • !QAB: QUANT threshold value deviation marker (method range) Value=0 (OK) Value=-1 (below lower range limit) Value=1 (above upper range limit) • !XPM: Experiment file

	Content	Definition
	Entry.i=*EntryKeyWord*	**Note:** If these entries are not available, the following standard values will be used: NrEntries=5 Entry.1=!DAT Entry.2=!PRN Entry.3=!PRD Entry.4=!IDR Entry.5=!QAE
[InterfaceLog]	Active=*ActiveMarker*	Marker which indicates whether an interface file has to be created. • Value range: YES = interface file is created. For all other values no interface file is created. • Format: Character string
	LogFilePath=*LogFilePath*	This entry indicates the path name in which the interface file is stored. • Value range: Name of an existing path • Format: Character string
	LogFileName=*LogFileName*	This entry indicates the name of the interface file. • Value range: OpusLab.csv • Format: Character string
	AddDateTimeToFileName=*AddDateTimeToFileName*	This entry indicates whether date and time is added to file name. • Value range: YES = date and time is added to file name. For all other values date and times is not added to file name. • Format: Character string
	NrEntries=*NrEntries*	Number of component analyses recorded in the log file. • Value:1 up to 100 • Format: Integer

	Content	Definition
	Entry.i=*EntryKeyWord*	*i* Index of the *i*-th analysis date • Value range: 1 up to *NrEntries* • Format: Integer *EntryKeyWord* Key word which is assigned to the *i*-th analysis date. Format: Character string The following key words are supported: • !PRD: Sample description • !PRG: Product group • !PRN: Product • !DAT: Time of measurement • !SPP: Spectra path • !SPN: Spectra file name • !IDR: Identity test result Ident;ID_OK or Ident;ID_NOT_OK • !QAR: QUANT results ComponentName; QuantResultValue; QuantResultUnit; • !QAE: QUANT extended results ComponentName; QuantResultValue; QuantResultUnit; MahDistValue; MahDistThreshold MDIIndex • !QAO: QUANT outlier marker (chemometric alarm) Value=0 (no outlier) Value=1 (outlier) • !QAB: QUANT threshold value deviation marker (method range) Value=0 (OK) Value=-1 (below lower range limit) Value=1 (above upper range limit) • !XPM: Experiment file **Note:** If these entries are not available, the following standard values will be used: NrEntries=5 Entry.1=!DAT Entry.2=!PRN Entry.3=!PRD Entry.4=!IDR Entry.5=!QAE

Log.ini file in OPUS LAB

File Edit Format View Help

```
[GENERAL]
Separator=;
CSVFile=NO
DateFormat=%Y-%m-%d
TimeFormat=%H:%M:%S
UTC_Offset=YES
UTC_Offset_SEPARATED=NO

[PDFReport]
Print=YES
PDFAsStandardPrintout=NO
Comment.1=PDF Comment 1
Comment.2=PDF Comment 2
;----------------------------------
[Art]
IDENT.SINGLE.TEMPLATE = ReportIdent.ART
QUANT.SINGLE.TEMPLATE = ReportQuant.ART
SPECTRUM.SINGLE.TEMPLATE = ReportSpectrumOnly.ART
QUANT.MULTISAMPLE.TEMPLATE = ReportQuantMultiSample.ART
;----------------------------------


[OverallReport]
PrintHitList=YES
AddToHitListOnlyResultNotOK=NO
IndexProductInfoLineInSummery=-1
SingleReportIfResultNotOK=NO

[GenericLog]
NrEntries=6
Entry.1=!DAT
Entry.2=!PRG
Entry.3=!PRN
Entry.4=!SPP
Entry.5=!SPN
Entry.6=!XPM

[ProductLog]
NrEntries=5
Entry.1=!DAT
Entry.2=!PRN
Entry.3=!PRD
Entry.4=!IDR
Entry.5=!QAE

[InterfaceLog]
Active=NO
LogFilePath=c:\OpusLabInterface
LogFileName=OpusLab.csv
AddDateTimeToFileName=NO
NrEntries=5
Entry.1=!DAT
Entry.2=!PRN
Entry.3=!PRD
Entry.4=!IDR
Entry.5=!QAE
```

Figure 100: *Log.ini* file in OPUS LAB

6.1.2 General log file

This file is created if the *Active* check box in the *General Log File* group field has been activated on the *Log/report* tab in the *Product Setup* (see chapter 3.8).

	Definition
Format:	ASCII. The format of a line is defined in the *Initialization* file (see chapter 6.1.1).
Path:	*Applicationpath*\Log\Meas_*MM_YYYY.Extension* With: • *Applicationpath*: Directory in which OPUS LAB has been installed. • *MM*: Placeholder for the month • *YYYY*: Placeholder for the year • *Extension*: The standard extension is **.log*. If the *CSVFile* flag is set to YES in the log ini file, the file extension will be **.csv*.
Content:	Results of the OPUS LAB analysis. For each analysis a line is attached, including the current results.

6.1.3 Product-specific log file

The product-specific log file created by OPUS LAB provides:

- Threshold (for mahalanobis distance parameter)
- MD parameter (MD = mahalanobis distance)
- MDI parameter (MDI = MD/Threshold)

This file is created if the *Active* check box in the *Product log file* group field has been activated on the *Log/report* tab in the *Product Setup* (see chapter 3.8).

	Definition
Format:	ASCII. The format of a line is defined in the *Initialization* file (see chapter 6.1.1).

	Definition
Path:	*Applicationpath\Log\Productgroup\Product_MM _YYYY.Extension* With: • *Applicationpath*: Directory in which OPUS LAB has been installed. • *Productgroup:* Placeholder for the name of the product group • *Product:* Placeholder for the name of the product • *MM*: Placeholder for the month • *YYYY*: Placeholder for the year • *Extension*: The standard extension is **.log*. If the *CSVFile* flag is set to YES in the log ini file, the file extension will be **.csv.*
Content:	Results of the OPUS LAB analysis. For each analysis a line is attached, including the current results.

6.1.4 Interface file

A setting in the *Initialization* file (see chapter 6.1.1) defines whether this file is created.

	Definition
Format:	ASCII. The format of a line is defined in the *Initialization* file (see chapter 6.1.1).
Path:	The path and file name are defined in the *Initialization* file (see chapter 6.1.1).
Content:	Results of the OPUS LAB analyses. The file contains only one line, including the results of the last analysis performed.

6.1.5 PDF log files

In addition to a hardcopy print-out you can create a PDF file when printing evaluation results.

The settings in the [PDFReport] section of the log initialization file (see chapter 6.1.1) are mandatory when creating the PDF file.

6.1.5.1 Single sample QUANT results

	Definition
Path:	*Applicationpath\Log\Productgroup\Product_MM* With: • *Applicationpath*: Directory in which OPUS LAB has been installed. • *Productgroup:* Placeholder for the name of the product group • *Product:* Placeholder for the name of the product • *MM*: Placeholder for the month • *YYYY*: Placeholder for the year
File name:	*Quant_YYYYMMDD_HHNNSS.pdf* With: • *YYYY:* Placeholder for the year • *MM:* Placeholder for the month • *DD:* Placeholder for the day • *HH:* Placeholder for the hour • *NN:* Placeholder for the minute • *SS:* Placeholder for the second **Note:** The time indicated in the file name specifies the time at which the PDF file has been created and not the measurement time.
Content:	Same as hardcopy print-out. Optionally, you can add PDF-specific comments (see [PDFReport] chapter in 6.1.1)

6.1.5.2 Single sample IDENT results

	Definition
Path:	*Applicationpath\Log\Productgroup\Product_MM _YYYY* With: • *Applicationpath*: Directory in which OPUS LAB has been installed. • *Productgroup:* Placeholder for the name of the product group • *Product:* Placeholder for the name of the product • *MM*: Placeholder for the month • *YYYY*: Placeholder for the year
File name:	*Ident_YYYYMMDD_HHNNSS.pdf* With: • *YYYY:* Placeholder for the year • *MM:* Placeholder for the month • *DD:* Placeholder for the day • *HH:* Placeholder for the hour • *NN:* Placeholder for the minute • *SS:* Placeholder for the second **Note:** The time indicated in the file name specifies the time at which the PDF file has been created and not the measurement time.
Content:	Same as hardcopy print-out. Optionally, you can add PDF-specific comments (see [PDFReport] chapter in 6.1.1)

6.1.5.3 Overall reports QUANT results

	Definition
Path:	*Applicationpath\Log\OverallReports_MM _YYYY* With: • *Applicationpath*: Directory in which OPUS LAB has been installed. • *MM*: Placeholder for the month • *YYYY*: Placeholder for the year

	Definition
File name:	*Quant_YYYYMMDD_HHNNSS.pdf* With: • *YYYY:* Placeholder for the year • *MM:* Placeholder for the month • *DD:* Placeholder for the day • *HH:* Placeholder for the hour • *NN:* Placeholder for the minute • *SS:* Placeholder for the second **Note:** The time indicated in the file name specifies the time at which the PDF file has been created and not the measurement time.
Content:	Same as hardcopy print-out. Optionally, you can add PDF-specific comments (see [PDFReport] chapter in 6.1.1)

6.1.5.4 Overall reports IDENT results

	Definition
Path:	*Applicationpath\Log\OverallReports_MM _YYYY* With: • *Applicationpath*: Directory in which OPUS LAB has been installed. • *MM*: Placeholder for the month • *YYYY*: Placeholder for the year
File name:	*Ident_YYYYMMDD_HHNNSS.pdf* With: • *YYYY:* Placeholder for the year • *MM:* Placeholder for the month • *DD:* Placeholder for the day • *HH:* Placeholder for the hour • *NN:* Placeholder for the minute • *SS:* Placeholder for the second **Note:** The time indicated in the file name specifies the time at which the PDF file has been created and not the measurement time.
Content:	Same as hardcopy print-out. Optionally, you can add PDF-specific comments (see [PDFReport] chapter in 6.1.1)

7 Measuring and evaluating FTIR spectra on microtiter plate

7.1 Preparing OPUS LAB for HTS-XT measurements

During the OPUS installation procedure select the *Custom* mode and activate the *HTS-XT* check box when selecting the instrument configuration. Follow the on-screen installation instructions.

If OPUS has already been installed and subsequently needs to be configured, the module has to be activated using the general parameters (chapter 2.8).

To control the *Twister* microtiter stack device directly from OPUS LAB the *Twister* and spectrometer have to be connected to the respective communication port (e.g. COM1).

7.1.1 Initialization file entries

The settings for measurements using the HTS-XT spectrometer have to be defined in the *OPUSLab.ini* file. This file is stored in the *Applicationpath\Data\OpusLab.ini* path. *Applicationpath* is the directory in which OPUS LAB has been installed.

Double click the file to open it directly from the Windows Explorer. The [EXTERNAL_ACC] section has to include the following entries:

```
[EXTERNAL_ACC]
ACTIVE=YES
ITYPE=HTS-XT
PATH=HTS-XT
FILE=HTS-XT.ini
```

7.1.2 Defining reference position

Define the individual HTS-XT reference position in the *HTS-XT.ini* file. Data path: *Applicationpath\HTS-XT*.

[GENERAL]
NAME=HTS-XT
REF_POS96_X_MOT_STEPS=*Number of motor steps in x-direction for pos. A1*
REF_POS96_Y_MOT_STEPS=*Number of motor steps in y-direction for pos. A1*
USE_OPUS_STAGECONTROL=NO
OPUS_STAGE_MICRONS_PER_MOTORSTEP=7.2
OPUS_STAGE_TYPE=1stephtsxt
USE_OPUS_STAGE_RAMAN_96_POS=NO

Note: To be able to access the HTS-XT by the Lang controller you have to set the *USE_OPUS_STAGECONTROL* variable to *YES*.

All the other settings can be directly defined on the OPUS LAB software interface. When storing these settings they will automatically be imported into the *OPUSLab.ini* or *HTS.ini* file.

7.1.3 Log initialization file entries

OPUS LAB also allows to create a so-called log file. This log file enables to report measurement parameters and evaluation results, and to import them into simple external worksheet programs. The *Log.ini* initialization file (data path: *Applicationpath\HTS-XT*) defines which one of the parameters available will be saved (see chapter 6.1).

Each OPUS LAB measurement is reported within the general log file, regardless of the product selected. Whereas the product-specific log file only reports OPUS LAB measurements which belong to a specific product.

In case of HTS-XT measurements it is possible to create a plate-specific log file, i.e. for each microtiter plate measured a separate text file will be created. This text file includes different kinds of information on each measurement position.

The plate-specific log file is stored by the *PlateDescription_ MeasurementDateTime* file name in the *Applicationpath\Log\Plates* path. This plate-specific log file can include the following parameters:

Parameter	Log file key word
Sample description	!PRD
Product group	!PRG
Product	!PRN
Time of measurement	!DAT
Spectra path	!SPP
Spectra file name	!SPN
Identity test result	!IDR
QUANT results	!QAR
QUANT outlier	!QAO
QUANT threshold deviation	!QAB
Spectra quality test result	!SQT
Experiment file	!XPM

Note: If the above mentioned entries are not available, the following standard values will be used:

Parameter for plate-specific log file
[PlateLog]
NrEntries=6
Entry.1=!DAT
Entry.2=!PRG
Entry.3=!PRN
Entry.4=!SPP
Entry.5=!SPN
Entry.6=!XPM

7.2 HTS-XT configuration

Product-specific settings, e.g. the measurement experiment to be used, evaluation methods desired as well as data storage are defined and stored in the *Product Setup* (see chapter 3).

Use the *HTS-XT* tab to define settings which specify the HTS-XT microtiter plate module.

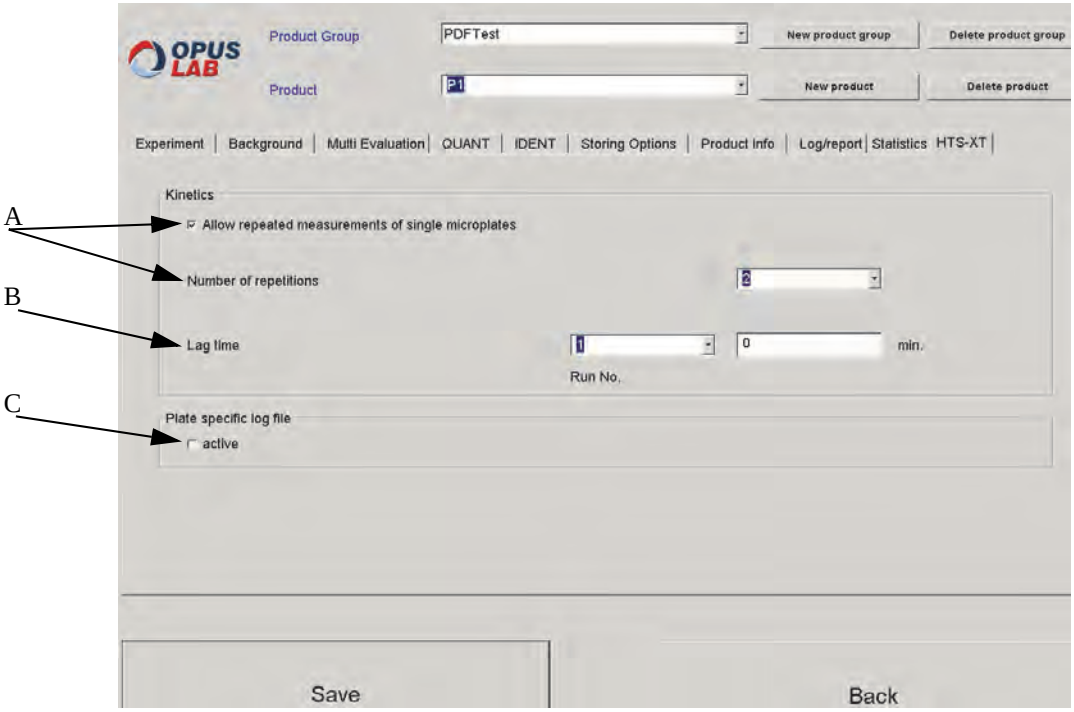


Figure 101: OPUS LAB Product Setup - HTS-XT

A) If you want to repeatedly measure one single microtiter plate, e.g. to measure kinetics, activate the check box. Use the *Number of repetitions* drop-down list to define the number of repeated measurements for this particular plate.

B) This drop-down list allows to set the delay before measurement after each measurement repetition, i.e. the measurement of all sample positions defined on the microtiter plate.

   It is possible, e.g. to measure a plate three times without any interruption, and define a 30-minutes' delay before the forth run and a 1-hour's delay before the fifth run.

C) If you activate the check box, an individual log file will be created for each microtiter plate measured. All measurement parameters and evaluation results defined in the *log.ini* initialization file will be imported into this log file (see chapter 3.8).

7.2.1 Calibrating *Twister* (a stacker for microtiter plates)

To be able to automatically measure several microtiter plates the *Twister* stacker can be coupled to the HTS-XT module.

This *Twister* stacker has to be calibrated before the initial operation. The calibration can be performed in OPUS by the *Twister Control/Calibration* command on the *Measure* menu. More detailed information is described in the OPUS Reference Manual.

7.3 HTS-XT measurements

1) On the *Measure* menu, select the *OPUS LAB* command.
2) Click the *Measurements* button. The *Measurement* dialog opens (figure 35 on page 53).
3) Click the *HTS-XT* button. Another dialog opens (figure 102).
4) Define the settings described in the following.

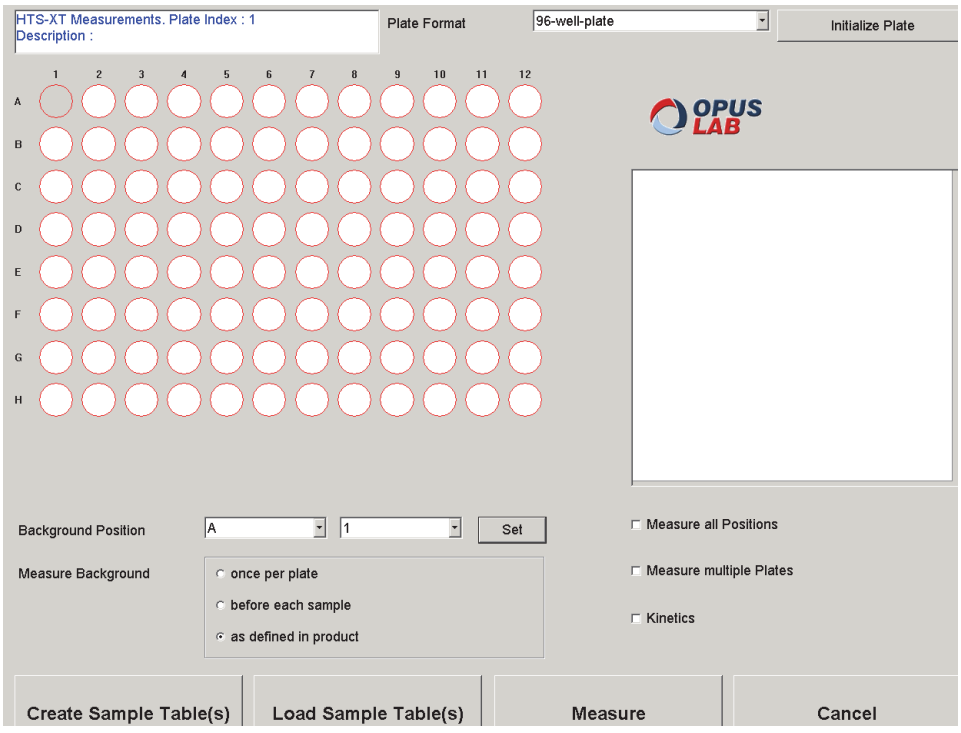


Figure 102: Define microtiter format and measurement positions

7.3.1 Selecting the microtiter format and setting measurement positions

1) Select the microtiter format to be measured (48, 96, 384 or 1,536 positions) from the *Plate format* drop-down list.

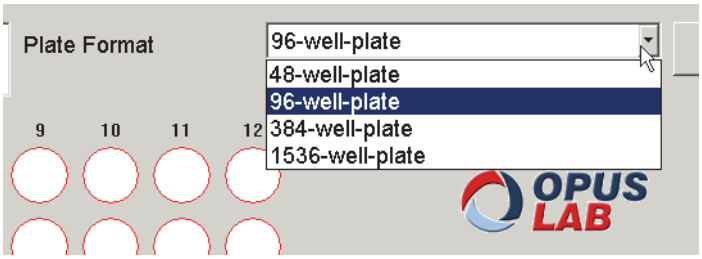


Figure 103: Selecting microtiter format

2) Set the position specified for the background measurement.

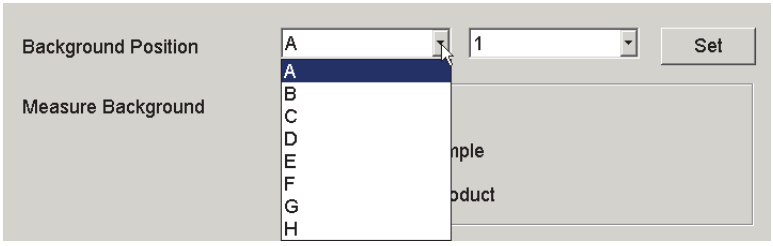


Figure 104: Setting background position

Click the *Set* button.

Note: The background position can be set on any microtiter plate position. Once set, the background position cannot be used for a sample measurement any more.

3) Specify when the background is to be measured.

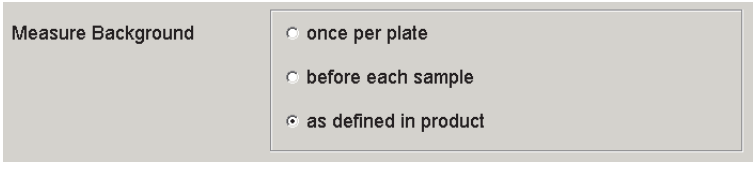


Figure 105: Setting time of background measurement

Activate the respective option button.

4) Select the sample positions directly on the microtiter plate display by a left mouse click. The positions selected are displayed in yellow.

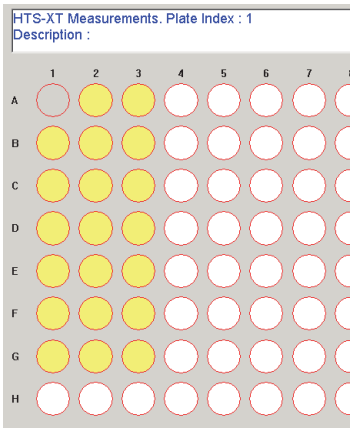


Figure 106: Selecting sample positions

To select several positions separately press the <*CTRL*> key. If you want to select an entire plate section, move the cursor to the initial position. Then, press the <*CTRL*> and <*SHIFT*> key and click the corresponding end position.

Activate the *Measure all positions* check box to select the entire microtiter plate.

To reset the plate positions selected click the *Initialize plate* button .

7.3.2 Measuring several microtiter plates

If you connect the *HTS-XT* to the *Twister* microtiter stack device, you can repeatedly measure several microtiter plates. The parameters for the *Twister* are defined using the *Twister Control/Calibration* command from the OPUS *Measure* menu. Detailed information is provided in the OPUS Reference Manual.

1) Activate the *Measure multiple plates* check box.
2) Select the number of plates from the drop-down list.

Figure 107: Measuring several plates

7.3.3 Repeating measurement

You can measure a particular microtiter plate several times. Activate the *Kinetics* check box.

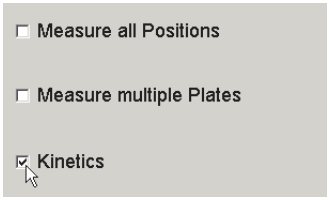


Figure 108: Repeating measurement

The *Kinetics* parameters are defined in the *Product Setup* (see *HTS-XT* tab in chapter 7.2).

7.3.4 Loading existing sample tables

Instead of a completely new setting of the microtiter plate positions (chapter 7.3.1), you can load a sample table which has been previously created and stored.

1) Click the *Load sample table(s)* button.

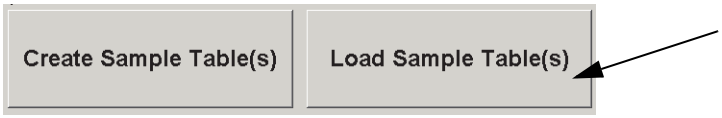


Figure 109: Loading sample table

2) Select the sample table from the dialog that opens. Sample tables have the file extension **.ini*.

7.3.5 Creating sample table

If you click the *Create sample table(s)* button, your settings made will be imported into a sample table (see figure 110).

7.3.6 Sample table

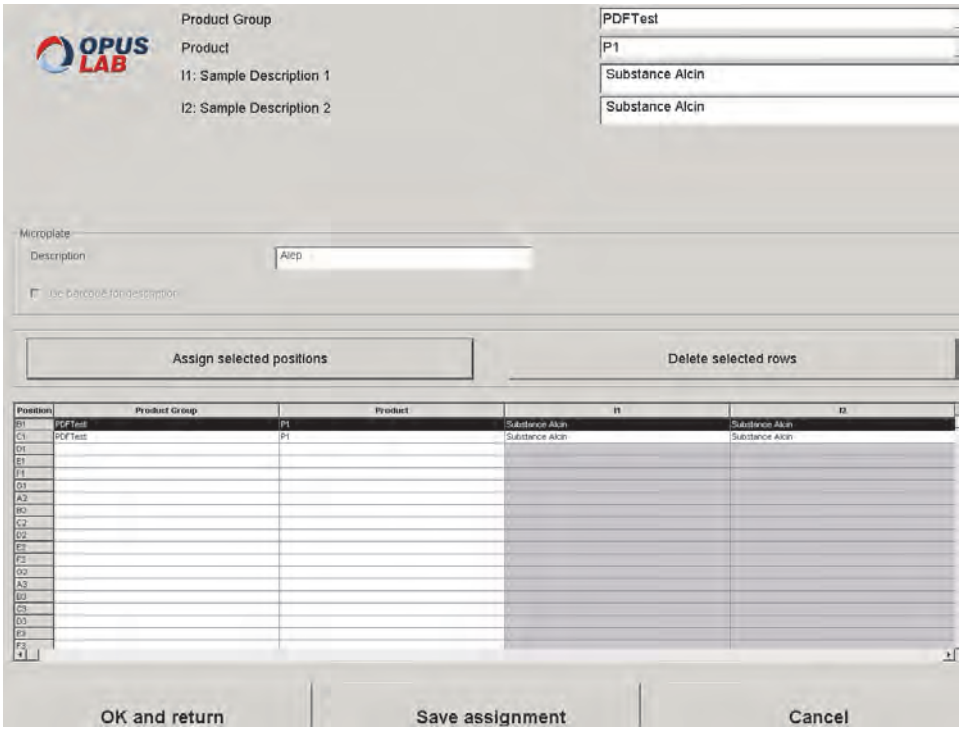


Figure 110: Assignment table

Each position on the table must contain an entry which describes the product to be measured on this position. This is important as the measurement experiment used defines the evaluation method and type of data storage (see those settings specified in the *Product Setup*).

7.3.6.1 Assigning positions

1) Select the desired product and product group from the drop-down lists.
2) Enter possible descriptions into the *Sample description 1* and *Sample description 2* text fields.
3) Each microtiter plate needs to have a title. Enter this title into the *Description* entry field on the *Microplate* group field. If you measure several plates, the total number of measurements is indicated next to the *Description* field on the right.
4) Select the respective lines of the sample table for which the entry has to be created.
5) Click the *Assign selected positions* button.
6) Click the *Save assignment* and then the *OK and return* button. The microtiter plate will be displayed again. The positions selected and assigned by a product will now be orange. Positions selected which are not assigned to any product will still be yellow.

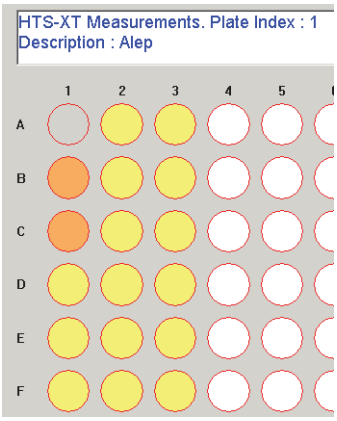


Figure 111: Assigned positions

The yellow positions cannot be measured as no product, i.e. no measurement experiment, has been defined.

If you place the cursor on any position, the assignment is indicated in the text field next to the microtiter plate.

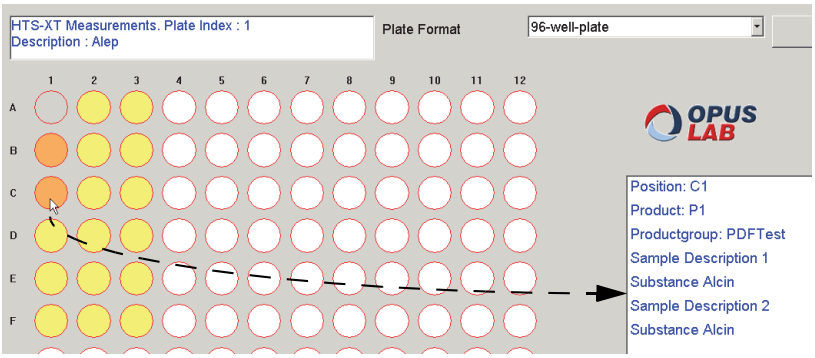


Figure 112: Position with defined assignment

7.3.7 Measuring plate

1) Click the *Measure* button.

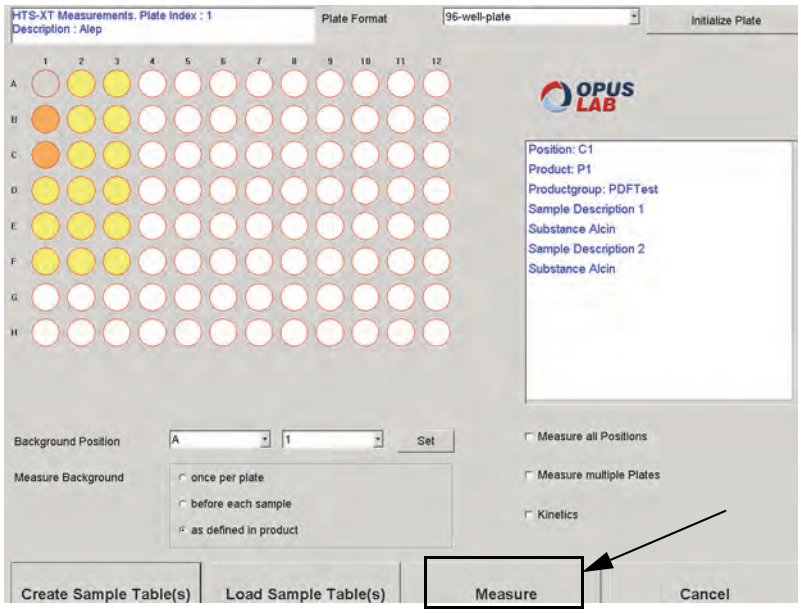


Figure 113: Position with defined assignment

Another dialog is shown.

2) Position the microtiter plate into the HTS-XT sample compartment.
3) Click the *Check Signal* button.

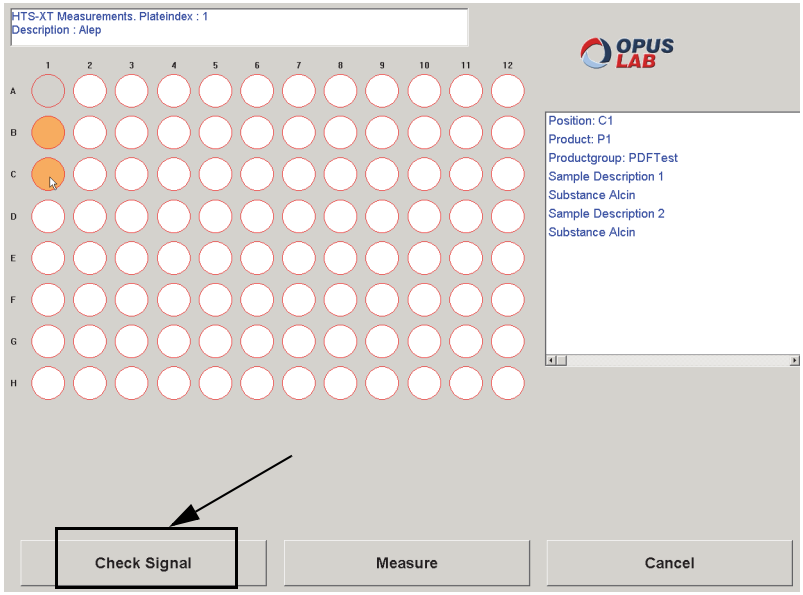


Figure 114: Measure dialog

The measuring signal on the microtiter plate is checked. Measurement starts on the *A1* position of the plate, using the current measurement experiment. During this measurement the signal intensity and peak posi-

tion of the interferogram will be diagnosed. If these features reveal to be all right, you will get the *OK* to start measurement. If problems arise, a warning will indicate the error.

4) Click the *Measure* button. The positions to be measured are displayed in orange.

   If you click the *Measure* button after the measurement has started, the positions already measured change their color. They turn to green or red, depending on whether the spectra quality test results have been positive or negative.

   The status bar below the microtiter plate always shows the current measurement position.

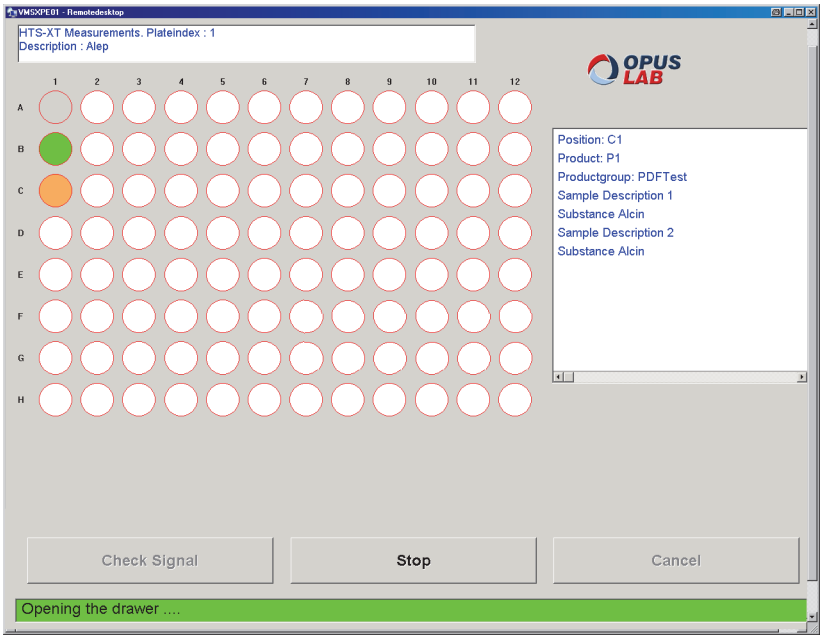


Figure 115: Current measurement display

Evaluation results obtained by IDENT and QUANT methods can be displayed during or after measurement. If you have made the settings required for IDENT and QUANT in the product setup, the dialog in figure 115 shows the respective buttons to have the evaluation result displayed. Click the *Show IDENT results* or *Show QUANT results* buttons.

The screen shows the corresponding evaluation results of one microtiter plate position. You can switch between each position using the scrollbar. The current position is shown in the *Sample description 1* field. You can get an overview of all measurement results by clicking the *Show overall report* button.

8 Measuring and evaluating Raman spectra on microtiter plate

8.1 Preparing OPUS LAB for HTS-R measurements

During the installation procedure select the *Custom* mode and activate the *HTS-R* check box when selecting the instrument configuration. Follow the on-screen installation instructions.

If OPUS has already been installed and subsequently needs to be configured, the module has to be activated using the general parameters (chapter 2.8).

8.1.1 Initialization file entries

The settings for measurements using the HTS-R spectrometer have to be defined in the *OPUSLab.ini* file. This file is stored in the *Applicationpath\Data\OpusLab.ini* path. *Applicationpath* is the directory in which OPUS LAB has been installed.

Double click the file to open it directly from the Windows Explorer. The [EXTERNAL_ACC] section has to include the following entries:

```
[EXTERNAL_ACC]
ACTIVE=YES
ITYPE=HTS-R
PATH=HTS-R
FILE=HTS-R.ini
```

8.1.2 Defining reference position

Define the individual HTS-R reference position in the *HTS-R.ini* file. Data path: *Applicationpath\HTS-R*.

[GENERAL]
NAME=HTS-R
REF_POS49_X_MOT_STEPS=*Number of motor steps in x-direction for pos. A1*
REF_POS49_Y_MOT_STEPS=*Number of motor steps in y-direction for pos. A1*

All the other settings can be directly defined on the OPUS LAB interface. When storing these settings they will automatically be imported into the *OPUSLab.ini* or *HTS-R.ini* file.

8.1.3 Log initialization file entries

OPUS LAB also allows to create a so-called log file. This log file enables to report measurement parameters and evaluation results, and to import them into simple external worksheet programs. The *Log.ini* initialization file (data path: *Applicationpath\HTS-R*) defines which one of the parameters available will be saved (see chapter 6.1).

Each OPUS LAB measurement is reported within the general log file, regardless of the product selected. Whereas the product-specific log file only reports OPUS LAB measurements which belong to a specific product.

In case of HTS-R measurements it is possible to create a plate-specific log file, i.e. for each microtiter plate measured a separate text file will be created. This text file includes different kinds of information on each measurement position.

The plate-specific log file is stored by the *PlateDescription_Measurement-DateTime* file name in the *Applicationpath\Log\Plates* path. This plate-specific log file can include the following parameters:

Parameter	**Log file key word**
Sample description	!PRD
Product group	!PRG
Product	!PRN
Time of measurement	!DAT
Spectra path	!SPP
Spectra file name	!SPN

Parameter	Log file key word
Identity test result	!IDR
QUANT results	!QAR
QUANT outlier	!QAO
QUANT threshold deviation	!QAB
Spectra quality test result	!SQT
Experiment file	!XPM

Note: If the above mentioned entries are not available, the following standard values will be used:

Parameter for plate-specific log file
[PlateLog]
NrEntries=6
Entry.1=!DAT
Entry.2=!PRG
Entry.3=!PRN
Entry.4=!SPP
Entry.5=!SPN
Entry.6=!XPM

8.2 HTS-R configuration

Product-specific settings, e.g. the measurement experiment to be used, evaluation methods desired as well as data storage are defined and stored in the *Product Setup* (see chapter 3).

Use the *HTS-R* tab to define settings which specify the HTS-R microtiter plate module.

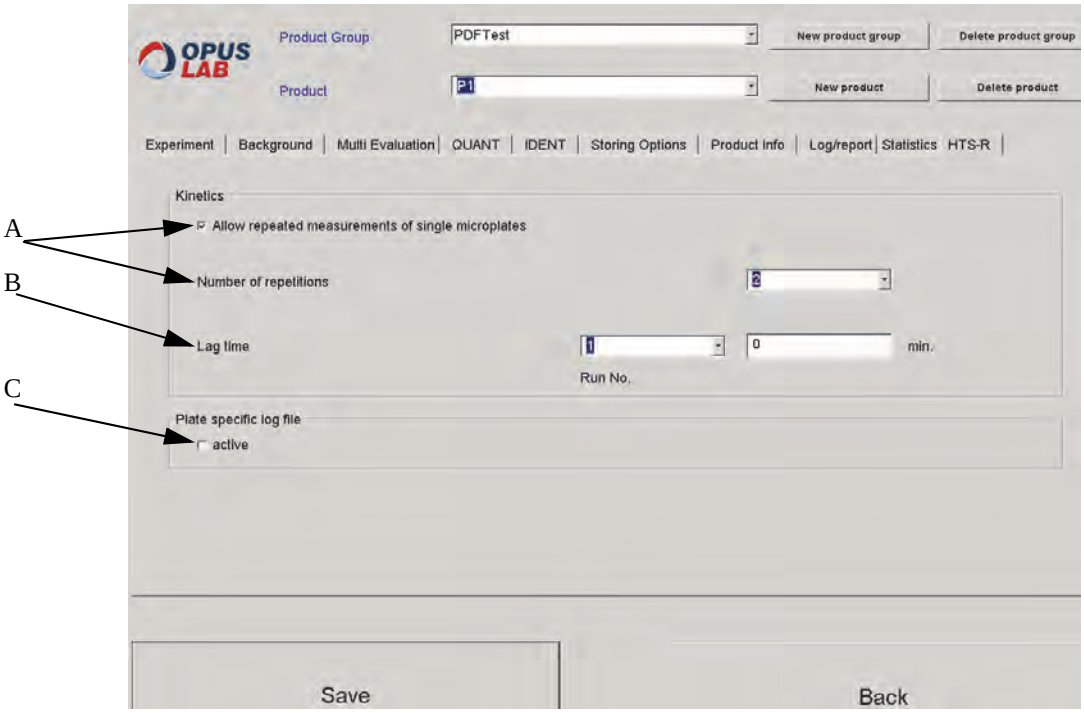


Figure 116: OPUS LAB Product Setup - HTS-R settings

A) If you want to repeatedly measure one single microtiter plate, e.g. to measure kinetics, activate the check box. Use the *Number of repetitions* selection box to define the number of repeated measurements for this particular plate.

B) This drop-down list allows to set the delay before measurement after each measurement repetition, i.e. the measurement of all sample positions defined on the microtiter plate.

   It is possible, e.g. to measure a plate three times without any interruption, and define a 30-minute's-delay before the forth run and a 1-hour's-delay before the fifth run.

C) If you activate the check box, an individual log file will be created for each microtiter plate measured. All measurement parameters and evaluation results defined in the *log.ini* initialization file will be imported into this log file (see chapter 3.8).

8.3 HTS-R measurements

1) On the *Measure* menu, select the *OPUS LAB* command.
2) Click the *Measurements* button. The *Measuring method selection* dialog opens (figure 35 on page 53).
3) Click the *HTS-R* button. Another dialog opens (figure 117)
4) Define the settings described in the following.

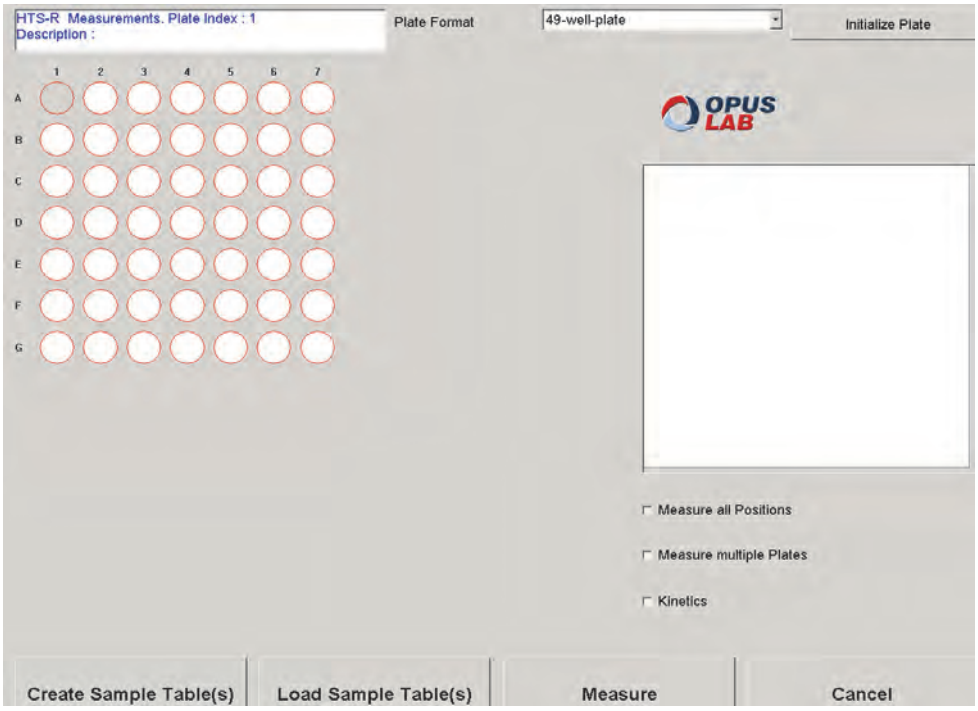


Figure 117: Define microtiter format and measurement positions

8.3.1 Selecting the microtiter format and setting measurement positions

1) Select the microtiter format to be measured (49 positions) from the *Plate format* drop-down list.

Figure 118: Selecting microtiter format

2) Select the sample position directly on the microtiter plate display by a left mouse click. The positions selected are displayed in yellow.

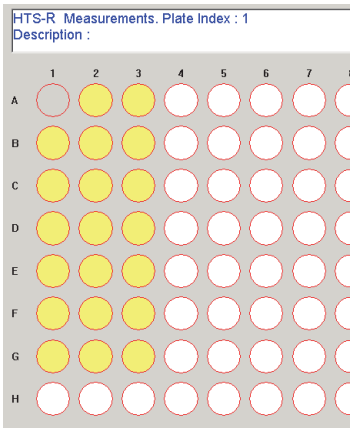
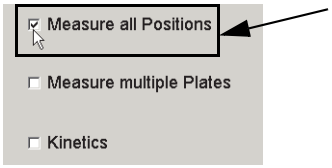


Figure 119: Selecting sample positions

To select several positions separately press the <*CTRL*> key. If you want to select an entire plate section, move the cursor to the initial position. Then, press the <*CTRL*> and <*SHIFT*> key and click the corresponding end position.

Activate the *Measure all positions* check box to select the entire microtiter plate.



To reset the plate positions selected click the *Initialize plate* button.

8.3.2 Repeating measurement

You can measure a microtiter plate several times. Activate the *Kinetics* check box.

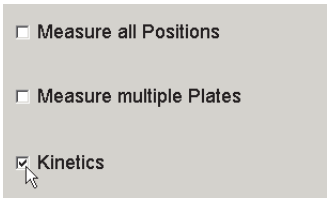


Figure 120: Repeating measurement

The *Kinetics* parameters are defined in the *Product Setup* (see *HTS-R* tab in figure 116).

8.3.3 Loading existing sample tables

Instead of a completely new setting of the microtiter plate positions, you can also load an assignment table which has been previously created and stored.

1) Click the *Load sample table(s)* button.

Figure 121: Loading sample table

2) Select the sample table from the dialog that opens. Sample tables have the file extension **.ini*.

8.3.4 Creating sample tables

If you click the *Create sample table(s)* button, your settings made will be imported into an assignment table (see figure 122).

8.3.5 Assignment table

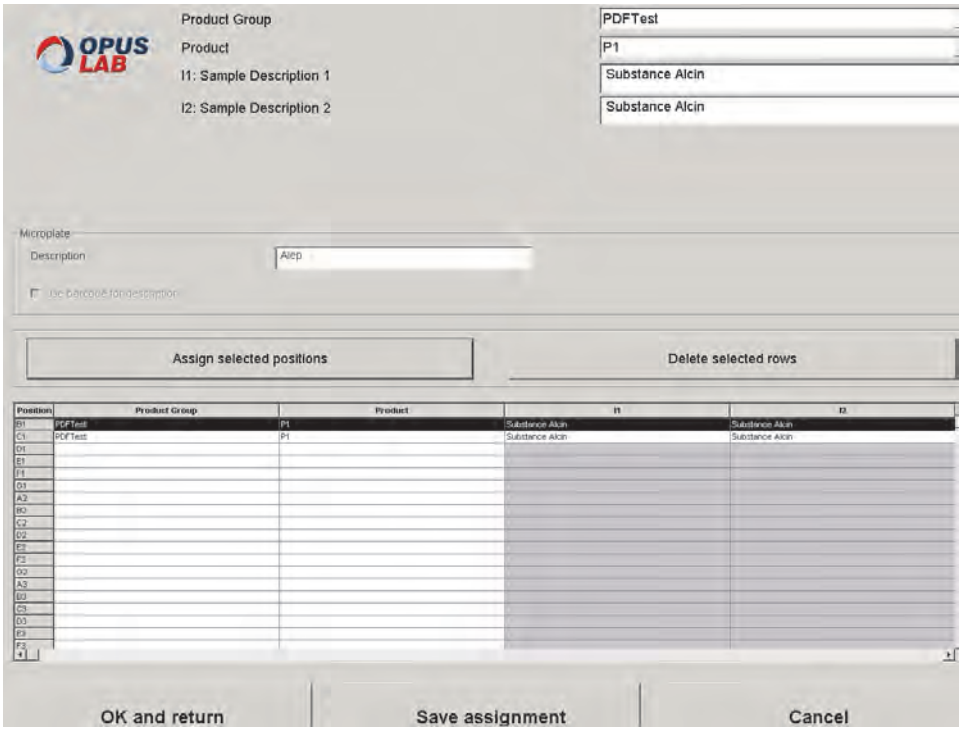


Figure 122: Assignment table

Each position on the table must contain an entry which describes the product to be measured on this position. This is important as the measurement experiment used defines the evaluation method and type of data storage (see those settings specified in the *Product Setup*).

8.3.5.1 Assigning positions

1) Select the desired product and product group from the drop-down lists.
2) Enter possible descriptions into the *Sample description 1* and *Sample description 2* text fields.
3) Each microtiter plate needs to have a title. Enter this title into the *Description* entry field on the *Microplate* group field. If you measure several plates, the total number of measurements is indicated next to the *Description* field on the right.
4) Select the respective lines of the sample table for which the entry has to be created.
5) Click the *Assign selected positions* button.
6) Click the *Save assignment* and then the *OK and return* button. The microtiter plate will be displayed again. The positions selected and assigned by a product will now be orange. Positions selected which are not assigned to any product will still be yellow.

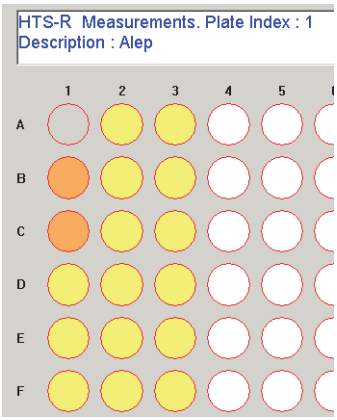


Figure 123: Assigned positions

The yellow positions cannot be measured as no product, i.e. no measurement experiment, has been defined.

If you place the cursor on any position, the assignment will be indicated in the text field next to the microtiter plate.

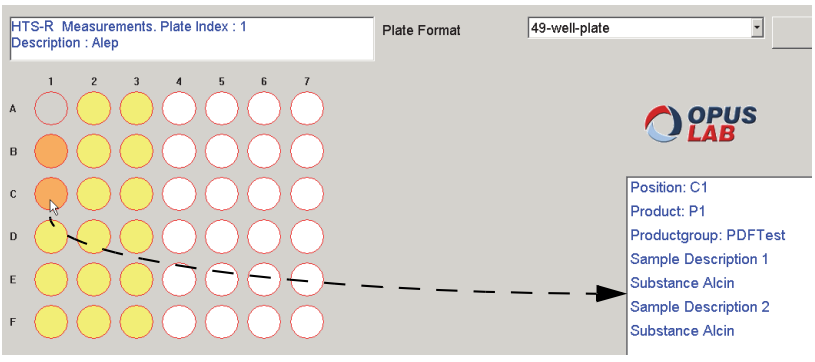


Figure 124: Position with defined assignment

8.3.6 Measuring plate

1) Click the *Measure* button

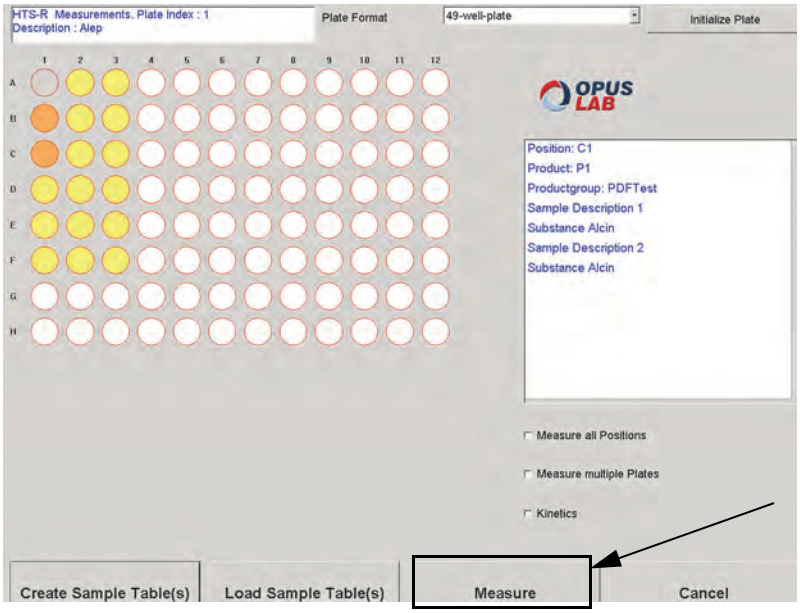


Figure 125: Positions with defined assignment

Another dialog is shown.

2) Position the microtiter plate into the HTS-XT sample compartment.
3) Click the *Check Signal* button.

   The measuring signal on the microtiter plate is checked. Measurement starts on the *A1* position of the plate, using the current measurement experiment. During this measurement the signal intensity and peak position of the interferogram will be diagnosed. If these features reveal to be all right, you will get the *OK* to start measurement. If problems arise, a warning will indicate the error.
4) Click the *Measure* button. The positions to be measured are displayed in orange.

   If you click the *Measure* button after the measurement has started, the positions already measured change their color. They turn to green or red, depending on whether the spectra quality test results have been positive or negative.

   The status bar below the microtiter plate always shows the current measurement position.

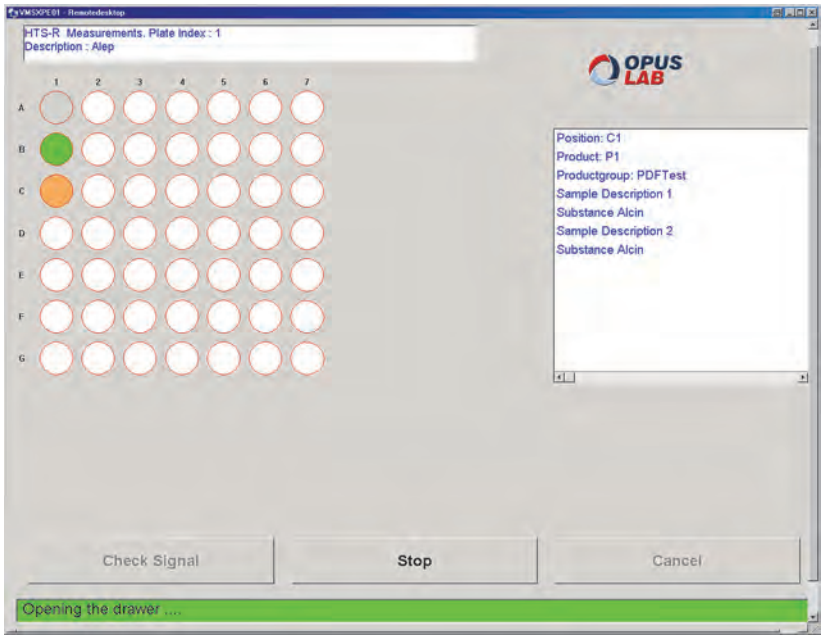


Figure 126: Current measurement display

Evaluation results obtained by IDENT and QUANT methods can be displayed during or after measurement. If you have made the settings required for IDENT and QUANT in the product setup, the dialog in figure 126 shows the respective buttons to have the evaluation result displayed. Click the *Show IDENT results* or *Show QUANT results* buttons.

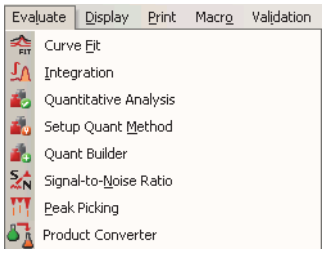
The screen shows the corresponding evaluation results of one microtiter plate position. You can switch between each position using the scrollbar. The current position is shown in the *Sample description 1* field. You can get an overview of all measurement results by clicking the *Show overall report* button.

9 Product Converter

The product converter, a feature implemented in OPUS 7 version, allows to convert single OPUS/LAB products generated in OPUS 7 or earlier versions, into the XML[1] and OPX[2] format.

There is also the possibility to copy the converted OPUS/LAB products to a different directory or external data storage medium (e.g. USB stick). The product converter is part of the OPUS *Manipulate* menu.

9.1 Starting product converter



Step 1:
- Switch to the OPUS interface.
- On the *Evaluate* menu, select the *OPUSLAB Product Converter* command.

➢The product converter opens.

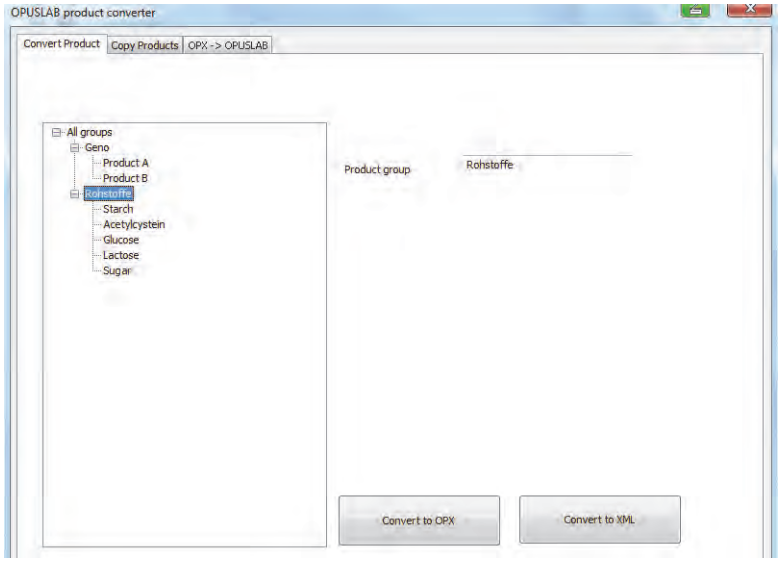


Figure 127: Product Converter

1. The XML file contains the product information.
2. The OPX file contains the product information and the binary file for the method.

9.2 Product converter view

The product converter consists of two tabs which allow to convert and copy products. You can convert either single products or all products belonging to one particular product group.

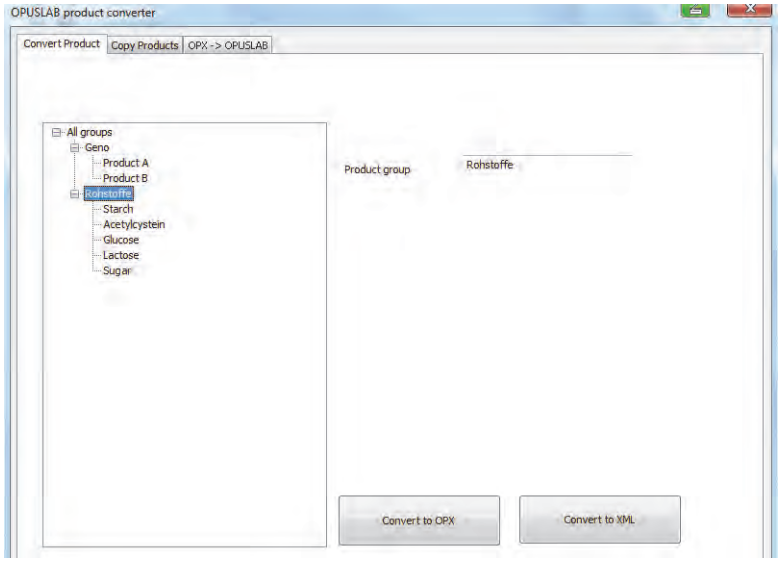


Figure 128: Product Converter - Convert Product tab

The list box on the left side of the *Convert Product* tab contains all product groups with their corresponding products available in OPUS/LAB.

The *Copy Products* tab allows to copy products, which have already been converted, to different directories or data storage mediums.

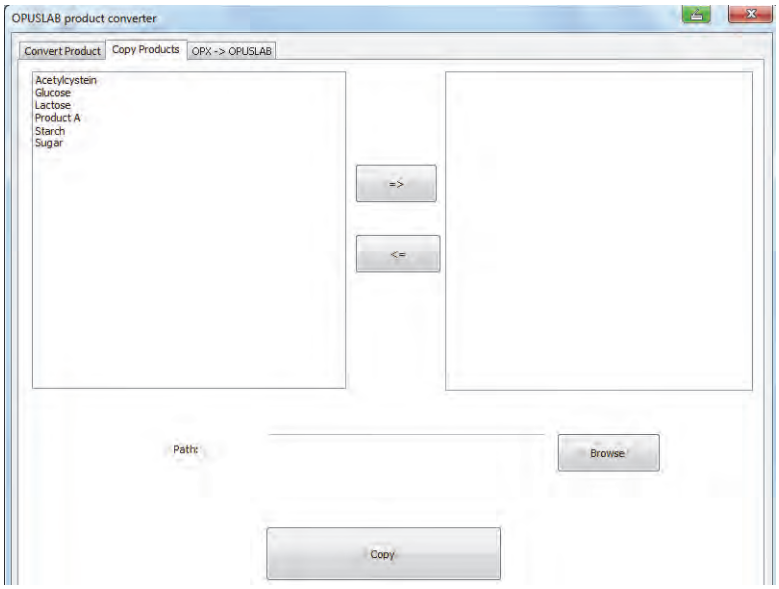


Figure 129: Product Converter - Copy Products tab

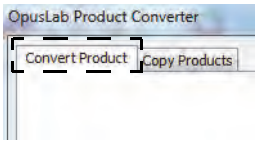
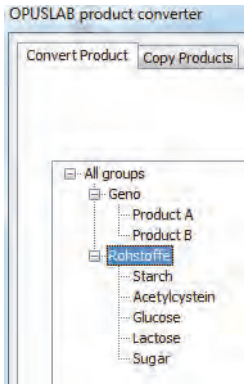
The list box on the left side of the *Copy Products* tab contains all the products converted.

9.3 Converting product

Basically, you can convert all OPUS/LAB products which have been generated in OPUS 7 or lower. There may be exceptional cases in which a conversion is aborted. This may be due to the fact that:

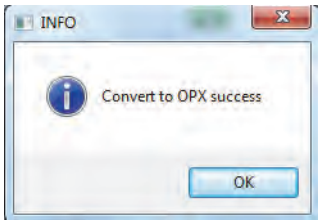
- in case of the IDENT analysis the hit list result option was activated[1]
- based on the *OpusLab* main directory, method files (e.g. XPM, Q2, FAA etc.) of the product to be converted are not available in the respective sub-directories
- an alias is assigned to a variable which is part of a multi evaluation method created by OPUS 7 or >7
- the multi evaluation method was created by using OPUS/STATISTICS and has the file extension **.me*

9.3.1 Converting into OPX format

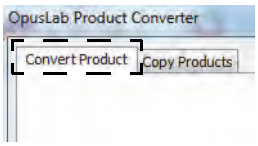
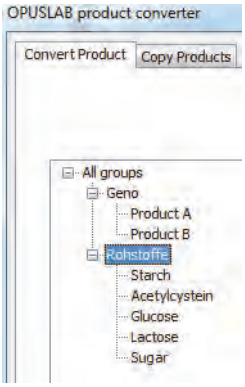
	**Step 1:** Select the *Convert Product* tab.
	**Step 2:** From the list box, select the product of the particular product group. **Note:** You can either select a single product or all products belonging to the product group. ➢The name of the particular product group is shown in the *Product Group* box on the right side.
	**Step 3:** Click the *Convert to OPX* button.

1. With this kind of setting made in the product setup of OPUS/LAB more than one IDENT method may have been used to perform IDENT analysis. When converting, only one IDENT method can be taken into account.

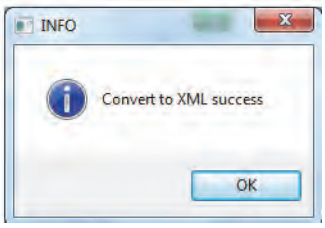
If the conversion has been successful, the following message is displayed:



9.3.2 Converting into XML format

	**Step 1:** Select the *Convert Product* tab.
	**Step 2:** From the list box, select the product of the particular product group. **Note:** You can either select a single product or all products belonging to the product group. ➢The name of the particular product group is shown in the *Product Group* box on the right side.
	**Step 3:** Click the *Convert to XML* button.

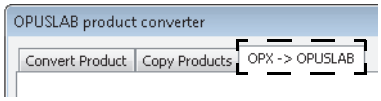
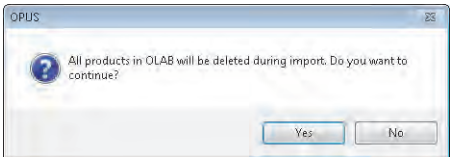
If the conversion has been successful, the following message is displayed:



9.3.3 Importing OPX products into OPUS LAB

Note: In case of this option, products with the **.opx* file extension are converted into files required by OPUS LAB. These files are saved in the particular sub-directories of *OPUS\OPUS LAB*. All the files which have already been available in the *OPUS\OPUSLab\DATA* directory will be deleted.

Before starting the import, save all the files already available in the *OPUS\OPUSLab\DATA* directory into a different directory to be able to copy these files into the *OPUS\OPUSLab\DATA* directory again after the import has finished.

	**Step 1:** Select the *OPX -> OPUSLAB* tab.
	**Step 2:** Click the *Browse* button and select the product path.
	**Step 3:** Click the *Import* button.
	**Step 4:** Confirm the message displayed if you have saved the existing OPUS LAB files into a different directory.

9.3.4 Directory structure of converted products in Windows explorer

If the conversion of products has finished, the *C:\ProgramFiles\OPUS\PRODUCTS* directory is generated. This directory contains all converted products. Below each product name the following sub-directories are created:

<Product name>
\Ident
\ME
\Quant

During conversion all methods used with the respective product are copied from the original *OpusLab* directory to the new directory structure.

The *<\ME* sub-folder may contain methods with different types of file extensions. Methods with the **.me* file extension have been created by OPUS/LAB <7, methods with the **.mev* file extension by OPUS/LAB 7 or >7.

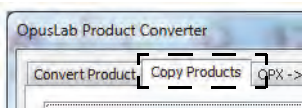
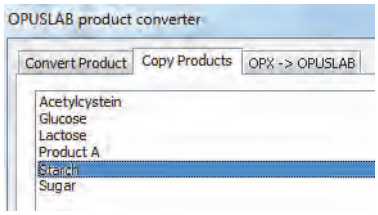
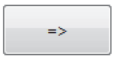
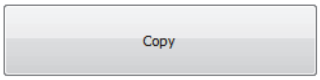
If the product has been converted, the corresponding OPUS/LAB method is stored in the *<\ME* sub-folder with the additional *_fromOLAB* term and the **.mev* file extension.

Example: *<Method name>_fromOLab.mev*

The converted files for the product with the **.opx*, **.xml* or **.xpm* file extension are stored in the *<\ME_Base* sub-directory.

9.4 Copying product

To copy products to a different directory or an external data storage medium (e.g. USB stick), the products must have been already converted.

	**Step 1:** Select the *Copy Products* tab.
	**Step 2:** From the left list box, select the product converted. ➢ The product is now highlighted.
	**Step 3:** Click the arrow button. ➢ The name of the product is now displayed in the right list box.
	**Step 4:** Enter the path of the directory or external data storage medium into the entry field. Alternatively, click the *Browse* button and select the correct path.
	**Step 5:** Click the *Copy* button.

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