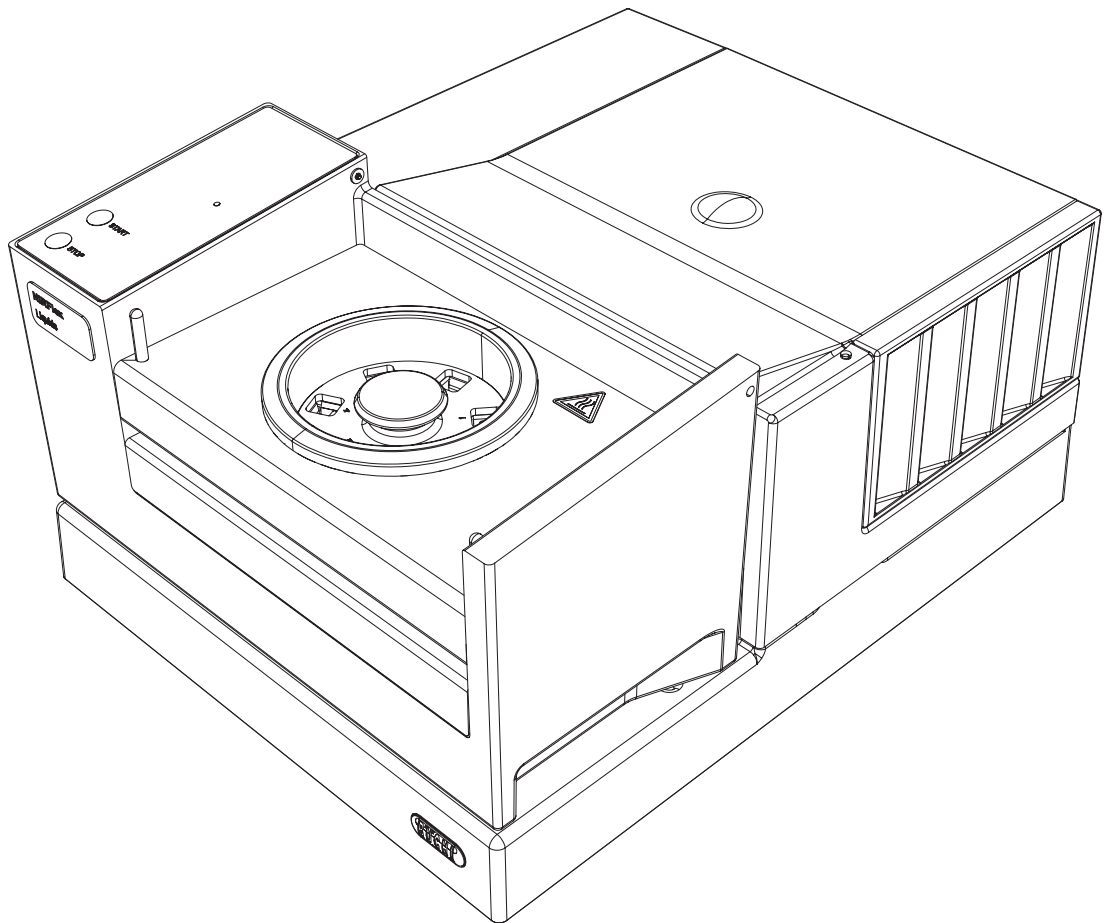




NIRWare 1.5

Operation Manual



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BUCHI reserves the right to make changes to the manual as deemed necessary in the interest of experience; especially in respect to structure, illustrations and technical depth.

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1. Welcome

Dear customer,

Thank you for choosing the BUCHI NIRFlex N-500 FT-NIR spectrometer with the NIRWare Software Suite. We are sure that it will be a valuable tool for solving your analytical requirements.

NIRWare has been developed to design your complete NIR applications, to manage your samples (spectra and reference values) and to customize the user interface for routine work. In addition it includes all necessary tools for administration including import and export of calibrations and applications, security and lifecycle settings.

The NIRWare Library Designer is an optional software module for identity control using direct spectral comparison methods.

NIRWare does not include a module for calibration development. This is done using the new version of the well-known and proven NIRCal 5 Chemometric Software. NIRCal and NIRWare are closely linked and both use the identical database. The interaction between both is described in detail throughout this manual.

BUCHI has made every effort to ensure the accuracy of the information given in this manual. We would appreciate very much to be informed as soon as you may detect any mistake or omission.

BUCHI is going to improve its products and documentations continuously. Therefore the information in this document will be subject to change without notice. It does not represent a commitment on the part of BUCHI.

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Should you come across any feature (important or minor), which needs improvement or extension, please do not hesitate to contact us. Your feedback helps us to continuously improve our software and is highly appreciated.

We are convinced that your new NIR system will be very helpful and beneficial for your daily work.

Flawil, March 2013

Warning notices used in this Online Help



ATTENTION

With the general "Read this" symbol, ATTENTIONs indicate the possibility of equipment damage, malfunctions or incorrect process results, if instructions are not followed.

NOTE

Useful tips for an easy operation of the software.




2. Introduction

NIR spectroscopy covers a wide variety of applications, which in turn place diverse demands on operation and calibration. Especially the software of the NIR system must take this point into account and should therefore be of modular and flexible design.

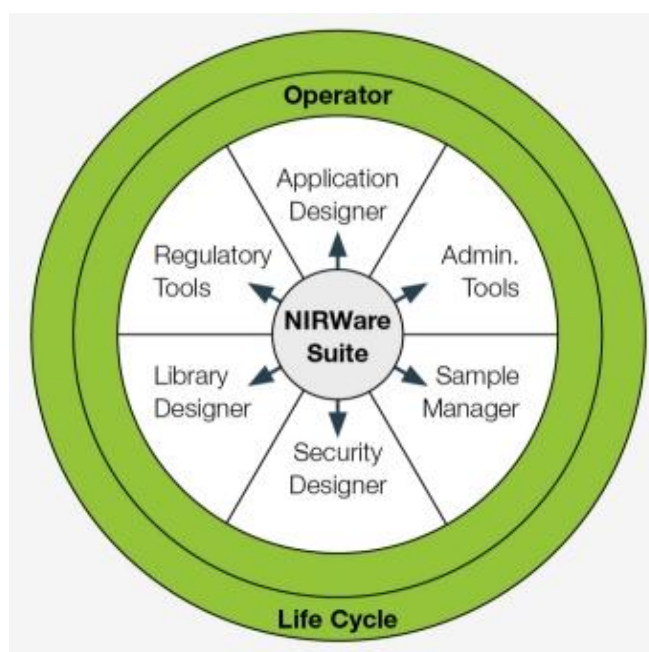
For years, the BUCHI NIRCal Chemometric Software has proven its worth as a powerful and flexible software package for creating calibrations. It has been substantially expanded and improved for the new generation now available. The wide variations in calibration creation requirements and routine use of NIR spectroscopy have been given special consideration.

The NIRWare Software Suite allows creating routine applications which fulfill a wide variety of needs in terms of data management and the necessary security settings. NIRCal and NIRWare are closely interlinked in one single database.

BUCHI NIRWare Suite bundles several applications:

-  NIRWare Management Console including:
 - Application Designer
 - Sample Manager
 - Administrative Tools
 - Security Designer
 - Library Designer
-  NIRWare Operator
-  NIRCal 5, the advanced chemometric software used for calibration development

All data like applications, calibrations, spectra are stored in a database and are controlled by the lifecycle management.



2.1. NIRWare Management Console

NIRWare Management Console is related to Microsoft Management Console (MMC). It hosts all Snap-In Modules of the NIRWare Suite except NIRWare Operator. The Management Console can be configured for different Users or User Groups. Closely linked to the NIRWare Software Suite is the NIRCal Chemometric Software.

2.1.1. Application Designer

The design of an application predominantly defines how the operator has to perform a specific analysis. It includes the definition of instrument configuration and instrument parameters and the definition of the required inputs (Batch number, sample name,...), the properties to estimate, the calibrations to be used, the Standard Operating Procedure (SOP) displayed in order to guide the operator and finally to select the report to be displayed.

The Application Designer is very flexible to customize a specific application. For easy use the basic mode is available in which only a few entries are necessary to develop an application. For the advanced user many options and features are available. Different report templates are available for qualitative and quantitative applications.

2.1.2. Sample Management

NIRWare Sample Manager is designed to check previous measurement results and to enter reference values.

The main concept of NIRWare Sample Manager is a software interface allowing to:

- Manage Samples (assign reference values and properties to the sample)
- Manage and Print-out results of previous measured samples and system tests
- sign results electronically
- Manage Properties (create and design properties)

For further details see section: [Introduction Sample Manager](#)

2.1.3. Administrative Tools

The entire software is database-oriented. In NIR spectroscopy, vast data volumes are processed. It must be possible to manage these data easily. The NIRWare Administrative Tools allow backups and updates to be made.

Audit Trail / System Logger

All relevant operations within all software modules, applications and calibrations are stored in the Audit Trail. With this tool all changes are traceable. Other log functions for the system and errors are also part of this tool. The Audit Trail is a required part of FDA's 21 CFR Part 11 regulations. Different filter functions are also available to select the requested entry.

Life Cycle Templates

Different Life Cycle Templates can be selected for configuration. In order to simplify the use of the lifecycle model there are three pre-defined lifecycle model templates: Unregulated, ER (Electronic Records), and ERES (Electronic Records/Electronic Signatures), which cover different requirements. The lifecycle involves all software modules, applications and calibrations.

NIRWare Configuration

In NIRWare Configuration, the IP address of the connected device and the database server to which NIRWare connects are specified. In addition, installed language packages can be activated and a reset of the grid configuration can be performed here.

Database Maintenance

Backup of the database and restore of previous backup files can be performed externally in the BUCHI Database Manager (BDM). An Archive function is available.

Customer Information

Company name and address can be entered. This information will be shown in the header of result reports.

Import / Export

The possibility of efficient and easy data exchange is highly significant. The import and export functions of the Administrative Tools offer the required and direct options.

Applications, calibrations and samples can be exported from the database to an XML-File.

Applications, calibrations and samples previously exported as an XML-File can be imported to the database.

For the selection different filter functions are available.

2.1.4. Security Designer

Especially in regulated environments, authorizations for access to the software or to individual software modules must be precisely defined. A basic precondition for this task is an integrated user management system.

Users and user groups

Access authorizations may be assigned exclusively to users and user groups registered in the integrated user management system. For this purpose, you can create and manage users and user groups with individual rights.

Security policies

All software components, including applications, can be fully protected against unauthorized access.

Account Policy

With the aid of the Account Policy, the rules are defined for user names and passwords. For example, it is possible to define the minimum length of the user name as well as the complexity

and period of validity of the passwords. A password history check and an automatic logout function are implemented as well.

2.1.5. Library Designer

For identity checking at goods receipt, it is not always necessary to apply chemometric procedures such as cluster analysis or SIMCA. Often, a direct comparison of spectra will also produce unambiguous results directly and require fewer reference samples than in chemometric models. With the aid of the Library Designer, it is possible to create and manage the necessary spectral libraries. On the basis of existing spectra, any number of libraries can be created which can be interlinked to allow spectra to be compared. The Library Designer enables you to select from ten different algorithms for spectral comparison and to define the acceptance criteria to ensure optimal matching to your specific task. At the push of a button, you can perform internal and external validations of the libraries.

2.2. NIRWare Operator

All measurements are performed using the NIRWare Operator. Its user interface can be tailored to user specific needs. The integrated standard operating procedures guides users through the application. In the routine mode, only a few sample-specific entries are required, which may also be entered using a barcode reader. The results are displayed directly in the report format on the monitor. Even users with little PC experience will be able to use this software after just a short introduction

Additionally there are tools for instrument tests implemented.

2.3. NIRCal 5

NIRCal 5 is the proven chemometric software. It is database oriented and includes an integrated user management feature. Calibrations of NIRCal 5 are incorporated directly in the application with the NIRWare Application Designer.

NIRCal is a chemometric software to analyze measured spectra and to develop calibrations.

General features of NIRCal:

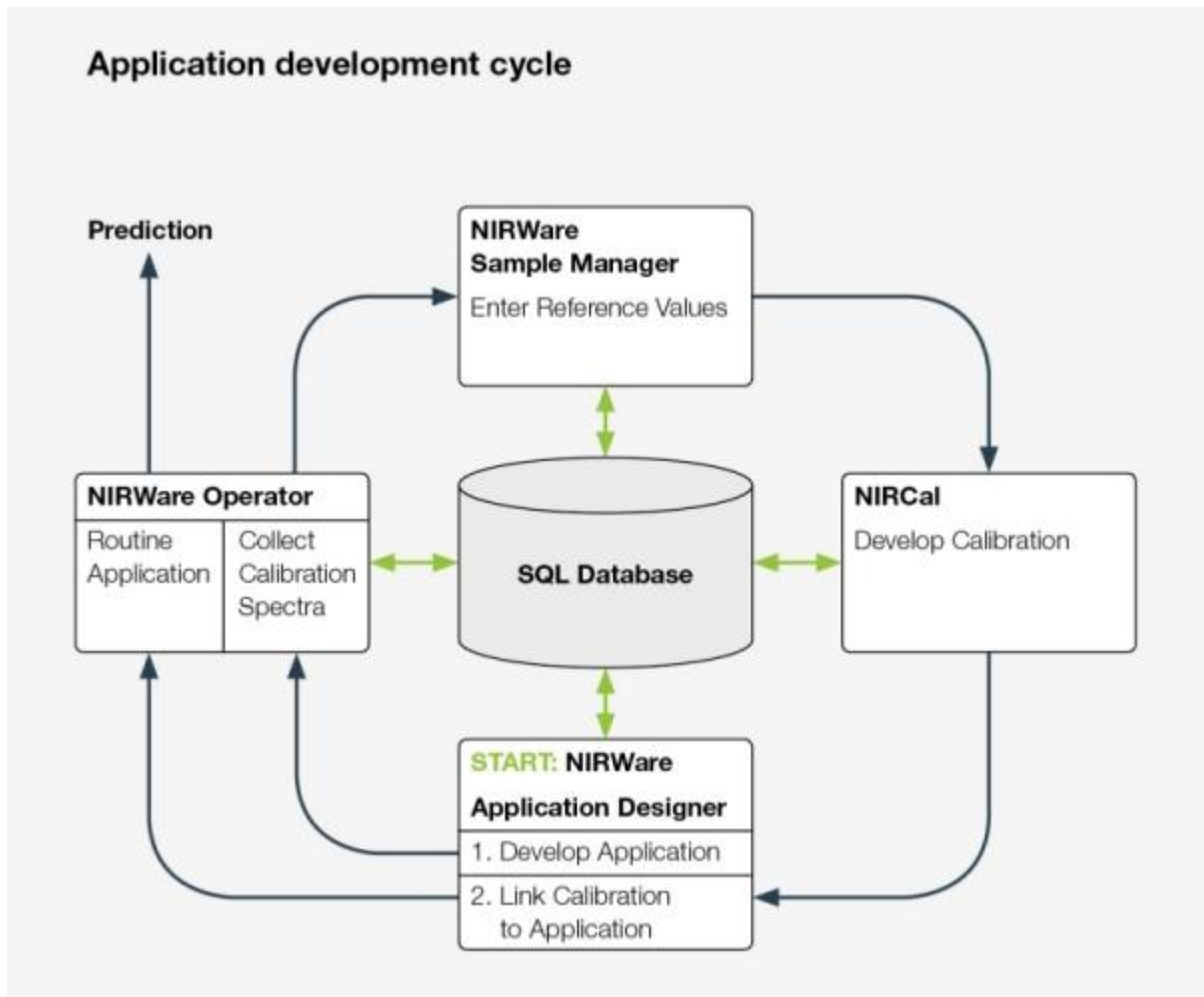
- Fully database oriented
- Internal User Management (via NIRWare Security Designer)
- Performance increase (up to 10 times faster than NIRCal 4.21)
- Integrated lifecycle model

Please confer to the dedicated NIRCal manual for detailed information.

3. General work flow




















In the development of a routine application, different software modules are used. The application development cycle is summarized below:

1. Develop an application with **NIRWare Application Designer**
2. Measure the calibration samples with **NIRWare Operator**
3. Assign reference values to each sample with **NIRWare Sample Manager**
4. Analyze spectral data and develop a calibration with **NIRCal 5**
5. Assign the calibration to the application with **NIRWare Application Designer**
6. Measure and predict measured samples in routine use with **NIRWare Operator**



Roadmap to Application Design



Design Ref.-Application <i>Set to 'Approved'</i> 		
Record spectra of ref. samples		
Define Properties & -values	 	
Calibrate <i>Set cal. to 'Approved'</i> 		
Copy appl. as template for routine appl. <i>(Adjust SOP & meas. per sample)</i>		
Integrate Calibration in Application <i>Set to 'Approved'</i> 	 	
Use for Prediction / Routine Measurement		

The shown roadmap illustrates the workflow under the Life Cycle Template "Unregulated".

The Life Cycle Template "ER" (Electronic Records) and "ERES" (Electronic Records/Electronic Signatures)", usually used in pharmaceutical industry, contains an additional step.

An application or calibration is set in the life cycle state "checked" for test runs before it can be set to the "approved" state, which is used for released applications and calibrations.

4. Software Installation

This chapter explains how to install or update the NIRWare Software Suite and introduces the license philosophy.

4.1. Important Notes

A new version of NIRWare cannot be installed at the same time as a previous version. In case of an existing installation of NIRWare it will be removed by the setup of the new version. An existing NIRWare database from a prior installation will be upgraded. Therefore it is recommended to backup all needed data prior to installation.

NIRWare 1.5 can run on 32-bit and 64-bit versions of Windows. NIRCal 5.5 runs **only** on the 64-bit versions of Windows. If you choose to install NIRWare 1.5 on a 32-bit operating system, NIRCal 5.5 will **not** be installed.

A user with administrator rights for the operating system is required to install the software.

4.2. System requirements

The PC must fulfill the following requirements:

- Windows 7 Professional / Enterprise / Ultimate (32-bit or 64-bit) SP1, 3 GB RAM or higher
- Windows 8 Pro (64-bit), .NET 3.5 recommended, 3 GB RAM or higher
- Intel Core i3 or higher and 1.4 GHz or faster
- 3GB RAM or higher
- 15GB free hard disk space
- DVD-ROM drive
- 1 x 100 Mbit/s LAN (2x 100 Mbit/s LAN recommend)
- 1280x1024 display resolution

The firewall needs to be stopped during the installation procedure



ATTENTION

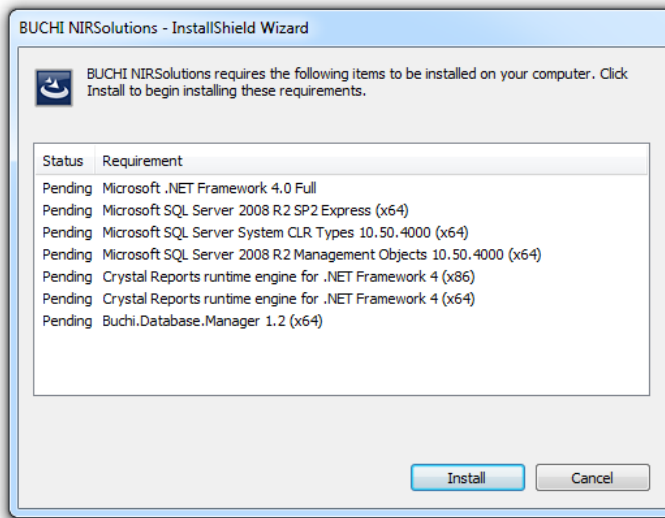
For security reasons, we highly recommend to disconnect from the internet before shutting down a firewall.

4.3. Installation procedure

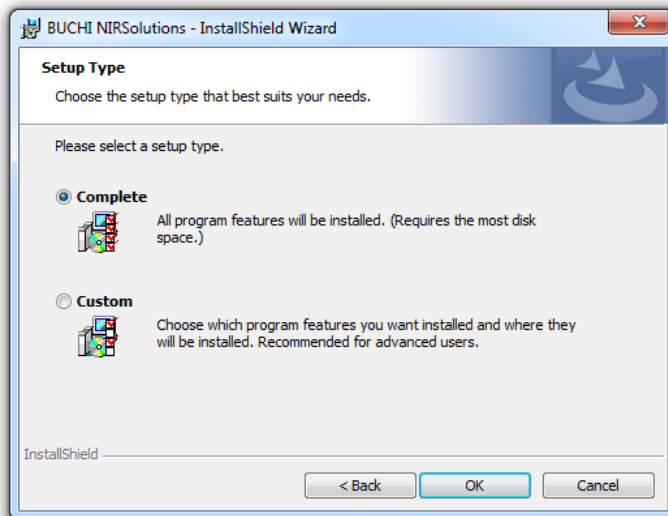
To install the NIRWare software, proceed as follows:

- Insert the Installation DVD. If the installation window does not start automatically, then manually run the executable 'Start.exe'. In the opening window, click on 'Install NIRWare 1.5 and NIRCal 5.5'.

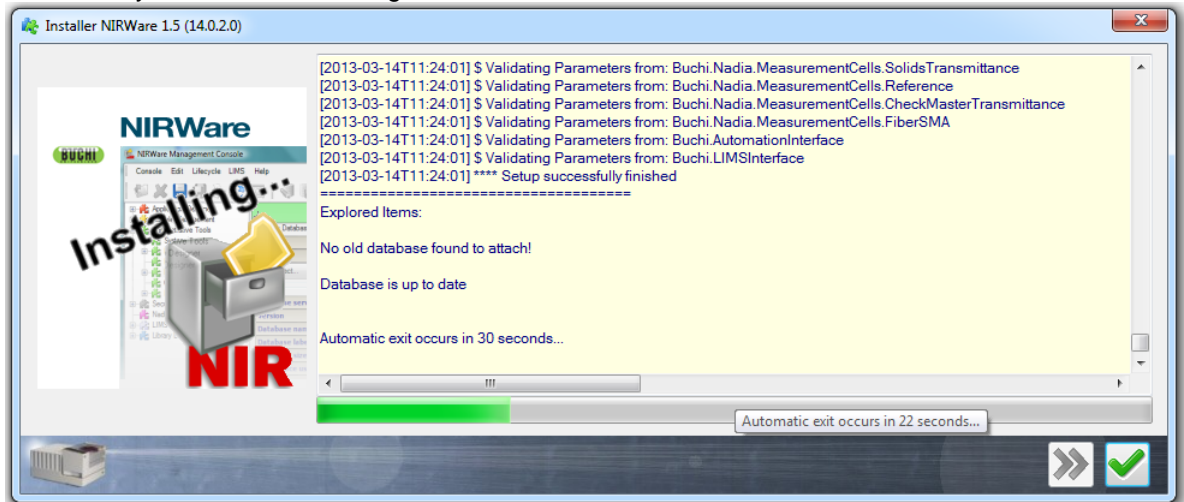
- The InstallShield Wizard with the list of software parts to be installed opens. Click 'Install' to start the installation.



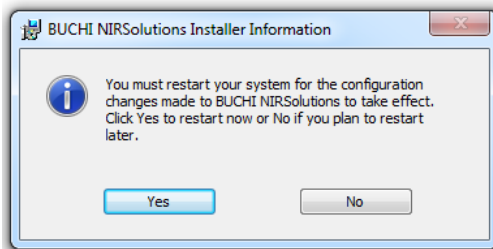
- Wait during installation of .NET 4.0 and MS SQL Server 2008 R2...
- After automatic installation of .NET 4.0 and MS SQL Server 2008 R2, click OK to confirm the warning that any older NIRWare version will be automatically uninstalled when installing NIRWare 1.5.
- Follow the installation wizard and use the default options.
- Click OK to confirm the complete installation of NIRsolutions.



- Click on green check mark to confirm or let the timer run its course. Ensure the setup finishes successfully and no error message is shown.



- Click Yes to confirm to restart your system

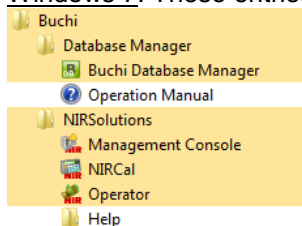


4.4. What has been installed

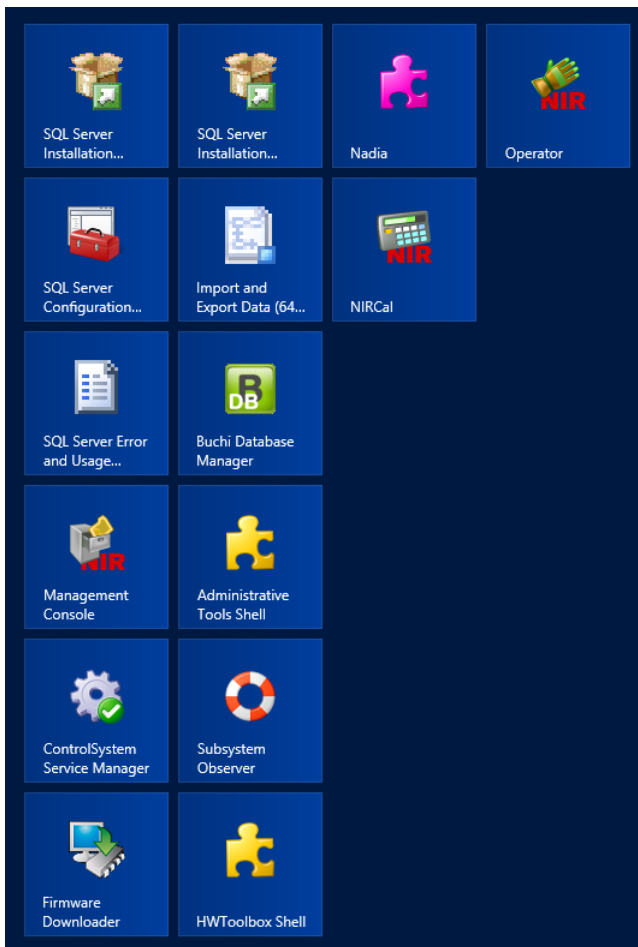
The following three shortcuts have been added to the desktop for all users (Windows 7 and Windows



Windows 7: These entries have been added to the start menu for all users

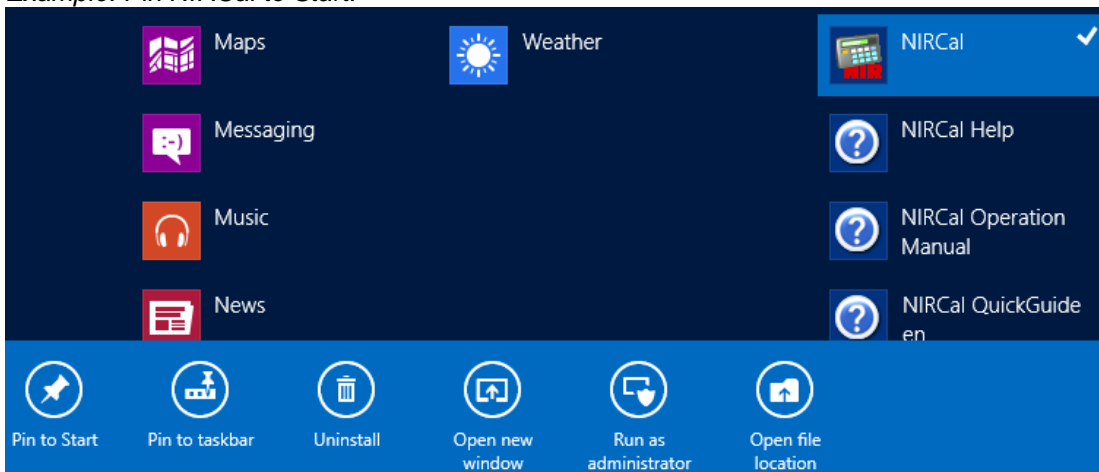


Windows 8: These tiles have been added to the Start screen of the user who has done the installation



The above tiles are only added to the Start screen of the user who installed NIRWare 1.5. Other users do not see automatically any NIRWare 1.5 tiles on their start screens. Users who want to add NIRWare 1.5 tiles to their start screen have to select the desired apps (right click on the start screen and click on 'All apps', or press the keys Windows-Q to open the search app view) and pin them to the start screen: Right click on the app and then click on 'Pin to Start'

Example: Pin NIRCAl to Start.



Management Console, Operator and NIRCAl

- Windows 7: These applications can also be started using the Start menu: Start / All Programs / Buchi / NIRsolutions / ...
- Windows 8: These applications can also be started using the Start screen, if they have been pinned to the Start screen. Alternatively, just start typing the name of the application on the Start screen until you see the desired application selected.

- These three applications are stored by default here:
C:\Program Files\Buchi\NIRSolutions

BUCHI Database Manager

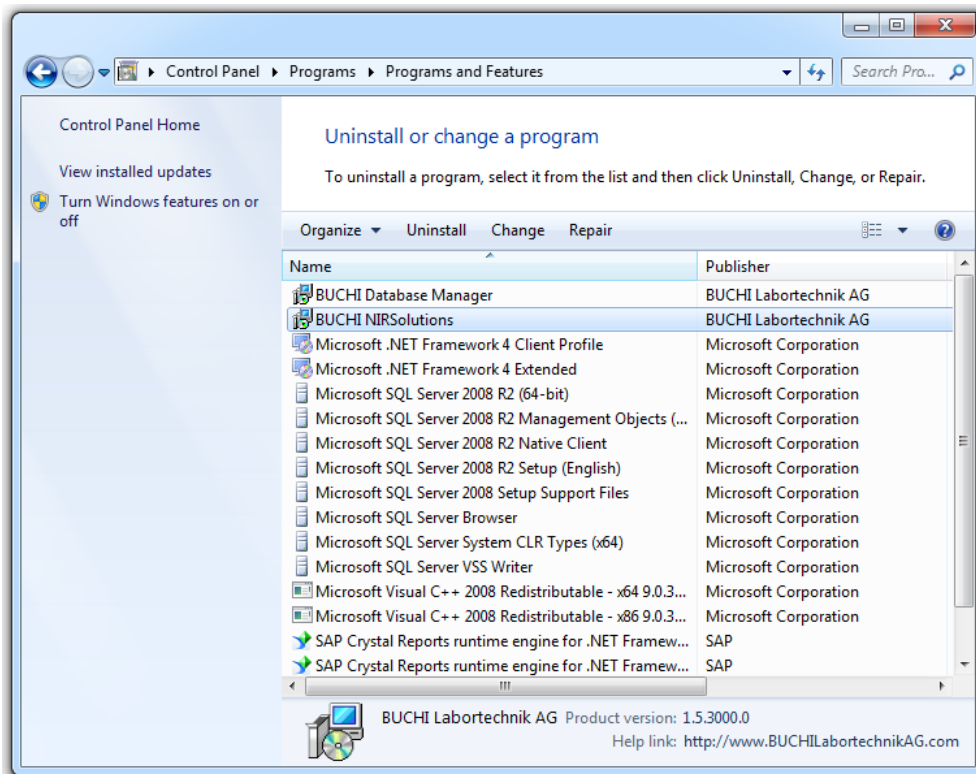
- Windows 7: This application can be started using the Start menu:
Start > All Programs > Buchi > Database Manager > Buchi Database Manager
- Windows 8: This application can also be started using the Start screen, if it has been pinned to the Start screen. Alternatively, just start typing the name of the application on the Start screen until you see the desired application selected.
- This application is stored by default here:
C:\Program Files\Buchi\Buchi Database Manager

4.5. Software removal

4.5.1. BUCHI NIRSolutions

Please uninstall the existing software version manually. For this purpose:

- Windows 7: Start > Control Panel > Uninstall a program
- Windows 8: On the Start screen start typing control panel until you see the app Control Panel selected, then hit the enter key, then click on Uninstall a program
- Select BUCHI NIRSolutions from the list and click Uninstall



- Confirm the next few dialog boxes to uninstall BUCHI NIRSolutions, including the one that asks for a reboot of your system.
- The default shortcuts are removed after the reboot. Manually added shortcuts remain and have to be deleted manually.

4.5.2. BUCHI Database Manager

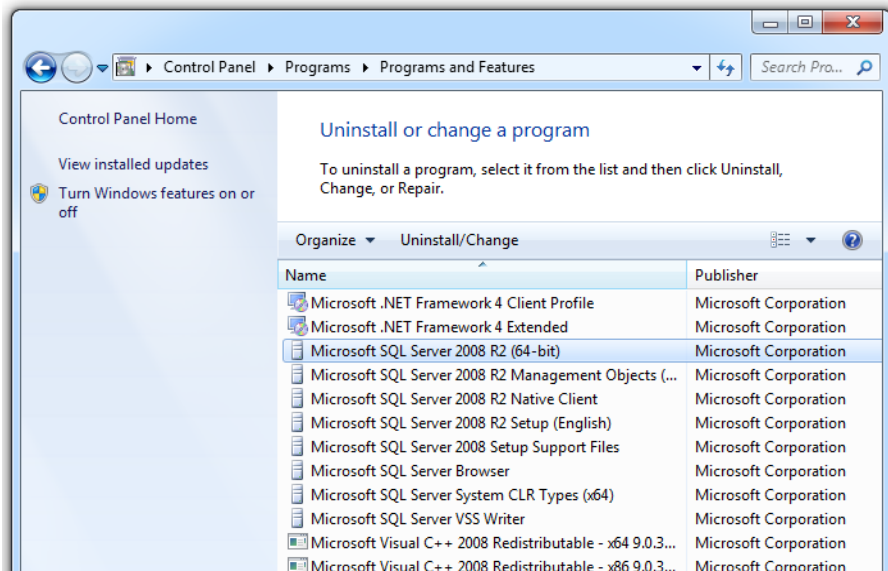
Please uninstall the existing software version manually. For this purpose:

- Windows 7: Start > Control Panel > Uninstall a program
- Windows 8: On the Start screen start typing control panel until you see the app Control Panel selected, then hit the enter key, then click on Uninstall a program
- Select BUCHI Database Manager from the list and click Uninstall
- Confirm the next few dialog boxes to uninstall BUCHI Database Manager

4.5.3. Microsoft SQL Server 2008 R2

Please uninstall the existing software version manually. For this purpose:

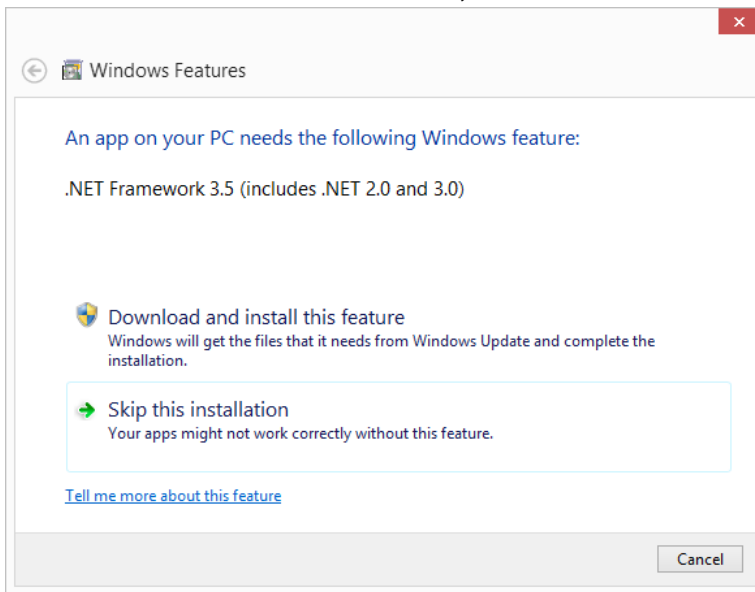
- Windows 7: Start > Control Panel > Uninstall a program
- Windows 8: On the Start screen start typing control panel until you see the app Control Panel selected, then hit the enter key, then click on Uninstall a program
- Select Microsoft SQL Server 2008 R2 (64-bit) from the list and click Uninstall/Change



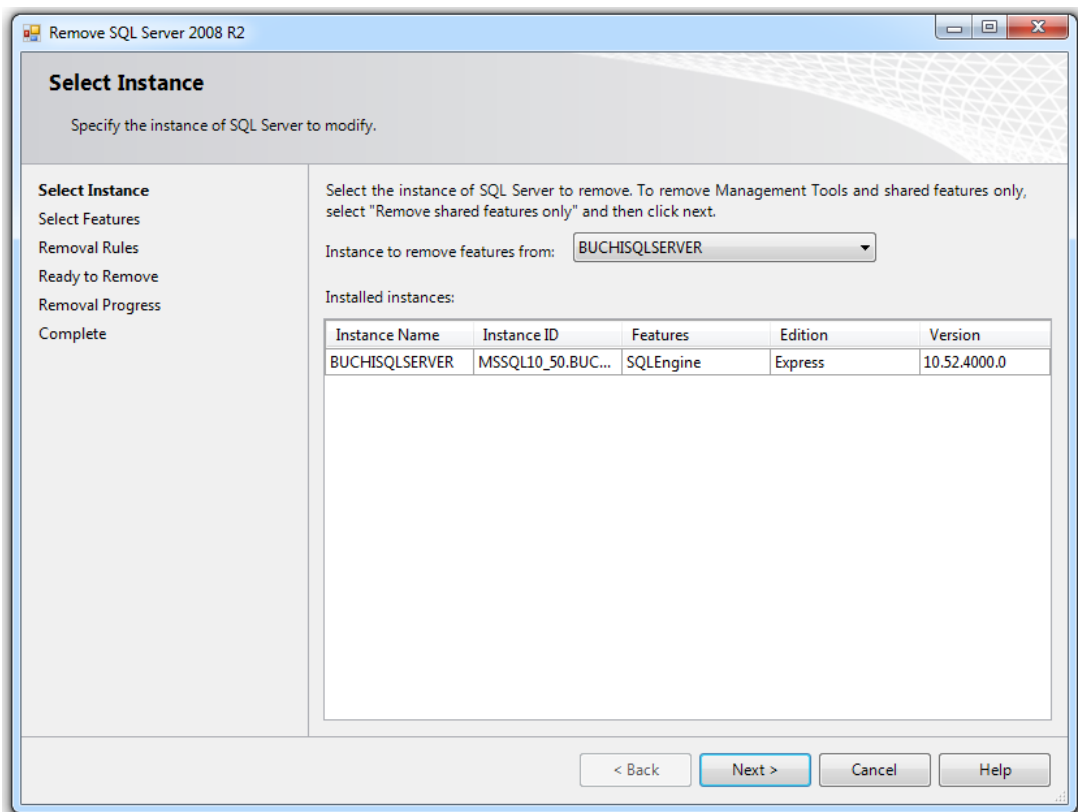
- Select Remove



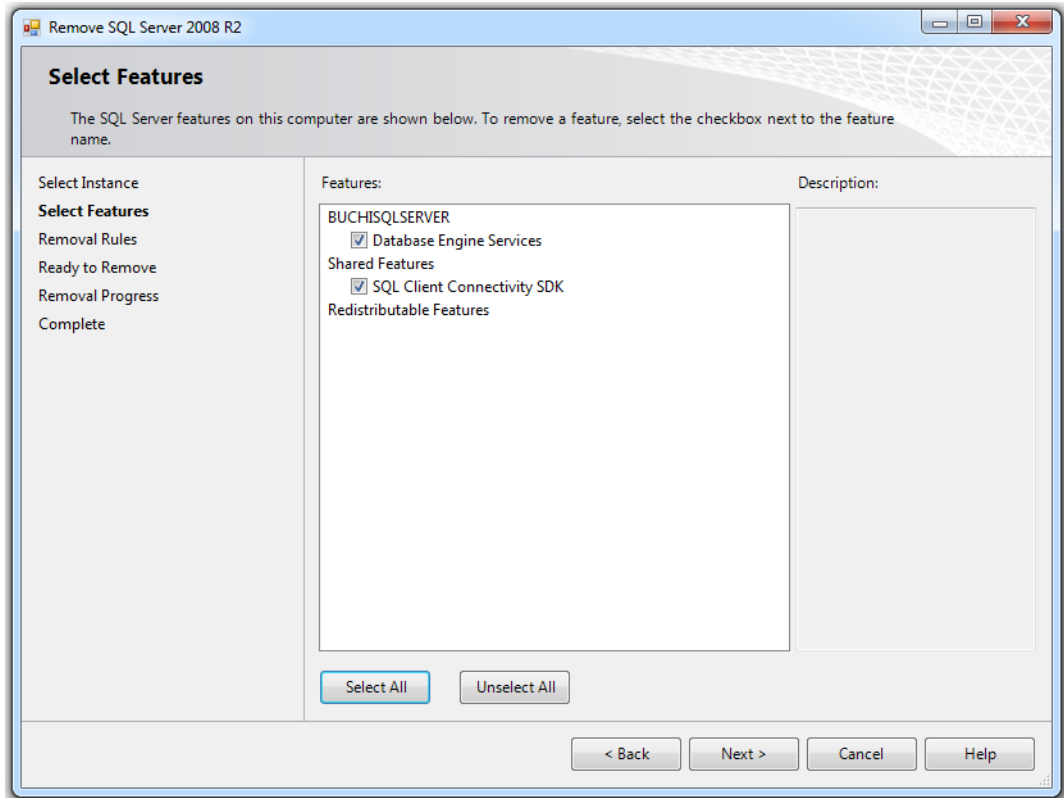
- **Windows 8:** If .NET 3.5 is not enabled then Windows asks to enable it. **To download and install this feature, an internet connection is needed.**



- Click OK to confirm the Setup Support Rules
- Select the instance BUCHISQLSERVER and click Next to remove it



- Click Select All to select all features and click Next to remove them



- Click Next to confirm Removal Rules
- Click Remove to confirm being Ready to Remove
- Click Close to finish the uninstallation of SQL Server 2008 R2

4.5.4. Remove further software

The following software versions can be uninstalled easily by going to

- Windows 7: Start > Control Panel > Uninstall a program
- Windows 8: On the Start screen start typing control panel until you see the app Control Panel selected, then hit the enter key, then click on Uninstall a program
- Select the program and click Uninstall
- Microsoft SQL Server 2008 R2 Management Objects (x64)
- Microsoft SQL Server 2008 R2 Native Client
- Microsoft SQL Server System CLR Types (x64)

The following software versions can also be uninstalled easily in the same way when they are not needed by other installed software

- SAP Crystal Reports runtime engine for .NET Framework 4 (32-bit)
- SAP Crystal Reports runtime engine for .NET Framework 4 (64-bit)

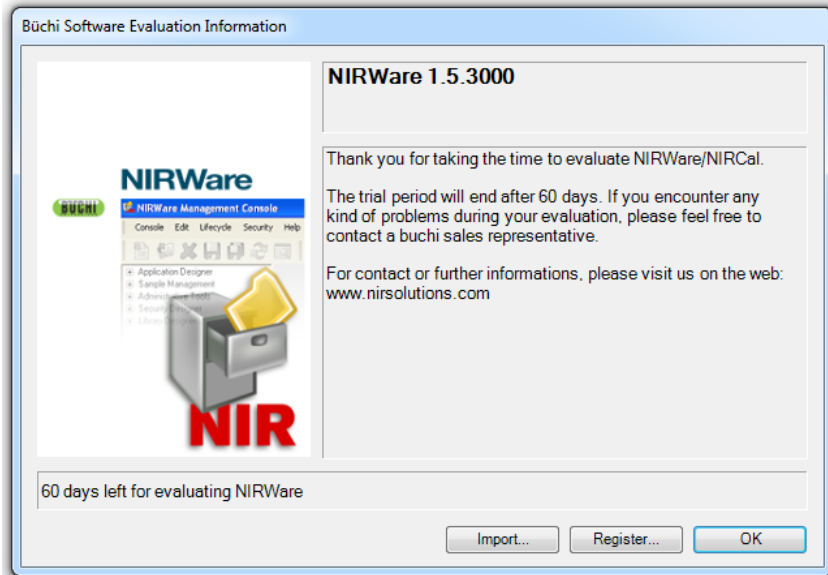
4.6. Software Licenses

After Installation of NIRWare or NIRCal the software can be used in DEMO mode for 60 days. Within these 60 days it is recommended to register the software and apply for a license.

4.7. Software Registration

The registration form can be saved as an *.xml file and needs to be sent to your BUCHI contact person, for example as an email attachment.

The form can be opened using the "NIRWare Management Console" → Menu: Help > Software Registration... or clicking the button "Register..." on the startup of a trial version.



The registration form:

Please fill out the bold mandatory fields. The AN and SN numbers are necessary for new registrations; they can be found on a sticker on the installation DVD.

Click OK and save the file in a convenient place. Email this saved file to your BUCHI sales representative.

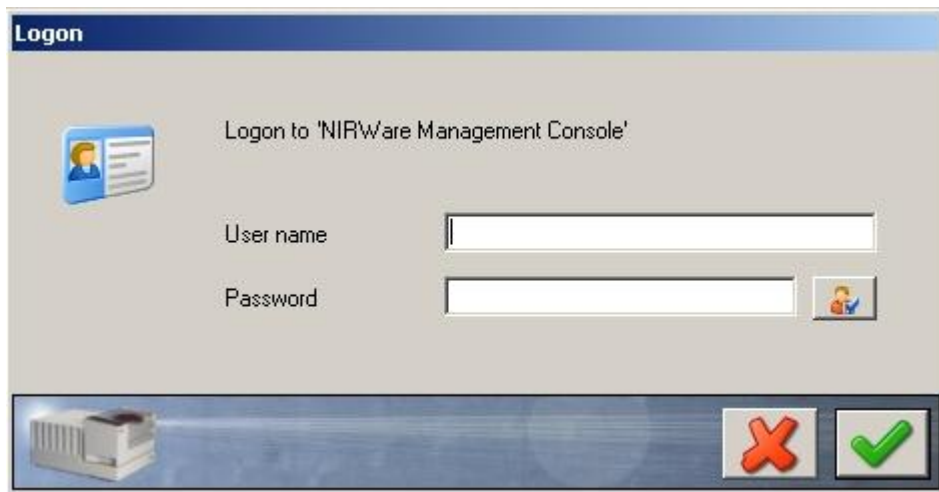
4.8. Activating the licenses

- To activate the demo mode start the Management Console and select Demo mode.
- When the software is in demo mode it is valid for 60 days.
- To activate the software and make it a fully valid version, licenses are required.
- Licenses are provided by BUCHI.
- The form can be opened using the "NIRWare Management Console" --> Menu: Help > Software Registration... or clicking the button "Register..." on the startup of a trial version.

5. Tutorial

5.1. Logon

The NIRWare Management Console, the NIRWare Operator and NIRCal 5 are protected by Logon.



After NIRWare is installed, four default users are provided, which do not require password entry at the beginning.

Just type in the corresponding user name and click the green checkmark to log on.

The four default users are:

- Administrator
- QManager
- Designer
- Operator

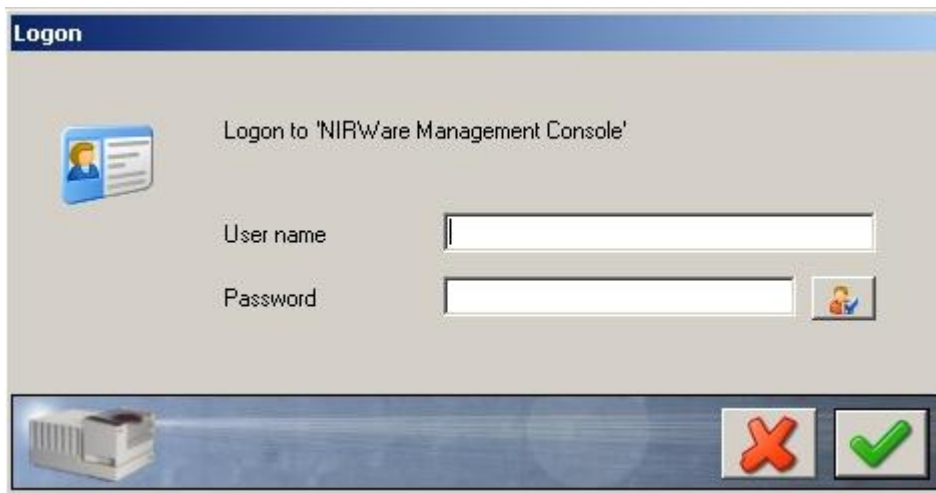
NOTE

We highly recommend to define passwords for the four default users or deactivate the accounts after creating new user accounts with password to control the software access.

5.2. Defining a new password

After a certain time, your password will expire. The number of password expiration days is defined in the submenu Account Policy. You might get a warning before your password expires when a number of days is defined for the property "Show Warning Before Expiration" in the submenu Account Policy.

When you are prompted to change your password, you can do so in the logon window:



Click on the icon behind the Password line. The logon window is extended:



Enter your new password in the corresponding line and confirm it below. Then click the check mark button to save your changes.

5.3. Creating a qualitative application

5.3.1. Introduction

This tutorial describes how to create an application for identity check.

As an example, the NIRFlex N-500 is used with the measuring cell Solids and the Vial Add-on.

The application should be able to check the identity of four different types / forms of sugar: Fructose (= fruit sugar), lactose (= milk sugar), sucrose (= crystal sugar) and fine sucrose (= sugar powder).

Note that sucrose and fine sucrose are of the same chemical composition and only differ in particle size.

The process of creating a ready-to-use NIR application requires reference samples. These are samples of doubtless identity and quality. In combination with their NIR spectra ('reference spectra') they provide the necessary data sets for calculating a chemometric calibration. The calibration can then be used for prediction, which means deriving the identity information from the spectra of substances to be tested.

A typical use of an NIR application with such a calibration is the identity check of incoming substances in a pharmaceutical plant.

It is recommended to use dedicated applications for reference measurement and routine use (= prediction).

NOTE

The terms 'reference measurement', 'reference samples' or 'reference spectra' used in the tutorial describes the data collected for calibration development.






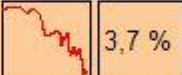












To ensure that reference and unknown samples are measured under identical spectrometric conditions, we suggest to start the development of the routine application with a copy of the application for reference measurement, which is then adjusted.

Please keep in mind that only applications in the 'Approved' Lifecycle state are visible to (and usable by) a user from the user group 'Operators'.

These considerations are visualized in the following scheme:

Roadmap to Application Design



Design Ref.Application <i>Set to 'Approved'</i> 		
Record spectra of ref. samples		
Define Properties & -values		
Calibrate <i>Set cal. to 'Approved'</i> 		
Copy appl. as template for routine appl. <i>(Adjust SOP & meas. per sample)</i>		
Integrate Calibration in Application <i>Set to 'Approved'</i> 	 	
Use for Prediction / Routine Measurement		

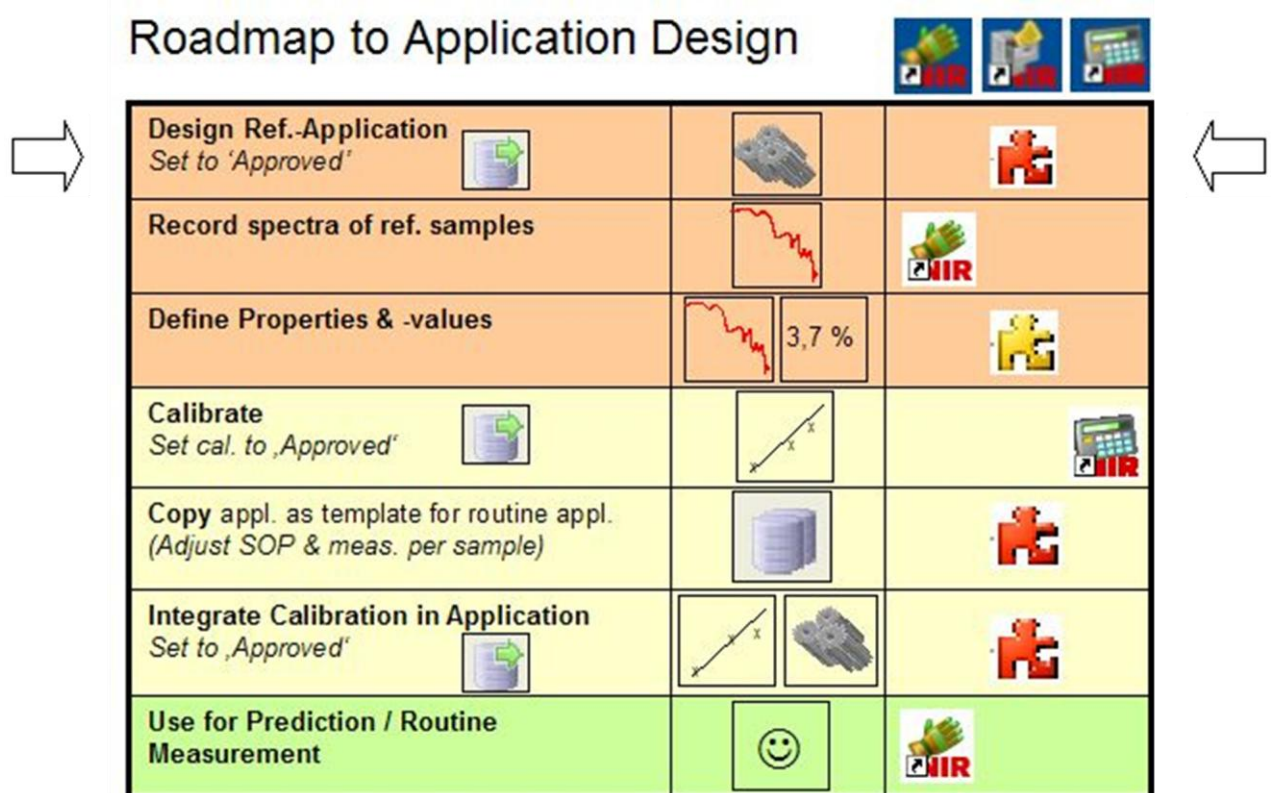
The upper part of the scheme includes all steps regarding the reference samples.
 The middle part shows the processes for designing an application for routine use.
 The last part indicates the routine use, which is the goal of the development process.

In the following, we will use the term 'Operator user' for a user account from the user group 'Operators', and 'Administrator' for one belonging to the user group 'Administrators'.

For Logon as such a user, the correct user name and password are required for the corresponding dialog.

5.3.2. Creating an application for reference measurement

This first part of the tutorial covers the development process for a method that allows an operator to collect spectra of reference samples. These are necessary for calculating a qualitative chemometric calibration.



The application development starts in the NIRWare Management Console (MC).


Start the program by clicking the icon shown above and log on as a 'Designer' (access to 'Application Designer' and 'Sample Management') or as an 'Administrator' (full access).



Left-click on 'Application Designer' in the tree menu on the left, then on the subtitle 'New'. A dialog appears for creating a new application



Fill in the application name and all other requested information into the white fields on the right side. The 'SOP Text' will later on tell the Operator how to perform the actual measurement, so it is important to give a complete description which is easily understandable.

Click the Save icon  to save the new application to the database.

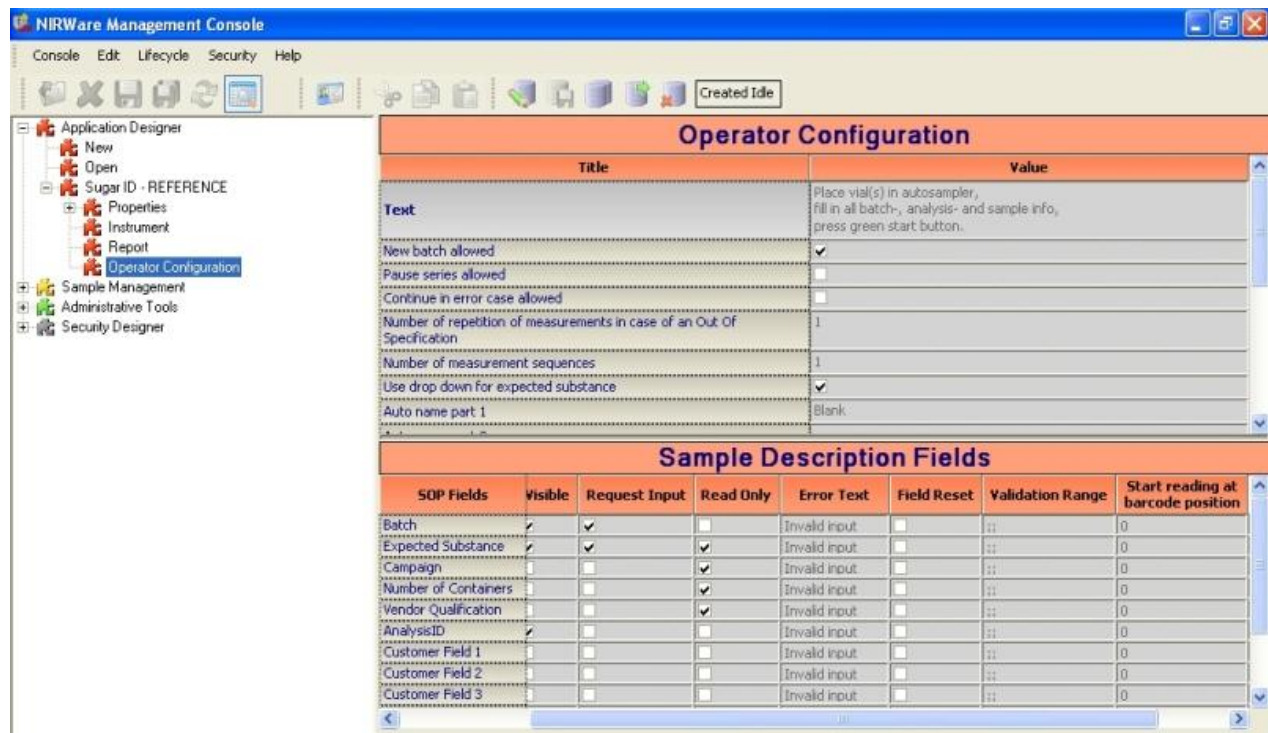


Your newly created application is now shown in the tree menu.

Open it by double-clicking on its field in the tree menu, or by clicking once on the plus-symbol in front of it. Then select its subtitle 'Operator Configuration'. You will now see only one field for the SOP text.

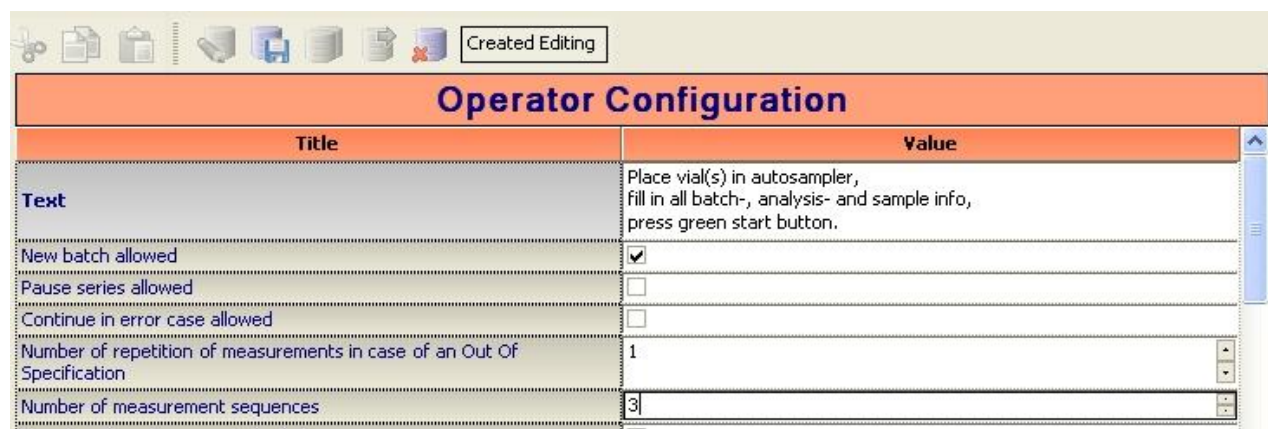
To see all of the information fields on the right, click on the 'Show Advanced Settings' icon in the menu

bar .



The fields on the right are greyed out, indicating that they cannot be changed right now.

To change the settings, first click on the 'Edit Data Set' icon .



Notice the change in the icon bar for Lifecycle state from 'Created Idle' to 'Created Editing' (see above).


You can now make changes to all white fields. For our example, we just change the 'Number of measurement sequences' from 1 to 3.

This will cause a triplicate measurement of every reference sample, which creates more variation in the spectra set later used for calibration. Thus, we will get more robust calibrations.

Save all changes you made to the database by clicking the respective icon .

The fields are greyed out again afterwards, indicating successful saving.

The method for triplicate calibration sample measurement is now still in the 'Created' state, where only a 'Designer' or 'Administrator' can see and use it in the operator software.

To provide this method for the operator user, 'Put the data set into the next state' by clicking on the corresponding icon .

Now the application is in the 'Approved' state.



NOTE

Approved applications cannot be changed anymore. To adjust something, you first have to create a copy of the application, which again starts in the 'created' state. Then you can apply changes to this new application.

The application is now ready for measurement of reference spectra with the Operator software.




















5.3.3. Measuring reference spectra

To measure spectra of reference samples, the Operator software is used.

Measurement of reference spectra is the second step in the development process.

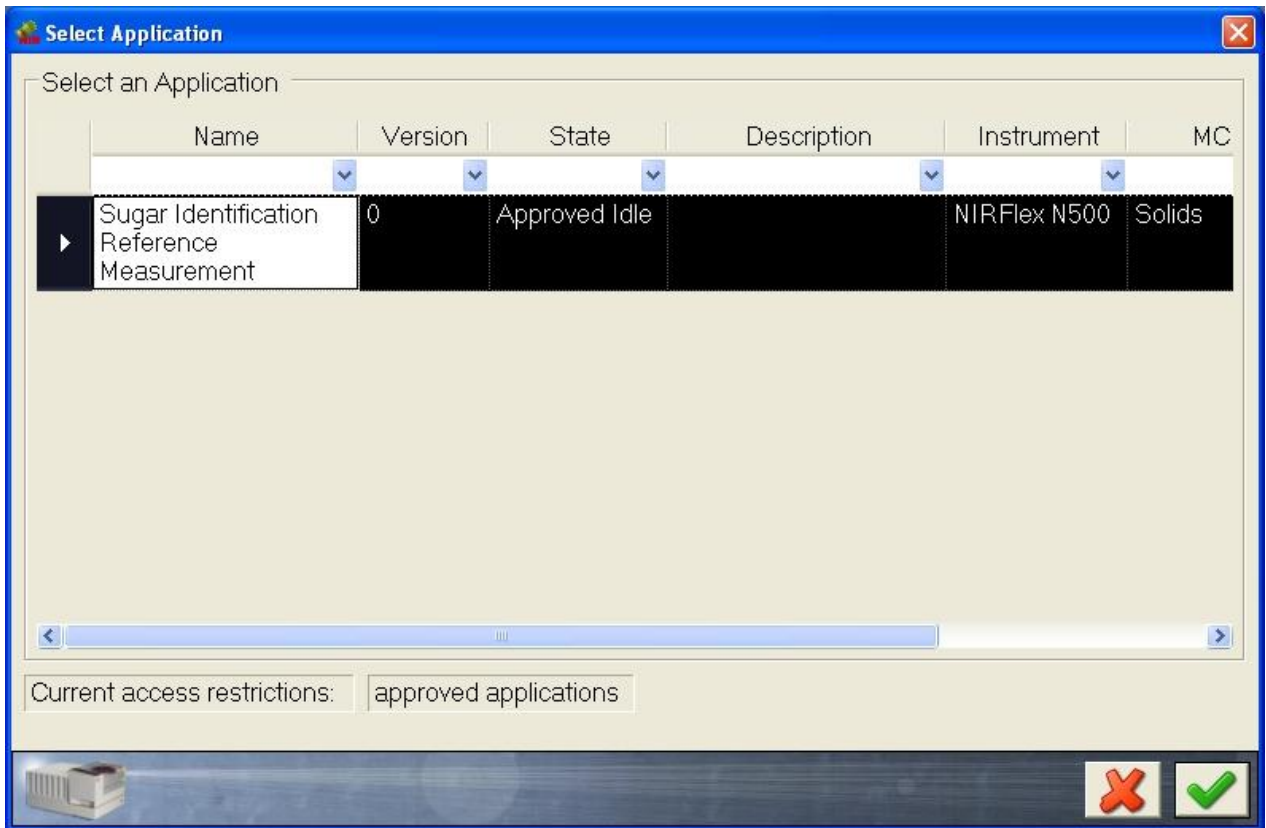
Roadmap to Application Design



Design Ref.-Application <i>Set to 'Approved'</i> 		
Record spectra of ref. samples		
Define Properties & -values	 	
Calibrate <i>Set cal. to 'Approved'</i> 		
Copy appl. as template for routine appl. <i>(Adjust SOP & meas. per sample)</i>		
Integrate Calibration in Application <i>Set to 'Approved'</i> 	 	
Use for Prediction / Routine Measurement		

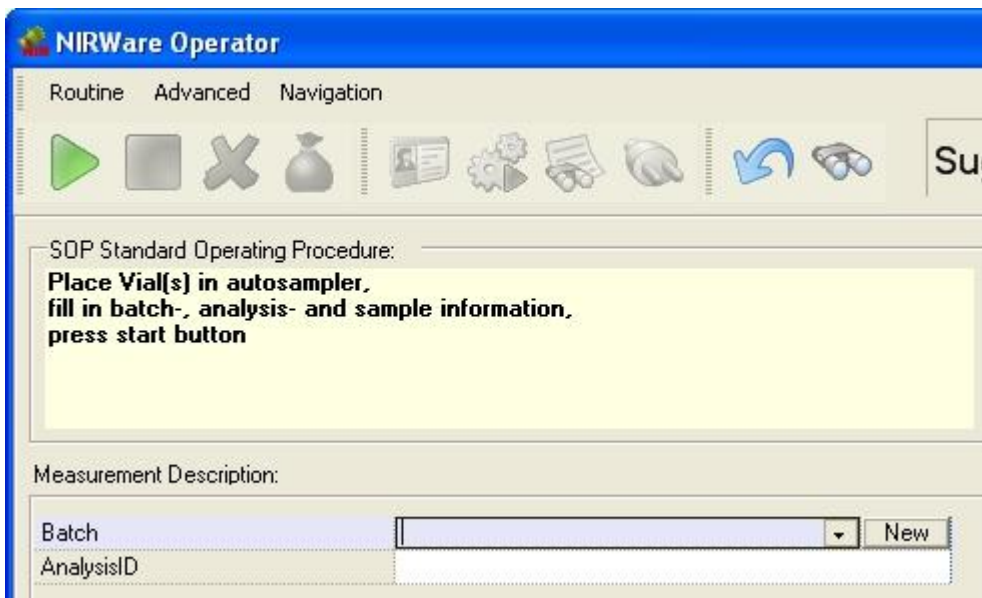
Start the operator software by clicking the corresponding icon  and log on as an operator user.

Click the 'Select application' icon:  .

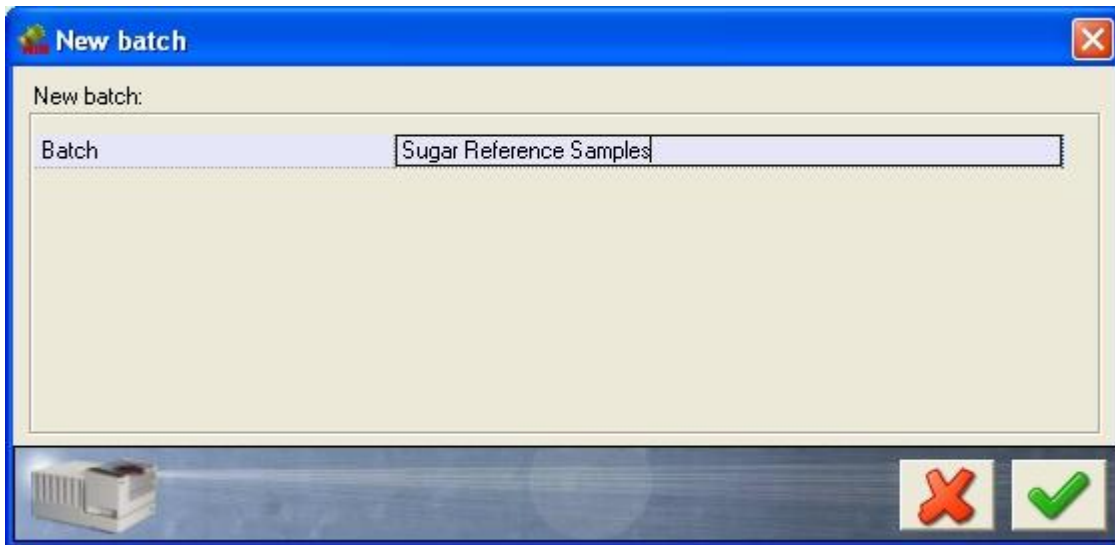


Select the application you created for spectra measurement of the calibration samples.

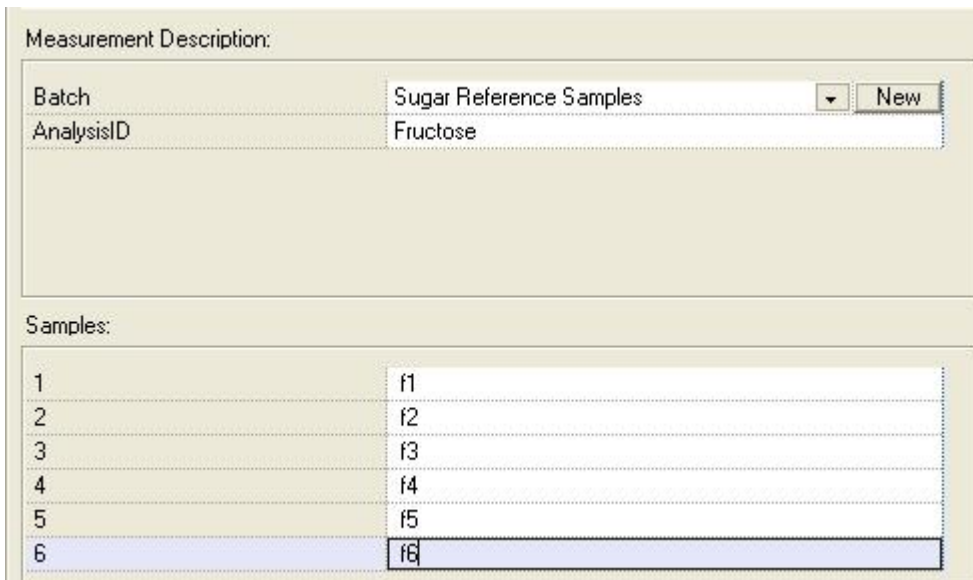
Notice the access restrictions for the Operator: He can only see and use 'Approved' applications.



Click on the 'New' icon of the 'Measurement description - Batch' field to create a new batch.



Type in the name of your batch, then click on the green check mark button.



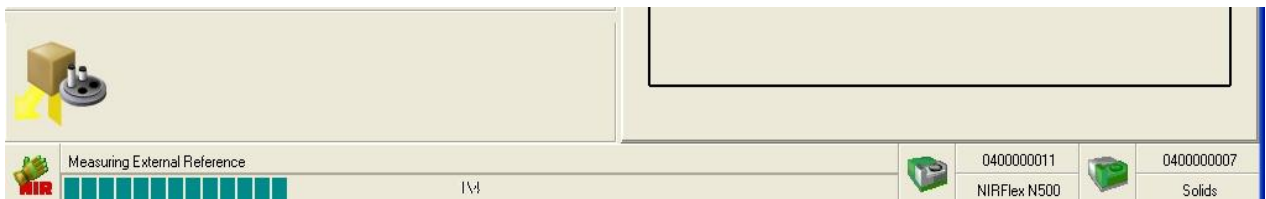
Then type in the information for AnalysisID and Sample names.

Note: For 'real' applications, use 'speaking' names that precisely identify each sample just from the name. Also think of using the autaname functions described in the NIRWare documentation.

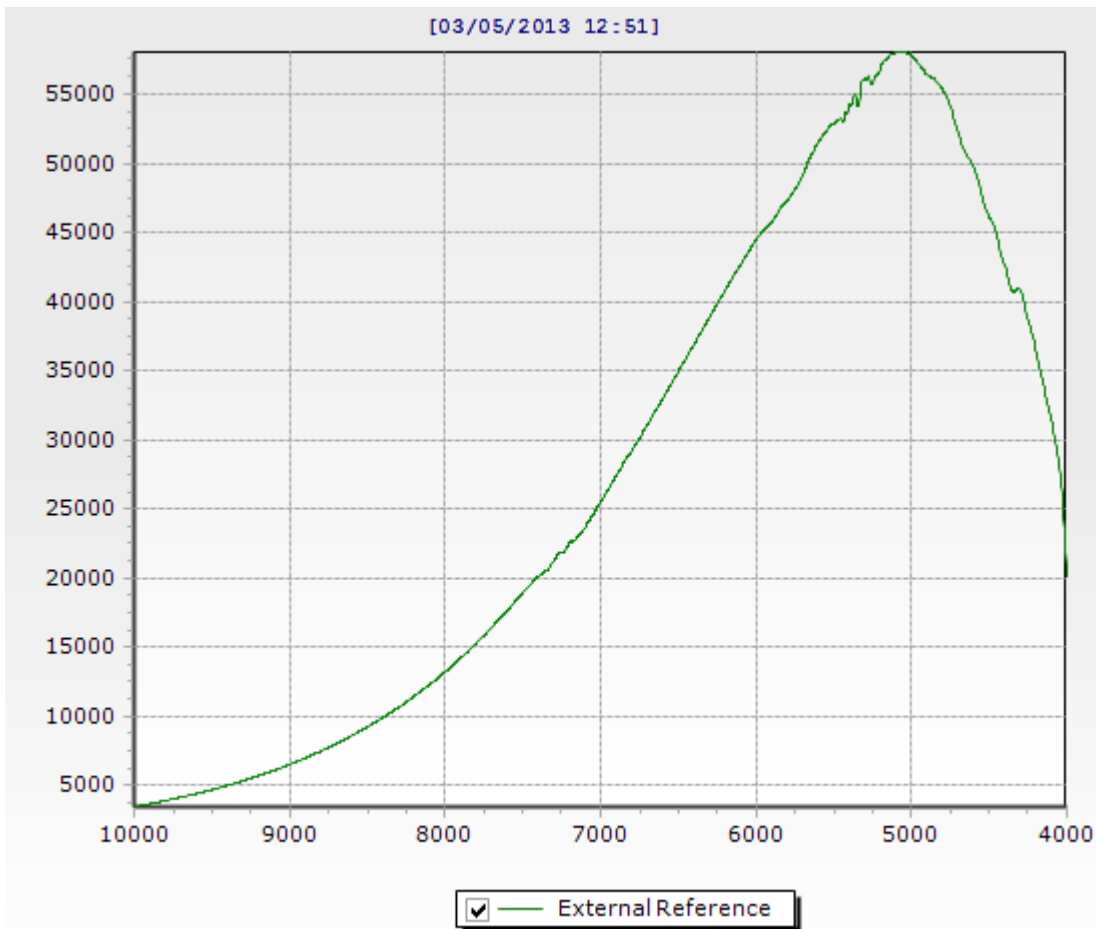
If you have filled in and checked all information, prepare the samples for measurement (i.e. place all vials in the Autosampler) and press the green arrow button.

During the measurement sequence, the SOP text field is greyed out.

If an 'Instrument Suitability Test' (SST) starts, just wait until it is finished. Then the instrument will start with the measurement sequence. This includes periodic measurement of internal and external references. In our example with the vial Autosampler option, these measurements are automatized. With other options, the software will give a description of what to do.



First, the external reference is measured.



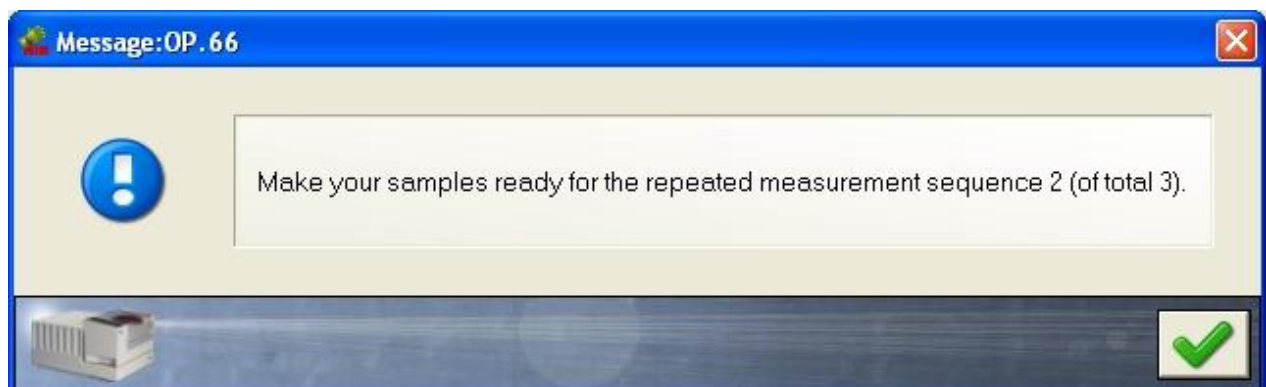
Then the samples are measured. All spectra are displayed in one window.

Since the intensity of the external reference is so much higher than that of the sample spectrum, the latter are just a flat line on the x-axis.

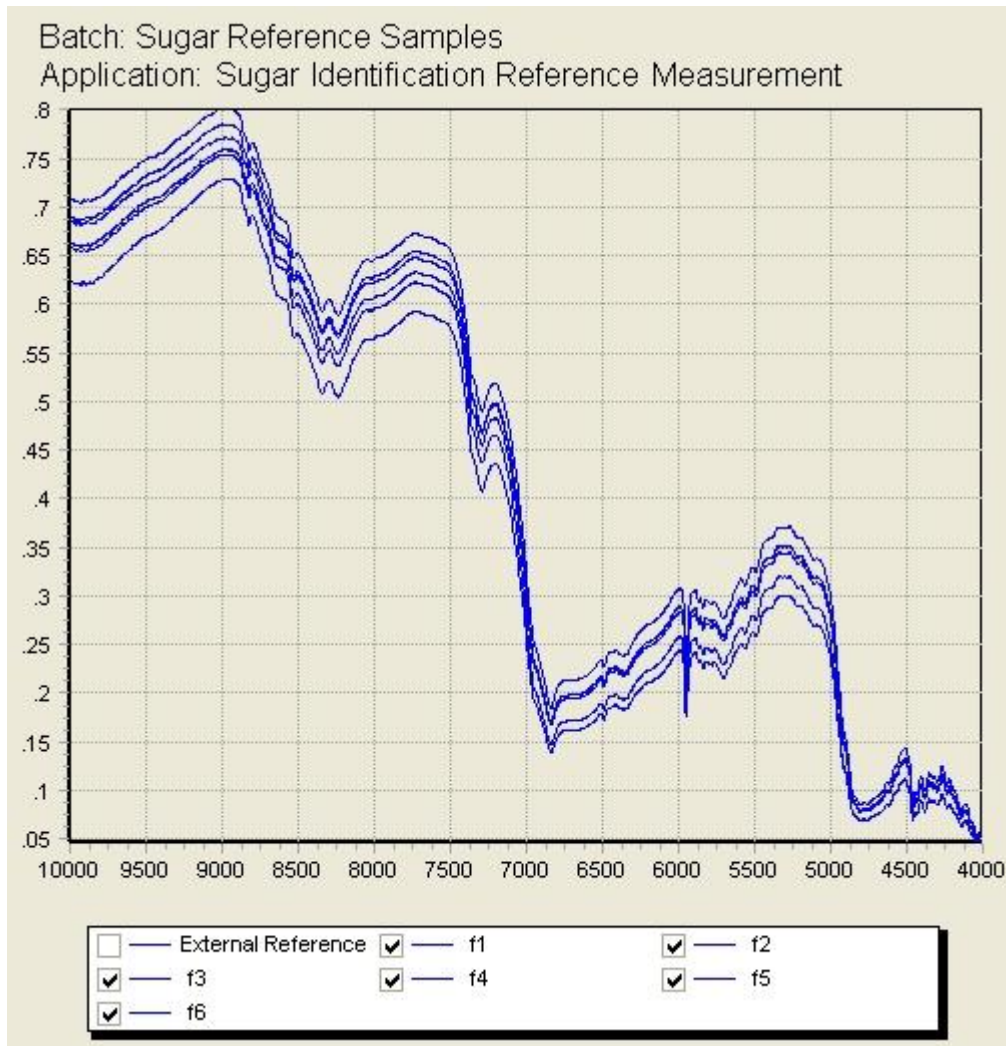


To have a closer look on the sample spectrum, deactivate the check box for 'External Reference' below the graphic.

The vial autosampler will automatically continue with the next samples after confirmation of the following message:

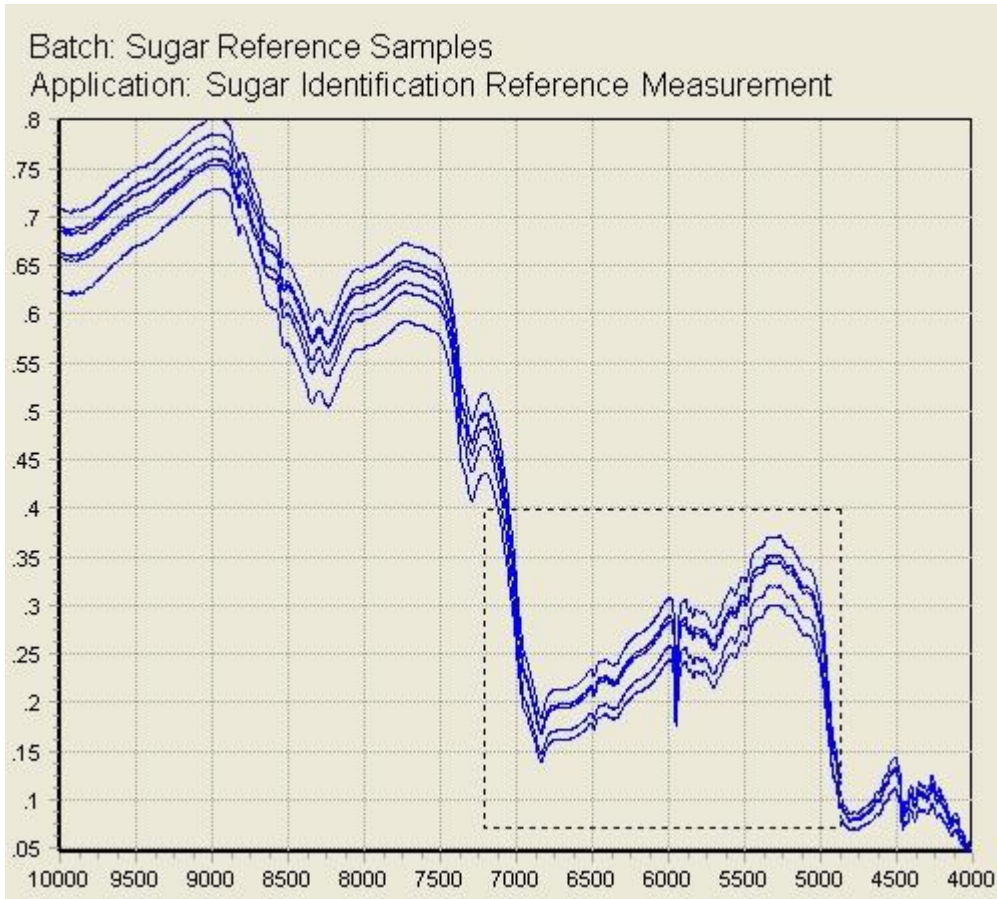


Turn the sample vials and click on the green check mark icon to start the next measurement sequence.

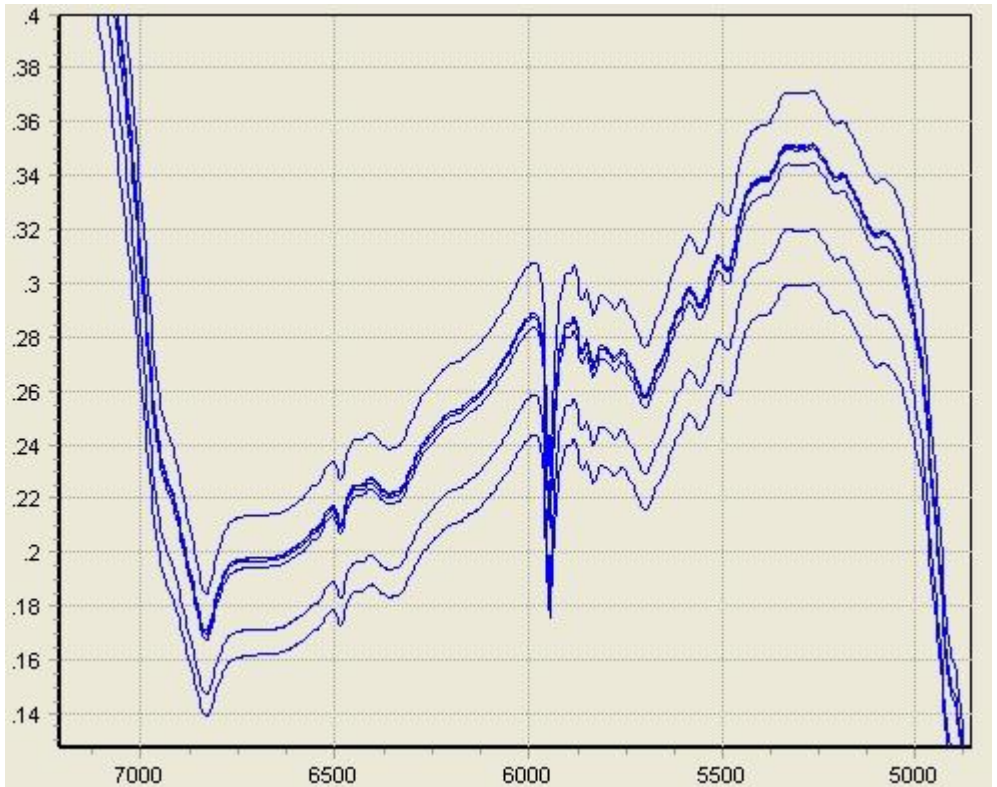


The spectra shown below are all from identical fructose samples.

The strong variations along the y-axis (shift) are typical for reflectance measurements of solids and result from variations in particle size and –orientation, and other sources of variation, e.g. thickness of the glass vials.



To zoom into the spectrum, click and hold the left mouse icon while dragging the cursor.



The selected frame will be magnified:

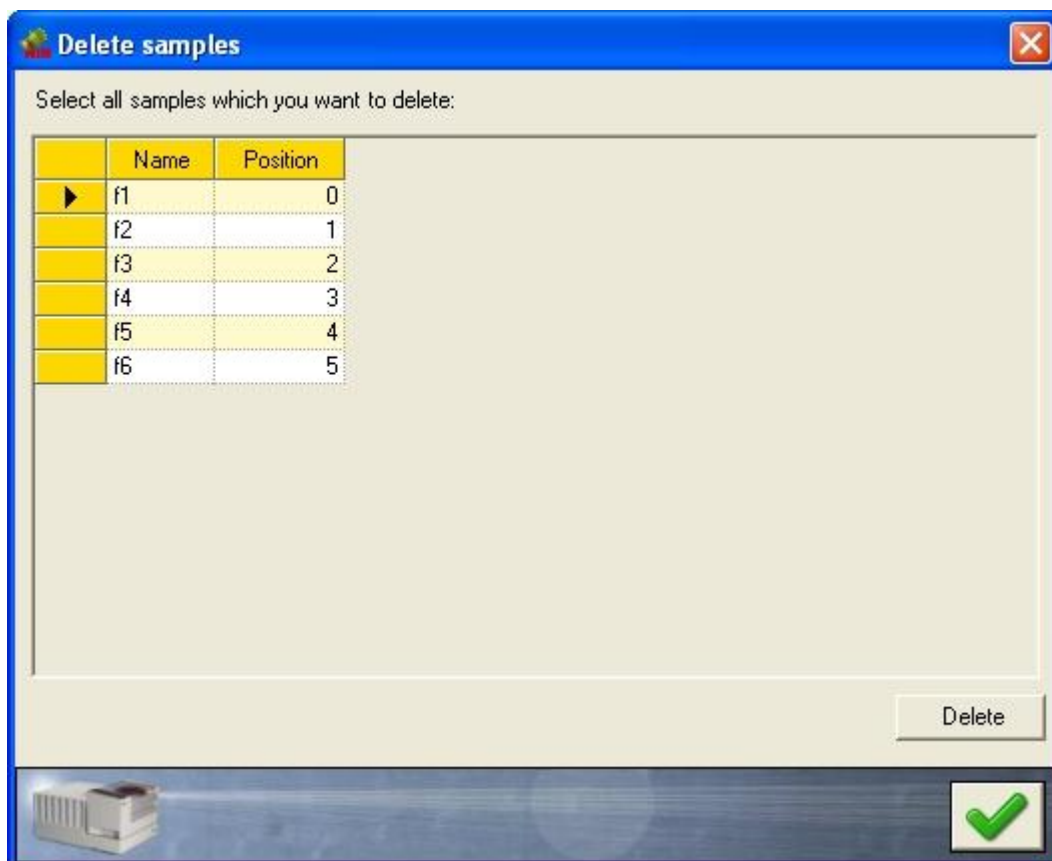


To change back to full view, click on the symbol with the magnification lens above the globus.

NOTE

In the Operator it is possible to delete spectra, but only right after they have been measured and if they are not used for prediction with a calibration. This might be desirable if e.g. a vial was not correctly positioned in the Autosampler. To delete a measurement, click the red cross button (red cross in the upper left corner, not the one next to the magnification lens icon).

You can now select samples from the last measurement sequence for deletion.

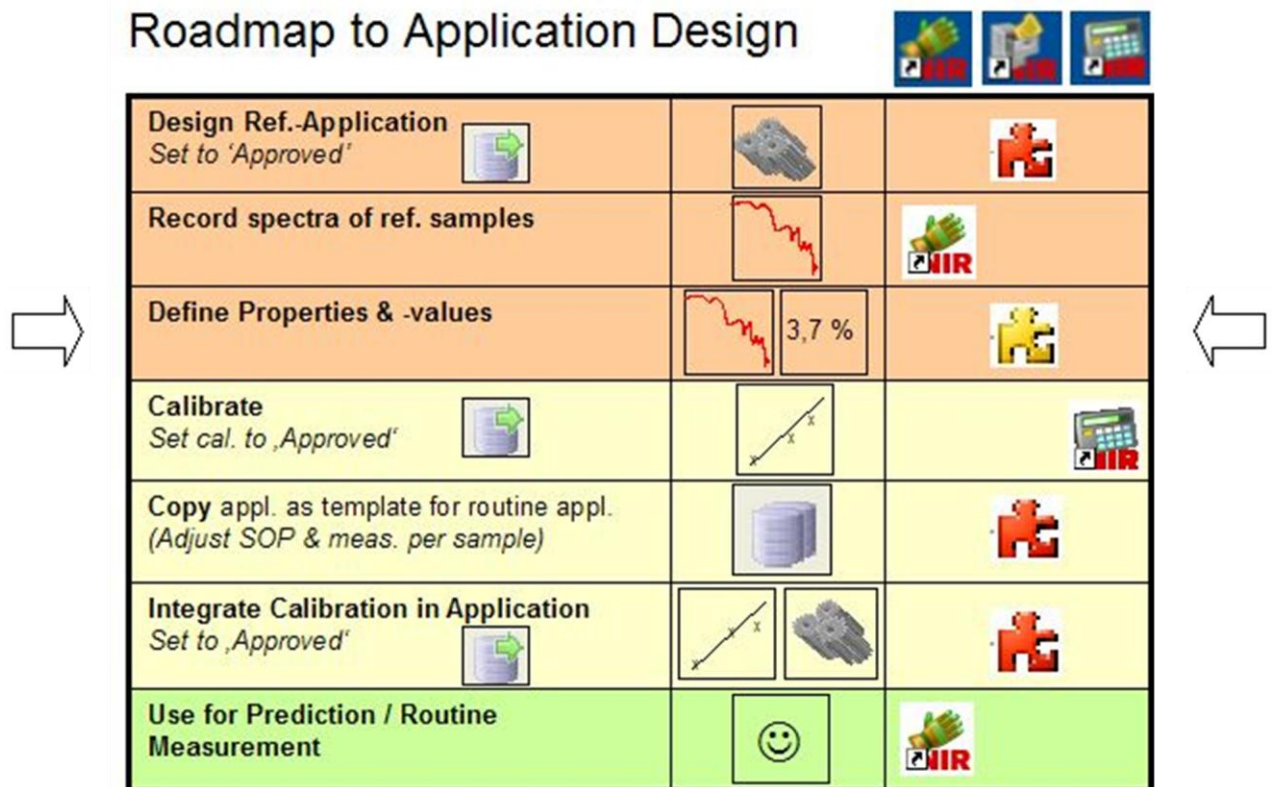


To select (or deselect) a line in the list, press and hold the Ctrl-icon on your keyboard while left-clicking on that line. Click on the red cross button to delete the selected measurements.

After completion of the measurement of your reference samples, switch to the NIRWare Management Console to continue with the next step in application development: the assignment of properties and property values. In this case, it means to add the substance identity behind each spectrum.

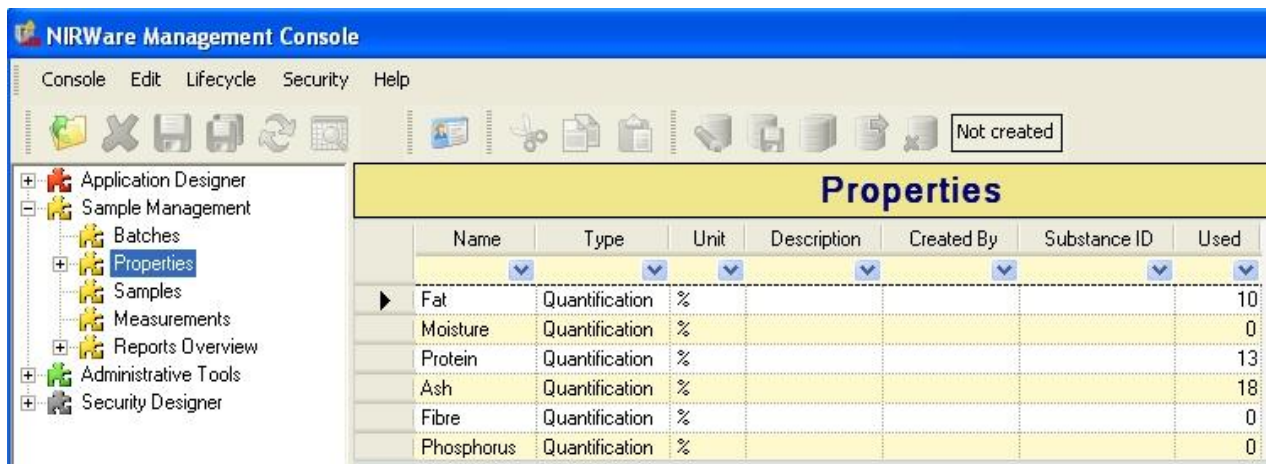
5.3.4. Defining a property and a property value

After the spectra of the reference samples have been measured, the properties (here: identities) have to be connected to the reference samples. This is done in the NIRWare Management Console (MC). The so created data sets are later on the basis for building a calibration in NIRCal.



Switch to the MC, and select 'Sample Management' from the tree menu.

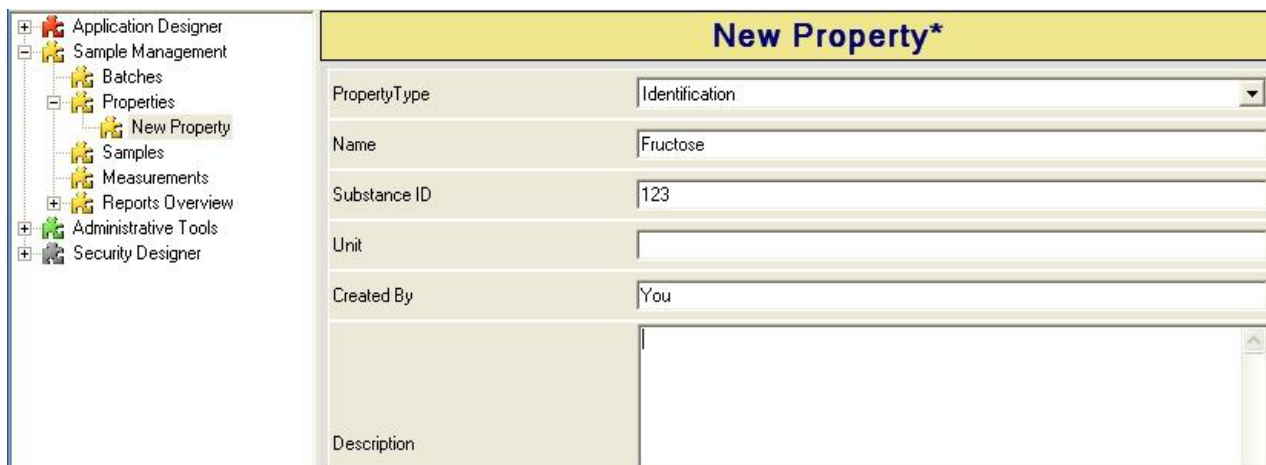




Select 'Properties' to open a list with all properties that have been defined so far.


NOTE

If the property you need is not in the list, create it by clicking on 'Properties' in the tree menu, and then selecting 'new property'.



Define the type (here: identification) and name of the property.

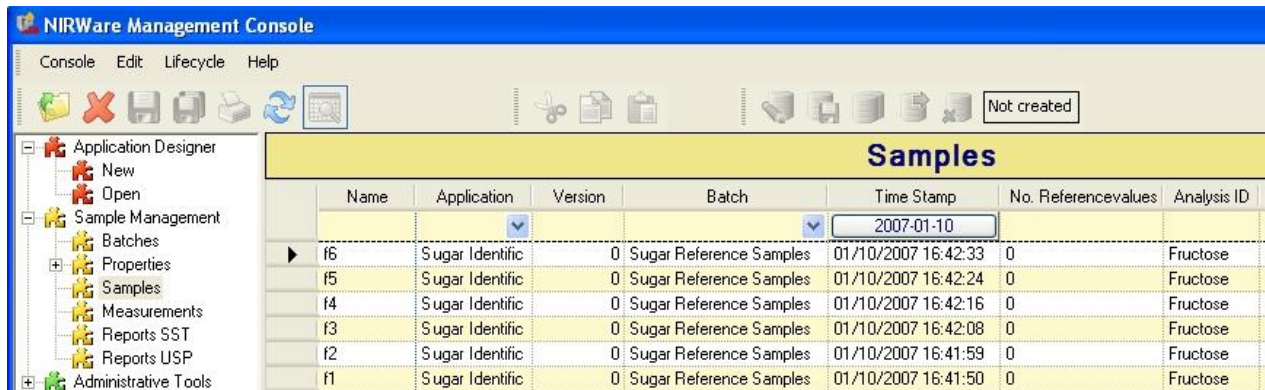
Note: Additionally, it is possible to define several Substance IDs, for example a company specific number code that is used as substance label. This code can be used later on in the Operator software to define the expected substance in the ID application, instead of the substance name. Also type in your name to document who created this property.

Click on the Save icon  to write this property definition to the database.

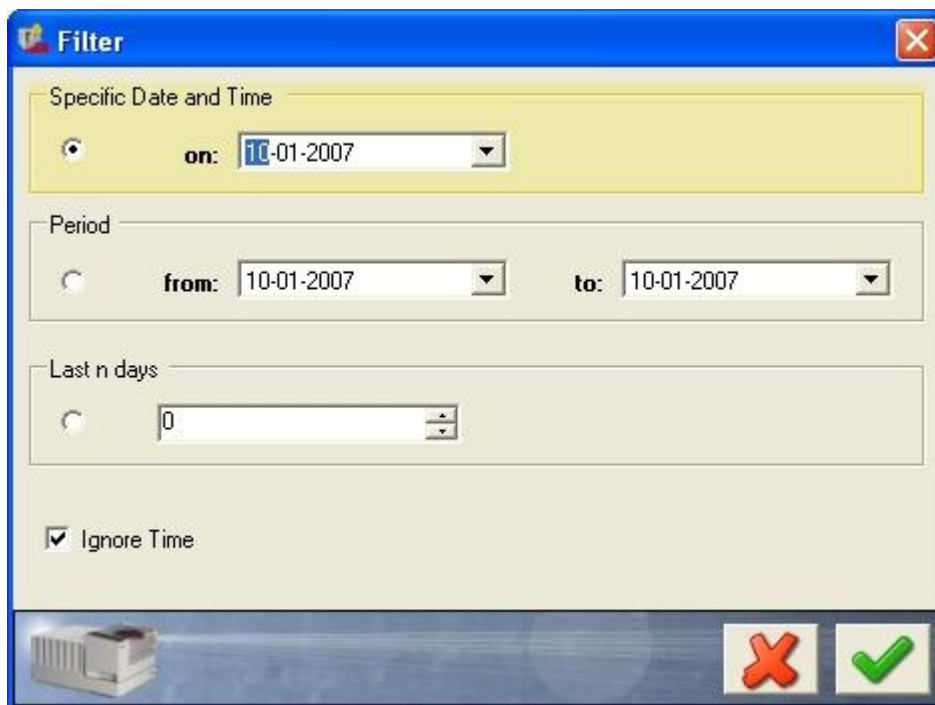
Create all new properties accordingly.

Now we want to tell the computer which sample belongs to which property.

Switch to 'Sample Management – Samples' to open a list with all samples that have been measured.

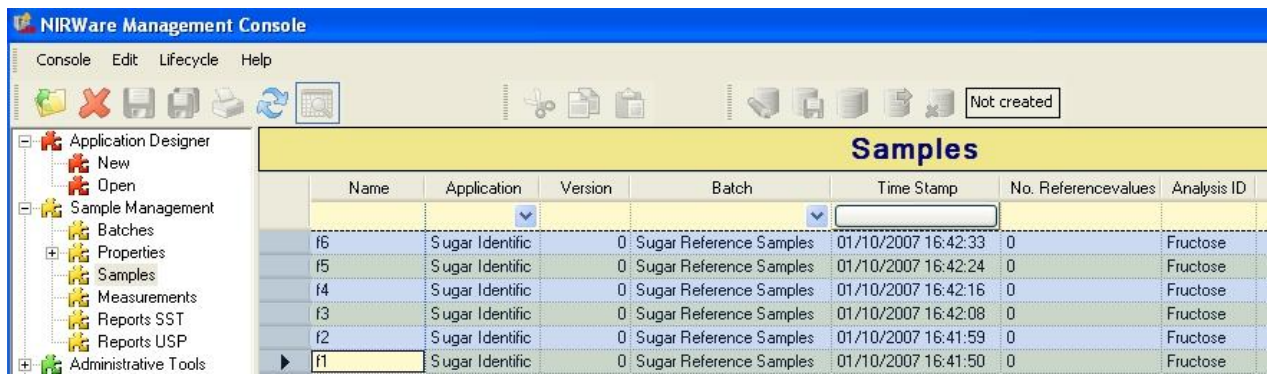


Notice that in the list the 'Time Stamp' filter is set to a specific date.



Right click the time stamp icon to ignore, or left click on it to edit the filter settings

To shorten the list of samples, you can also use additional filters, e.g. on the 'Application' column. This can be helpful if you used dedicated applications for reference spectra measurement of each sample type.

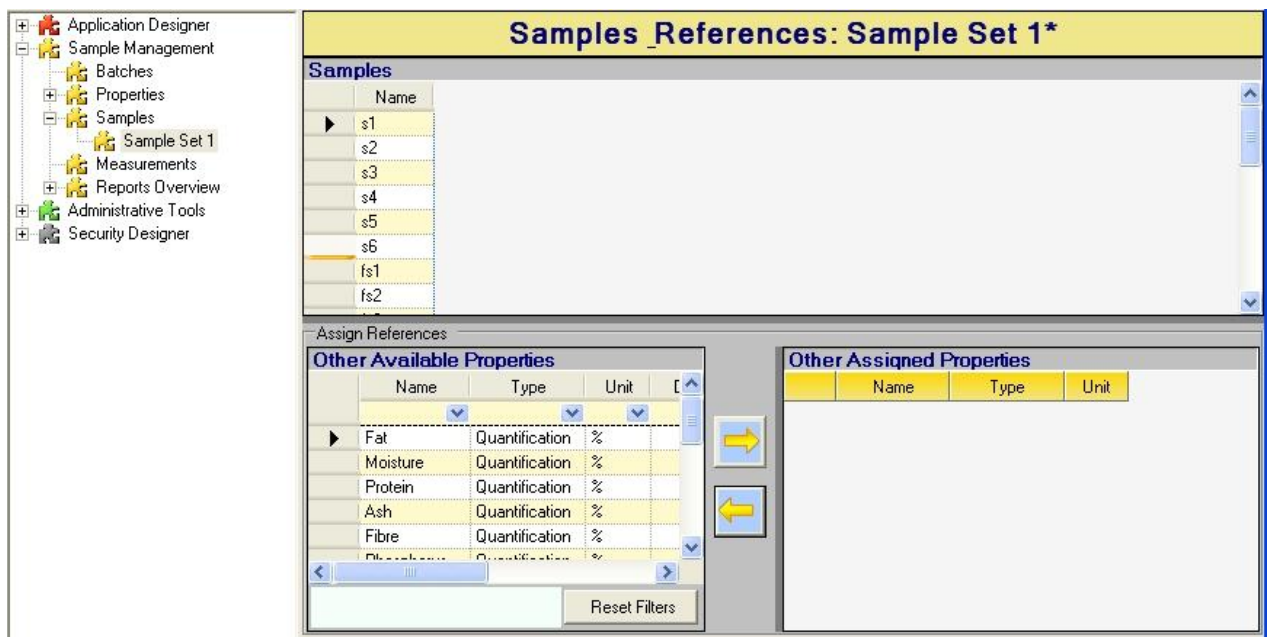


Select your reference samples by clicking on the topmost reference sample in the list. Then press and hold the Shift-button on your keyboard while scrolling down the list (using the mouse or the arrow keys on your keyboard). Alternative: By pressing 'Ctrl-Shift-End' on your keyboard you can highlight everything from the first selection down to the end of the list.



Then click on the 'Open existing data set'-icon in the upper left corner to create a new Sample Set.

A window with three lists opens: 'available properties', 'assigned properties', and 'samples'.



This allows you to select properties for the samples by shifting them from the 'available' to the 'assigned' list.

Samples_References: Sample Set 1*

Samples

	Name	Fructose	Lactose	Fine Sucrose	Sucrose
▶	s1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	s2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	s3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	s4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	s5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	s6	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	fs1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	fs2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Assign References

Other Available Properties

	Name	Type	Unit	D
▶	Fat	Quantification	%	
	Moisture	Quantification	%	
	Protein	Quantification	%	
	Ash	Quantification	%	
	Fibre	Quantification	%	
	...	Quantification	%	

Reset Filters

Other Assigned Properties


	Name	Type	Unit
	Fructose	identification	
	Lactose	identification	
	Fine Sucrose	identification	
▶	Sucrose	identification	

Select a property that you want to assign to your samples. Then click on the right-arrow key to shift it to the 'assigned' list. Repeat this process for all your properties.

Samples

	Name	Fructose	Lactose	Fine Sucrose	Sucrose
	s4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	s5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	s6	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	fs1	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
	fs2	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
	fs3	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
	fs4	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
✎	fs5	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Notice that this assignment created a matrix with check icons in the 'Samples' window. By activating the check icons you can now easily create a matrix that connects sample (=row) and property (=column).

Save these data by clicking on the corresponding icon .

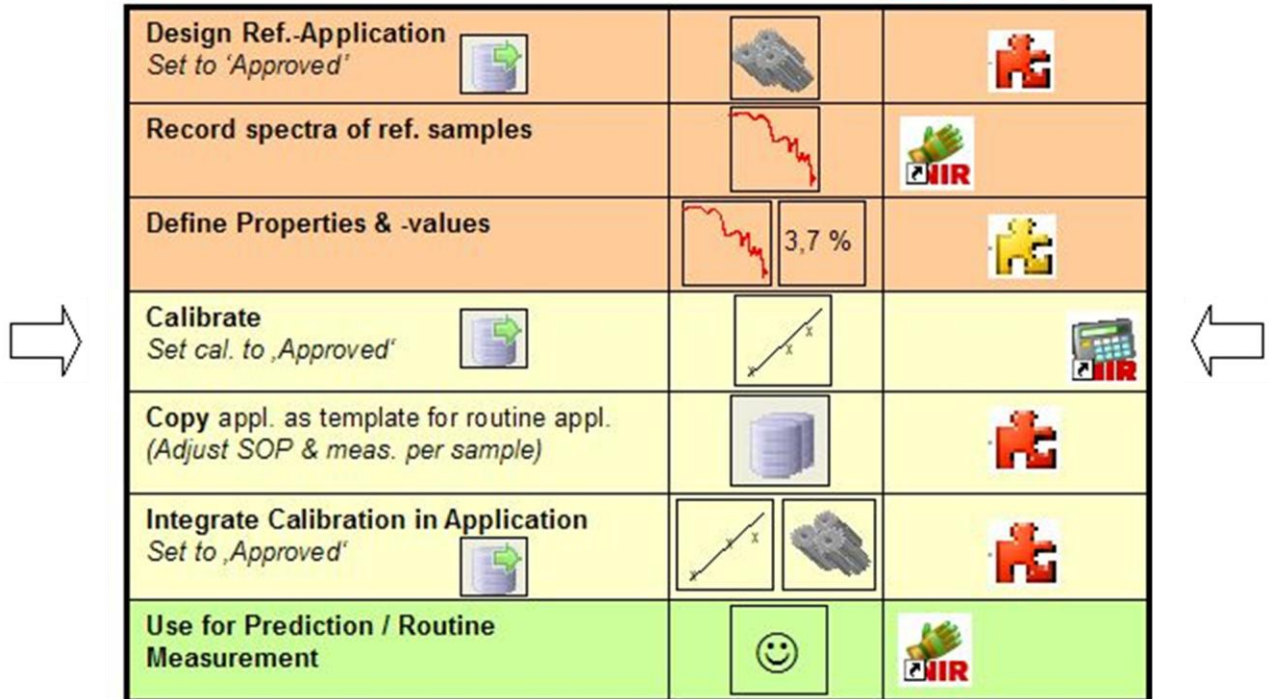
You can now switch to NIRCal to build a calibration based on this data set.

5.3.5. Creating a basic calibration by using the NIRCal wizard

This chapter describes how to create a calibration with NIRCal, using the data set of reference spectra with previously assigned properties. The description here is limited to the use of the NIRCal wizard, since

detailed optimization procedures and description of NIRCal features are described in the NIRCal documentation.

Roadmap to Application Design




Start NIRCal and log on as an administrator.





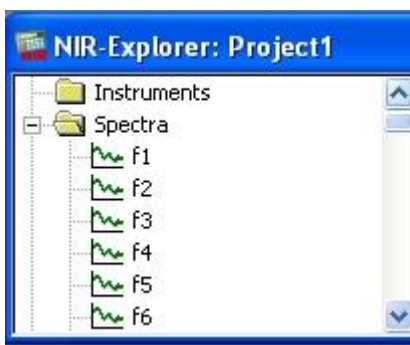
From the menu, select View/Toolbars and select the Toolbars as shown in the picture

To load spectra from the database into your empty project, click on the binocular icon .

Select the spectra from the list, and click on the green check mark icon.



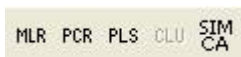
To simplify the selection, use appropriate filter settings, especially for 'Time' and 'Application'. (Time: right click to ignore time filter, left click to set time filter settings.)




Since we performed triplicate spectra measurement of each sample, we now find three spectra for each individual sample.

Select the NIR-Explorer window, select 'spectra' from the tree menu and check if all spectra have been correctly loaded.

Before calculating a first calibration, make sure that 'CLU' (for 'cluster calibration') is selected in the menu bar



Click on the Overview icon  to start a first calculation.

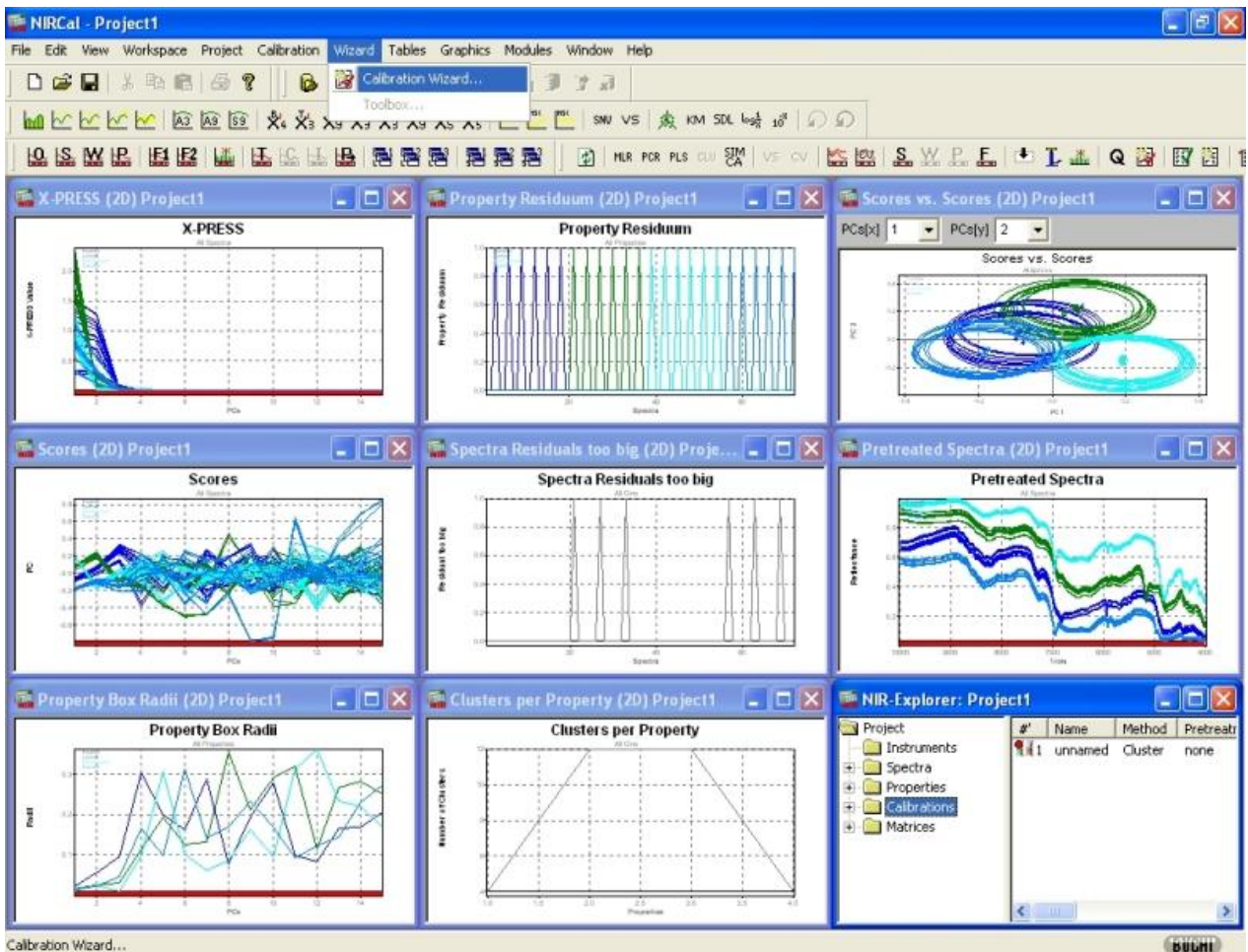
A message appears regarding Calibration- and Validation set selection (C-Set and V-Set):



Click on YES to let the C/V-selection wizard create a selection.

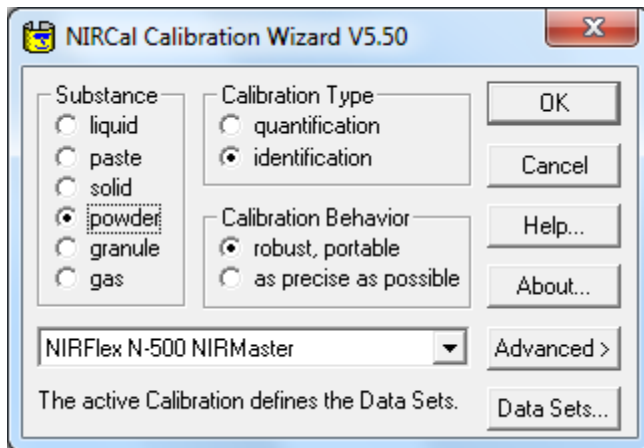
Note: It is highly recommended to perform the selection sample wise, so that ALL spectra of one individual sample are EITHER in the C- OR V-Set. This is described in detail in the NIRCal documentation. For our example, we will leave the result from the selection wizard untouched.

A full calculation is performed, and the result is visualized in nine windows.

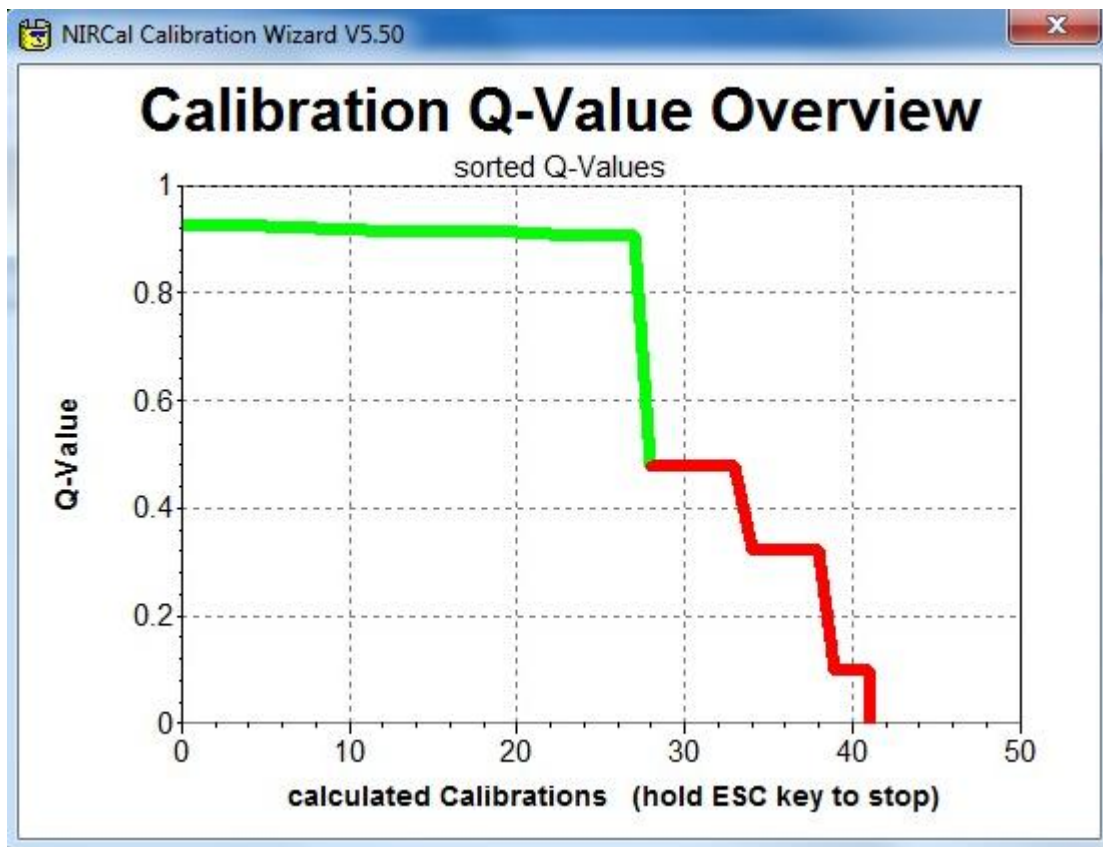


In case that your spectra are all shown in the same color, they are all marked as selected. Press the 'C' icon to unselect, so that you can differentiate between the different property colors.

From the menu, select 'Wizard - Calibration Wizard' (see above). A dialog appears for defining general parameters.



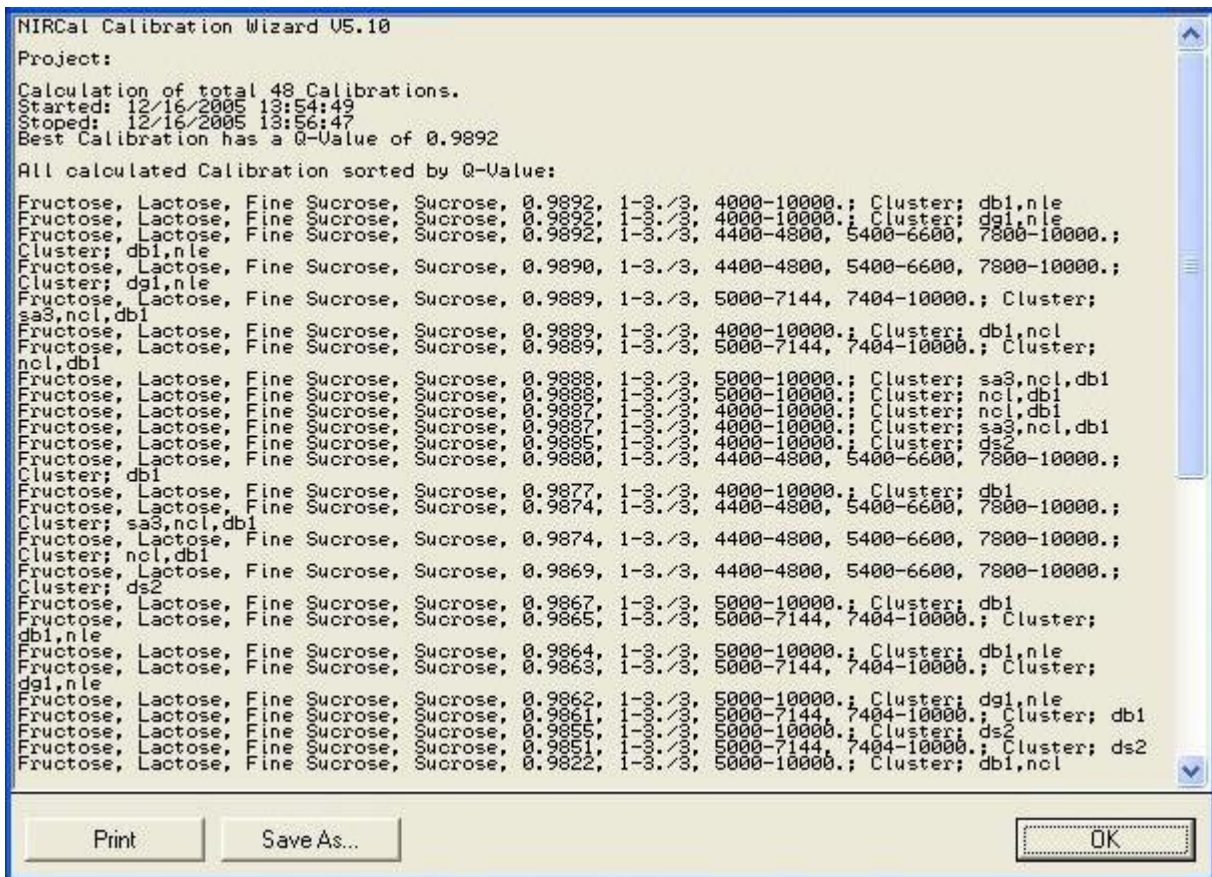
Select 'identification' as calibration type, and click on 'OK'.



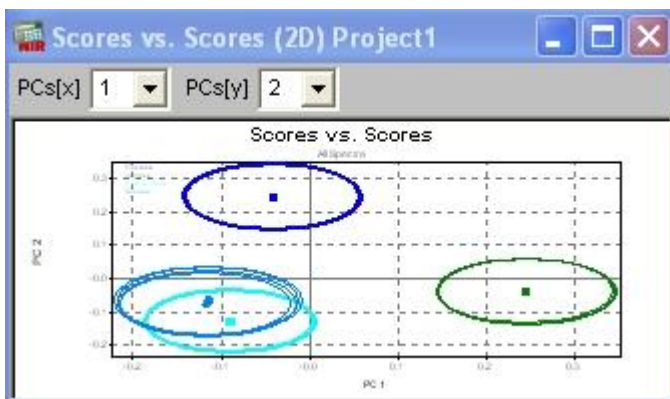
The wizard now starts with the optimization process, which will take a few minutes. The progress is visualized in the 'Calibration Q-Value overview'.

In the course of the optimization process, you see the Q-Value rise from zero (no working calibration) up close to 1 (=perfect calibration).

After the wizard is finished, the results are shown in a list where the best calibrations (with the highest Q-values) are found on top of the list.



The ten best results are stored in the NIRCAl Explorer, and the one with the highest Q-value is set to 'active'.



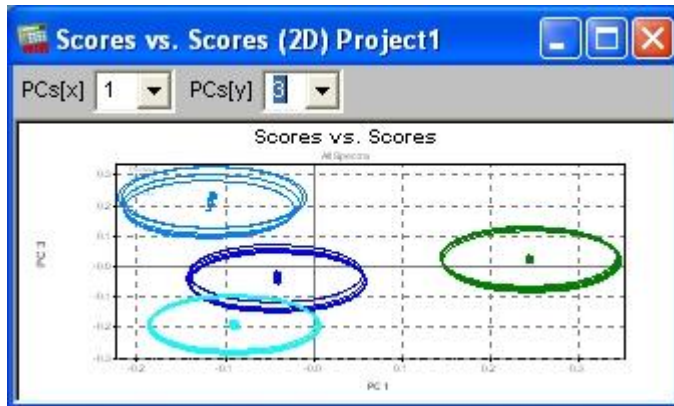
From the plot 'Scores vs. Scores' of PC1 vs. PC2 you can see an excellent separation for two of the four properties.

Only one overlap is displayed.

But since we look at a 2-dimensional projection of a multidimensional space, we have to keep in mind that an overlap might only result from the projection, and not from a spatial interpenetration of the clusters in

the multidimensional space. In other words: we have to check if the overlap is only a question of perspective.

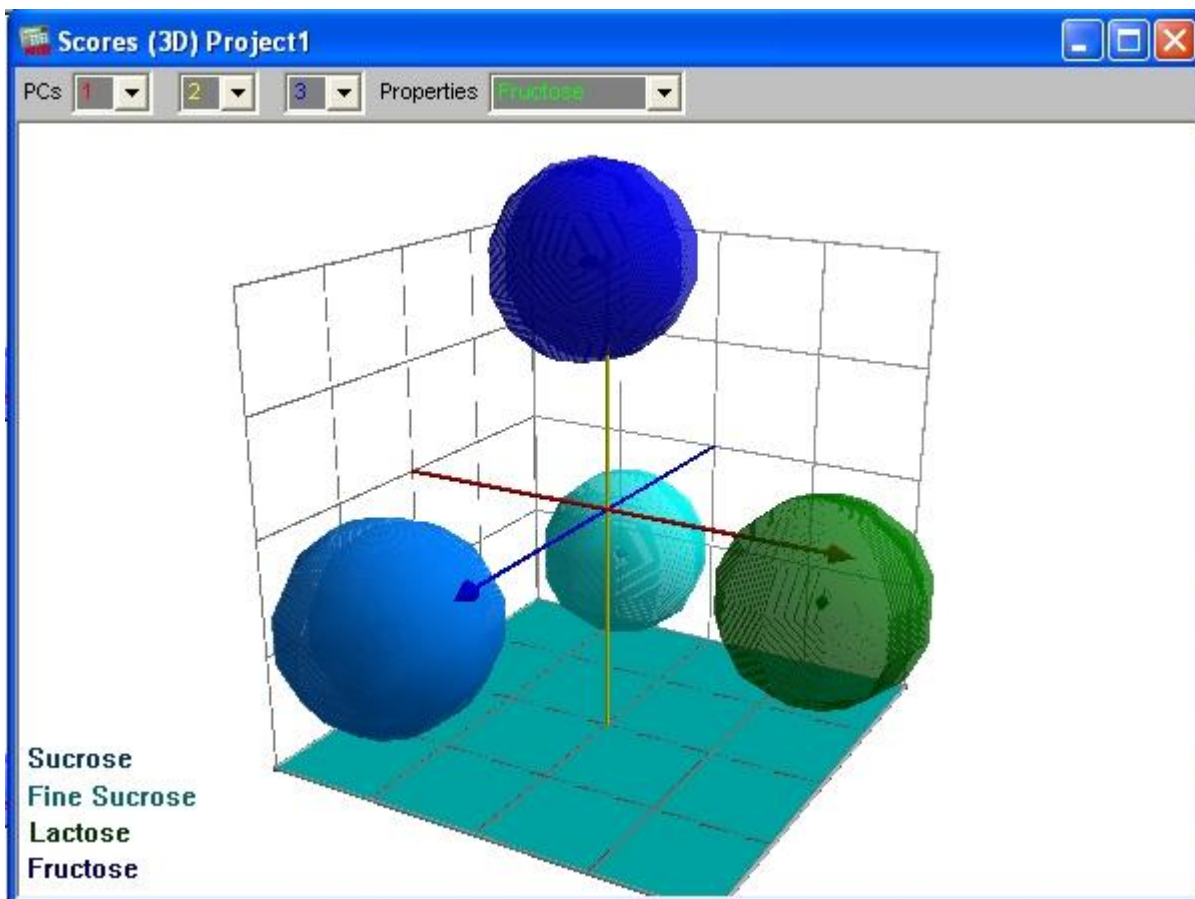
For this purpose, we select a projection to PC1 vs. PC3.



Notice that we see an overlap again, but of different clusters. The overlap from the first projection is now resolved. This proves that the four clusters are in fact separated from each other.

This can be clearly demonstrated by using a 3D- instead of a 2D-projection:

Select from the menu 'Graphics – Scores – 3D-Scatter', and have a look at a 3D-projection on PC 1, 2 and 3



Click on the 'R' icon on your keyboard to start (and stop) the autorotation function.

The plot confirms that the calibration from the wizard is well capable to differentiate between all four sugar types.

(Comment: For more complex examples, the same rule for overlap checking applies to 3D- as for 2D-projections: Look at every overlap from different perspectives.)

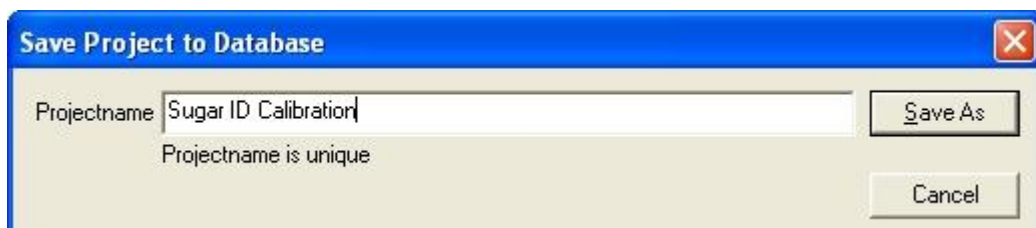
Now switch again to the NIRCal Explorer window and have a look at the 'Calibrations'

Project	#'	Name	Method	Pretreatments	Creator Login	Created	Q-Value
	1	unnamed	Cluster	none	Administrator	16.12.2005 13:49:11	0.01880
	2	Q-value, secondary/primary PCs, wave selection	Cluster	none	Administrator	16.12.2005 13:54:44	0.14157
	3	Fructose, Lactose, Fine Sucrose, Sucrose, 0.9889, 1-3./3, 5000-7144, 7404-10000.	Cluster	sa3,ncl,db1	Administrator	16.12.2005 13:55:32	0.98894
	4	Fructose, Lactose, Fine Sucrose, Sucrose, 0.9890, 1-3./3, 4400-4800, 5400-6600, 7800-10000.	Cluster	dg1,nle	Administrator	16.12.2005 13:56:03	0.98902
	5	Fructose, Lactose, Fine Sucrose, Sucrose, 0.9892, 1-3./3, 4400-4800, 5400-6600, 7800-10000.	Cluster	db1,nle	Administrator	16.12.2005 13:56:11	0.9891E
	6	Fructose, Lactose, Fine Sucrose, Sucrose, 0.9892, 1-3./3, 4000-10000.	Cluster	dg1,nle	Administrator	16.12.2005 13:56:34	0.9891E
	7	Fructose, Lactose, Fine Sucrose, Sucrose, 0.9892, 1-3./3, 4000-10000.	Cluster	db1,nle	Administrator	16.12.2005 13:56:42	0.9891E

Note that the ten best calibrations are stored here. The one with the highest Q-value is set to active (indicated by a red dot).

Since we only need one calibration, we select everything except for the one we want to keep. This is done by holding down the Ctrl-Key while clicking in the list on the calibration to be selected. Then right-click on the selection and choose 'delete'. A confirmation message appears, which you will answer with YES.

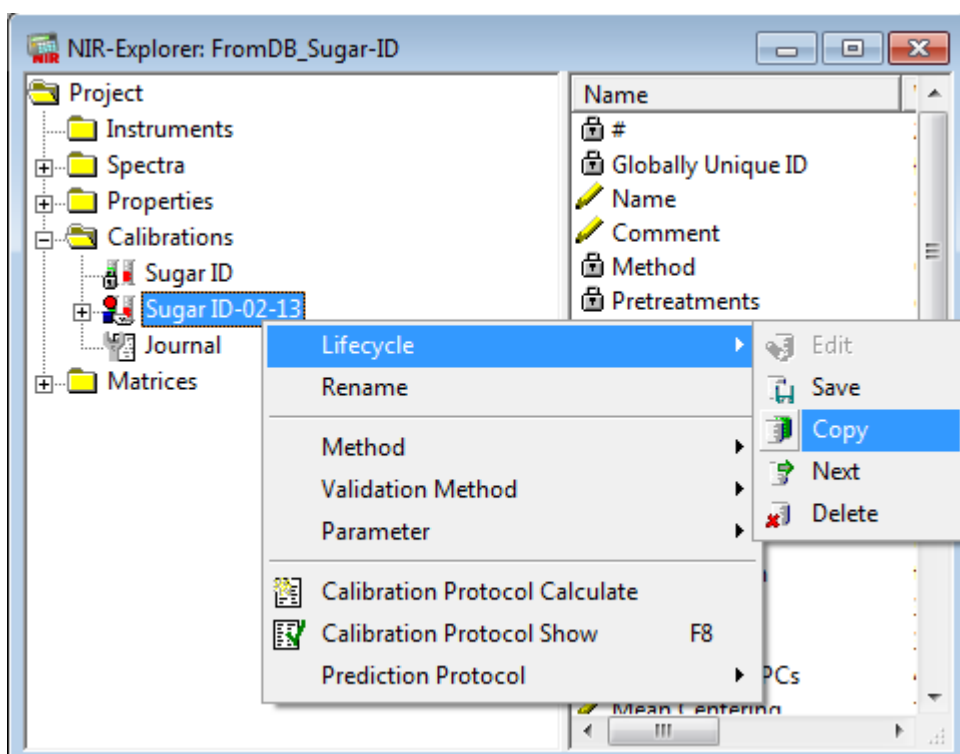
To save the calibration to the database, click on the 'save' icon in the menu bar .



Type in a name for your NIRCal project and click on the 'Save As' icon.

So far the calibration is still in the 'created' state. If you would try to use it in an application, this would prevent you from changing your application (!) into the next state, because an approved application requires an approved calibration.

It is suggested to recalculate the first calibration. This is a master calibration, which organises the spectra in the project and can never be put the approved LC state. Copy this calibration, open the copy (LC: Edit), rename this: give a short name preferable with date at the end. Make a new calculation after renaming. Put this calibration to "approved" state.



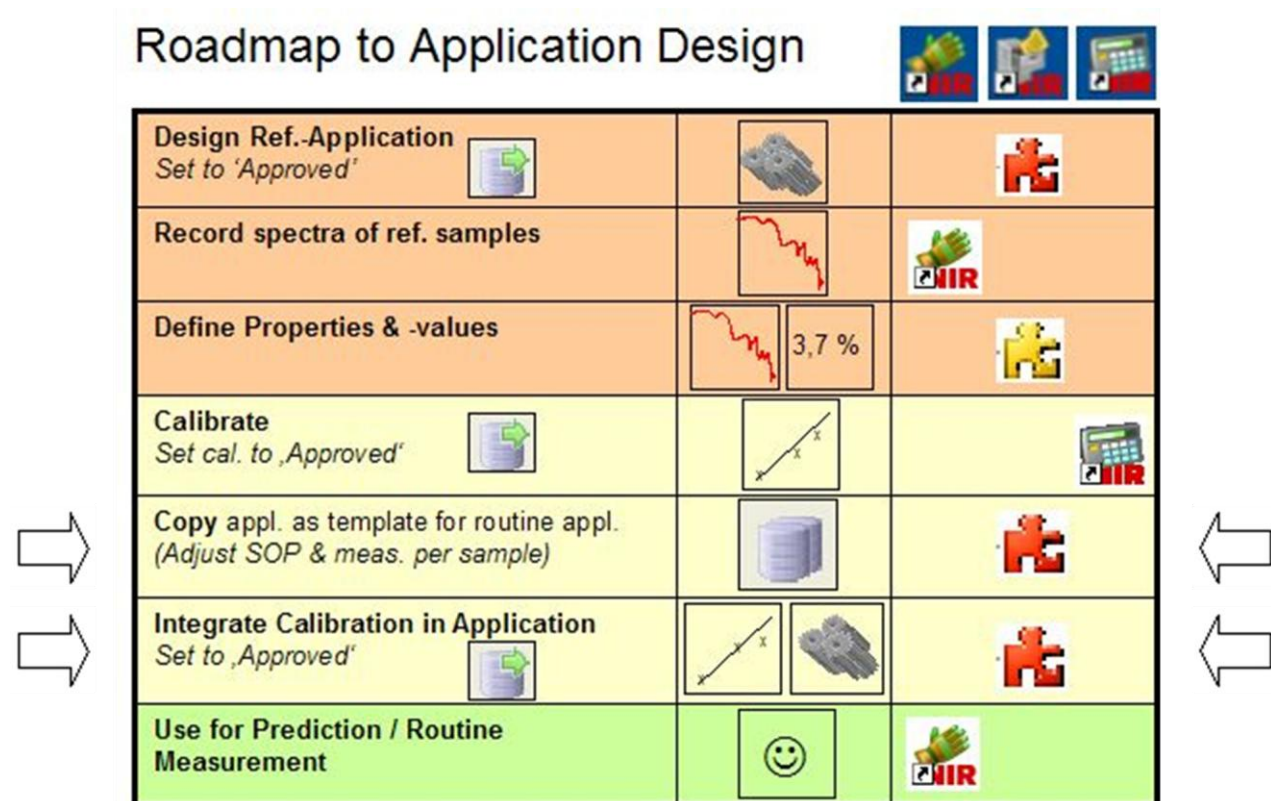
To put your application into the next state, right-click on the name of the calibration in the NC Explorer, select 'Lifecycle' and 'Next'.

Now your calibration is finished and in the approved state, so it can be used for integration into an application. This is done in the NIRWare Management Console. (Please remember that only applications with an approved calibration can be approved.)

5.3.6. Integrating a qualitative calibration into an application

The final step in creating an application for identity control with NIR is to integrate the calibration into the application.

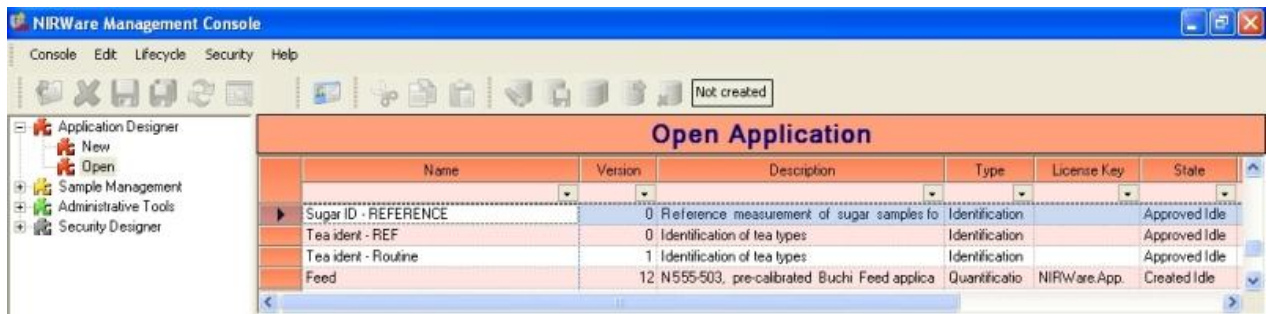
Remember that we started with an application for triplicate measurement of reference substances. This serves now as a template for the routine application. In effect, we create a copy of the reference method, make adjustments to this, and integrate the calibration. Adjustments involve mainly the number of measurements per sample, the SOP text, and Reports. All instrument parameters remain untouched, ensuring identical spectral conditions for both reference samples and those to be tested.




Both the creation of the routine use application and the integration of the calibration into this is performed in the NIRWare Management Console (MC).



Load the existing application for data acquisition by choosing 'Open' from the 'Application Designer' in the tree list. Then select the application from the list on the right:




The application is now available as a new point in the tree menu.

Click on the 'Copy' icon  to create a copy of this application.

This copy starts in the 'created' state, while the original application remains 'approved'.




To change the name, you first have to click on the 'Edit' icon .

This causes a change from 'idle' to 'edit' mode.

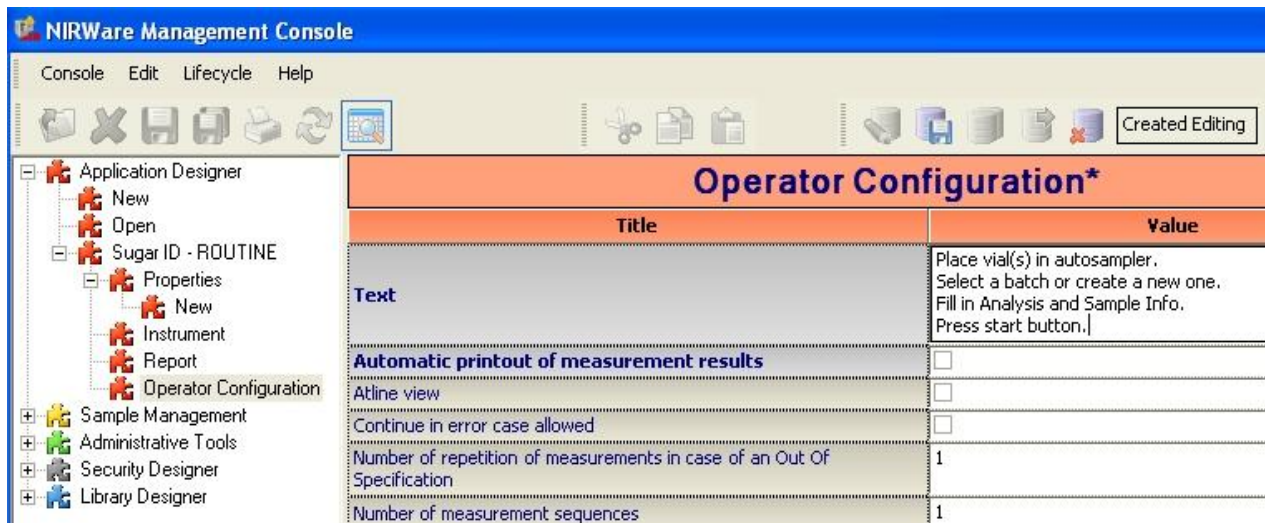
Now you can change application name and description

Copy of Sugar ID - REFERENCE*	
Title	Value
Application name	Sugar ID - ROUTINE
Application type	Identification
Application description	Enter here the name of the new application

Save this change to the database by clicking on the 'Save' icon .

Next we change the 'number of measurement sequences' from 3 to 1.

From the tree menu, select the 'Operator configuration' menu of your application

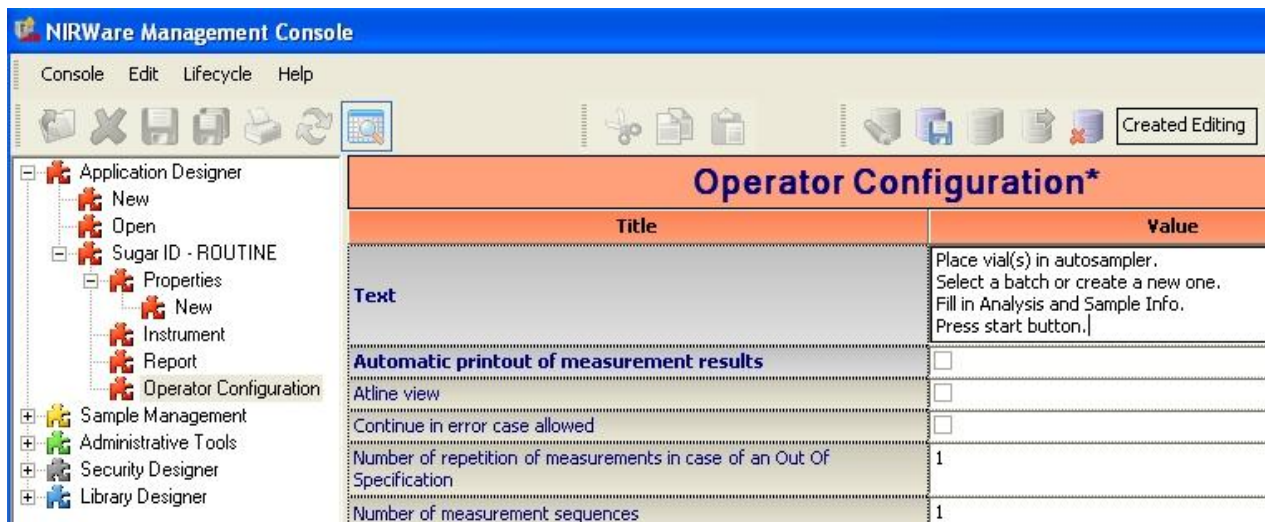



Remember that the complete view as shown above is only visible if the icon 'show advanced settings'



was activated.

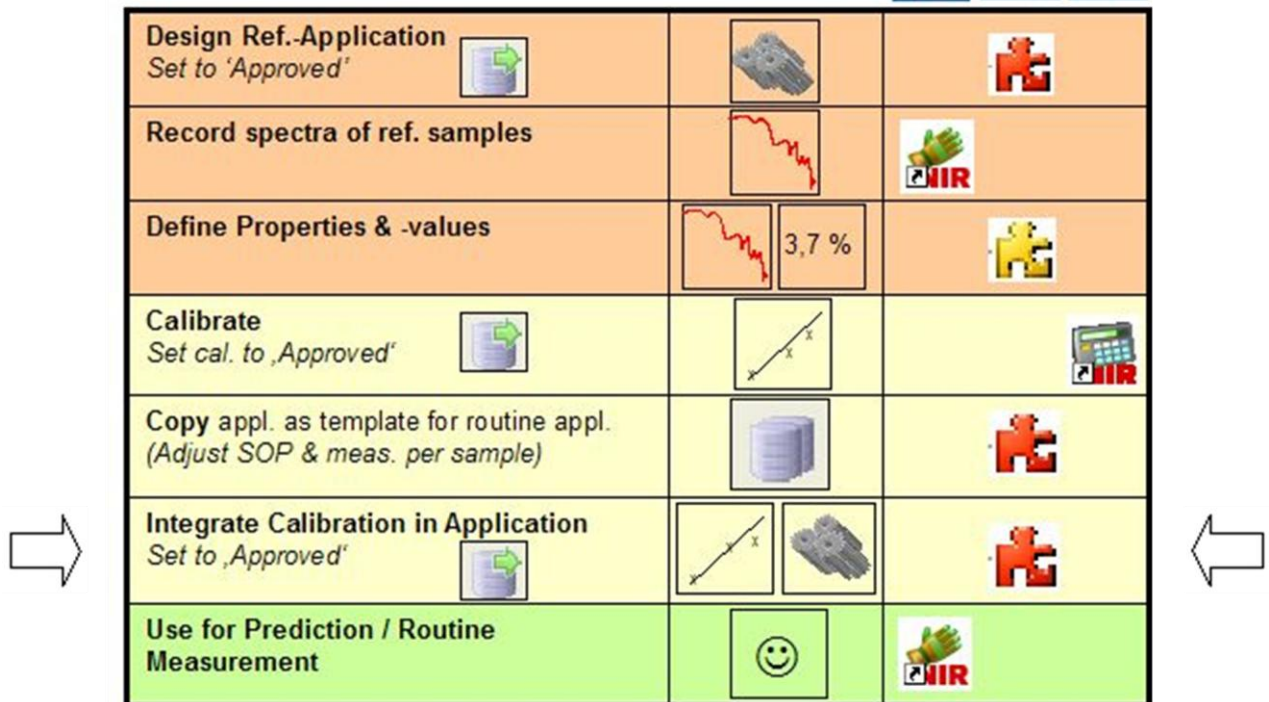
Again, first change to 'edit' mode. Then change the number of measurement sequences to '1'. Also type in an appropriate Standard Operation Procedure (SOP) description:



Save this dataset by clicking on the save icon  again.

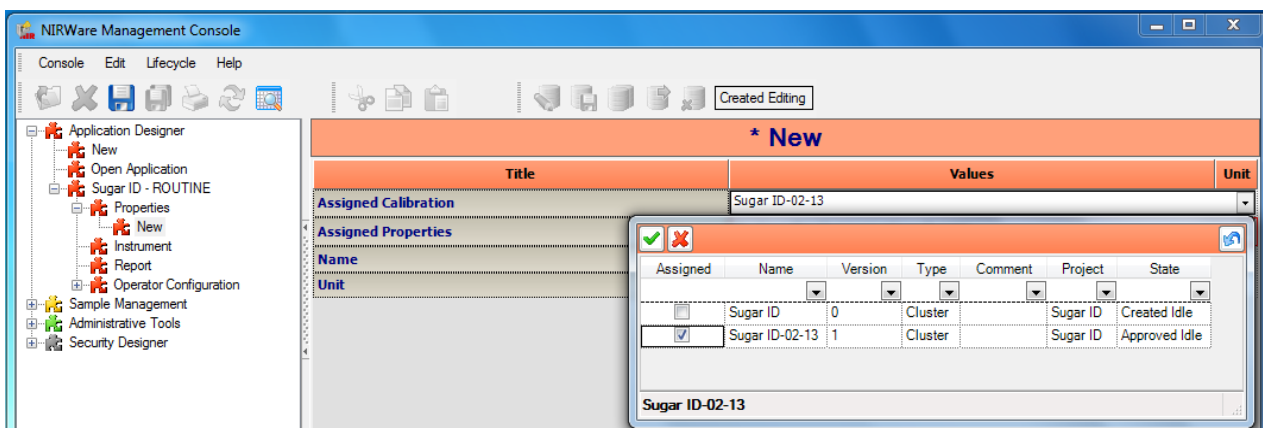
The application for routine use has been prepared, and the calibration can now be assigned to it.

Roadmap to Application Design

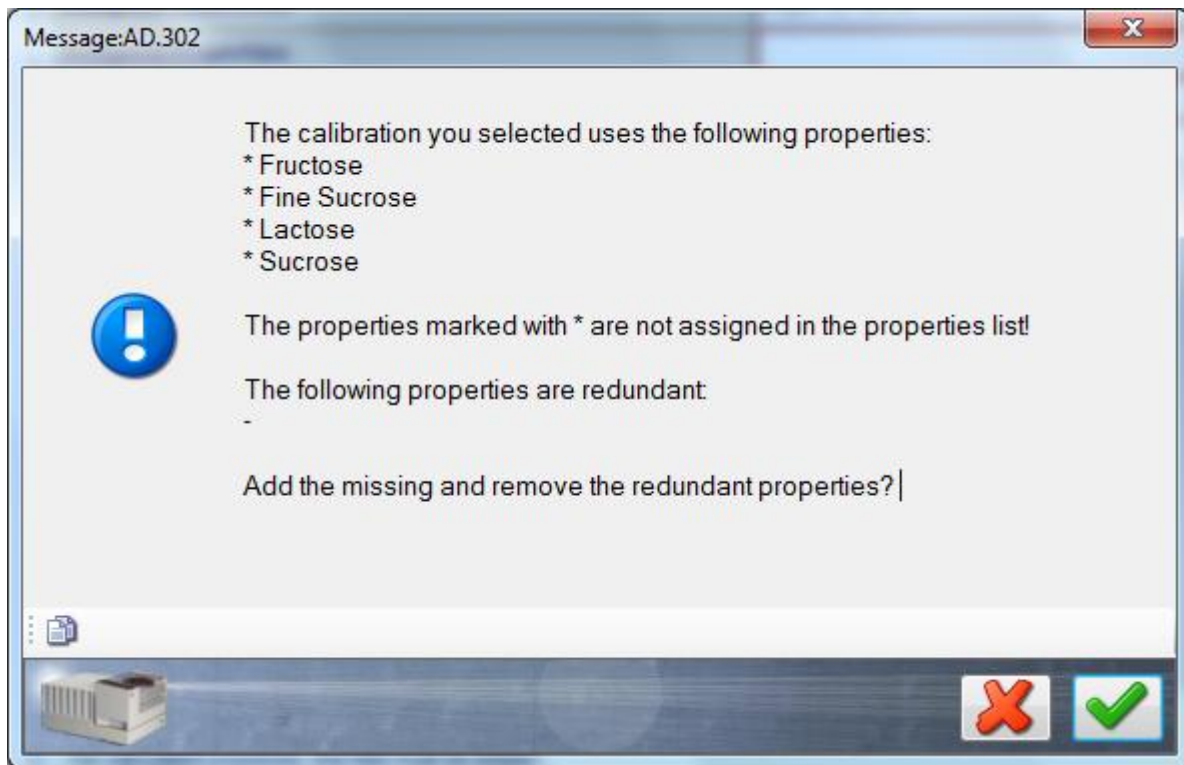


On the Properties level click the button to make the property editable.

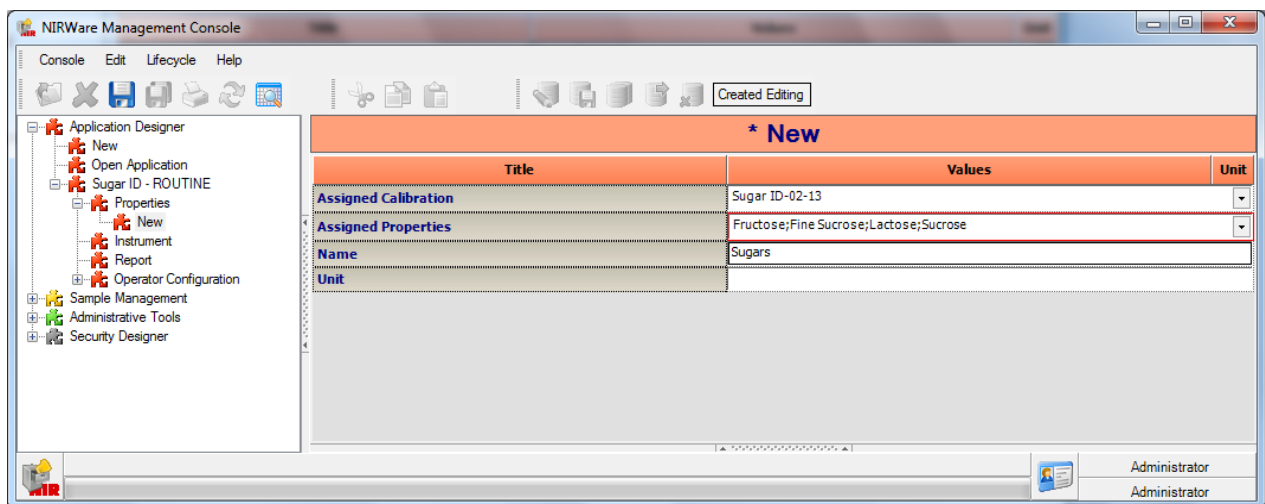
Select 'Properties - New' menu from the tree menu of your application and select the drop down-menu for 'Assigned Calibration'.



In the 'Assigned' column, set a check-mark in front of the calibration you want to use. Click on the green check-mark button to assign the chosen calibration to the application. A message appears, which you just confirm:




The properties defined in the selected calibration are now automatically assigned to the application.



A 'Name' can be entered as a label to e.g. translate a foreign property name.


The 'Unit' field should be left blank, since we do not create a quantitative application.

Save all changes made to this data set .

Then select your application from the tree and save it also to the database .

Now this newly created application is ready for use in the operator software, but only for administrators.

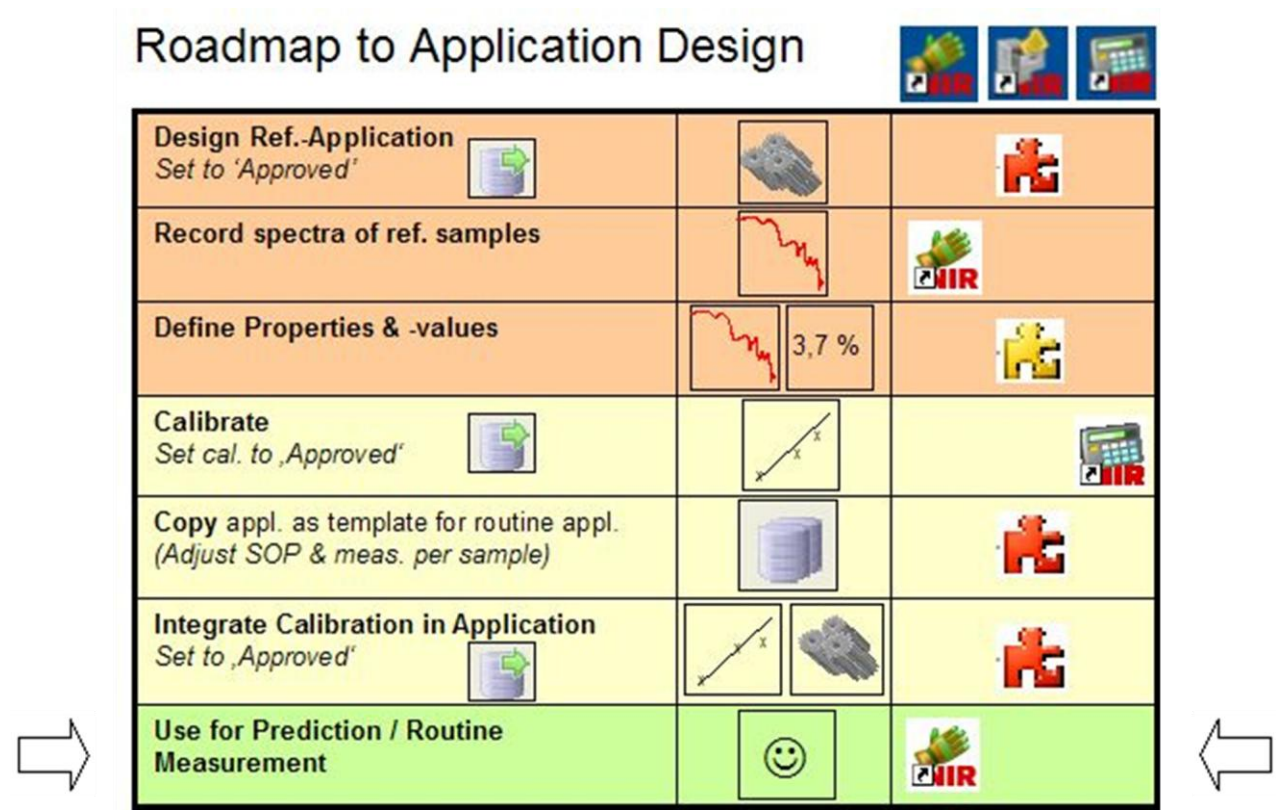
NOTE:

To make this application also available for operators, select the application and put it in the approved state .

You can now start with routine ID checking of sugar samples with the Operator software.


5.3.7. Routine use for ID check

The previously developed application was designed for routinely testing of the identity of sugar samples. Similar applications are performed in the pharmaceutical industry, especially for ID testing of incoming raw materials.



To use the previously created application for sugar ID check, switch to the Operator software and log on as an 'Operator'.



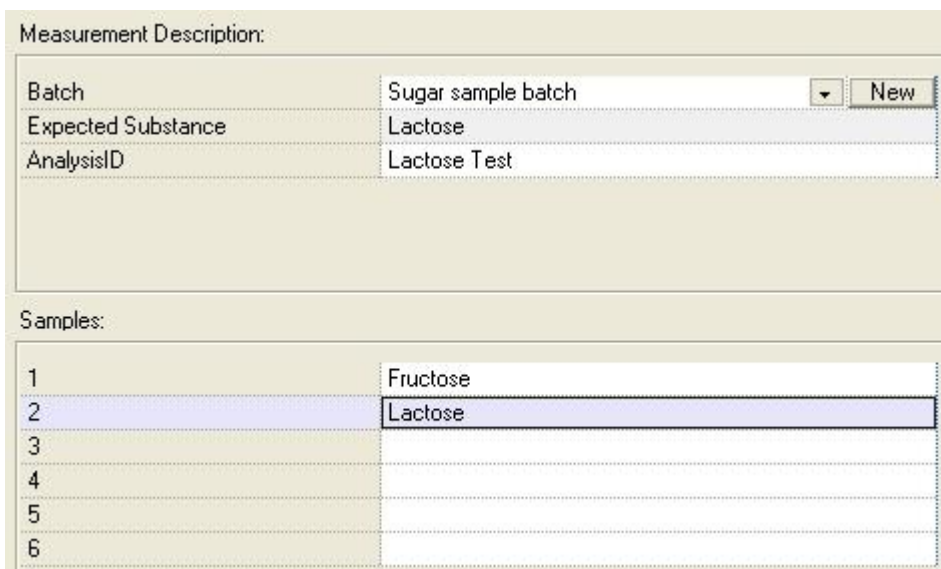
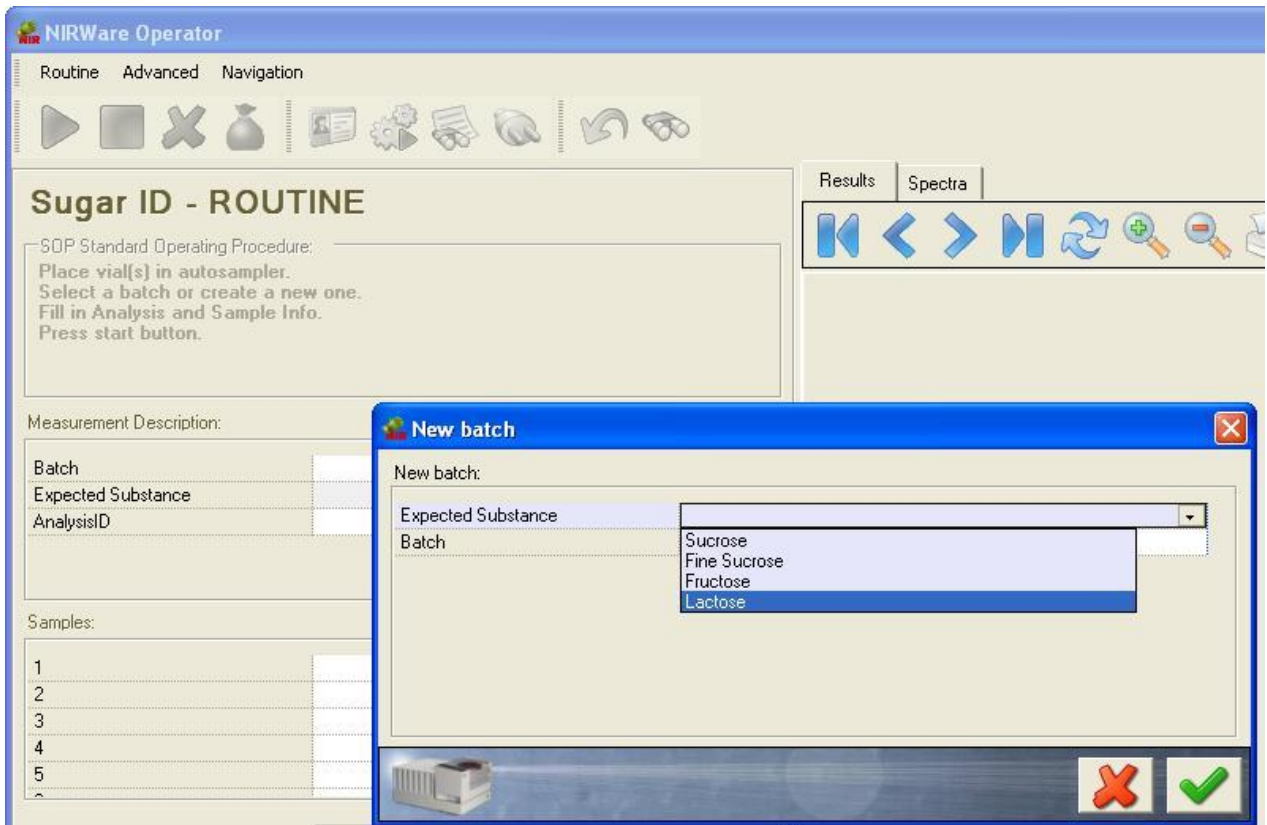
Select your application for routine measurement by clicking on the binocular icon .

Select your application from the list:

Select an Application

Name	Version	State	Description
Sugar ID - Routine use			
Sugar ID - Routine use	1	Approved Idle	Routine use for ID testing of sug

Create a new batch and define name and expected identity of the substance(s) you want to test:

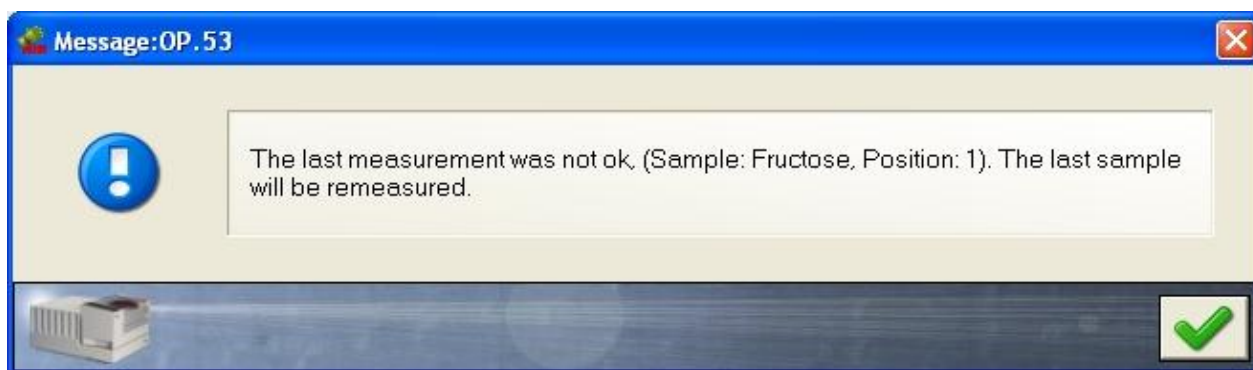


We want to use the application to check if our sugar samples really consist of lactose ('milk sugar'). For demonstration purposes, we choose a sample of fructose ('fruit sugar') and one of lactose

As expected substance we choose lactose. If our calibration is working properly, the first sample will be rejected, and the second one accepted.

Press the green arrow button to start the measurement sequence.

Since the identity of the first substance is (deliberately) not the expected one, the following message appears:



Confirm by clicking on the green check mark button. The sample will then be measured a second time. This is the default setting in case of a failed ID test, and can be adjusted in the Management console.

The second sample is accepted, since name, spectral deviations (residual) and distance to cluster are all within the allowed limits of the calibration.

Sample: Lactose			
Identity:	ok		
Expected substance		Lactose	
Found substance	ok	Lactose	
Distance:	ok	0.002007	
Spectrum residual	ok	0.000334	
		Max. distance:	0.100089
		Max. allowed residual	0.000917
Hitlist			
-hit	Substance	Distance allowed	Distance
1	_lactose	0.100089	0.002007 ok
2	_lactose	0.100124	0.002082 ok
3	_lactose	0.100111	0.003053 ok

In the report of the rejected sample, we find also more information than just the fact that this sample was rejected:

Sample: Fructose		Measurement No.: 1	
Identity:		not ok	
Expected substance		Lactose	
Found substance	x	Fructose	
Distance:	ok	0.010827	Max. distance: 0.105788
Spectrum residual	ok	0.000450	Max. allowed residual: 0.000917
Hitlist			
Hit	Substance	Distance allowed	Distance
1	Fructose	0.105788	0.010827 ok
2	Fructose	0.105816	0.011759 ok
3	Fructose	0.106081	0.012277 ok

The spectrum residual is judged to be OK, which indicates that the spectrum is very similar to those that the calibration was built on.

'Distance OK' tells us that the spectral representation falls within the boundaries of a cluster, but because 'found' and 'expected' substance differ, the sample is falling into the wrong cluster and is thus rejected.

So from the report you can be sure that the sample is not lactose, but -with high probability- fructose. With this information a further investigation is now possible to check if just the label was wrong, or an independent analytical method can be used to confirm the ID suggestion of the NIR application.

This example clearly shows that ID testing with NIR integrates a label check!

5.4. Creating a quantitative application

5.4.1. Introduction

This tutorial describes how to create an application for quantification. As an example, the NIRFlex N-500 is used with the solids cell and the vials (autosampler) option.

The application shall be capable of quantifying

- the concentration of Lactose ('milk sugar') and
- the concentration of Fine Sucrose ('powder sugar')

in a mixture of both substances. Concentrations are expressed in % wt. (g / 100 g). In NIRWare 1.5 if there is a 2 component system like this, one property can be calibrated and the other calculated, e.g. Fine Sucrose concentration = 100-Lactose concentration.

The process of creating a ready-to-use NIR application requires calibration samples. These are samples of doubtless quality and composition. In combination with their NIR spectra ('calibration spectra') they provide the necessary data sets for calculation of a chemometric calibration. The calibration can then be used for prediction, which means deriving the identity information from the spectra of substances to be tested.

It is recommended to use two dedicated applications for acquisition of calibration data and routine use (=prediction).

NOTE

The terms 'reference measurement', 'reference samples' or 'reference spectra' used in the tutorial describes the data collected for calibration development.



















To ensure that all samples are measured under identical spectrometric conditions, we suggest to start the development of the routine application with a copy of the application for acquisition of calibration data, which is then adjusted.

Please keep in mind that only applications in the 'approved' Lifecycle state are visible to (and usable by) a user of the 'Operators' user group.

These considerations are visualized in the following scheme:

Roadmap to Application Design



Design Ref.-Application <i>Set to 'Approved'</i> 		
Record spectra of ref. samples		
Define Properties & -values		
Calibrate <i>Set cal. to 'Approved'</i> 		
Copy appl. as template for routine appl. <i>(Adjust SOP & meas. per sample)</i>		
Integrate Calibration in Application <i>Set to 'Approved'</i> 	 	
Use for Prediction / Routine Measurement		

The upper part of the scheme includes all steps regarding the calibration samples.

The middle part shows the processes for designing an application for routine use.

The last part indicates the routine use, which is the goal of the development process.

In the following, we will use the term 'Operator user' for a user account from the user group 'Operators', and 'Administrator' for one belonging to the user group 'Administrators'.




















To log on as such a user, the correct user name and password are required for the corresponding dialog.

5.4.2. Creating an application for acquisition of calibration spectra

This first part of the tutorial guides you through the development process for a method that allows an operator to collect spectra of calibration samples. These are required for calculation of a quantitative chemometric calibration.

Roadmap to Application Design



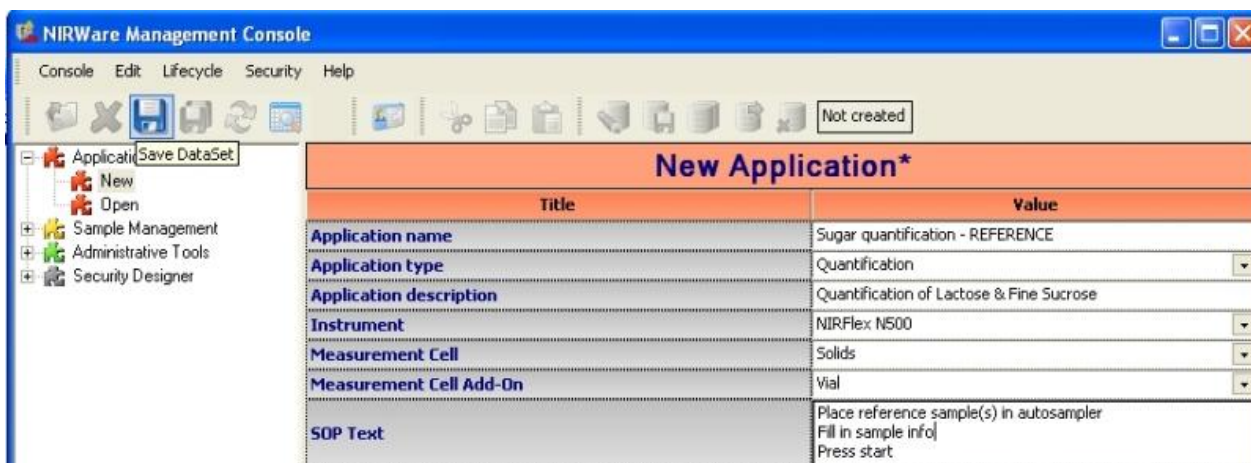
Design Ref.-Application <i>Set to 'Approved'</i> 		
Record spectra of ref. samples		
Define Properties & -values	 	
Calibrate <i>Set cal. to 'Approved'</i> 		
Copy appl. as template for routine appl. <i>(Adjust SOP & meas. per sample)</i>		
Integrate Calibration in Application <i>Set to 'Approved'</i> 	 	
Use for Prediction / Routine Measurement		



The application development starts in the NIRWare Management Console (MC).

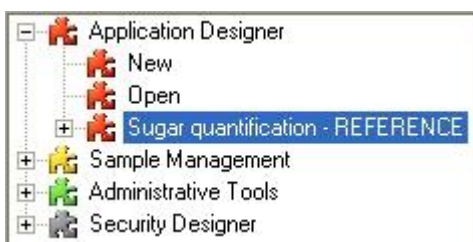


Start the program and log on as an 'Administrator'. Left-click on 'Application Designer' in the tree menu on the left, then on the subtitle 'New'. A dialog appears for creating a new application



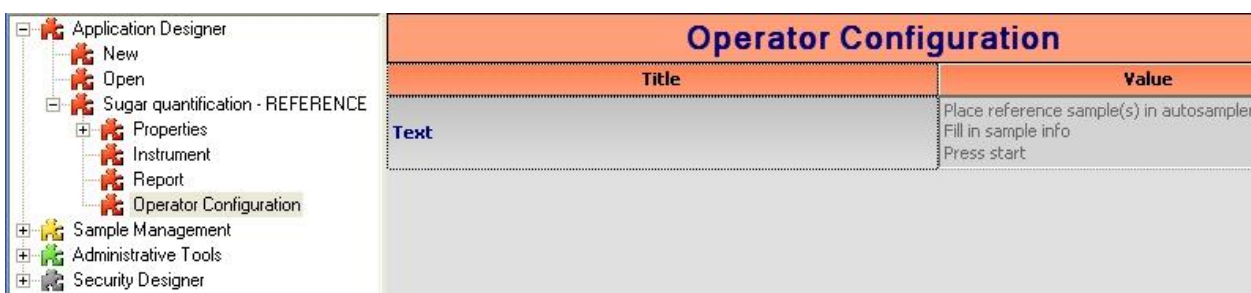
Fill in the application name and all other requested information into the white fields on the right side. The 'SOP Text' will later on tell the Operator how to perform the actual measurement, so it is important to give a complete description which is easily understandable.

Click the Save icon to save the new application to the database .



Your newly created application is now shown in the tree menu.

Open it by double-clicking on its field in the tree menu, or by clicking once on the plus-symbol in front of it. Then select its subtitle 'Operator Configuration'. You will now see only one field for the SOP text.

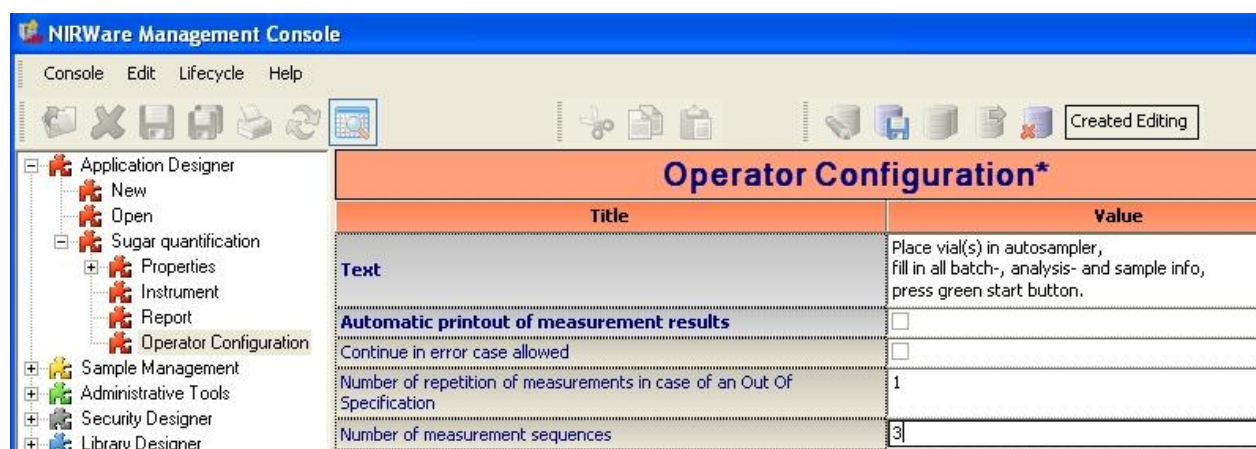


To see all of the information fields on the right, click on the 'Show Advanced Settings' icon in the menu



The fields on the right are grayed out, indicating that they cannot be changed right now.

To change the settings, first click on the 'Edit Data Set' icon  .



Notice the change in the icon bar for Lifecycle state from 'Created Idle' to 'Created Editing' (see above).


You can now make changes to all white fields. For our example, we just change the 'Number of measurement sequences' from 1 to 3.

This will cause a triplicate measurement of every reference sample, which creates more variation in the spectra set later used for calibration. Thus, we will get more robust calibrations.

Save all changes you made to the database by clicking the respective icon  .

The fields are greyed out again afterwards, indicating successful saving.

The method for triplicate reference sample measurement is now still in the 'Created' state, where only an 'Administrator' can see and use it in the operator software.

To provide this method for the operator user, 'Put the data set into the next state' by clicking on the corresponding icon  .

Now the application is in the 'Approved' state.

NOTE

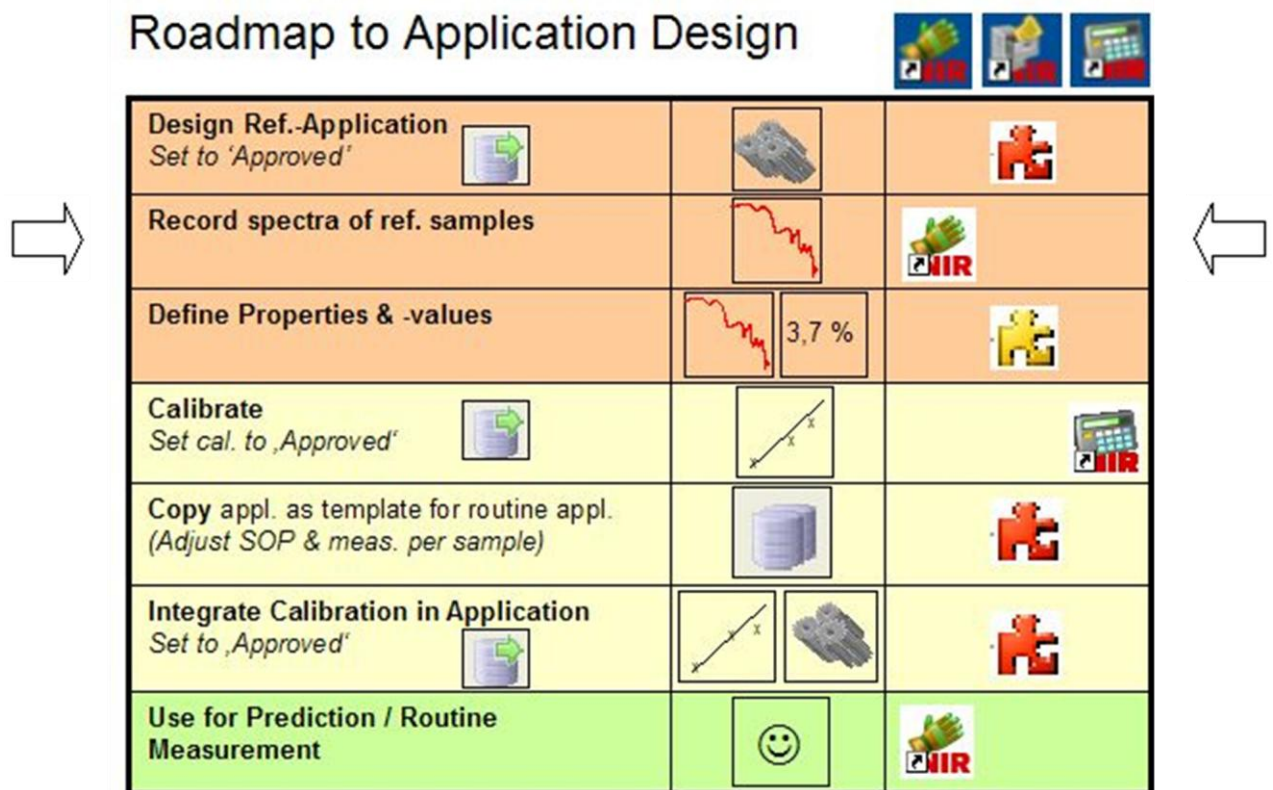
Approved applications cannot be changed anymore. To modify any settings or parameters, create a copy of the application. The copy will be generated in LC state "created" and can be edited.

The application is now ready for measurement of reference spectra with the Operator software.

5.4.3. Measuring reference spectra

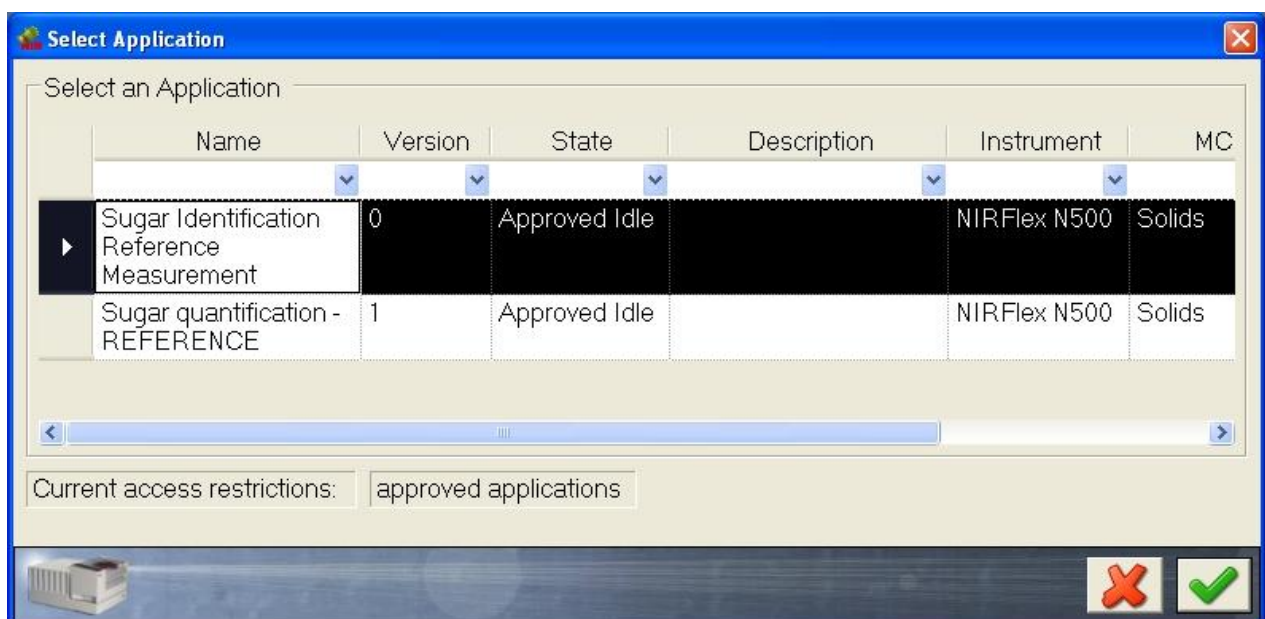
To measure spectra of reference samples, the Operator software is used.

Measurement of reference spectra is the second step in the development process.

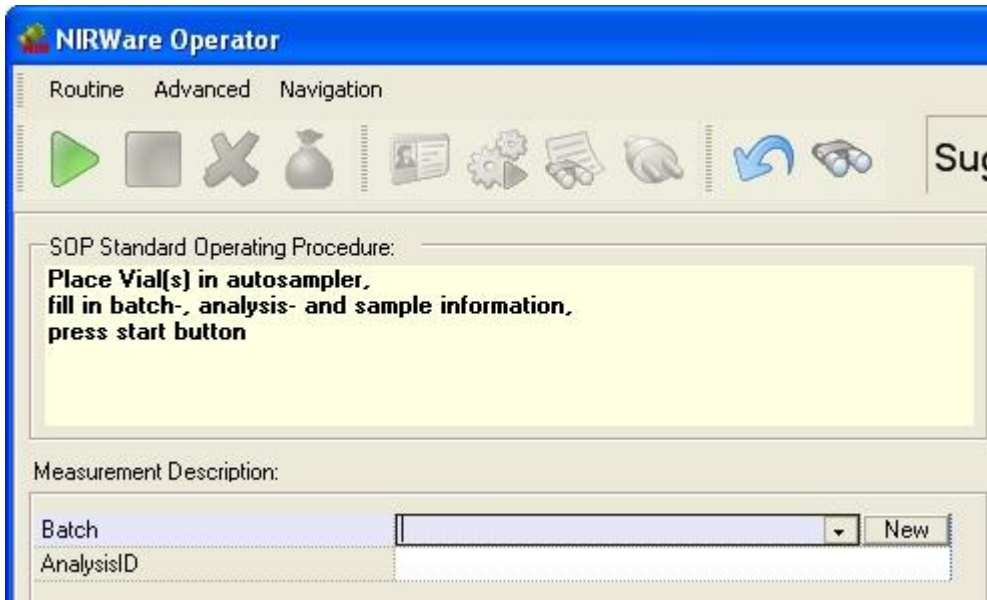


Start the operator software and log on as an 'Operator'.

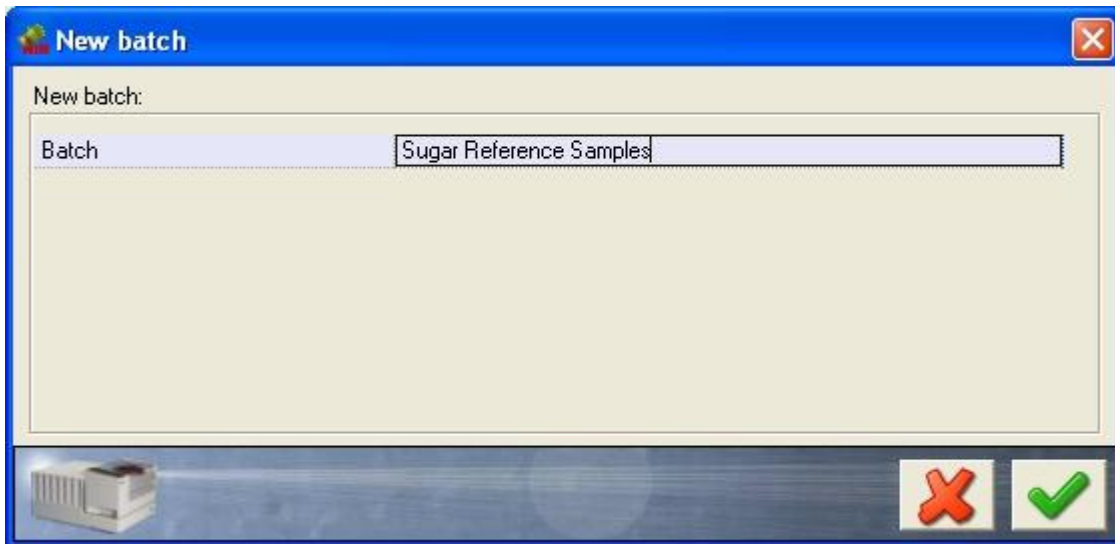
Then press the 'Select application' button and select the application you created for the measurement of reference spectra:



The application is now loaded to the Operator. At the left side, you see fields to fill in information about batch, analysis sequence and samples. Click on the 'New' button of the 'Batch' field to create a new batch:



Type in the name of your batch, then click on the green check mark button:



Then type in the information for AnalysisID and Sample names:

Batch	Sugar Reference Samples	New
AnalysisID	First Sequence	

Samples:

1	Lac 100 FSuc 0
2	Lac 90 FSuc 10
3	Lac 70 FSuc 30
4	Lac 50 FSuc 50
5	Lac 30 FSuc 70
6	Lac 10 FSuc 10

NOTE

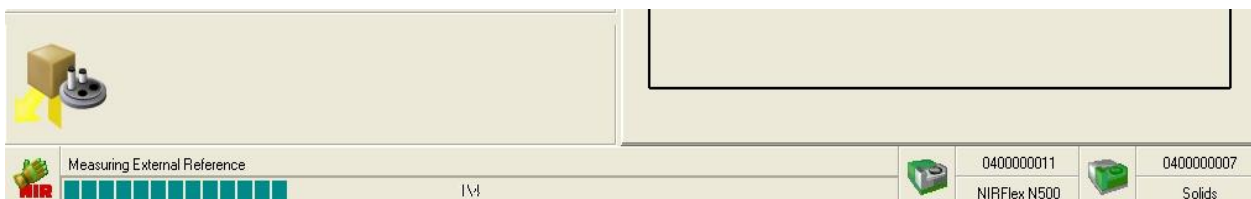
For 'real' applications, use 'speaking' names that precisely identify each sample just from the name! Also think of using the autoname functions described in the NIRWare documentation.

If you have filled in and checked all information, prepare the samples for measurement (i.e. place all vials in the autosampler) and press the green check mark button.

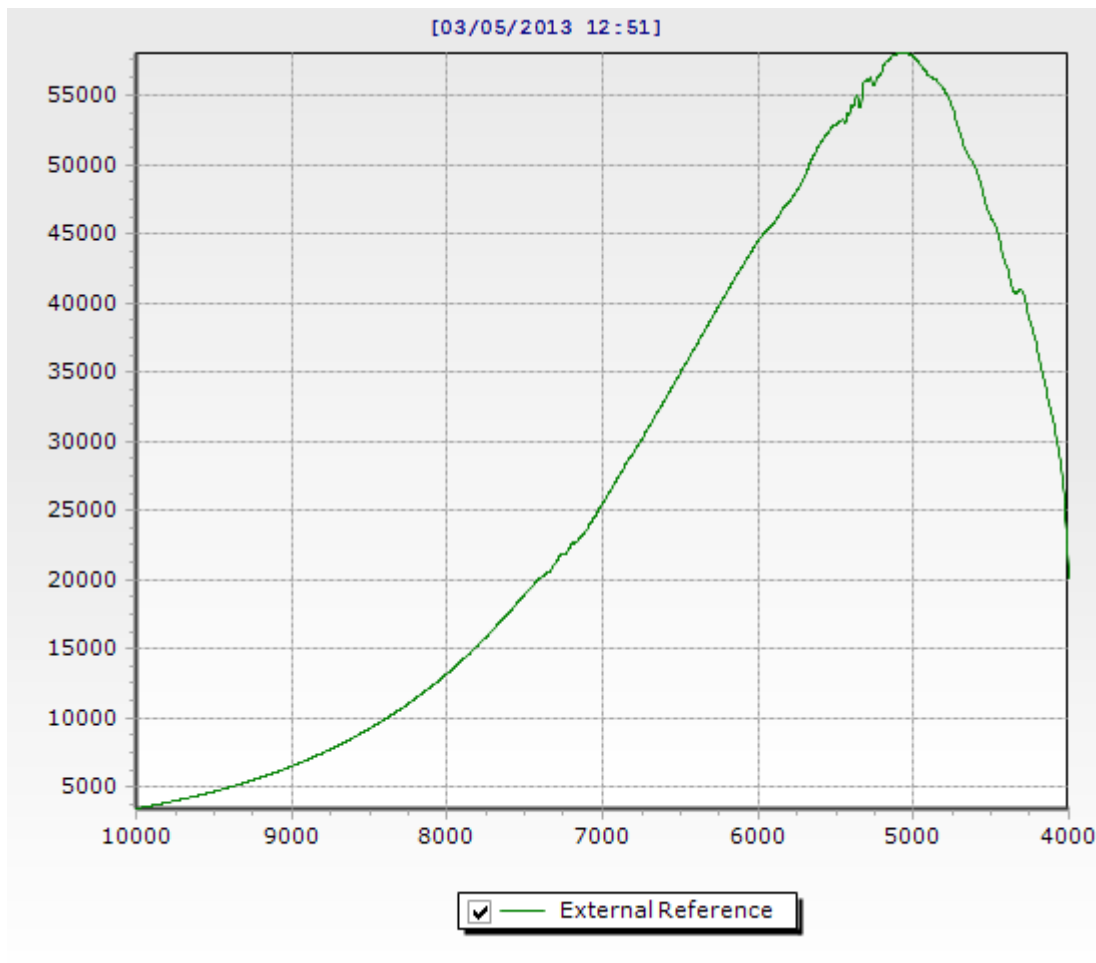
During the measurement sequence, the SOP text field is greyed out.

If an 'Instrument Suitability Test' (SST) starts, just wait until that is finished. Then the instrument will start with the measurement sequence. This includes periodic measurement of internal and external references. In our example with the vial autosampler option, these measurements are automatized. (With other options, the software will give a description of what to do.)

First, the external reference is being measured:

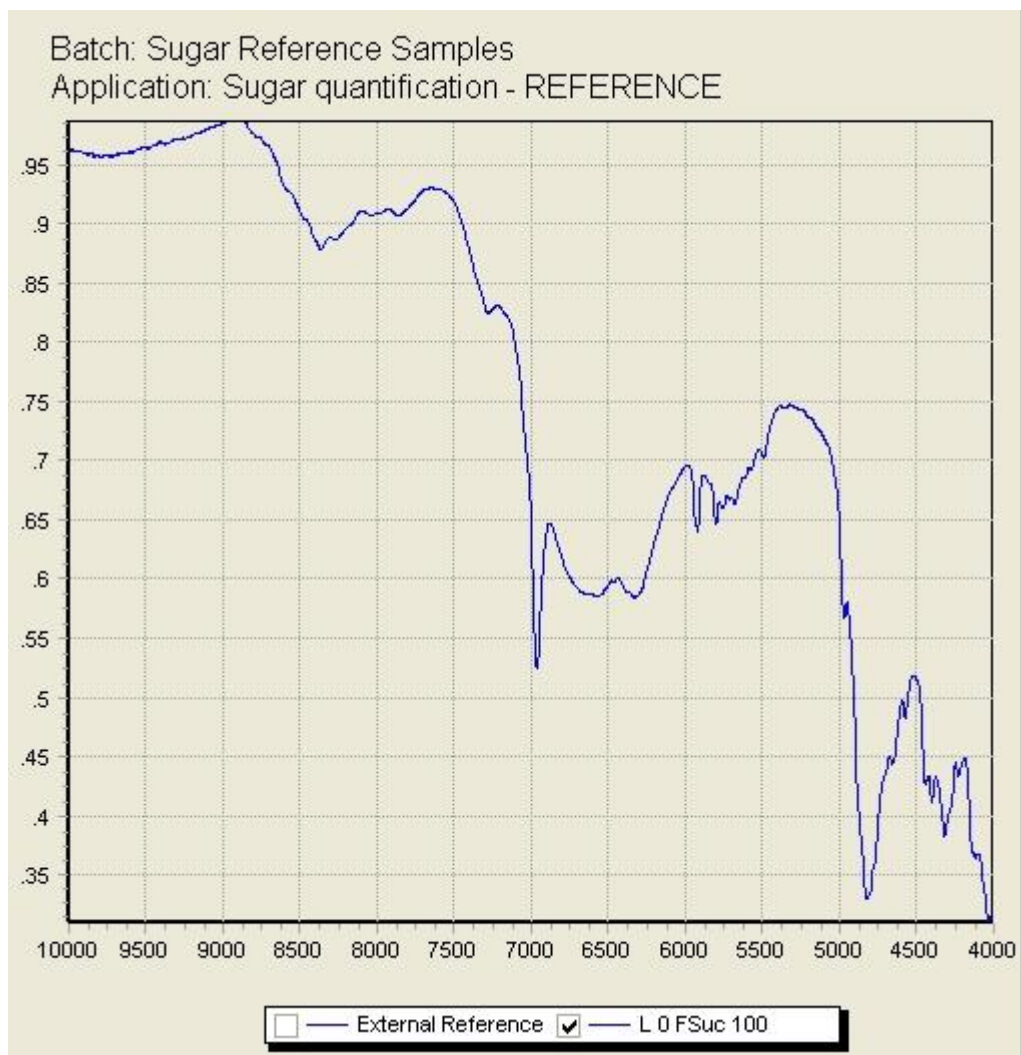


Then the samples are being measured. All spectra are displayed in one window:

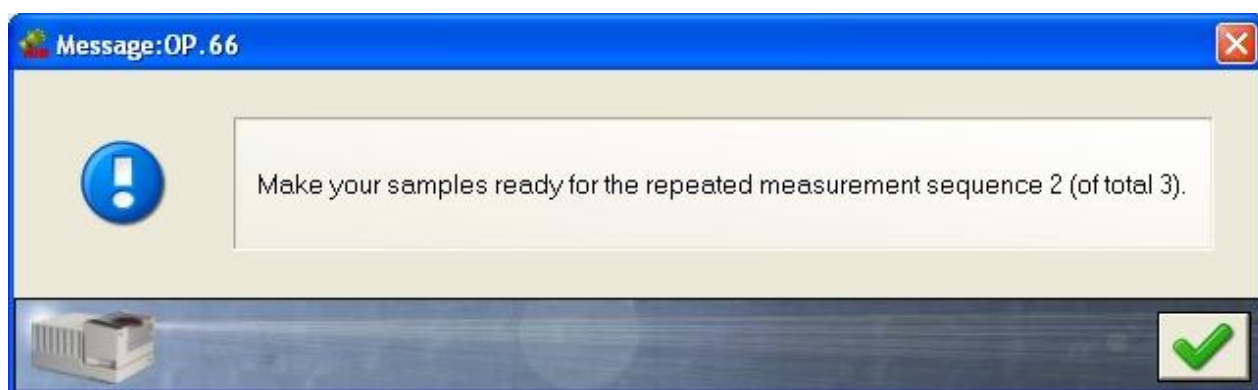


Since the intensity of the external reference is so much higher than that of the sample spectrum, the latter are just a flat line on the x-axis.

To have a closer look on the sample spectrum, deselect the check box for 'External Reference' below the graphic:



The vial autosampler will automatically continue with the next samples after confirmation of the following dialog:



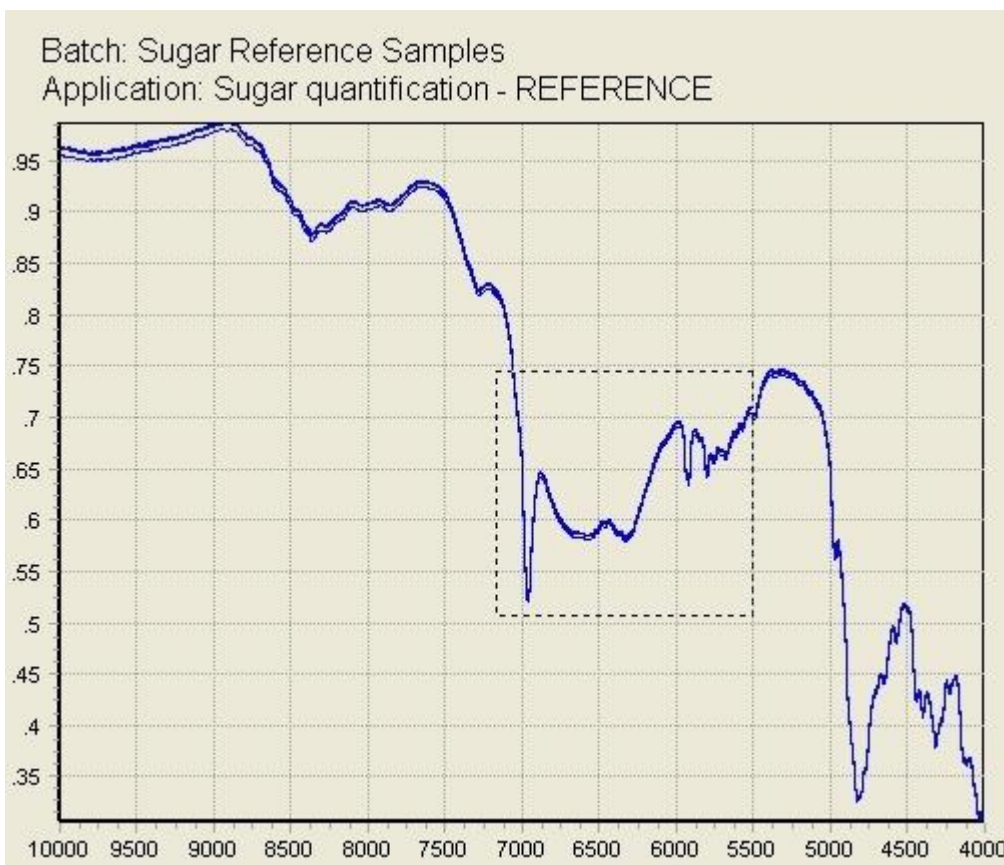
Click on the green check mark button to start the next measurement sequence.

The spectra shown below are all from identical sugar samples:

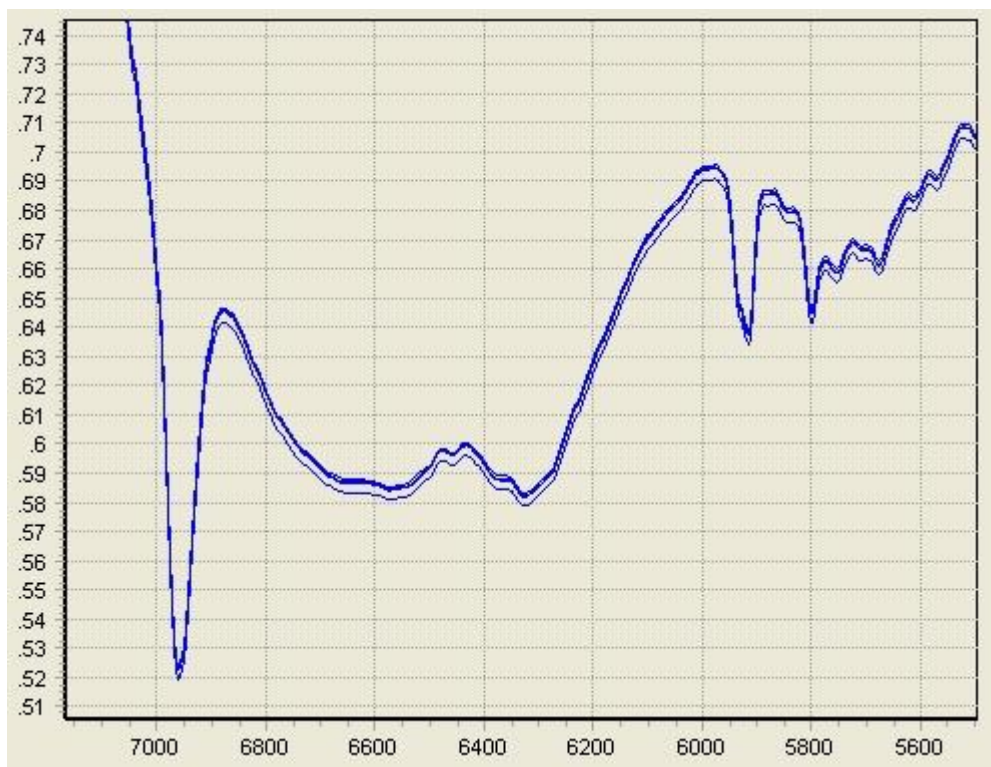


Variations in the spectra result from differences in size and orientation of the particles, and from variations between the glass vials.

To zoom into the spectrum, click and hold the left mouse button while dragging the cursor.



The so defined frame will be magnified:



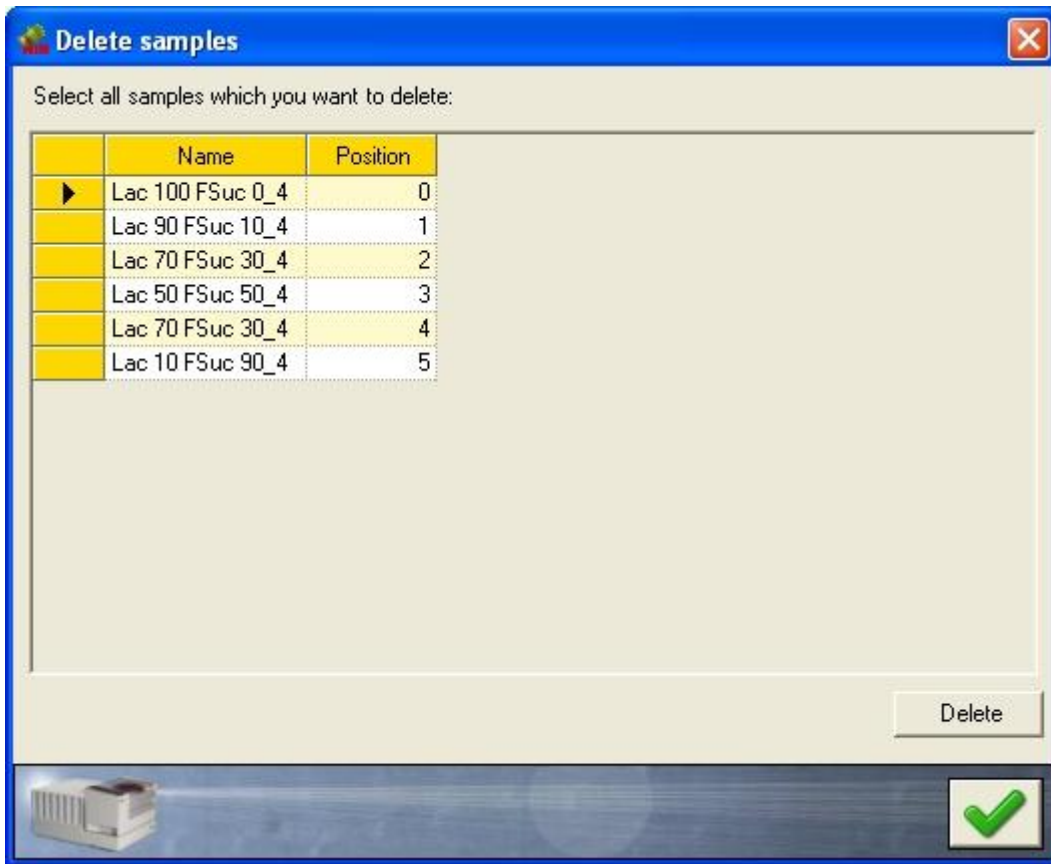
To change back to full view, click on the symbol with the magnification lens above the globus:



NOTE

It is possible to delete spectra, but only right after they were measured. This might be desirable if for example a vial was not correctly positioned in the autosampler. To delete a measurement, click on the red cross button (red cross in the upper left corner, not the one next to the magnification lens icon).

You can now select samples from the last measurement for deletion:



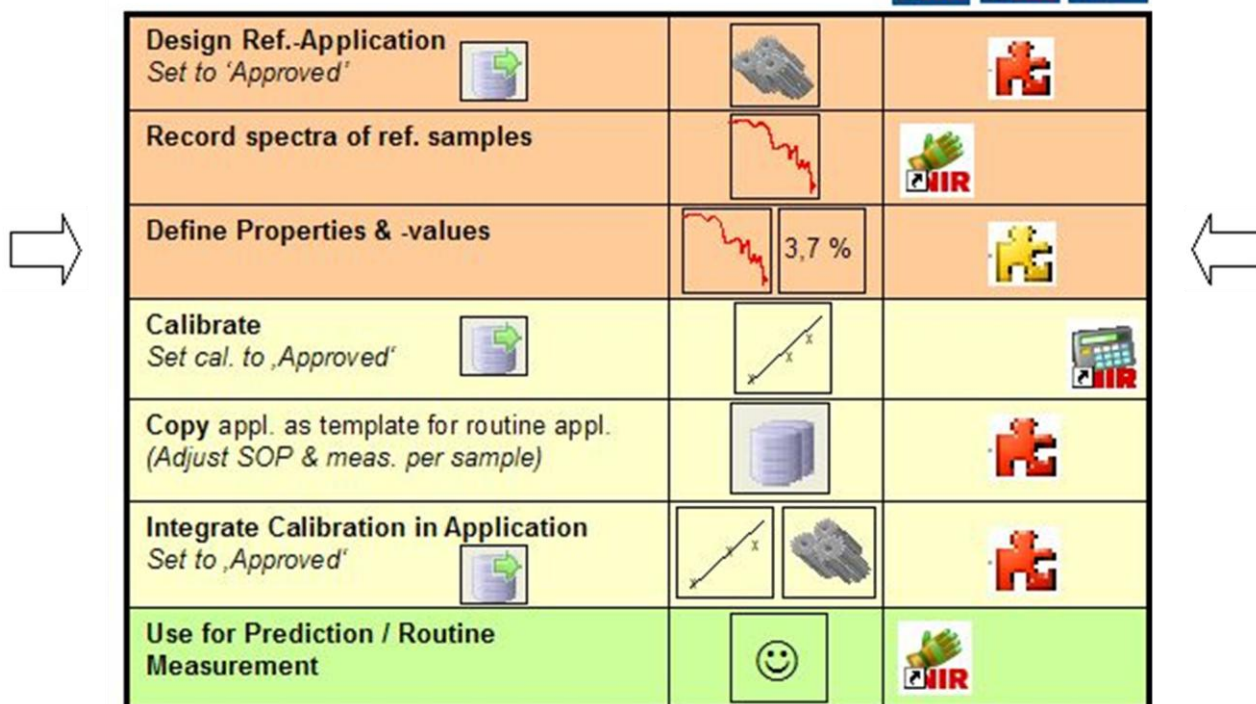
To select (or deselect) a line in the list, press and hold the Ctrl-button on your keyboard while left-clicking on that line. Click on the 'Delete' button to delete the selected measurements.

After completion of the measurement of your reference samples, switch to the NIRWare Management Console to continue with the next step in application development: the assignment of properties and property values. (here: concentration values)

5.4.4. Defining a property and a property value

After the spectra of the reference samples have been measured, the properties (here: concentration values) have to be connected to the calibration samples. This is done in the NIRWare Management Console (MC). The so created data sets are later on the basis for building a calibration in NIRCal.

Roadmap to Application Design



Switch to the NIRWare Management console, and select 'Sample Management' from the tree menu.

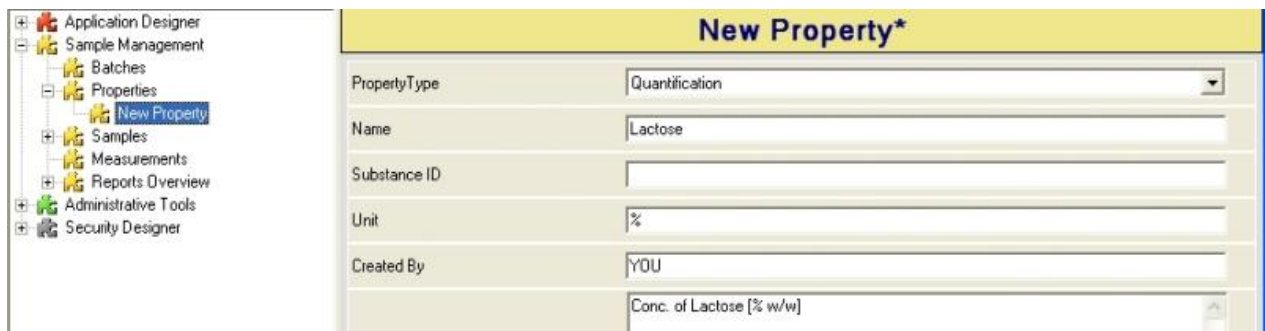


Switch to the MC, and select 'Sample Management' from the tree menu.

Select 'Properties' to open a list with all properties that have been defined so far:

Properties					
	Name	Type	Unit	Description	Created By
		Quantificat			
▶	Fat	Quantification	%		
	Moisture	Quantification	%		
	Protein	Quantification	%		
	Ash	Quantification	%		
	Fibre	Quantification	%		
	Phosphorus	Quantification	%		
	Salt	Quantification	%		

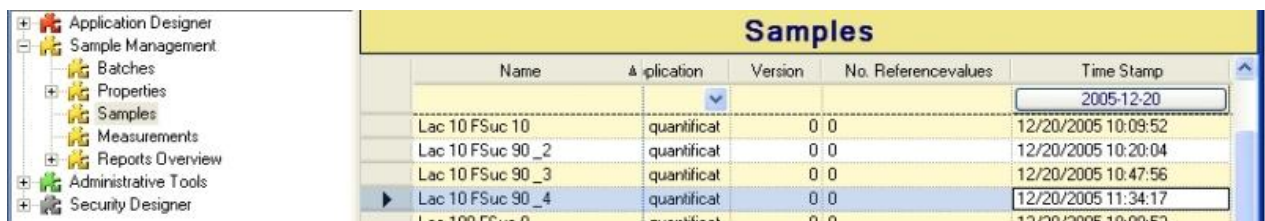
If the property you need is not in the list, create it by clicking on 'Properties' in the tree menu, and then selecting 'new property'.



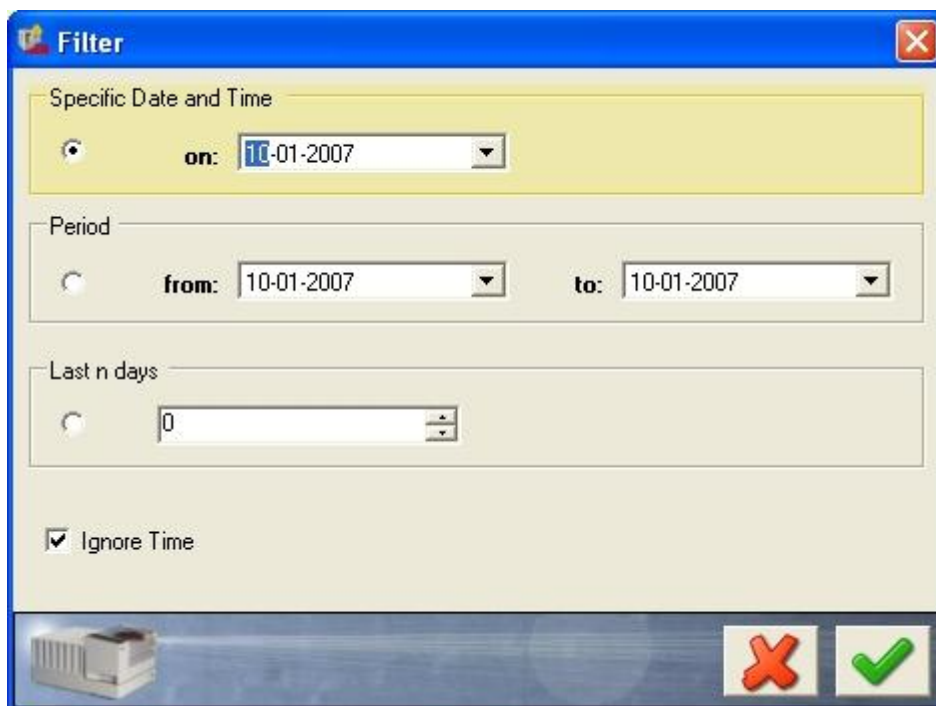
Define the type (here: qualification) and edit the name and unit of the property. Also type in your name to document who created this property. Click on the Save icon to write this property definition to the database. Create all new properties accordingly.

Now we want to tell the computer which sample belongs to which property.

Switch to MC – Sample Management – Samples to open a list with all samples that have been measured.



Notice that in the list the 'Time Stamp' filter is set to a specific date. Right click the time stamp button to ignore, or left click on it to edit the filter settings:

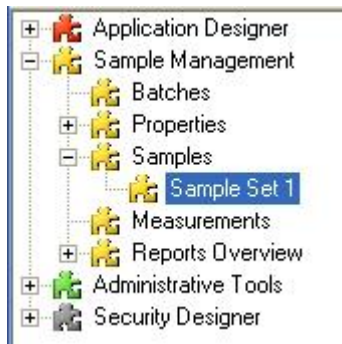


To shorten the list of samples, you can also use additional filters, e.g. on the 'Application' column. This can be helpful if you used dedicated applications for reference spectra measurement of each sample type.

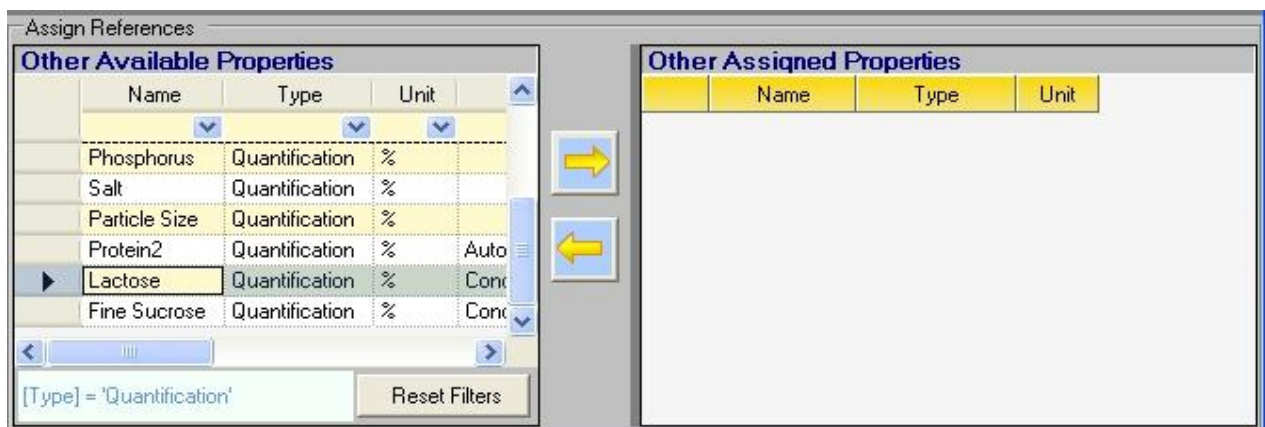
Select your reference samples by clicking on the topmost reference sample in the list. Then press and hold the Shift-button on your keyboard while scrolling down the list (using the mouse or the arrow keys on your keyboard). Alternative: By pressing 'Ctrl-Shift-End' on your keyboard you can highlight everything from the first selection down to the end of the list.

Samples					
Name	Application	Version	No. Referencevalues	Time Stamp	
	Sugar quantification - REFERENCE				
Lac 100 FSuc 0_3	Sugar quantification - REFERENCE	0 0		12/20/2005 10:47:56	
Lac 100 FSuc 0_4	Sugar quantification - REFERENCE	0 0		12/20/2005 11:34:17	
Lac 30 FSuc 70	Sugar quantification - REFERENCE	0 0		12/20/2005 10:09:52	
Lac 30 FSuc 70_2	Sugar quantification - REFERENCE	0 0		12/20/2005 10:20:04	
Lac 30 FSuc 70_3	Sugar quantification - REFERENCE	0 0		12/20/2005 10:47:56	
Lac 50 FSuc 50	Sugar quantification - REFERENCE	0 0		12/20/2005 10:09:52	
Lac 50 FSuc 50_2	Sugar quantification - REFERENCE	0 0		12/20/2005 10:20:04	
Lac 50 FSuc 50_3	Sugar quantification - REFERENCE	0 0		12/20/2005 10:47:56	
Lac 50 FSuc 50_4	Sugar quantification - REFERENCE	0 0		12/20/2005 11:34:17	
Lac 70 FSuc 30	Sugar quantification - REFERENCE	0 0		12/20/2005 10:09:52	
Lac 70 FSuc 30_2	Sugar quantification - REFERENCE	0 0		12/20/2005 10:20:04	
Lac 70 FSuc 30_3	Sugar quantification - REFERENCE	0 0		12/20/2005 10:47:56	
Lac 70 FSuc 30_4	Sugar quantification - REFERENCE	0 0		12/20/2005 11:34:17	
Lac 70 FSuc 30_4	Sugar quantification - REFERENCE	0 0		12/20/2005 11:34:17	
Lac 90 FSuc 10	Sugar quantification - REFERENCE	0 0		12/20/2005 10:09:52	
Lac 90 FSuc 10_2	Sugar quantification - REFERENCE	0 0		12/20/2005 10:20:04	
Lac 90 FSuc 10_3	Sugar quantification - REFERENCE	0 0		12/20/2005 10:47:56	
Lac 90 FSuc 10_4	Sugar quantification - REFERENCE	0 0		12/20/2005 11:34:17	

Then click on the 'Open existing data set'-button in the upper left corner to create a new Sample Set

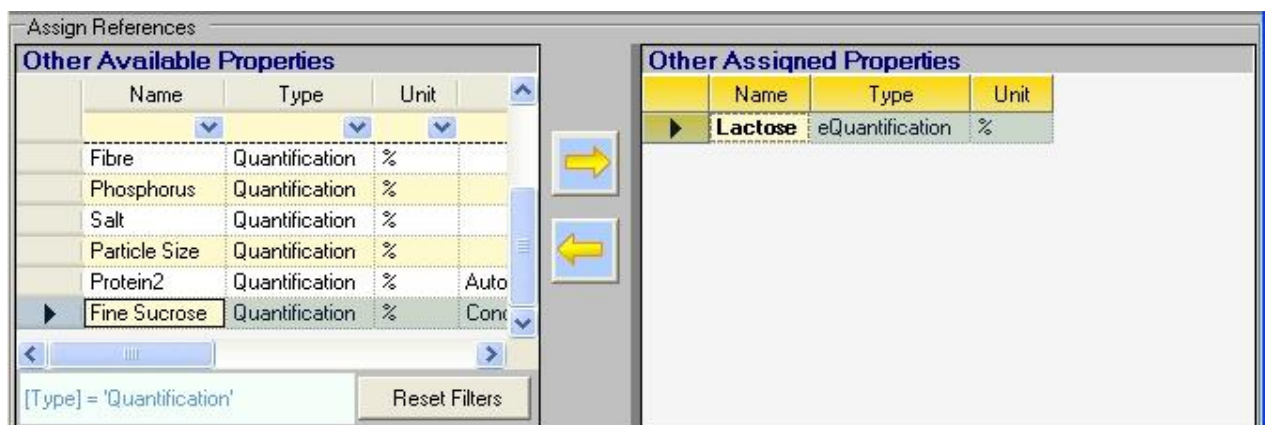


This opens a window with three lists: 'available properties', 'assigned properties', and 'samples'. This allows you to select properties for the samples by shifting them from the 'available' to the 'assigned' list. Select a property that you want to assign to your samples:



followed by a click on the arrow key to the right.

The property 'Lactose' has now been shifted to the 'assigned' list.



Repeat this process for all of your properties:

Samples_References: Sample Set 1*

Samples

Name	Lactose	Fine Sucrose
Lac 10 FSuc 90_2		
Lac 10 FSuc 90_3		
Lac 10 FSuc 90_4		
Lac 100 FSuc 0		
Lac 100 FSuc 0_2		
Lac 100 FSuc 0_3		
Lac 100 FSuc 0_4		
Lac 30 FSuc 70		
Lac 30 FSuc 70_2		
Lac 30 FSuc 70_3		

Assign References

Other Available Properties

Name	Type	Unit	De
Fat	Quantification	%	
Moisture	Quantification	%	
Protein	Quantification	%	
Ash	Quantification	%	
Fibre	Quantification	%	
Phosphorus	Quantification	%	

[Type] = 'Quantification'

Other Assigned Properties


Name	Type	Unit
Lactose	eQuantification	%
Fine Sucrose	eQuantification	%

The highlighted matrix cells allow you to define the lactose- and fine sucrose concentrations of each sample:

Samples_Referen

Samples

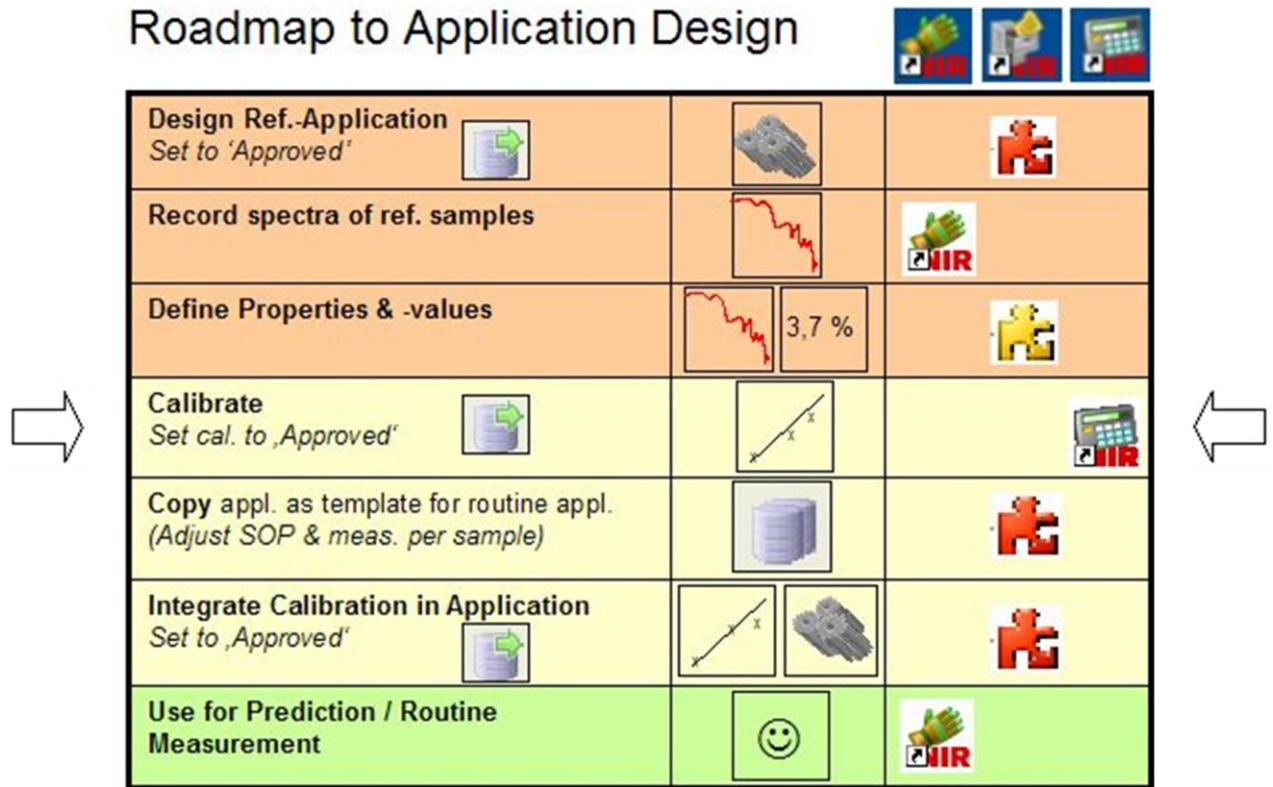
Name	Lactose	Fine Sucrose
Lac 10 FSuc 90_2	10	90
Lac 10 FSuc 90_3	10	90
Lac 10 FSuc 90_4	10	90
Lac 100 FSuc 0	100	0
Lac 100 FSuc 0_2	100	0
Lac 100 FSuc 0_3	100	0
Lac 100 FSuc 0_4	100	0
Lac 30 FSuc 70	30	70
Lac 30 FSuc 70_2	30	
Lac 30 FSuc 70_3		

Complete the matrix list, and save these data to the database by clicking on the save button .

You can now switch to NIRCal to build a calibration on this reference data set.

5.4.5. Creating a basic calibration by using the NIRCal wizard

This chapter describes how to create a calibration with NIRCal, using the reference spectra with previously assigned properties.




The description here is limited to the use of the NIRCal wizard, since detailed optimization procedures and description of NIRCal features are described in the NIRCal documentation.

Start NIRCal

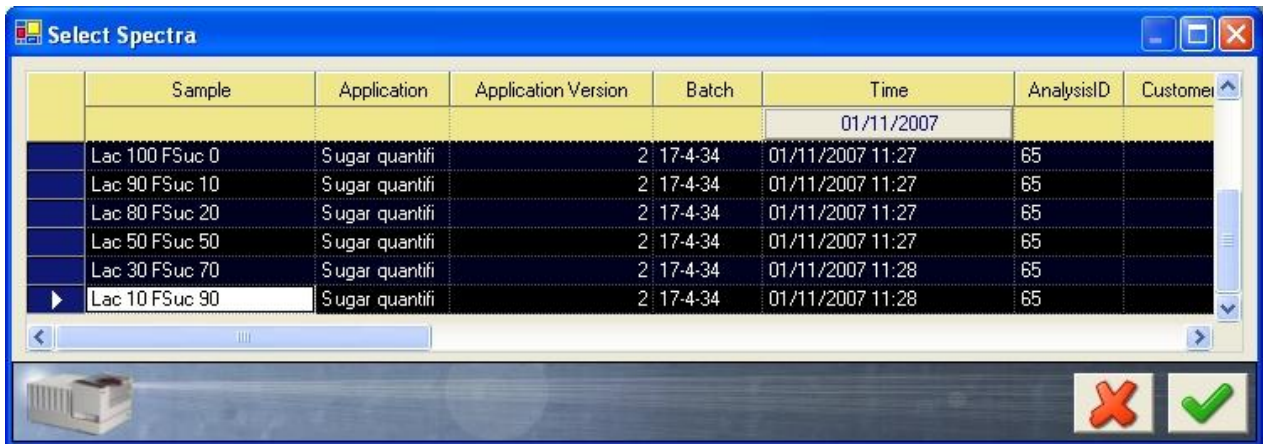


and log on as an 'Administrator'.

From the menu, select 'View' - 'Toolbars' and select the toolbars: Calibration, Database, File & Edit, Life Cycle, Pretreatments, Wizard Workspace, Status Bar.

To load spectra from the database into your empty project, click on the binocular icon .

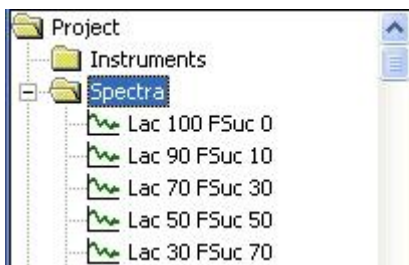
Select the spectra from the list, and click on the green check mark button:



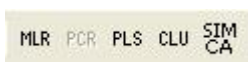
To simplify the selection, use appropriate filter settings, especially for 'Time' and 'Application'. (Time: right click to ignore time filter, left click to set time filter settings.)

Since we performed triplicate spectra measurement of each sample, we now find three spectra for each individual sample.

Select the NIR-Explorer window, select 'spectra' from the tree menu and check if all spectra have been correctly loaded:



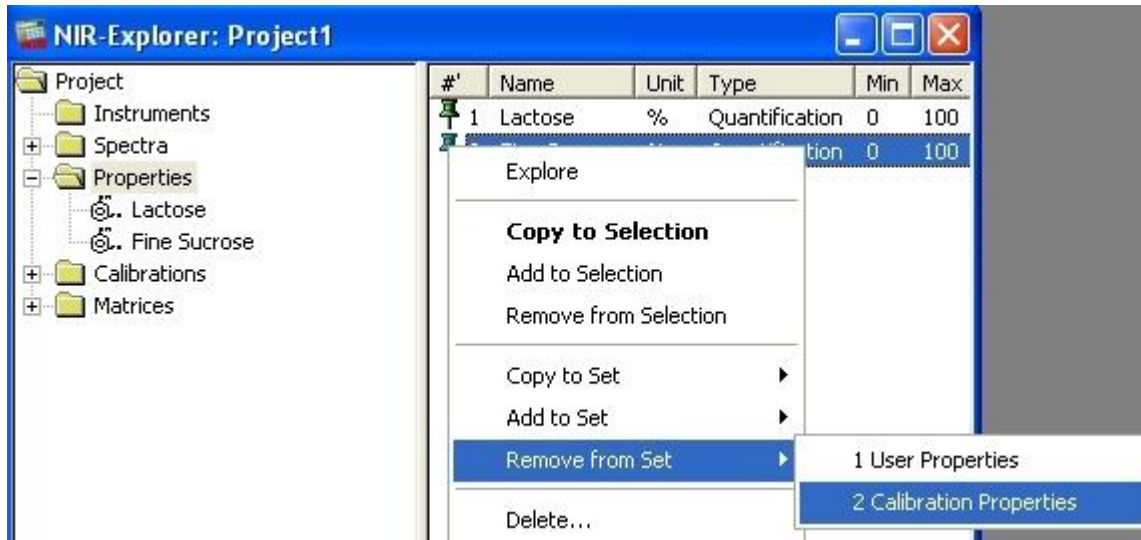
Now make sure that a quantitative method is selected ('MLR', 'PCR' or 'PLS') is selected in the menu bar:



Before we start with the calculations, let's reconsider that we have reference samples with two property values. And to this point, both are selected for calibration, as you can see in the NIRCal explorer:



It is not possible to develop only one calibration for determination of both properties. So we need to create two calibrations, one for each property. First we start with a calibration for Lactose quantification, so we deselect the unwanted property 'Fine Sucrose'. This is done by selecting 'Properties' in the NIRCal tree menu, followed by a right-click on the respective property name in the right part of the explorer window. From the menu, select 'Remove from Set' – 'Calibration Properties':



Notice the change in the symbol in front of the property name 'Fine Sucrose':



Now we are ready for a first calculation with default settings by clicking on the 'Overview' button.



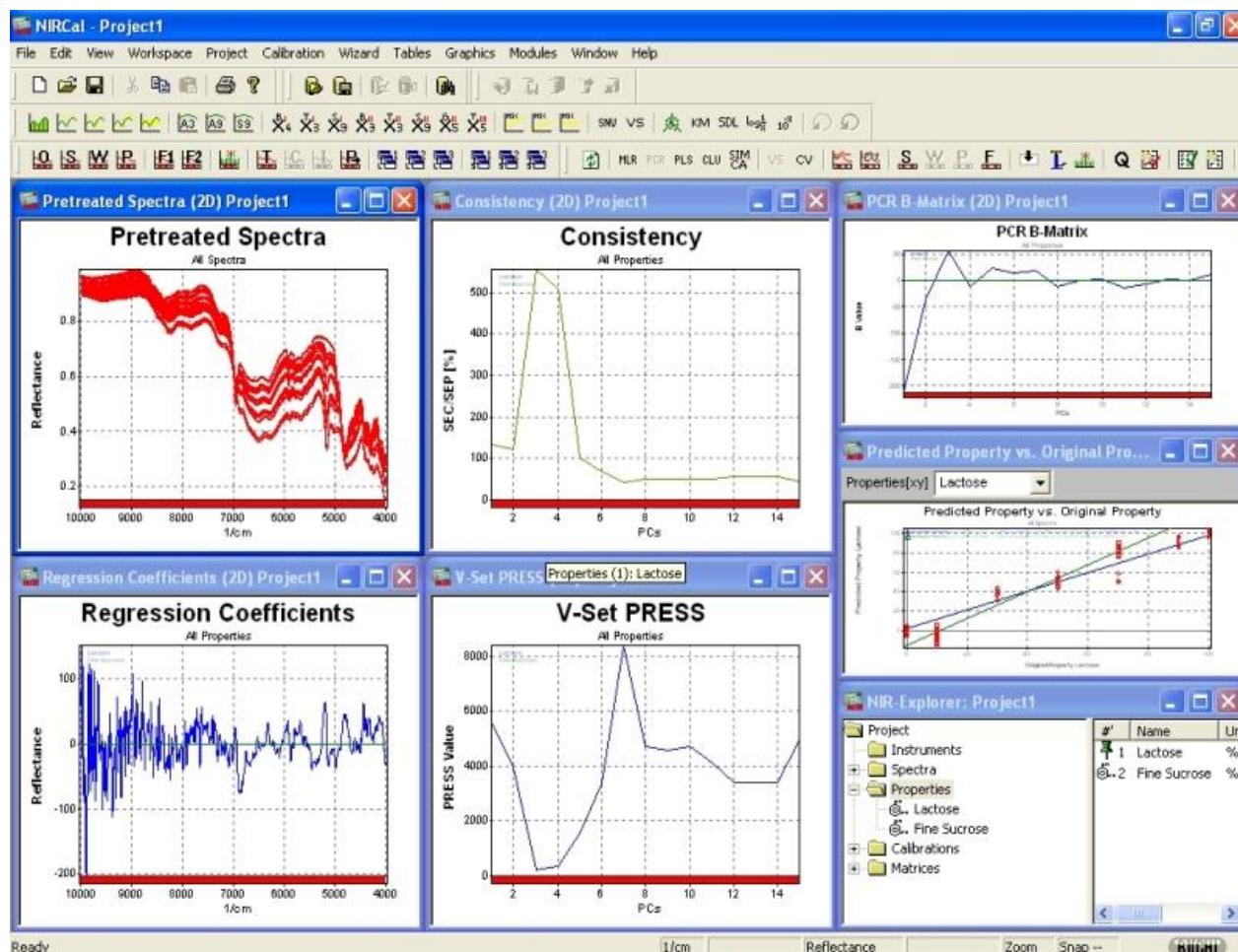
A message appears regarding Calibration- and Validation set selection (C-Set and V-Set):



Click on YES to let the C/V-selection wizard create a selection.

Note: It is highly recommended to perform the selection sample wise, so that ALL spectra of one individual sample are EITHER in the C- OR V-Set. This is described in detail in the NIRCal documentation.

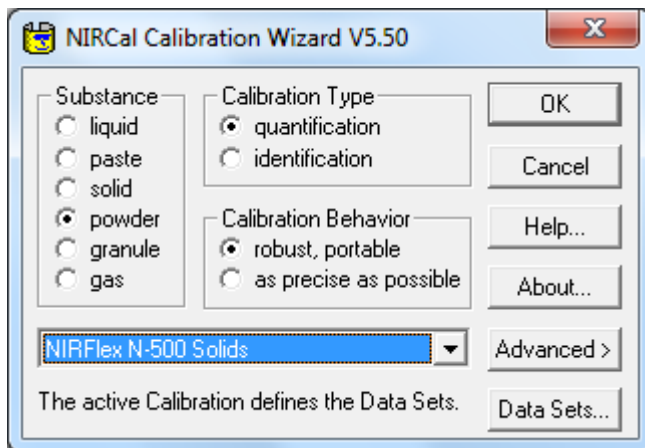
A full calculation is performed, and the result visualized in seven windows.



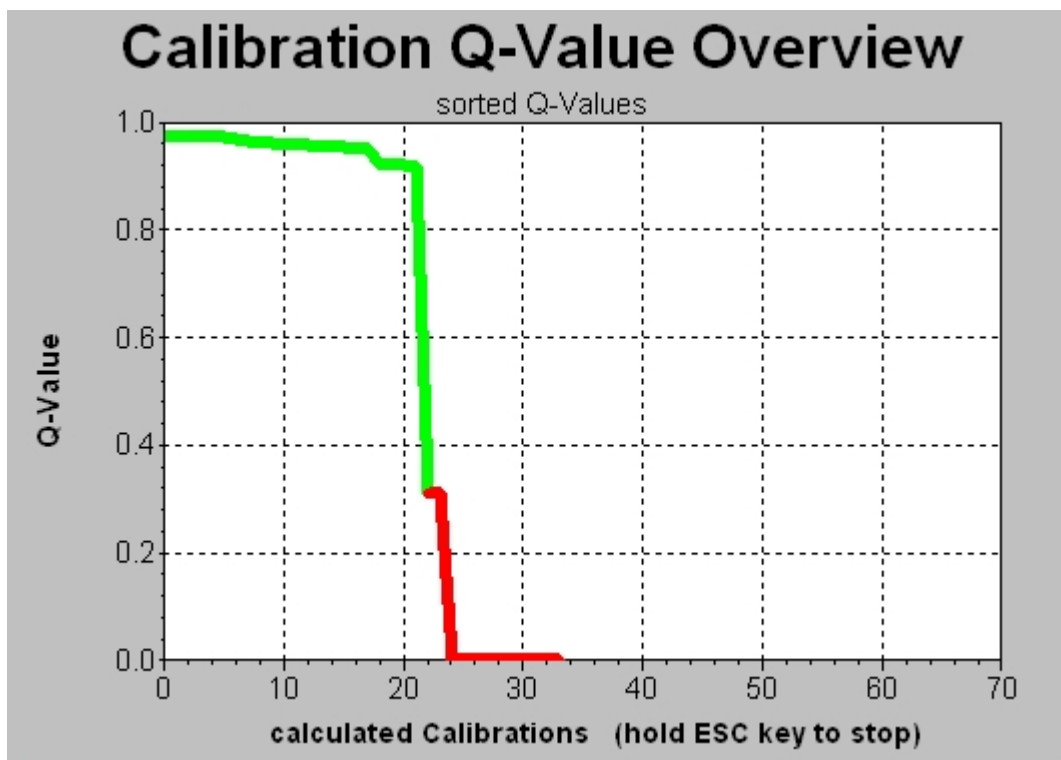
Notice that in the 'Predicted property vs. original property' window a diagonal calibration curve is shown for the Property Lactose.

This is a good check for successful deselection of the unwanted property, because it confirms that the actual calibration has only been calculated with regard to Lactose.

Optimization of the calibration is not a topic here, so we leave this job to the patented NIRCal Calibration Wizard: from the menu, select Wizard/Calibration Wizard. A dialog appears for definition of general parameters:

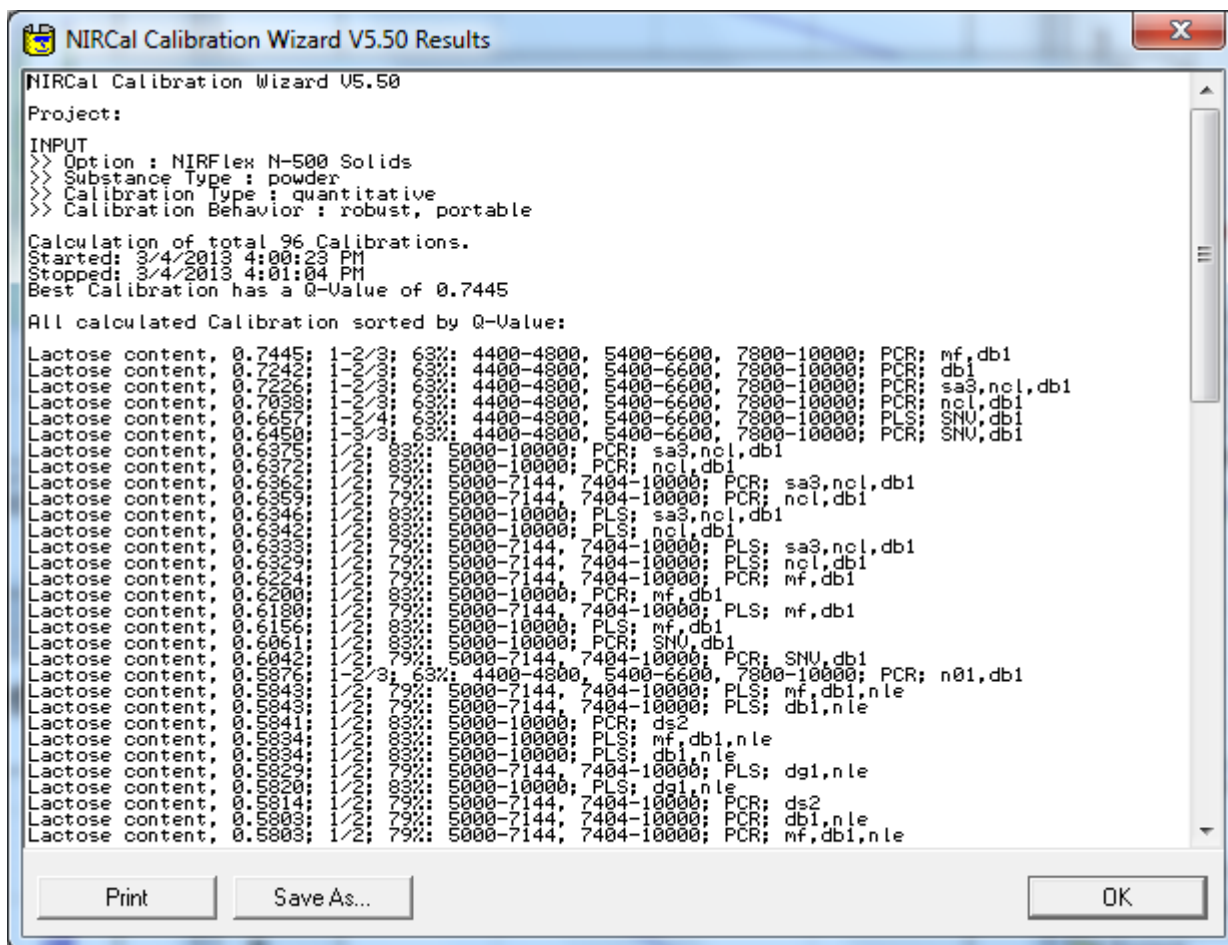


Select 'quantification' as calibration type, and click on 'OK'. The wizard now starts with the optimization process, which will take a few minutes. The progress is visualized in the 'Calibration Q-Value overview':

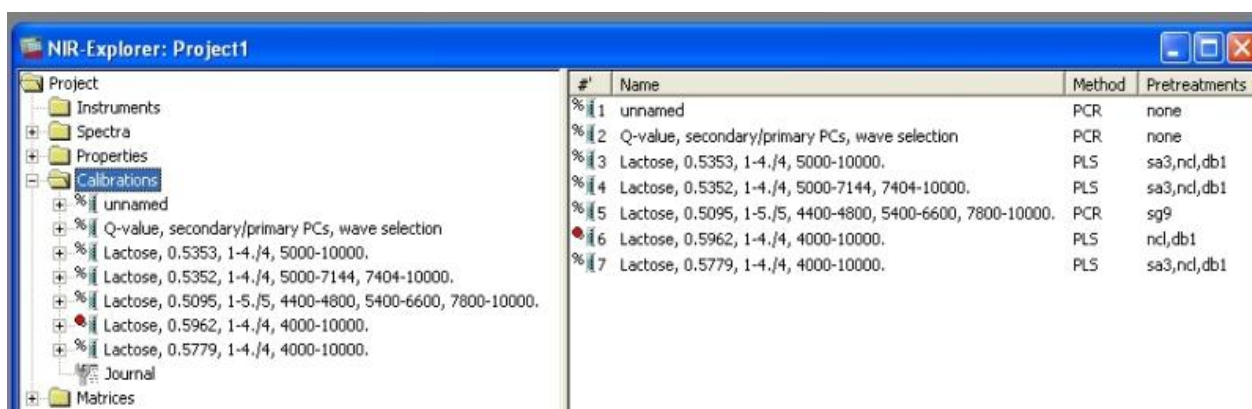


In the course of the optimization process, you see the Q-Value rise from zero (no working calibration) up close to 1 (=perfect calibration).

After the wizard is finished, the results are shown in a list where the best calibrations (with the highest Q-values) are found on top of the list:

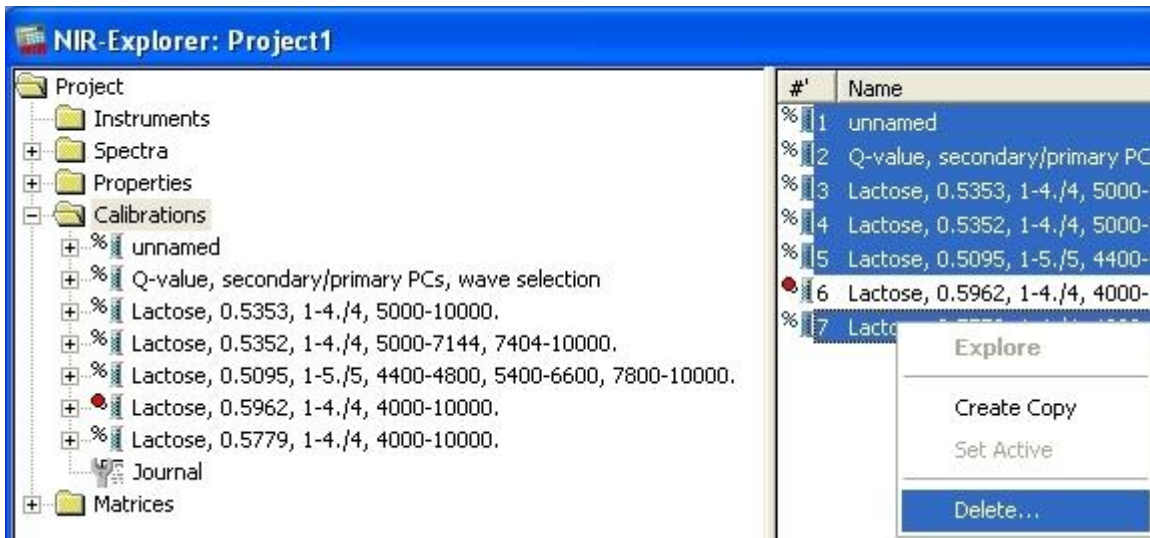


Now switch again to the NIRCal Explorer window, and have a look on the 'Calibrations':

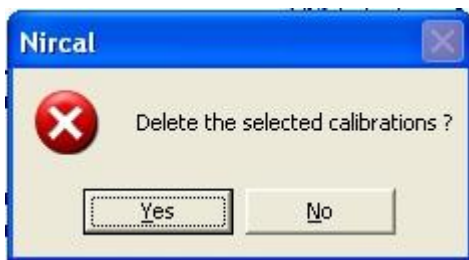


Note that the ten best calibrations are stored here. The one with the highest Q-value is set to active (indicated by a red dot). Since we only need one calibration, we select everything, except for the one we want to keep.

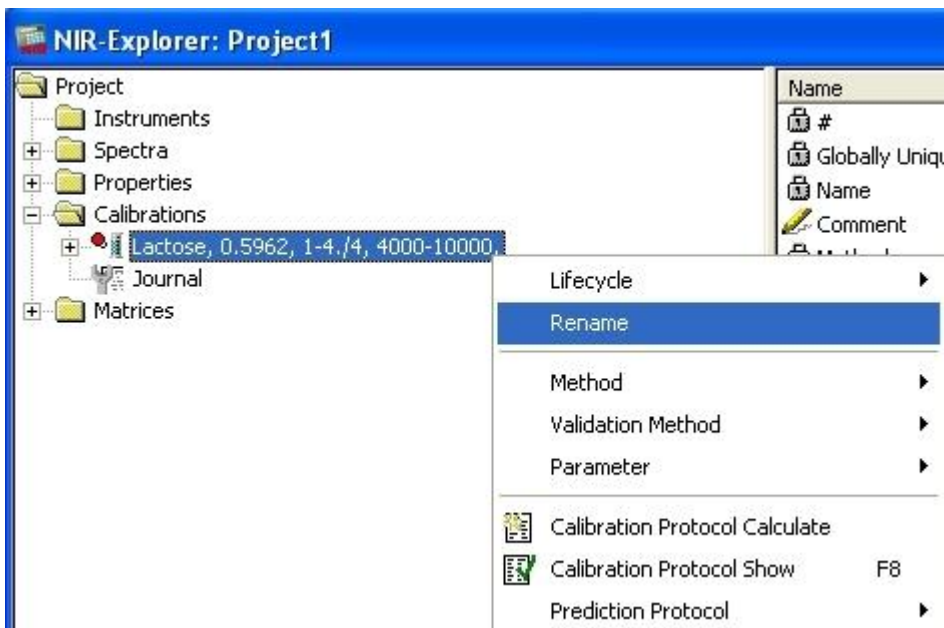
This is done by holding down the Ctrl-Key while left-clicking in the right window pane on the calibration to be selected:



Right-click on the selection and choose 'delete'. A confirmation message appears, which you will answer with 'YES':



To change the name of the calibration, right-click on the calibration name in the left window pane and select 'Rename' from the context menu:



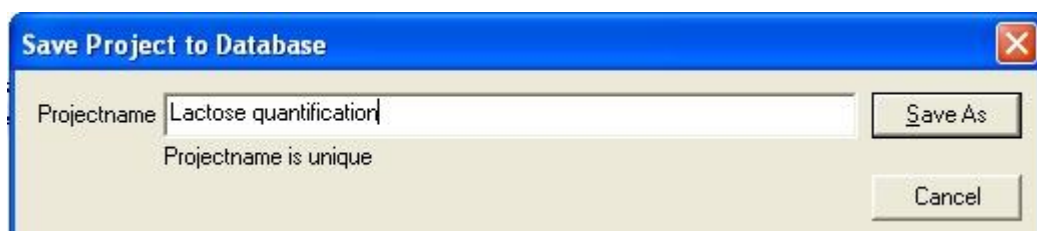
In this case, we rename it to 'Lactose Quan'.



(Hint: With more complex projects it is also a good idea to start with an identical project name for the calibration name and then just add a suffix for the respective property. Example: 'Sugar mixture – lactose' and 'Sugar mixture – fine sucrose'.)

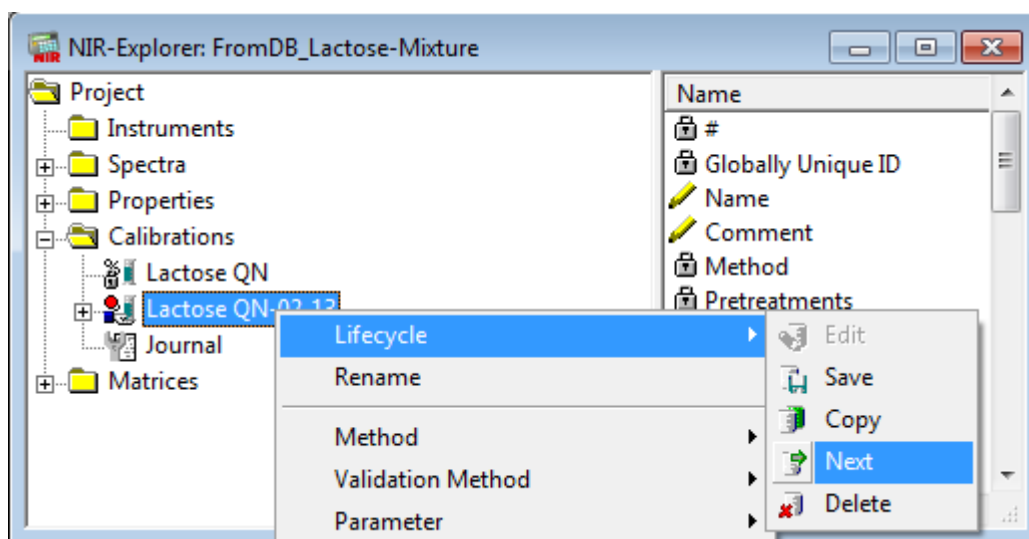
To save the calibration to the database, click on the 'Save' button in the menu bar .

Type in a name for your NIRCal project and click on the 'Save As' button:




So far the calibration is still in the 'created' state. If you would try to use it in an application, this would prevent you from changing your application (!) into the next state, because an approved application requires an approved calibration.

It is suggested to recalculate the first calibration. This is a master calibration, which organise the spectra in the project and can never be put the approved LC state. Copy this calibration, open the copy (LC: Edit), rename this: give a short name preferable with date at the end. Make a new calculation after renaming. Put this calibration to "approved" state.



and 'Next' .

Now your calibration is finished and in the approved state, so it can be used for integration into an application.

Remember that the just created calibration works only for lactose. So we need to start over again to create a second calibration project for fine sucrose. Create a new project by clicking on the respective button  and start over again with spectra loading etc.

In the end, you have two calibrations in individual projects, one specialised in Lactose quantification, the other for Fine Sucrose. For 2 component system a second calibration is not necessary, the second property can be calculated like: $\text{Property2} = 100 - \text{Property1}$.

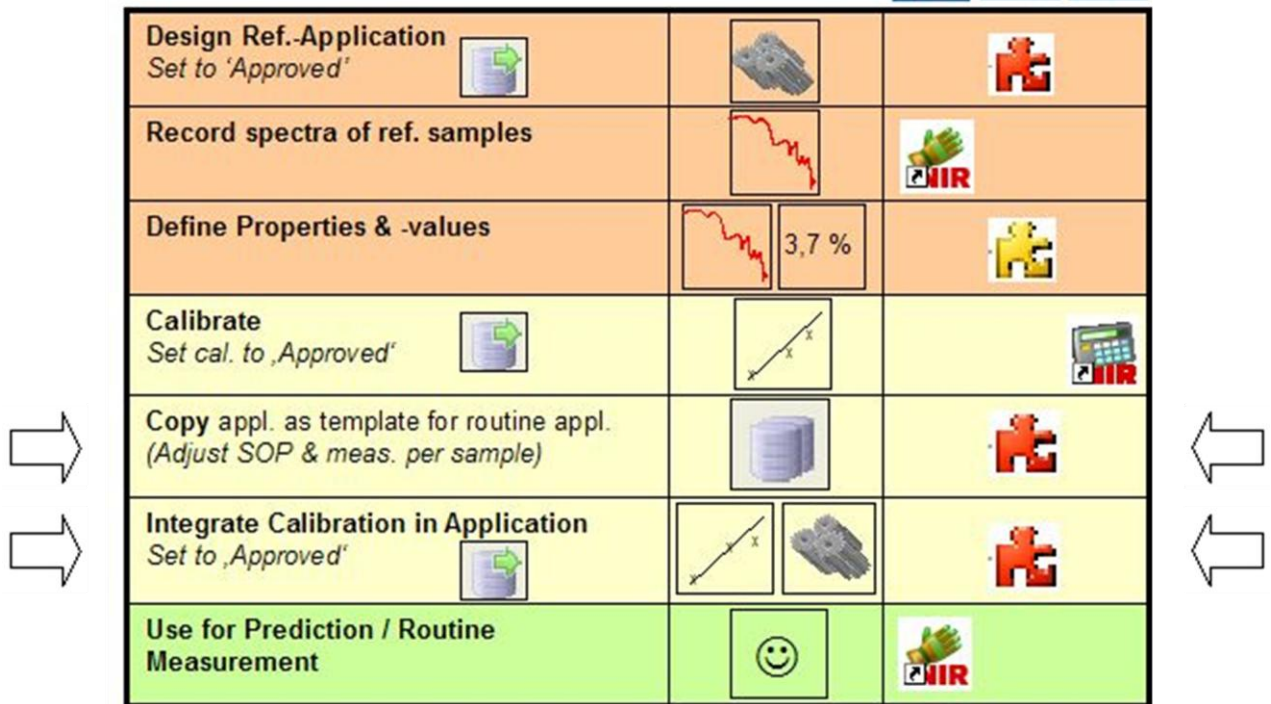
After creation of your calibrations in NIRCAl, these have now to be integrated to your application. This is done in the NIRWare Management Console.

5.4.6. Integrating a quantitative calibration into an application

The final step in creating an application for quantitative determination with NIR is to integrate the calibration into the application.

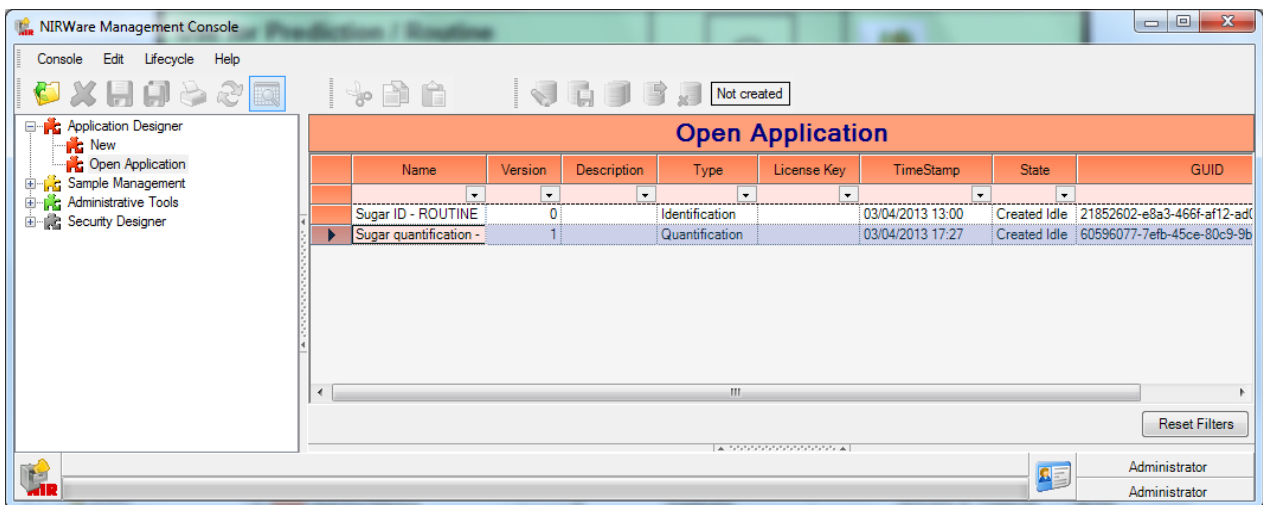
Remember that we started with an application for triplicate measurement of reference substances. This serves now as a template for the routine application. In effect, we create a copy of the reference method, make adjustments to this, and integrate the calibration. Adjustments involve mainly the number of measurements per sample, the SOP text, and Reports. All instrument parameters remain untouched, granting identical spectral conditions for both reference samples and those to be tested.

Roadmap to Application Design




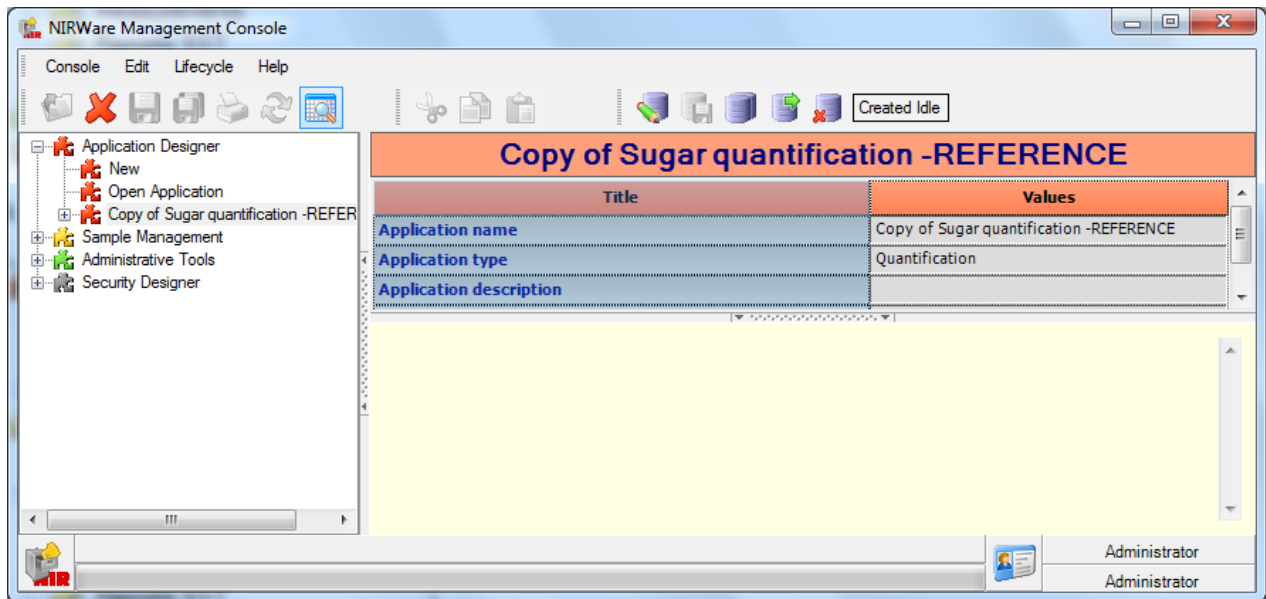
Both the creation of the routine use application and the integration of the calibration into this is performed in the NIRWare Management Console (MC)

Load the application for reference measurement by choosing 'Open' from the 'Application Designer' in the tree list. Then select the reference application from the list on the right:




The application is now available as a new point in the tree menu:


Click on the 'Copy' icon  to create a copy of this application:



This copy starts in the 'created' state, while the original application remains 'approved':

To change the name, you first have to click on the 'Edit' icon .

This causes a change from 'Idle' - to 'Edit' mode, allowing you now to make changes to the 'Value' -fields.

Change the application name, then save .

The application for routine use has been prepared, and the calibration can now be assigned to it.

Roadmap to Application Design

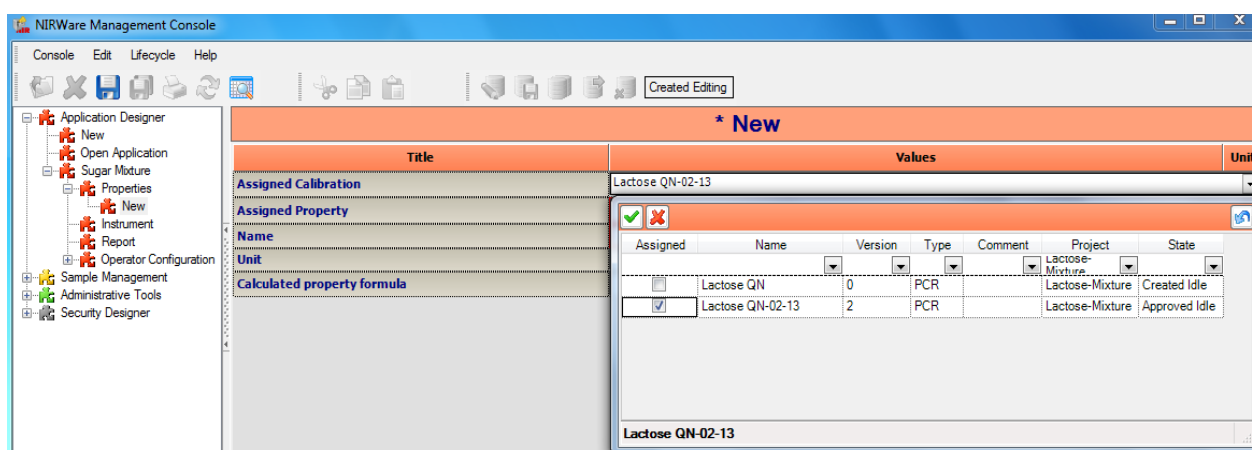


Design Ref.-Application <i>Set to 'Approved'</i>		
Record spectra of ref. samples		
Define Properties & -values		
Calibrate <i>Set cal. to 'Approved'</i>		
Copy appl. as template for routine appl. <i>(Adjust SOP & meas. per sample)</i>		
Integrate Calibration in Application <i>Set to 'Approved'</i>		
Use for Prediction / Routine Measurement		

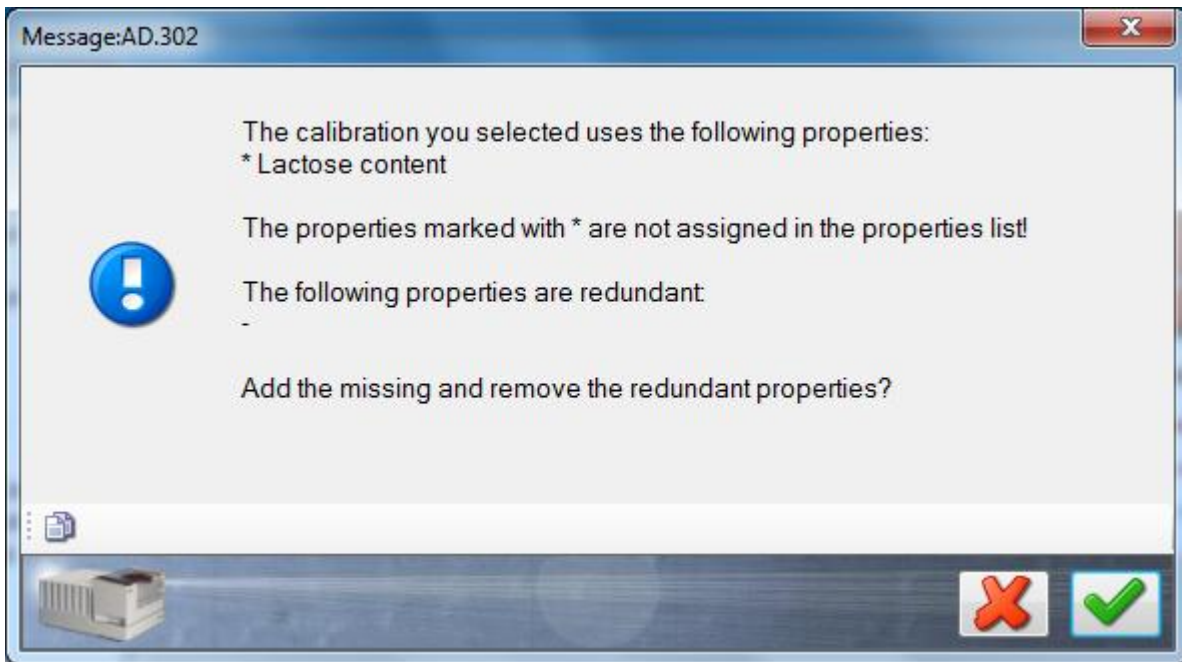


On the Properties level click the button to make the property editable.

Select 'Properties - New' menu from the tree menu of your application and select the drop down-menu for 'Assigned calibration' by clicking on the down arrow symbol at the end of the corresponding value field:



In the 'Assigned' column, set a check-mark in front of the calibration you want to use. Click on the green check-mark button to assign the chosen calibration to the application. A message appears, which you just confirm:




The property defined in the selected calibration is now automatically assigned to the application ('Assigned Property').

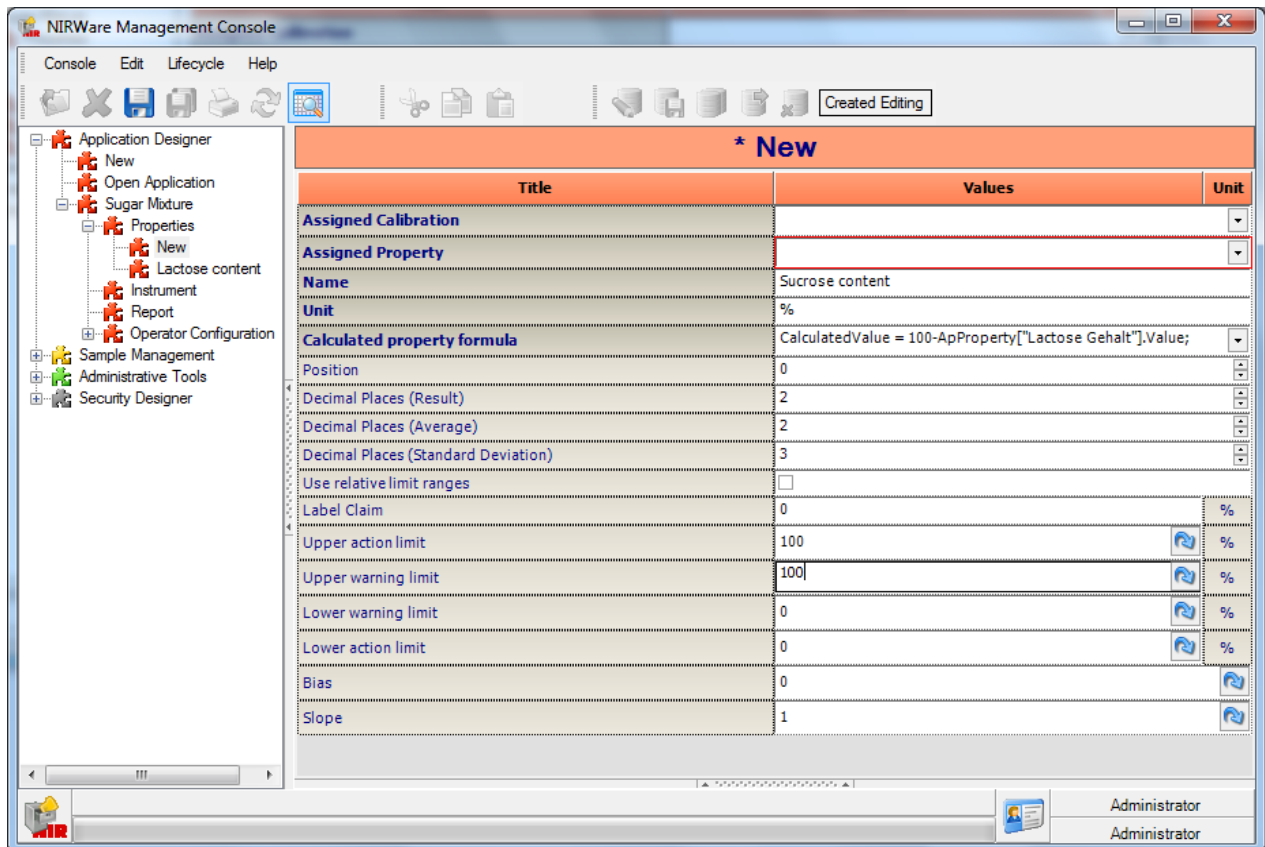
* Lactose content		
Title	Values	Unit
Assigned Calibration	Lactose QN-02-13	
Assigned Property	Lactose content	
Name	Lactose Gehalt	
Unit	%	
Calculated property formula		
Position	0	
Decimal Places (Result)	2	
Decimal Places (Average)	2	
Decimal Places (Standard Deviation)	3	
Use relative limit ranges	<input type="checkbox"/>	
Label Claim	0	%
Upper action limit	100	%
Upper warning limit	100	%
Lower warning limit	0	%
Lower action limit	0	%
Bias	0	
Slope	1	

A 'Name' can be entered as a label to e.g. translate a foreign property name.


The 'Unit' field has to be filled out as well.

Save all changes to the database by clicking on the icon .

These steps have to be repeated for every other calibration to be used in the application. In this example the Fine Sucrose is calculated = 100-Lactose content. Edit also the lower, upper, warning and action limits beside the property name, unit.



Now you can already use this newly created application as an administrator user in the operator software.

To make this application visible to the operator user, you have to put it in the approved state .

Congratulations! You just finished the application development process! You can now start with routine measurement of the contents of Lactose and Fine Sucrose in a mixture of both by using the Operator software.

Sugar quantification-ROUTINE USE
SOP Standard Operating Procedure:
1. Place sample on cell
2. Start measurement

Measurement Description:
Batch: Sugar Mixture
AnalysisID: [New]

Samples:

Sample No.	Value	Residual
1	82.18 %	0.000290
2	81.33 %	0.000288
3	80.71 %	0.000282
Lactose Gehalt	81.41 %	0.000282
1	17.82 %	0.000000
2	18.67 %	0.000000
3	19.29 %	0.000000
Sucrose content	18.59 %	0.000000

Containers Left: 0

Previous Measurements:

Date	Time	Batch
03/05/2013	12:55:21	Sugar Mixture_82_2013-03-05_12-54-11
03/05/2013	12:54:41	Sugar Mixture_82_2013-03-05_12-54-11
03/05/2013	12:54:11	Sugar Mixture_82_2013-03-05_12-54-11
03/05/2013	12:53:14	Sugar Mixture_5/5_2013-03-05_12-51-50

Calibration

Property	Value
Calibration name:	Lactose QN-02-13
Calibration range:	0.00 - 100.00 [%]
Action range:	0.00 - 100.00 [%]
Warning range:	0.00 - 100.00 [%]
Max. Residual:	0.000361
GUID:	{28AEE4E8-70F2-4F8A-8CFB-36C98E93122F}
Version:	2
Method:	PCR
SEP:	2.552099
Bias:	0.000000
Slope:	1.000000

Property	Value
Calibration name:	CalculatedValue = 100-ApProperty["Lactose Gehalt"] Value:
Calibration range:	0.00 - 100.00 [%]
Action range:	0.00 - 100.00 [%]
Warning range:	0.00 - 100.00 [%]
Max. Residual:	0.000000
GUID:	
Version:	Calculated
Method:	Calculated
SEP:	0.000000
Bias:	0.000000
Slope:	1.000000


Current Page No.: 1 Total Page No.: 1 Zoom Factor: 110%

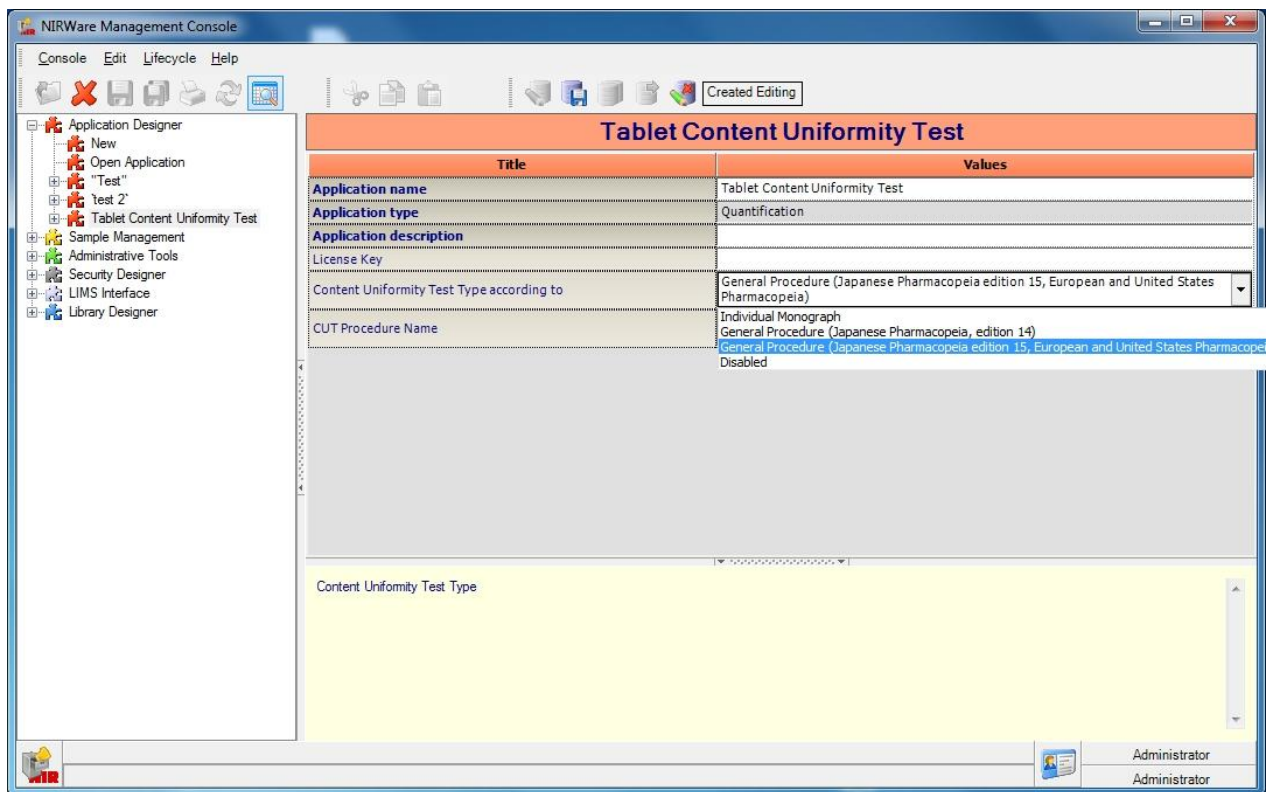
Administrator Administrator 1000044915 0400000004
NIRFlex N500 Solids

5.5. Content Uniformity Test (CUT)

5.5.1. Development of an application for Content Uniformity Testing (CUT) of Solid Dosage Forms

The US Pharmacopeia, the European Pharmacopoeia and the Japanese Pharmacopoeia describe detailed procedures to test the content uniformity of single dosage units. The test indicates the uniformity of the active pharmaceutical ingredient (API) in the dosage unit, such as tablets or capsules, based on the assay of a defined number of samples. This test is requested for batch release.

- Develop a quantitative application as described in the chapter “Creating a quantitative application” for the API.
- After the quantitative application is successfully developed and tested, create a copy of the application.
- To activate the CUT procedure, click on  to show the advanced settings of the application.



From the dropdown list under “Content Uniformity Test according to”, select the procedure you wish to use for testing (e.g. General Procedure (Japanese Pharmacopeia, edition 14)

General Procedure (Japanese Pharmacopeia edition 15, European and United States Pharmacopeia)). For details, please refer to the parameter list of the Application Designer.

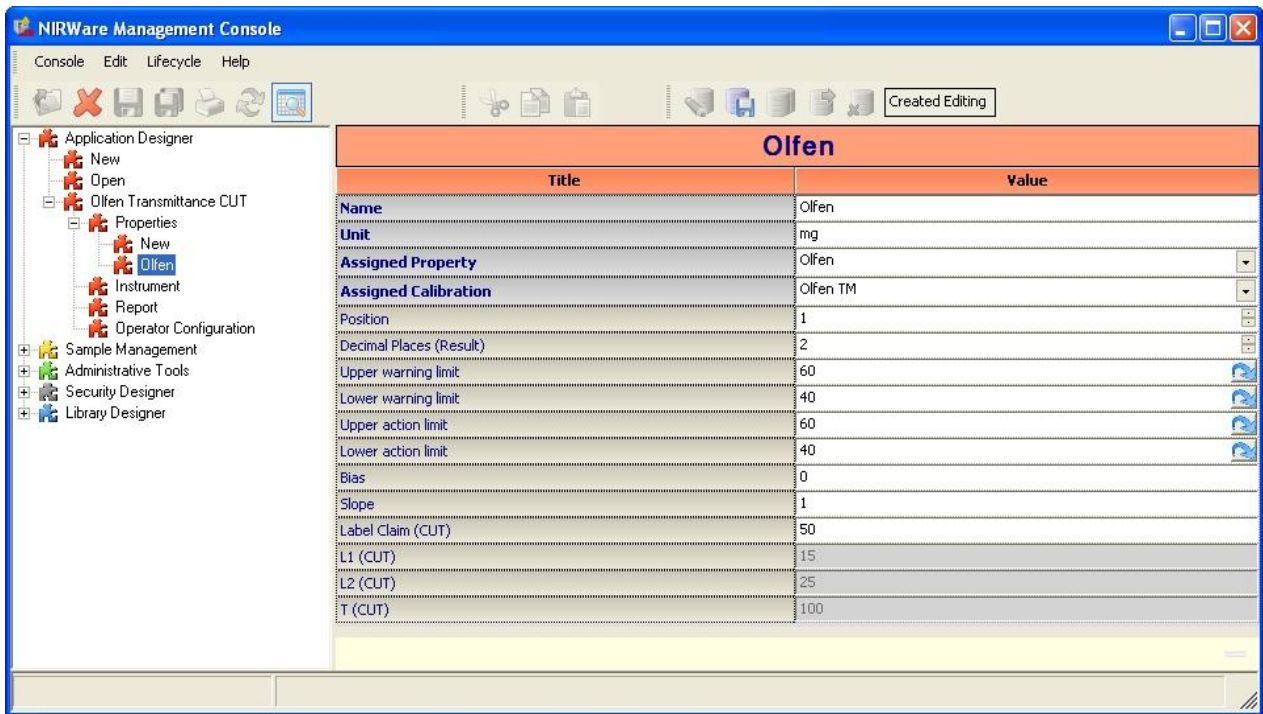
Please note.

Content Uniformity Test is only available for quantitative applications and for the modules NIRFlex Solids Transmittance and NIRFlex Solids with Tablet Add-on.

- For each calibrated property (e.g. API), enter the Label Claim for the CUT under “Properties”.

NOTE:

A value different to 0 has to be entered.



The parameters L1, L2 and T are given by the respective Pharmacopeia.

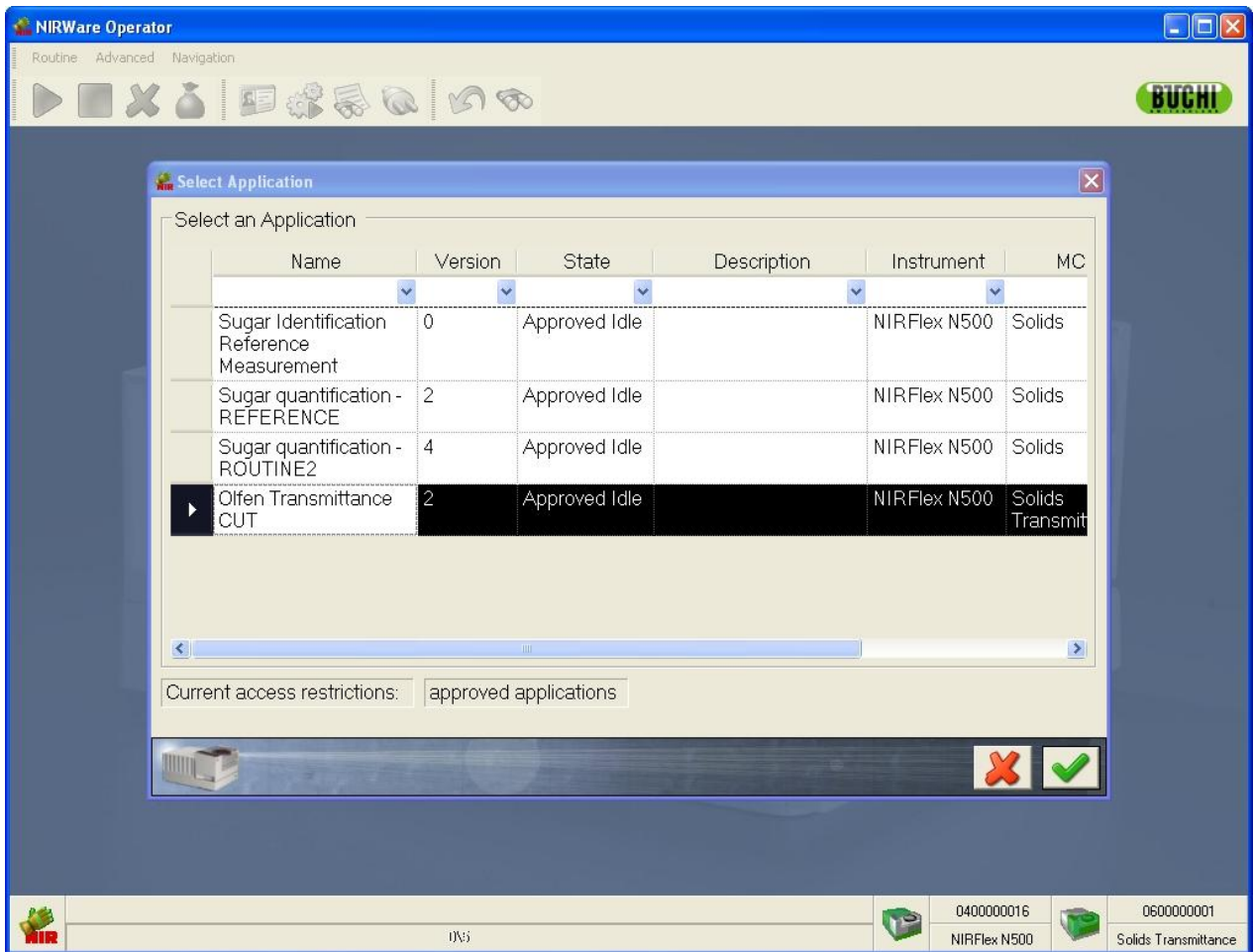
Choosing "Individual Monograph", the values for L1, L2 and T can be edited.

- It is recommended to use the Autaname function of the Operator Configuration to create sample names automatically from basic entries as shown in the below example (autaname part 1 = Batch information; autaname part 2 = none; autaname part 3 = Counter).

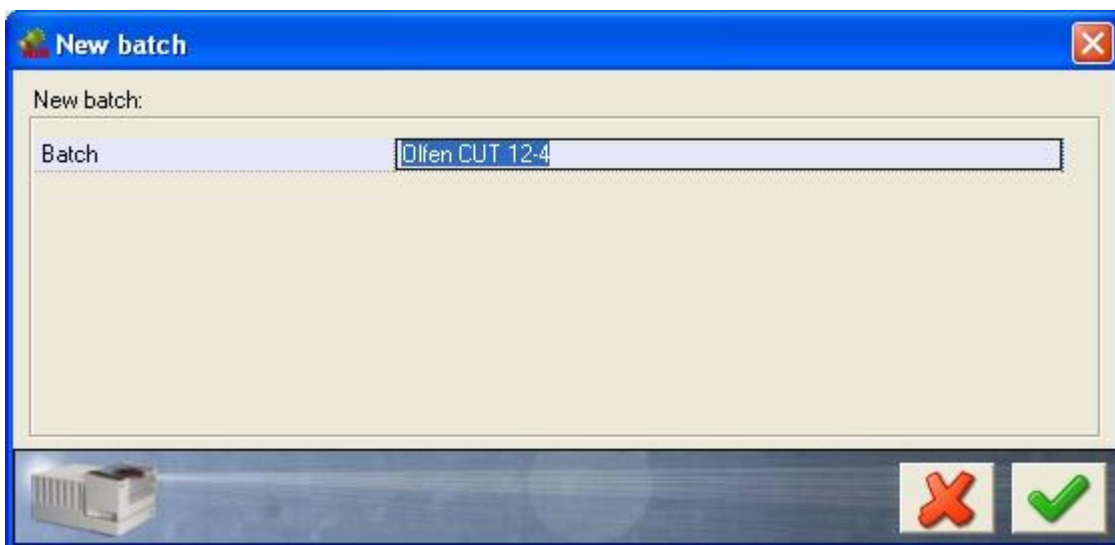
Operator Configuration	
Title	Value
Text	
Automatic printout of measurement results	<input type="checkbox"/>
Continue in error case allowed	<input type="checkbox"/>
Number of repetition of measurements in case of an Out Of Specification	0
Number of measurement sequences	1
Use drop down for expected substance	<input checked="" type="checkbox"/>
Sample Plan	
Auto name part 1	Batch
Auto name part 2	
Auto name part 3	Counter

If CUT is activated in the application, the settings for "Number of repetition of measurements in case of an Out Of Specification" case will be always 0 and "Number of measurement sequences" will be always 1 (even if specified otherwise in the application).

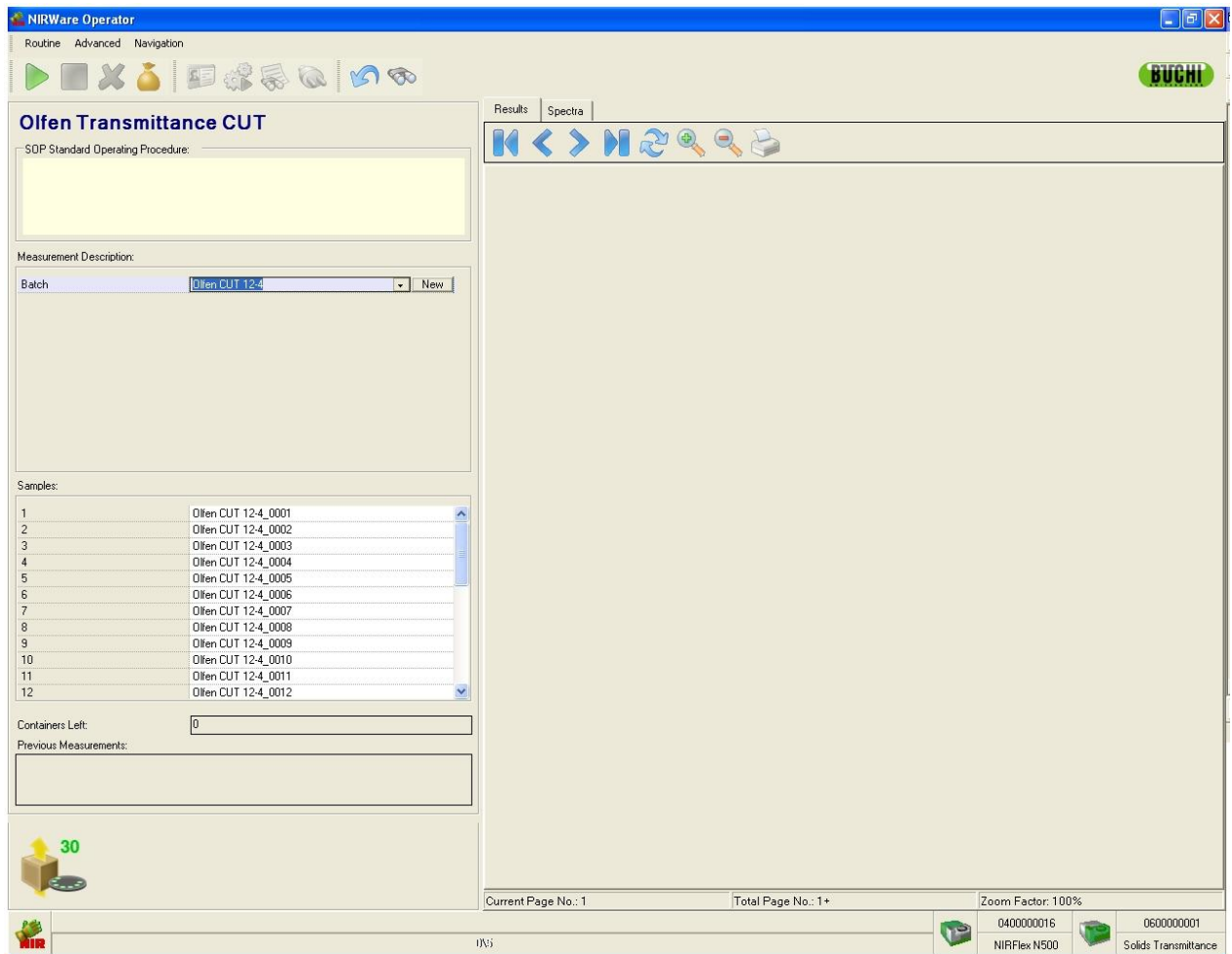
- After all changes on settings are made, set the application in the approved state.
- Start the operator and select the developed application for CUT.



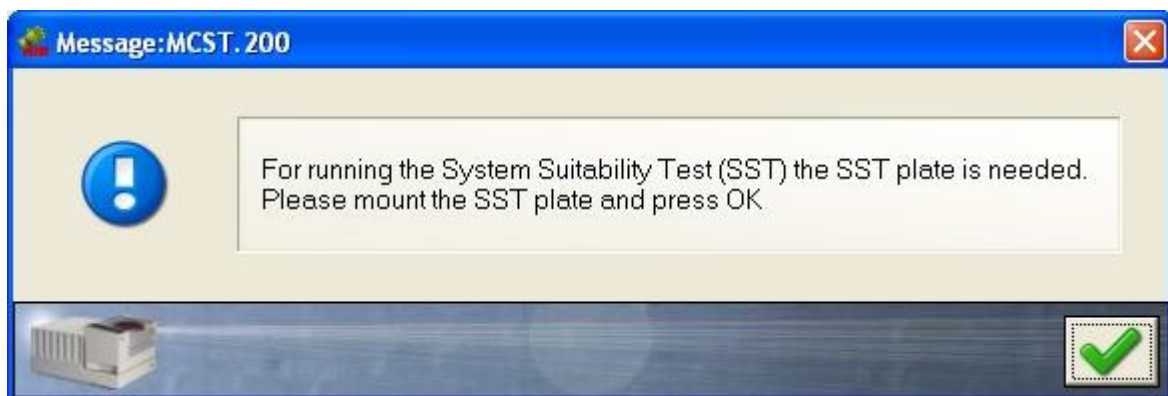
- Create a new batch. Each CUT is handled as an individual batch. When the CUT is finished, the batch will be closed.



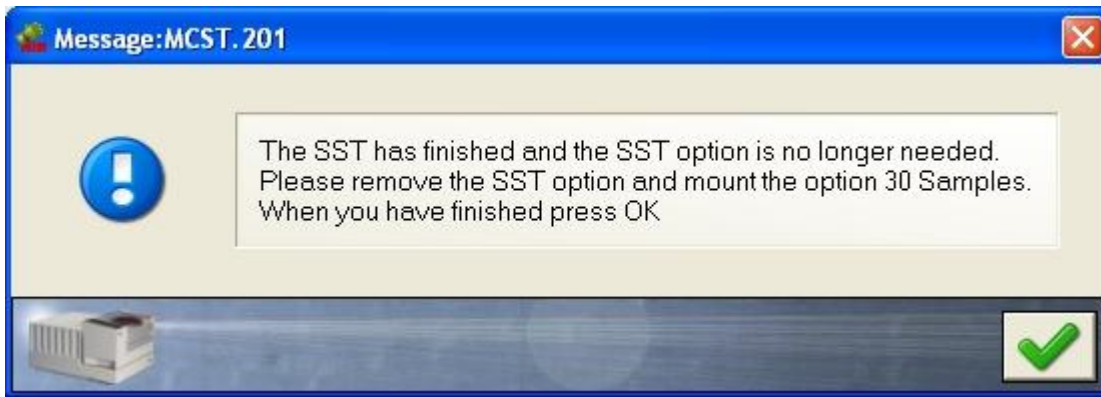
- With the autaname function, the sample names are generated automatically.



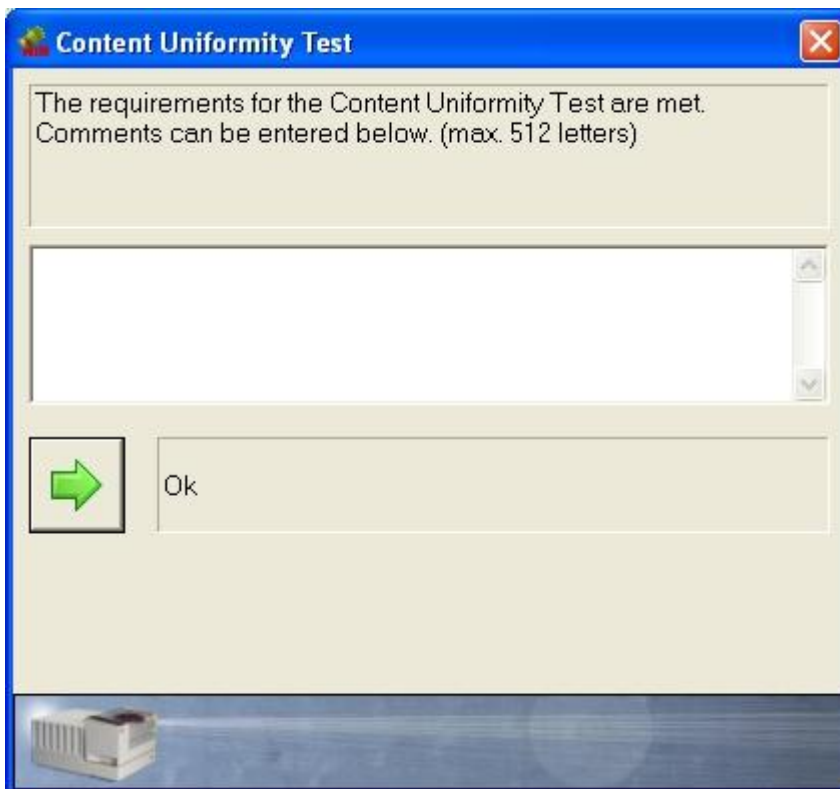
- Press on the Start Button to start the CUT. In case a SST is necessary, the following message appears:



- Follow the instructions and click OK. After the SST is finished successfully, the following message appears:



- Follow the instructions and click OK. Now the CUT starts. When the results of the 10 tested samples are conform, the following message appears:



Comments entered in the entry field will appear on the report.

After confirmation, the report will be displayed on the right, containing a detailed statistical evaluation of the data according the chosen Pharmacopoeia procedure.



UNIFORMITY OF DOSAGE UNITS

Tested according to:

General Procedure (Japanese Pharmacopela edition 16, European and United States Pharmacopela)

Application: **CUT Test SCHC**
 Version: 4 GUID: (4679D538-743F-4131-B7CE-ASCAD6C419D1) State: Approved Idle
 Batch: **Caffein Tablets**
 Tested at (Date, Time): **10/01/2010 10:50:33**
 Tester: **Customer System Maintenance**
 Test Comment: **Test successfully finished**

Caffein

Label Claim: **100.00 mg** L1: (max. allowed acceptance value) **16.0 %**
 T: (test sample amount) **100.0 %** L2: (max. allowed range for deviation) **26.0 %**
 Residual: (max. allowed) **0.011678**

Test n = 10

Sample Name	Residual	Actual Value [mg]	Percent of Label Claim
1 Caffein Tablets	0.004021	95.64 ok	95.6
2 Caffein Tablets	0.003099	98.17 ok	98.2
3 Caffein Tablets	0.002890	99.81 ok	99.8
4 Caffein Tablets	0.003606	97.63 ok	97.6
5 Caffein Tablets	0.002226	97.00 ok	97.0
6 Caffein Tablets	0.003631	99.91 ok	99.9
7 Caffein Tablets	0.003223	98.07 ok	98.1
8 Caffein Tablets	0.002422	99.08 ok	99.1
9 Caffein Tablets	0.002638	98.10 ok	98.1
10 Caffein Tablets	0.003550	99.54 ok	99.6

Mean of individual contents: (mean) **98.0 %**
 Sample standard deviation (s) **1.1 %**

Criteria:

Reference value M = **98.6 %**
 Acceptance value (k= L1: 15.0) **8.1**

RESULT: The requirements are met. (n = 10)

ok

RESULT: The requirements are met.

ok

Calibration Details			
Caffein	Calibration name:	Caffein_Transmittance	Version: 5
	Calibration range:	75.00 - 125.00 [mg]	Method: PLS
	Action range:	75.00 - 125.00 [mg]	SEP: 1.445703
	Warning range:	75.00 - 125.00 [mg]	Bias: 0.000000
	Max. Residual:	0.011678	Slope: 1.000000
	GUID:	(762714F5-32D7-4180-8FFE-34C080C21330)	

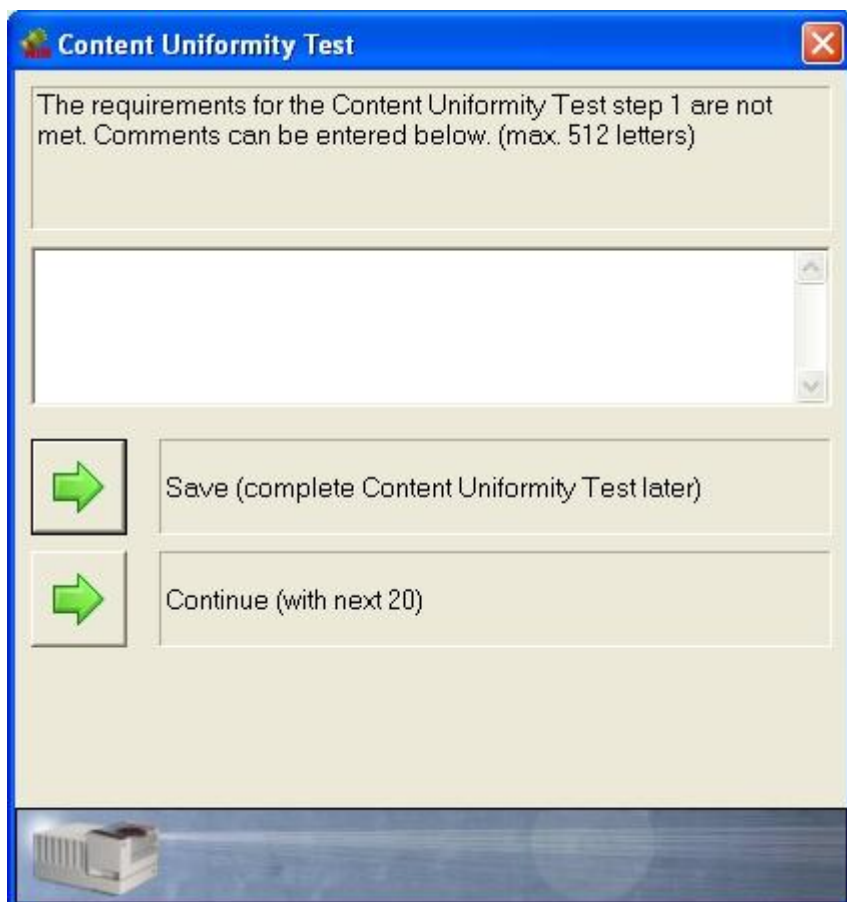
Electronic Signature

10/01/2010 10:55:05

Measurement done by:

Customer System Maintenance

- In case the results of the 10 tested samples were not conform, the following message appears:



Click the arrow in front of Continue if you wish to continue with the required 20 additional samples immediately or complete the test at a later time by selecting the batch from the drop down menu in the Operator.

After the CUT with the 20 additional samples is completed, a report will be displayed on the right, containing a detailed statistical evaluation of the data according the chosen Pharmacopoeia procedure.



UNIFORMITY OF DOSAGE UNITS

Tested according to: General Procedure (European and United States Pharmacopoeia)

Applicator: Olfen Transmittance CUT 2
 Version: 4 GUID: 713FCC9A-8489-4787-8A05-AD12EE8660C9 State: Approved MLE
Batch: Olfen CUT 12-8-54
Tested at (Date, Time): 12.01.2007 08:15:10
Tester: Holger Keller
Test Comment: Release of Batch not possible.

Olfen

Label Claim: 66.00 mg L1: (msd, allowed acceptance value) 16.0 %
T: (per sample amount): 100.0 % L2: (msd, allowed range for deviation) 26.0 %
Residual: (msd, allowed): 0.034028

Test n = 10

Po #	Sample Name	Residual	Actual Value [mg]	Percent of Label Claim
1	Olfen CUT 12-8-54_0001	0.014991	45.03 ok	81.8
2	Olfen CUT 12-8-54_0002	0.013539	45.44 ok	82.8
3	Olfen CUT 12-8-54_0003	0.012331	47.06 ok	86.8
4	Olfen CUT 12-8-54_0004	0.012179	46.67 ok	84.8
5	Olfen CUT 12-8-54_0005	0.010639	46.36 ok	84.3
6	Olfen CUT 12-8-54_0006	0.014265	44.55 ok	81.0
7	Olfen CUT 12-8-54_0007	0.010535	46.44 ok	84.4
8	Olfen CUT 12-8-54_0008	0.012953	43.63 ok	78.3
9	Olfen CUT 12-8-54_0009	0.014836	45.09 ok	82.0
10	Olfen CUT 12-8-54_0010	0.013866	45.93 ok	83.6

Mean of individual contents: (mean) 82.8 %
 Sample standard deviation(s) 1.8 %

Criteria:

Reference value M = 88.6 %
 Acceptance value (<= L1: 15.0) 20.2

RESULT: The requirements are not met. (n = 10)



Test n = 30

Po #	Sample Name	Residual	Actual Value [mg]	Percent of Label Claim
1	Olfen CUT 12-8-54_0001	0.014991	45.03 ok	81.8
2	Olfen CUT 12-8-54_0002	0.013539	45.44 ok	82.8
3	Olfen CUT 12-8-54_0003	0.012331	47.06 ok	86.8
4	Olfen CUT 12-8-54_0004	0.012179	46.67 ok	84.8
5	Olfen CUT 12-8-54_0005	0.010639	46.36 ok	84.3
6	Olfen CUT 12-8-54_0006	0.014265	44.55 ok	81.0
7	Olfen CUT 12-8-54_0007	0.010535	46.44 ok	84.4
8	Olfen CUT 12-8-54_0008	0.012953	43.63 ok	78.3
9	Olfen CUT 12-8-54_0009	0.014836	45.09 ok	82.0
10	Olfen CUT 12-8-54_0010	0.013866	45.93 ok	83.6
11	Olfen CUT 12-8-54_0011	0.012786	46.25 ok	84.1
12	Olfen CUT 12-8-54_0012	0.013821	45.11 ok	82.0
13	Olfen CUT 12-8-54_0013	0.015684	46.55 ok	84.8
14	Olfen CUT 12-8-54_0014	0.013501	46.61 ok	84.7
15	Olfen CUT 12-8-54_0015	0.012324	46.48 ok	84.6
16	Olfen CUT 12-8-54_0016	0.015078	46.24 ok	84.1
17	Olfen CUT 12-8-54_0017	0.009989	54.63 ok	89.3
18	Olfen CUT 12-8-54_0018	0.013230	46.04 ok	83.7
19	Olfen CUT 12-8-54_0019	0.013633	46.20 ok	84.0
20	Olfen CUT 12-8-54_0020	0.015766	50.83 ok	82.4

21	Oten CUT 12-8-54_0021	0.012502	45.26 <small>OK</small>	82.3
22	Oten CUT 12-8-54_0022	0.012908	43.45 <small>OK</small>	78.0
23	Oten CUT 12-8-54_0023	0.010104	46.20 <small>OK</small>	84.0
24	Oten CUT 12-8-54_0024	0.012744	44.93 <small>OK</small>	81.7
25	Oten CUT 12-8-54_0025	0.010868	46.44 <small>OK</small>	84.4
26	Oten CUT 12-8-54_0026	0.010819	46.19 <small>OK</small>	84.0
27	Oten CUT 12-8-54_0027	0.011674	47.35 <small>OK</small>	88.1
28	Oten CUT 12-8-54_0028	0.012647	45.15 <small>OK</small>	82.1
29	Oten CUT 12-8-54_0029	0.014122	45.10 <small>OK</small>	82.0
30	Oten CUT 12-8-54_0030	0.013274	46.46 <small>OK</small>	84.6

Mean of individual contents: (mean) 84.1 %
Sample standard deviation(s) 3.7 %

Criteria:

Reference value (M) = 88.6 %
Acceptance value (<= L1: 15.D) 21.8
Range for deviation low side (<= 73.9) 78.0
Range for deviation high side (<= 123.1) 88.8

RESULT: The requirements are not met (n = 30)

X

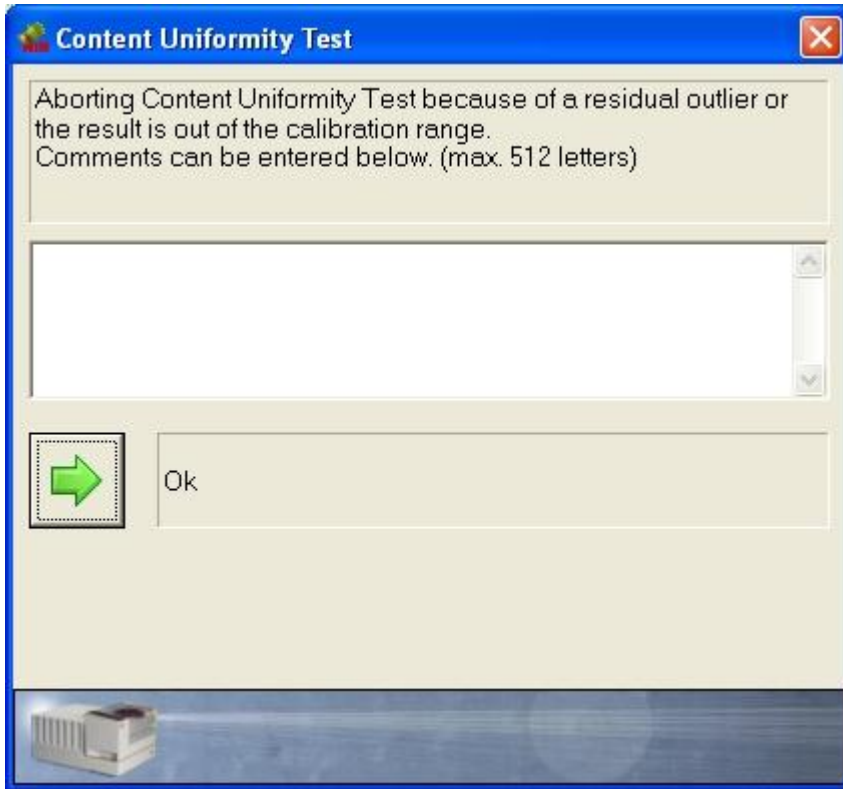
RESULT: The requirements are not met.

X

Calibration Details

Oten	Calibration name:	Oten TM	Version:	2
	Calibration range:	40.00 - 80.00 mg	Method:	PL8
	Action range:	40.00 - 80.00 mg	SEP:	0.783188
	Warning range:	40.00 - 80.00 mg	Bias:	0.000000
	Max. Residual:	0.0340283224	Slope:	1.000000
	GUID:	{1B834730-E41A-4300-8C07-F4D44E11B80D}		

- In case a sample measurement results in a residual outlier or is outside the calibration range, a prediction of this sample is not possible. In this case the CUT stops with the following message:



The corresponding report states the reason for the aborted test.



UNIFORMITY OF DOSAGE UNITS

Tested according to:
General Procedure (Japanese Pharmacopela edition 16, European and United States Pharmacopela)

Application: CUT Test SCHC
Version: 4 GUID: (4679D538-743F-4131-B70E-ASCAD6C419D1) State: Approved Idle
Batch: Tablets 2
Tested at (Date, Time): 10/01/2010 11:01:52
Tester: Customer System Maintenance
Test Comment: Residual outlier

Caffein

Label Claim: 100.00 mg L1: (max. allowed acceptance value) 16.0 %
T: (test sample amount) 100.0 % L2: (max. allowed range for deviation) 26.0 %
Residual: (max. allowed) 0.011678

Test n = 10

Table with 5 columns: Sample Name, Residual, Actual Value [mg], Percent of Label Claim. Contains 10 rows of test data for 'Tablets 2'.

Test aborted, because one or more samples are out of tolerance. (n = 10) !

Test aborted, because one or more samples are out of tolerance. !

Calibration Details table with columns for Caffein, Calibration name, Calibration range, Action range, Warning range, Max. Residual, GUID, Version, Method, SEP, Bias, Slope.

Electronic Signature
10/01/2010 11:06:58 Measurement done by: Customer System Maintenance

5.6. Using applications and calibrations in Life Cycle state "Created"

The calibrations and applications can be used in the Life Cycle state 'created'.

This can be helpful to test a calibration during calibration development or to adjust instrument and application parameters before setting it into the 'checked' state (only Life Cycle 'Electronic Records' or 'Electronic Records'/Electronic Signatures') or 'approved' state for routine use.

5.6.1. Application for development (Life Cycle state "Created")

For applications in the life cycle state 'created', all application parameters are accessible and can be modified. This can be used to define application parameters and test them directly with the Operator. Calibrations can be assigned in the life cycle state 'created' and used for predictions in the Operator module. Once the application fulfills all requirements for the routine, it will be necessary to secure the settings and set the calibrations and the application into an 'approved' state.

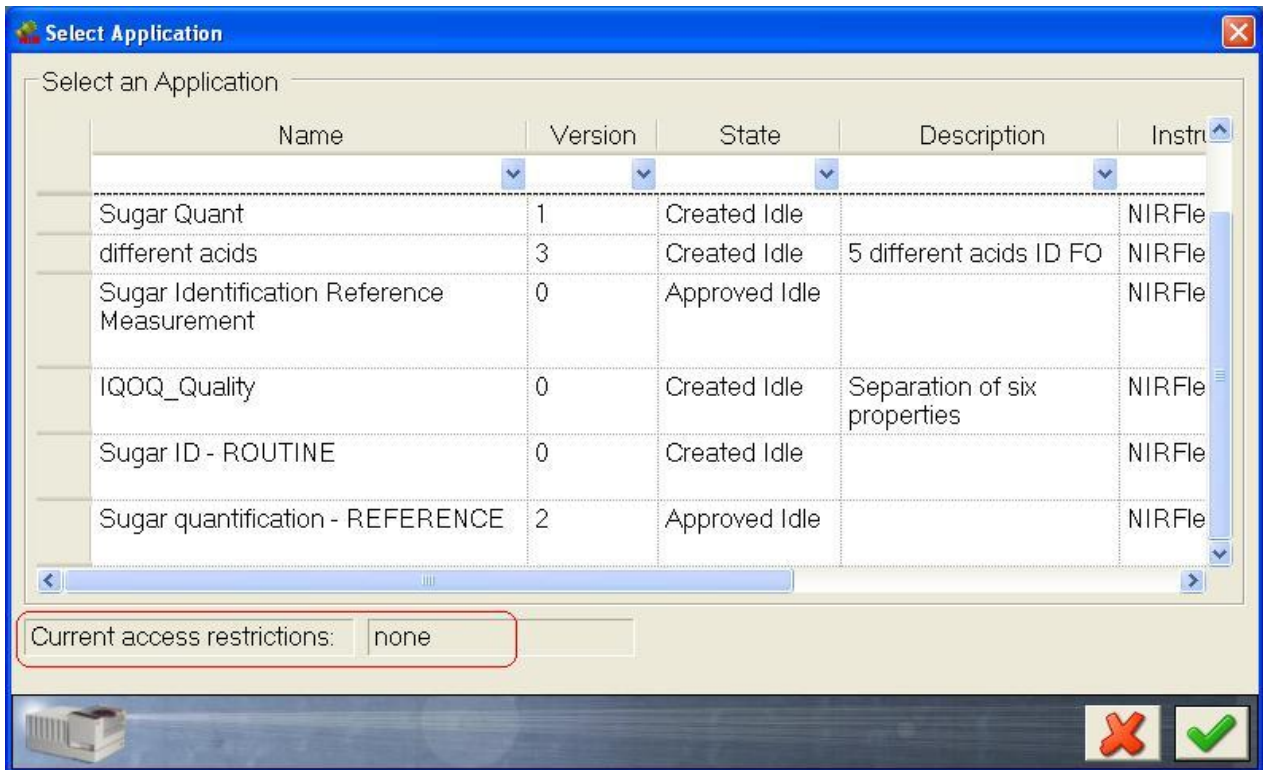
A test before release can be done with the application in Life Cycle state 'checked' (Life Cycle template 'Electronic Records' or 'Electronic Records'/Electronic Signatures' only).

NOTE:

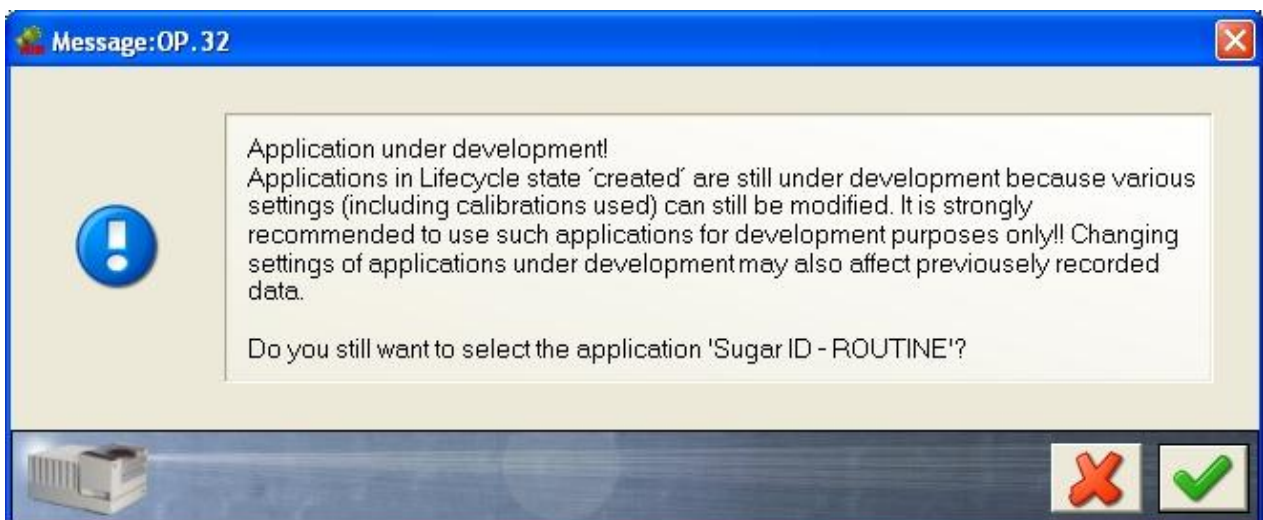
Applications or calibrations in the Life Cycle state 'Created' should not be used for routine measurements at any time, because relevant information that has direct influence on the result and performance of the method can be modified.

Applications in the Life Cycle state 'Created' have the following attributes:

- Only Designers or Administrators have access to applications in the Life Cycle state 'Created'.



If you select an application which is in the Life Cycle State 'Created' the following message appears:



- Under Life Cycle model 'Electronic Records'/Electronic Signatures' it will not be possible to apply an electronic signature on results.
- Under Life Cycle model 'Electronic Records'/Electronic Signatures' the measurement sequence will remain in the life cycle state 'created', therefore it can be differentiated from measurement sequences generated with 'approved' applications.
- It will be possible to modify application parameters such as operator entry fields, SOP text, number of measurements sequences or used report templates. The resulted change can be tested directly in the Operator module.
- Calibrations can be modified and tested in the Operator module.

NOTE:

If you modify a calibration in life cycle state 'created' that was used for predictions already, all previous measurement sequences and result reports generated with that calibration will be modified according to the new calibration setting.

To update the calibration in the application, you need to de-select the calibration and re-assign the calibration new to the corresponding property or property group.

After an application has been tested and is ready to be released for routine use, the following steps have to be followed:

- the used calibrations have to be set to life cycle state 'approved'
- the application has to be set to life cycle state 'approved'
- all generated measurement sequences during testing and development should be archived.

5.6.2. Application in routine use (Life Cycle state 'Approved')

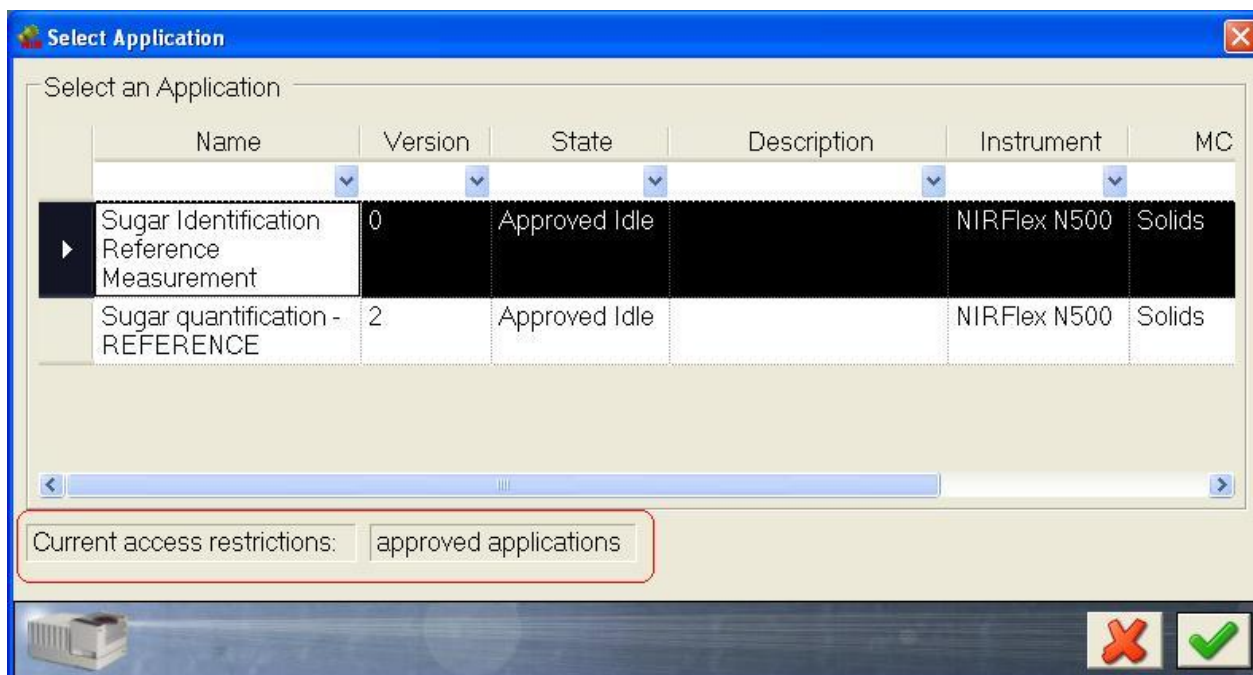
For routine measurements it is necessary to ensure the traceability between results, spectra, measurement methods and calibrations. Therefore applications and calibrations for routine use can not be modified anymore.

An application or calibration can be locked by setting them to the Life Cycle state 'Approved'. With the Life Cycle template 'Electronic Records' or 'Electronic Records'/ 'Electronic Signatures', a test of the application before release in approved state can be done by using the intermediate Life Cycle state 'checked'.

To bring an application in a higher Life Cycle state, the linked calibrations have to be put into approved Life Cycle state first.

An application for routine use in Life Cycle state 'approved' has the following attributes:

- The access for the user group 'Operators' is limited to applications in 'approved' state for routine use.



- Results generated with these applications are logged in the database. Depending on the life cycle state, it will be possible to disable or delete the results but they can not be modified afterwards.
- With the use of life cycle model 'Electronic Records'/'Electronic Signatures', it will be possible to use the electronic signature to sign results and reports.
- To update the calibration or modify application parameters (e.g. SOP, sample name), a copy of the application (version index increase) has to be made. This copy can be modified and logged by setting it into the life cycle state 'approved' again.
- Under Life Cycle state 'Electronic Records'/'Electronic Signatures' a finished measurement sequence will be moved in the life cycle state 'checked'

5.7. Importing license protected applications (e.g. BUCHI or Ingot Pre-Calibrated Applications)

BUCHI is offering various **licence protected applications**, i.e. **BUCHI or INGOT Pre-Calibrated Applications** for Food & Feed. These applications come along as a file that can be imported using the 'Import general' functionality of the NIRWare Management Console. To make the application visible within the Operator software, it must be licensed.

Thus, the licence request form has to be filled out. For this purpose, in the NIRWare Management Console select Help > Software Registration... Fill out the required fields, and click on OK.

(Note: Article- and Serial Number (AN & SN) apply only for prepaid licences, and can then be found on a sticker on the inside of your CD cover).


Software Registration

Buchi software is license protected. The software will only be available on the computer where you fill out this registration form, because the license will be bound to the HostID of this computer. The HostID is a unique machine identifier that will be used by the software to ensure the license agreement. Please fill out the registration form below and send the registration to your buchi sales representative. Thank you for using buchi software!

Software:

AN:

SN:

AN and SN numbers are mandatory if the sticker is in the DVD-Box! 

HostID of this computer:

Hostname of this computer:

Company:

Name and surname:

Title:

eMail:

Phone:

Address:

Postal code:

City:

Country:

Remark:

A licence request file will be generated and saved to your disk (ending '.xml'). Send this file to your BUCHI distributor. BUCHI will then create a licence file which is bound to the name and HostID of your computer ('nodelocked'), so that the application will only run on that specific PC. This licence file (ending '.lic') will then be sent to you. Just import it to your software by choosing Help > Import license in the NIRWare Management Console. Use the file explorer to select the licence file to import, then click on 'Open'. The licence file is now being imported. Restart the PC to activate the new licence.

5.8. Measuring an SST

The System Suitability Test (SST) is a short instrument test and serves as quick validation. It is suggested to perform SST regularly, the best after each start (can be adjusted with "Interval: 12 hours").

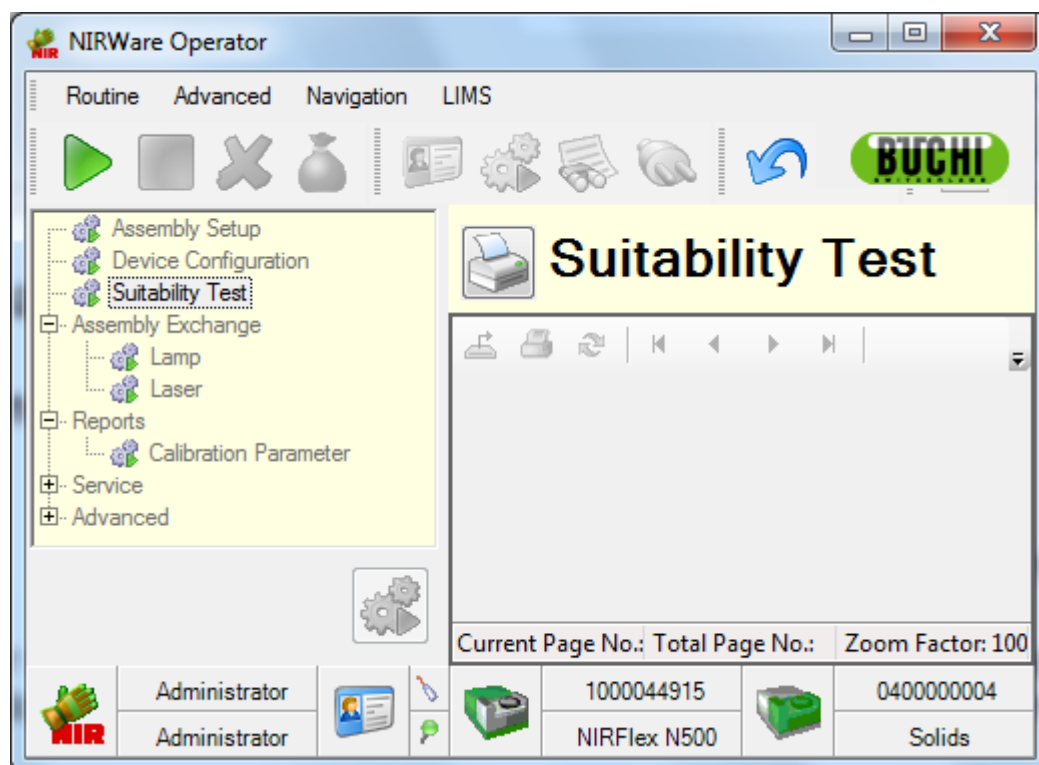
NOTE

Use N-500 only with successful SST.

5.8.1. Manual SST measurement

1. Start **NIRWare Operator**
2. select an Application from the DB
3. In the menu under **Advanced** select "Perform Suitability Test."

Or start NIRWare Operator, use "Open service tool" and choose "Suitability test".



After completion of the System Suitability Test a Report is displayed on the right side of the Operator window. A detailed Report can be viewed in the NIRWare Sample Manager.

5.8.2. Automatic SST measurement

By default, a SST will be measured automatically before the first sample measurement in an application, if the set time limit (every 24h) is exceeded.

The time interval can be set in the [Application Designer](#).

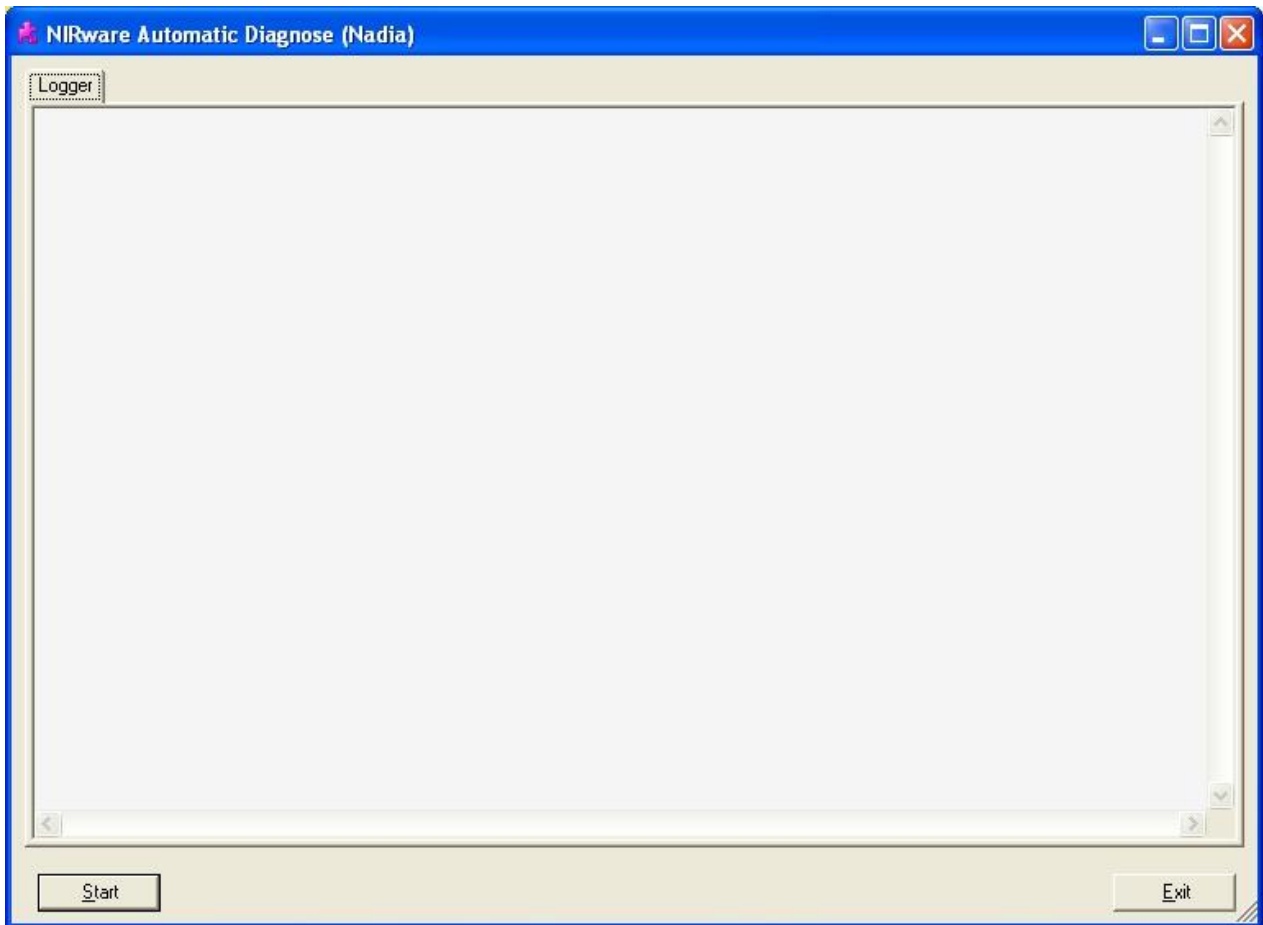
5.9. Measuring a NADIA

NADIA stands for „NIRWare Automatic Diagnose“ and is a service tool to examine the basic functions of the BUCHI NIRFlex-N500.

It will be used from Service Technicians to evaluate malfunctions of the instrument or to do a performance check of the instrument as part of a service contract.

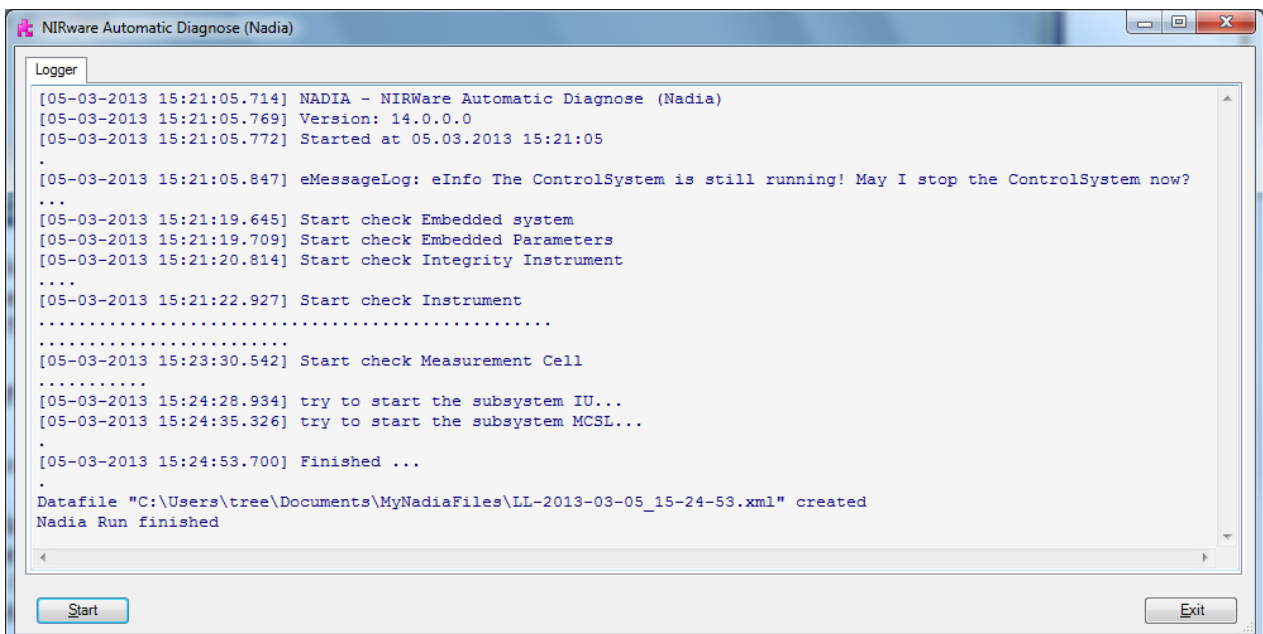
The NADIA is started via the Windows Start Menu (Start\All programs\ BUCHI\ NIRsolutions\ Tools\ Nadia)

The following window opens:



Press start to execute the NADIA test and follow the instructions on the screen.

Once the test is finished, the window shows the following information:



An *.xml file is generated and stored in the directory shown in the report window (example: "C:\Users\

Send this file to a service technician for evaluation. To archive the file, copy it to another location.

5.10. Measuring a reference

To measure a reference spectrum, proceed as follows:

1. Start the **NIRWare Operator**.
2. Select an Application from the DB
3. In the menu under **Advanced** select "Internal Reference" or "External reference" to measure references manually.

5.10.1. Internal / External Reference

Frequent reference measurements increase the stability of a spectrometer. Each measuring cell offers a channel for the reference measurement, which is called external reference. Some measuring cells additionally have an internal reference as the measurement of the external reference is not carried out at exactly the same spot as the sample measurement later on.

External reference

The external reference has the 100% light intensity, which is available at that moment with the NIR unit. In order to measure the transmittance or the reflectance of a sample, the measured intensity spectrum of the sample is divided by a reference spectrum. This reference spectrum is either recorded without a sample (in case of transmittance) or with a white standard in the sample position (reflectance). We call this an external reference. An external reference is always required. The white standard should be absolutely clean for the measurement.

Internal reference

The internal reference is measured to eliminate the minor changes of e.g. moisture content change in the air. While the acquisition of an external reference can be automated in some cases (NIRFlex Solids Transmittance, NIRFlex Liquids, Vial and Tablet add-on for NIRFlex Solids), in other cases the measurement of an external reference requires user interaction (Petri dish and XL add-on for NIRFlex Solids and Fiber Optic Solids).

With internal referencing an alternate measurement channel, which differs in optical path layout from the normal channel (internal reference channel) is measured automatically and more often than external references are taken. Spectral drift is reduced by calculating the following:

$T = (\text{sample}) / (\text{last internal reference}) \times (\text{first internal reference}) / (\text{external reference})$,

$$\text{Spectrum} = \frac{\text{sample spectrum } (I_S)}{\text{external reference spectrum } (I_{ER})} \cdot \frac{\text{internal reference spectrum } (I_{IR,S})}{\text{internal reference spectrum } (I_{IR,ER})}$$

where the first internal reference was recorded right before the external reference. Internal referencing minimizes the need for (inconvenient) user interaction in situations where no automatic placement of the reference is possible.

NOTE

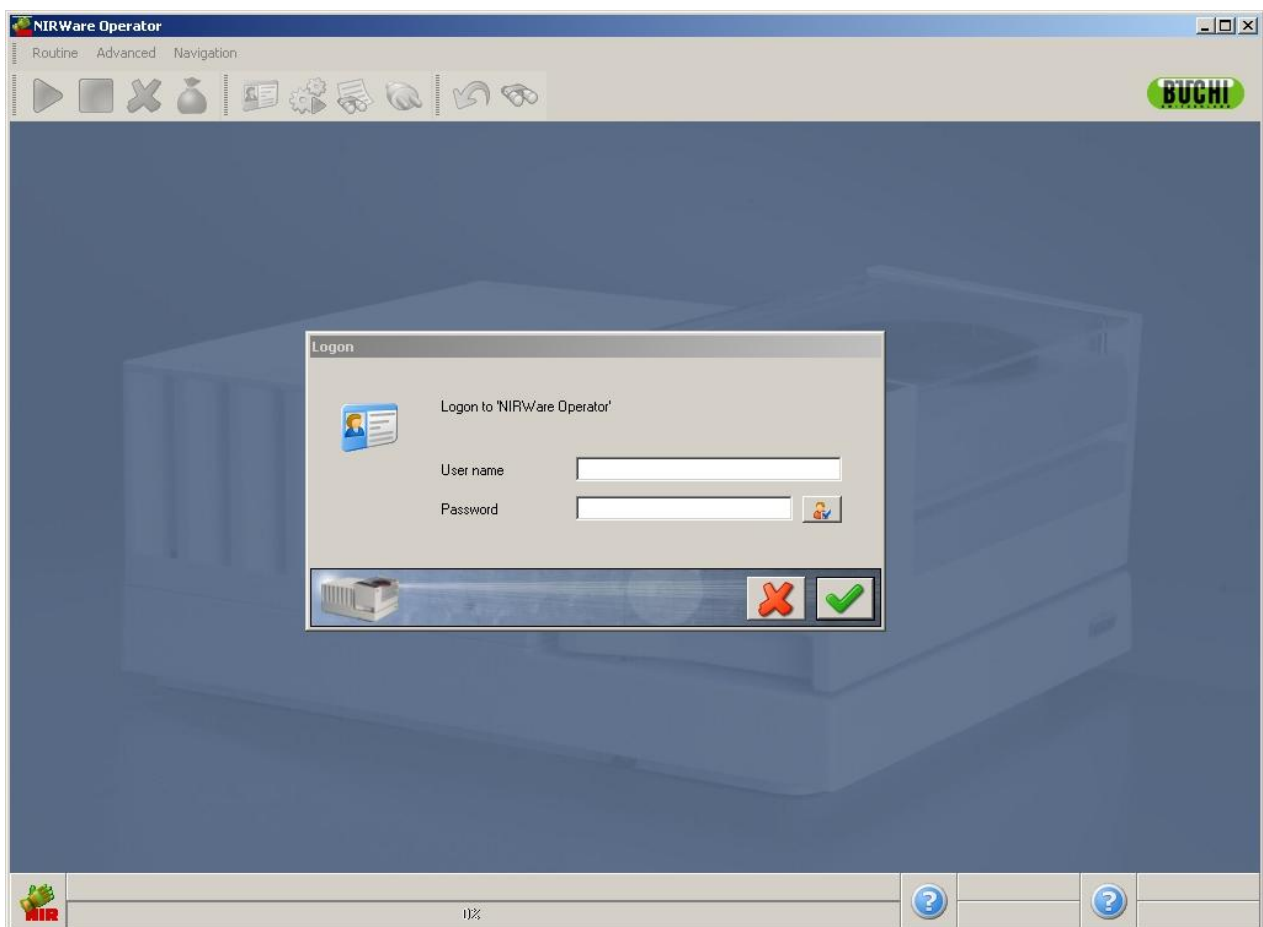
Different modes for reference measurements are available. Batch, Manual, Temperature Drift, Once a day, Measure Sequence, Interval and Disabled.

In case you plan to switch between different applications and want to avoid external reference spectra during each change, it might be useful to set the external referencing to “Manual” or “Once a day”.

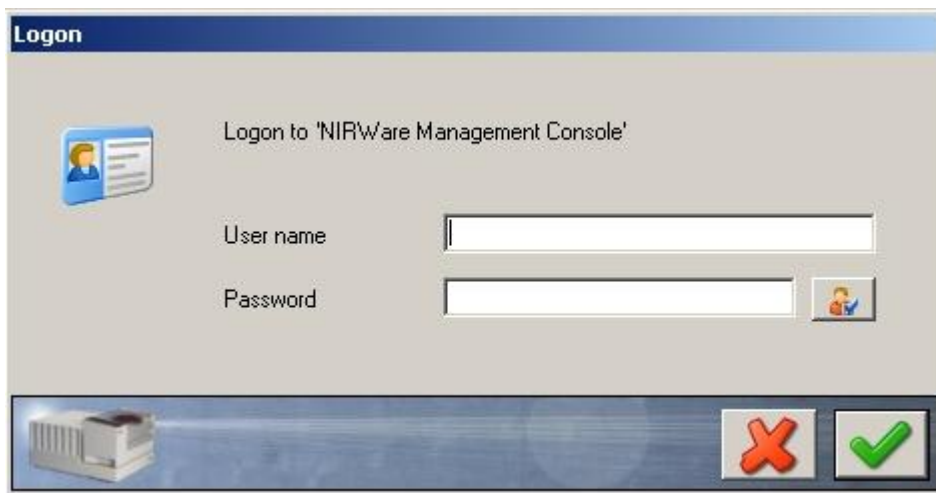
It is not recommended to disable the external referencing as that means that the spectrum is not taken into account for the calculation according to the above formula.

5.11. Carrying out a measurement with the Operator

- The measurement sequence should start with the N-500 warmed up for at least 30 minutes and with reference cap in place on the probe. The NIRWare Operator software is started by double-clicking the respective icon, or from the Windows Start-Menu. The window below appears:



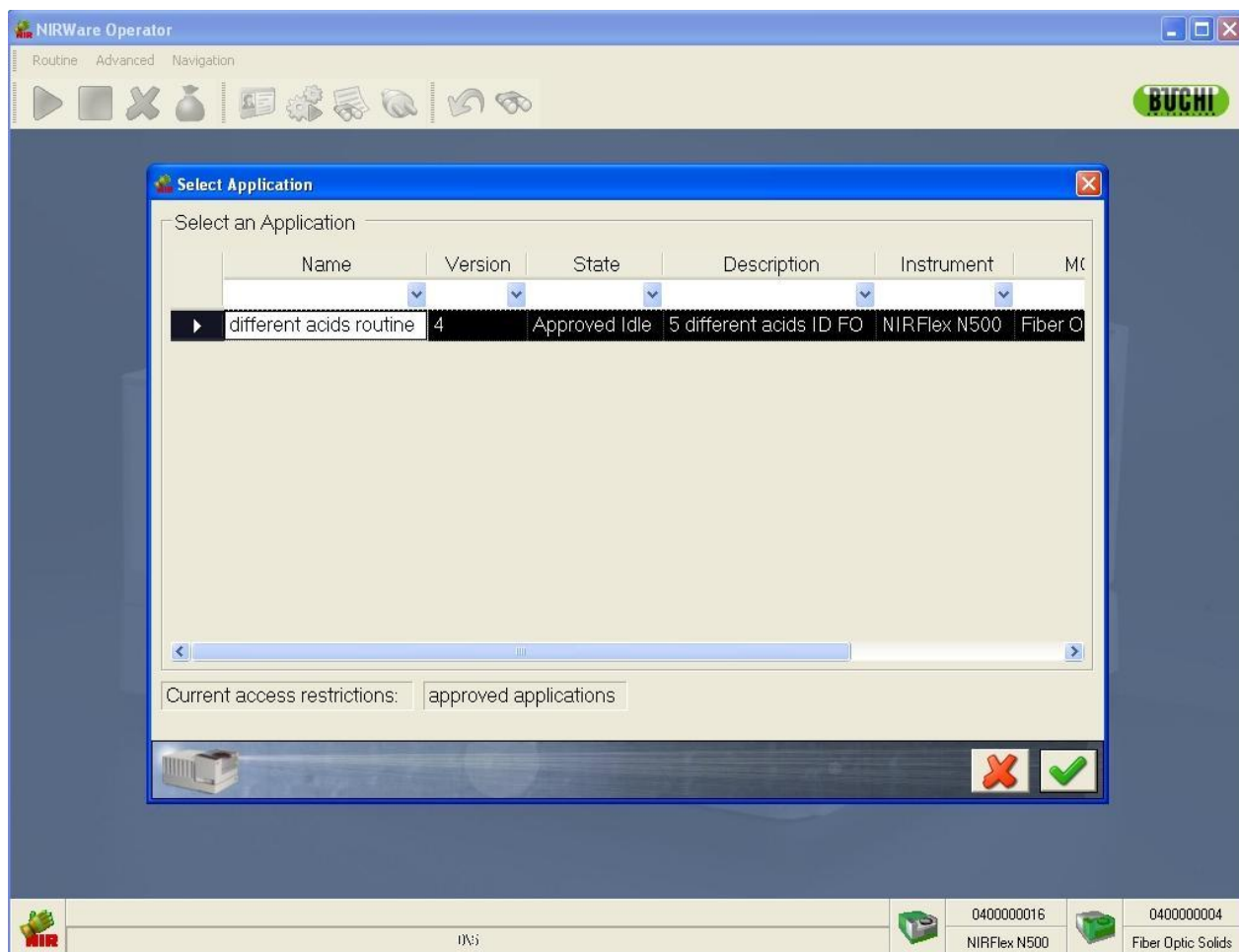
- The user then types in his user name and password in the fields indicated



- The Logon window will close if the user name and password are accepted.



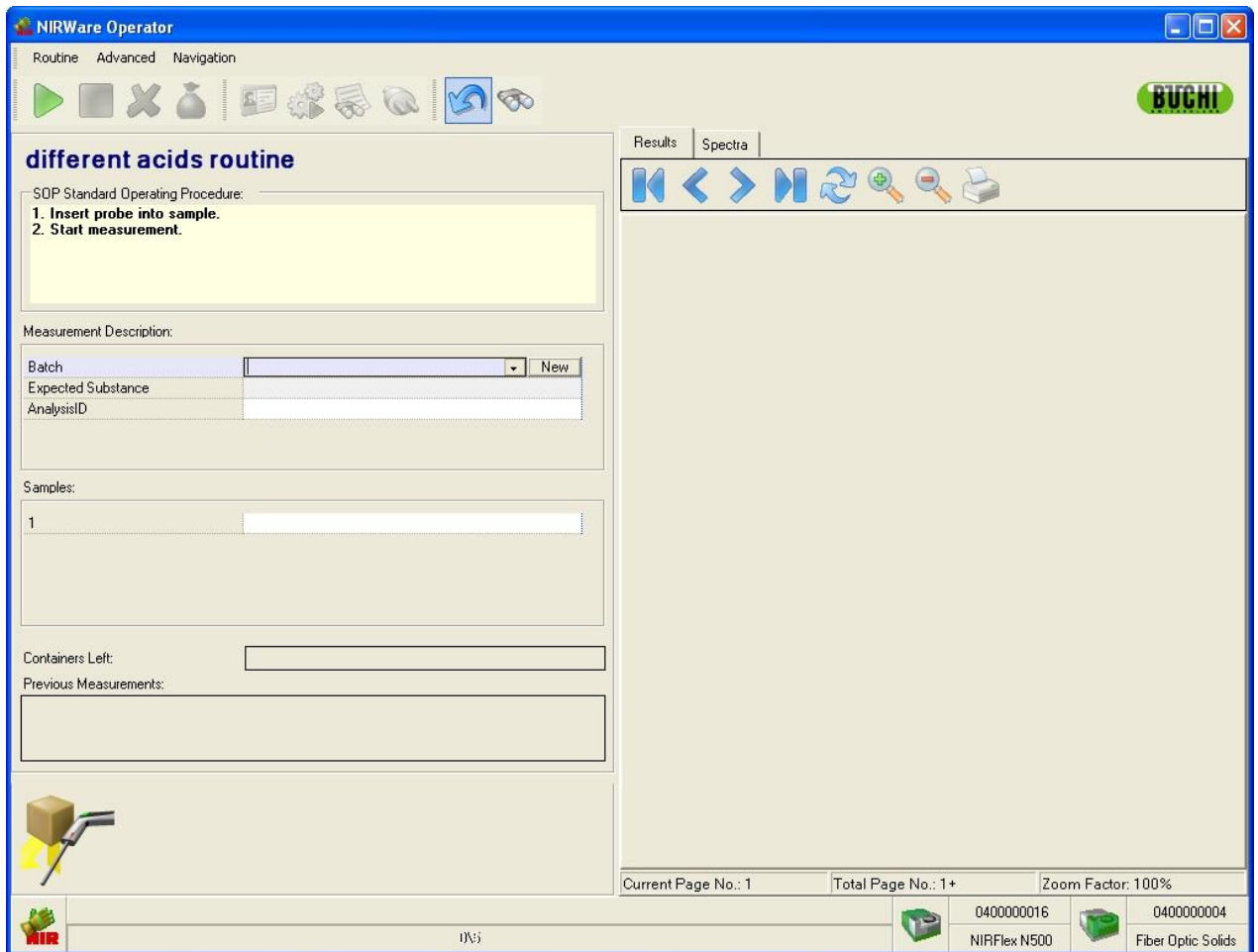
The user then clicks on the “Binoculars” icon to see the available Applications.



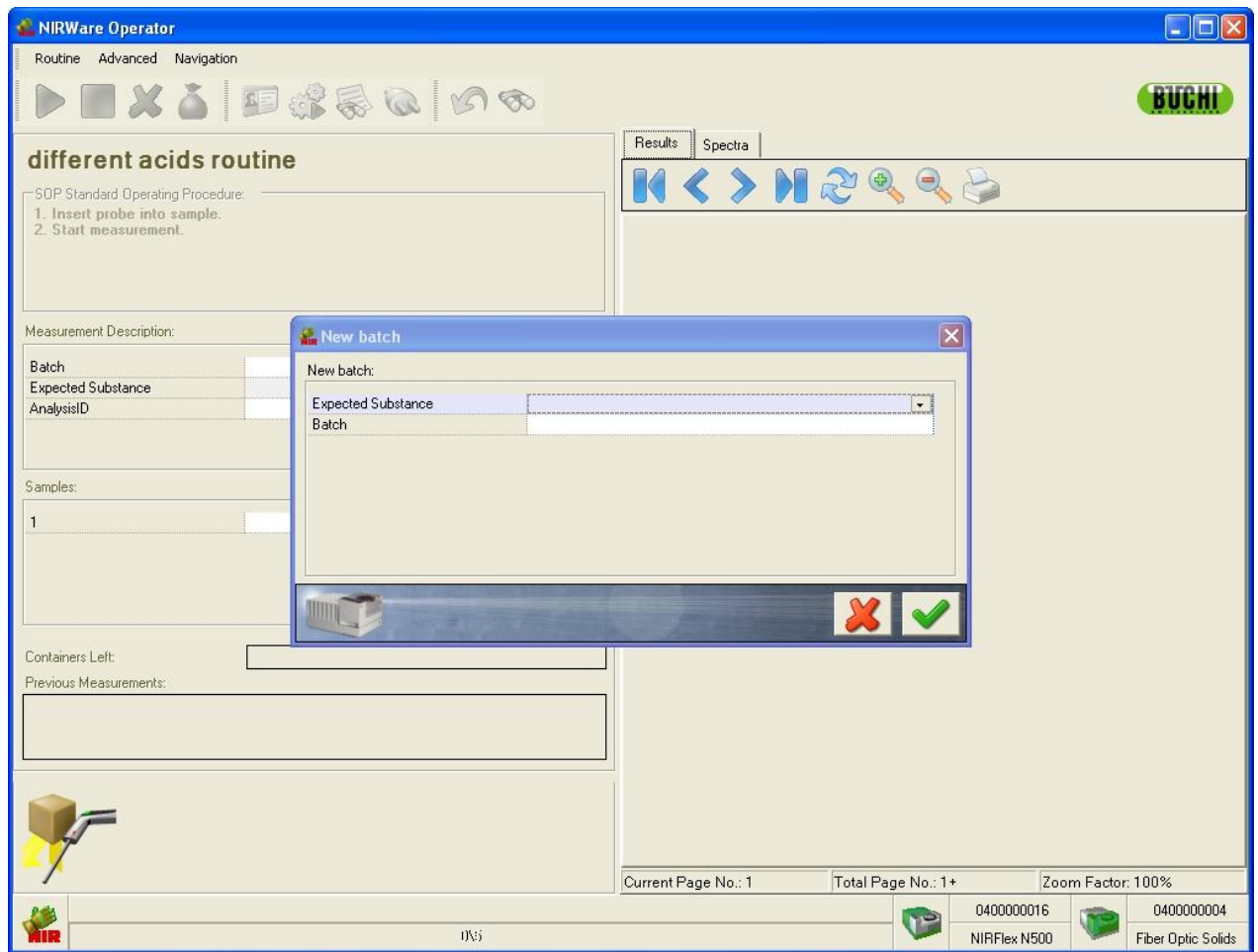
NOTE

Applications which are not saved in the Management Console remain in the Life Cycle state '...Editing'. Applications in this state will not be shown in the selection window.

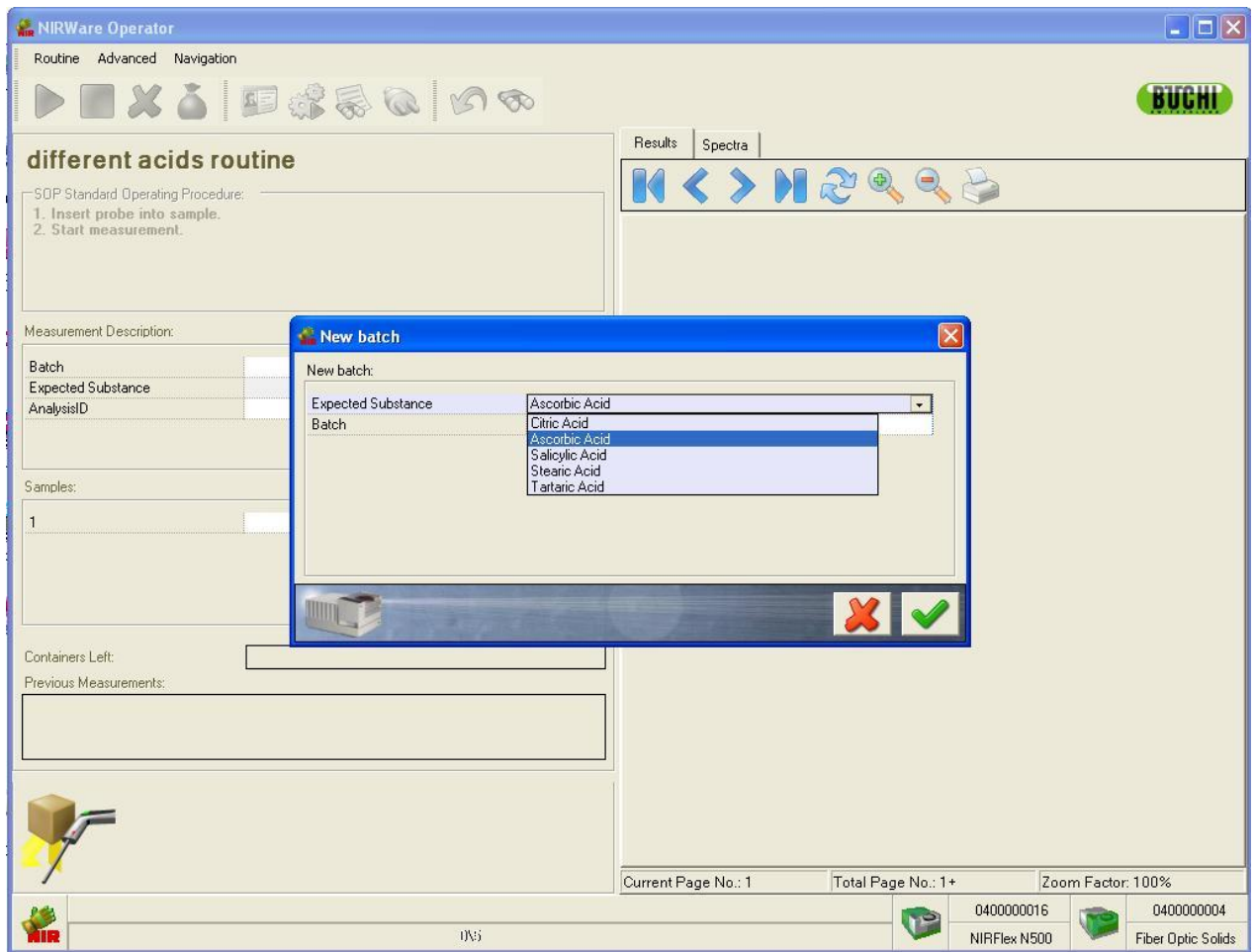
- The user selects the row for the desired application, then clicks the green check mark at the bottom right corner of the “Select Application” window. The windows appearance changes as shown below (particular fields and their labels may vary, depending on how your Application has been configured).



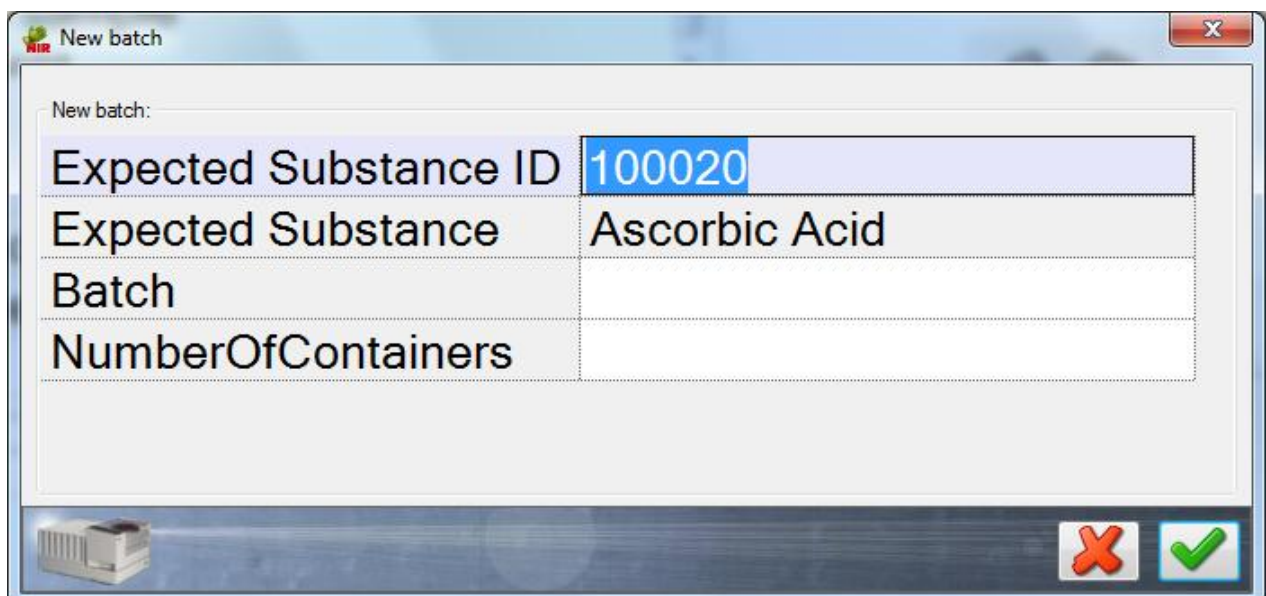
- If this batch (or lot) has already been entered in a past measurement, the user now proceeds to the selection of the batch that he is running. If this batch (or lot) is being measured now for the first time on the N-500, the user clicks on the “New” near the center of the screen, next to the empty “Batch” field. The “New Batch” window opens as shown below.



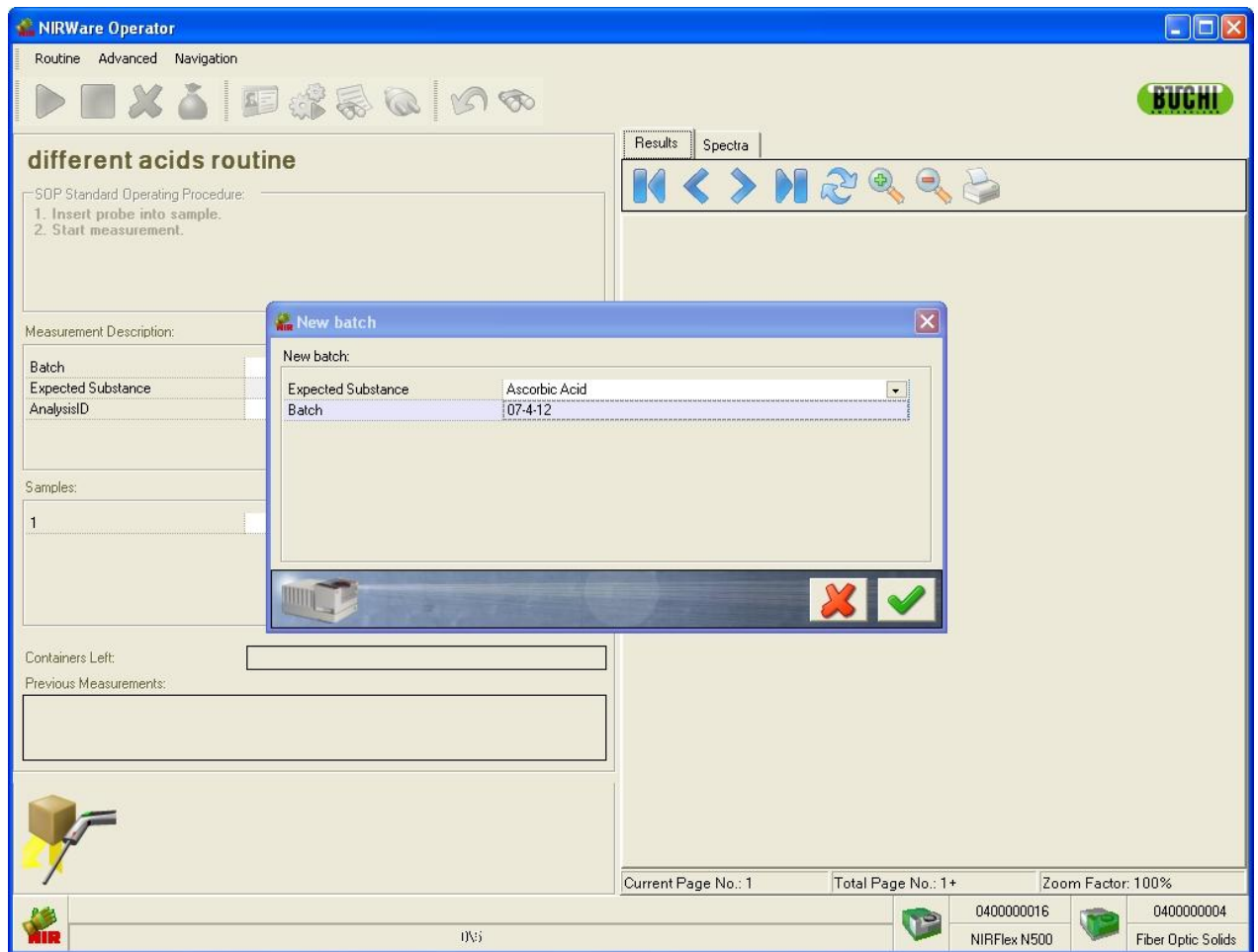
- Click on the "Expected substance" field, the substance name, which should be identified should be selected.



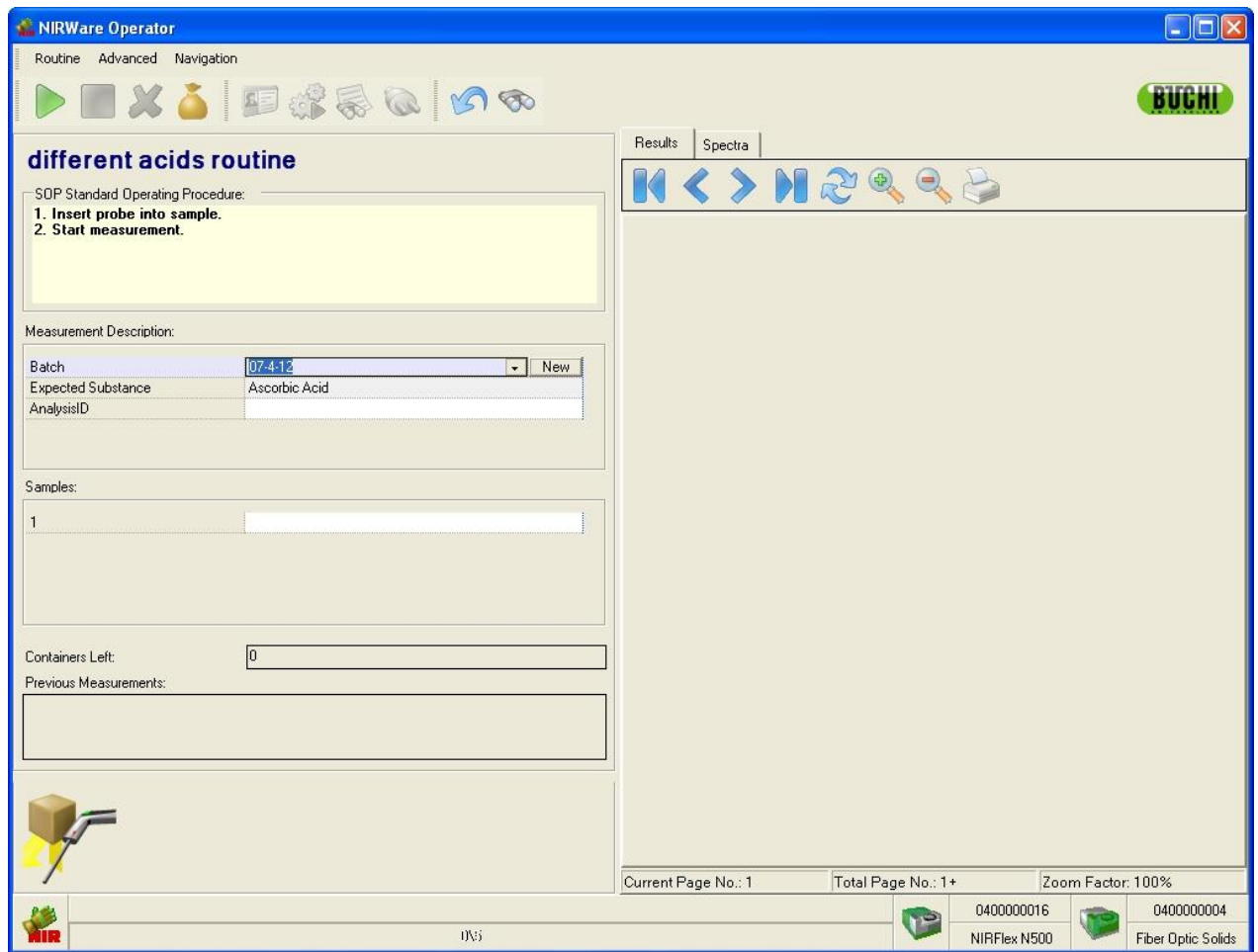
- If the Substance ID is used (deactivate "Use drop down for expected substance" filed in the application), the user has to enter the substance code (article number). Several codes can be used for the same substance (enter them in "MC: Sample Manager/ Properties"). This code with many other substance information can be entered also by barcode.



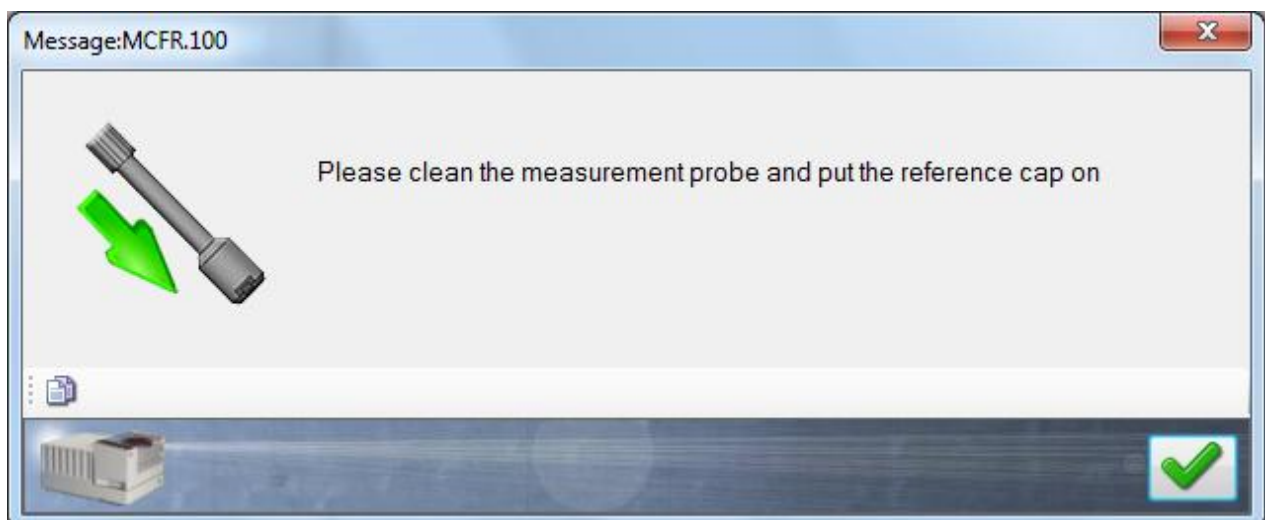
- The user types in the Batch (or Lot) number in the “Batch” field.



- The user goes to the batch dropdown menu and selects the batch that he is running. Since this batch was run previously, the Expected Substance field will fill in automatically.
- The user now sees the sample's Batch number and Expected Substance appear on the screen.

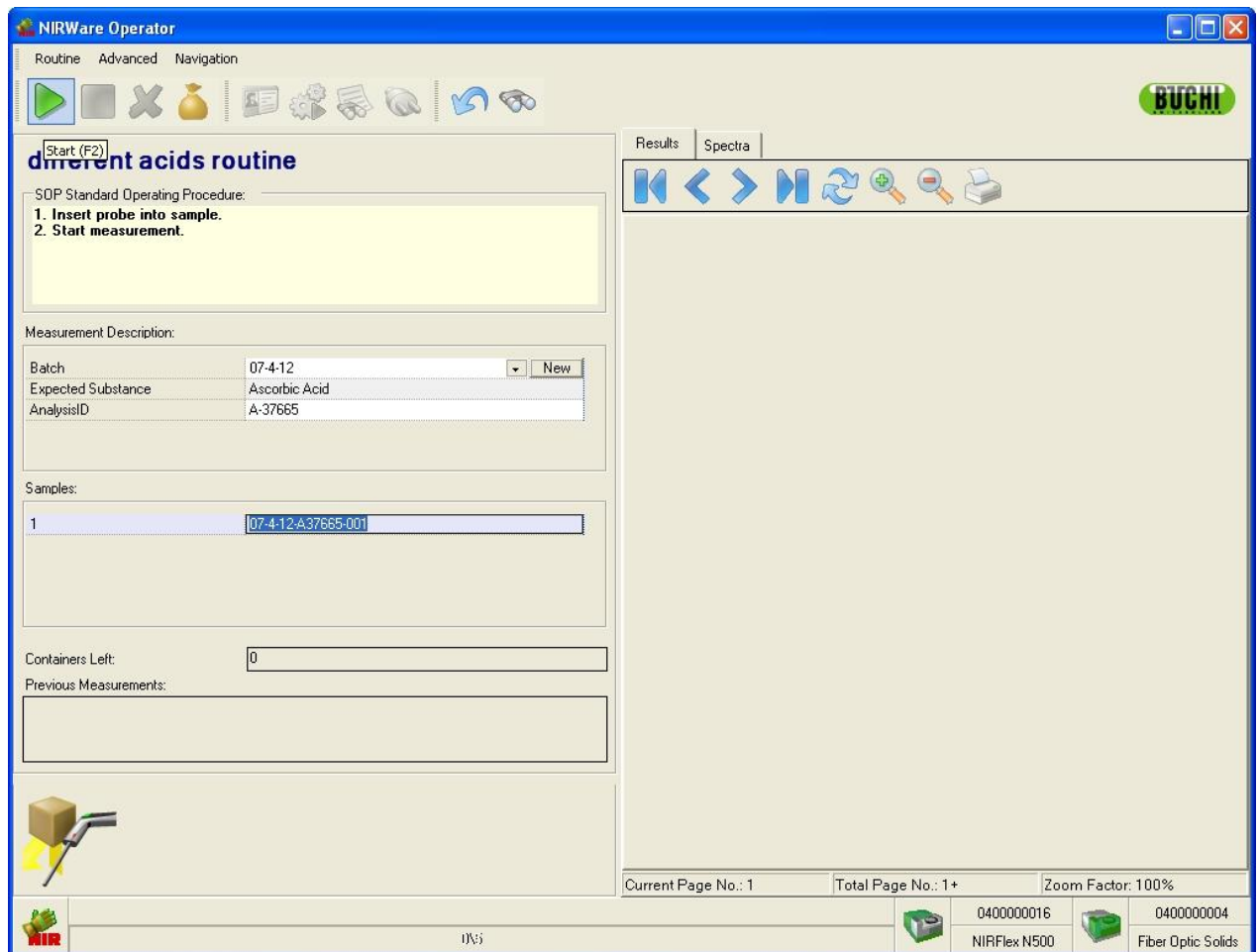


- Any additional required fields (such as “Analysis ID” and “Sample”) now need to be filled in by the operator.
- To start the measurement, the user clicks the green arrow in the top left corner, or clicks the button on the fiber optic probe.

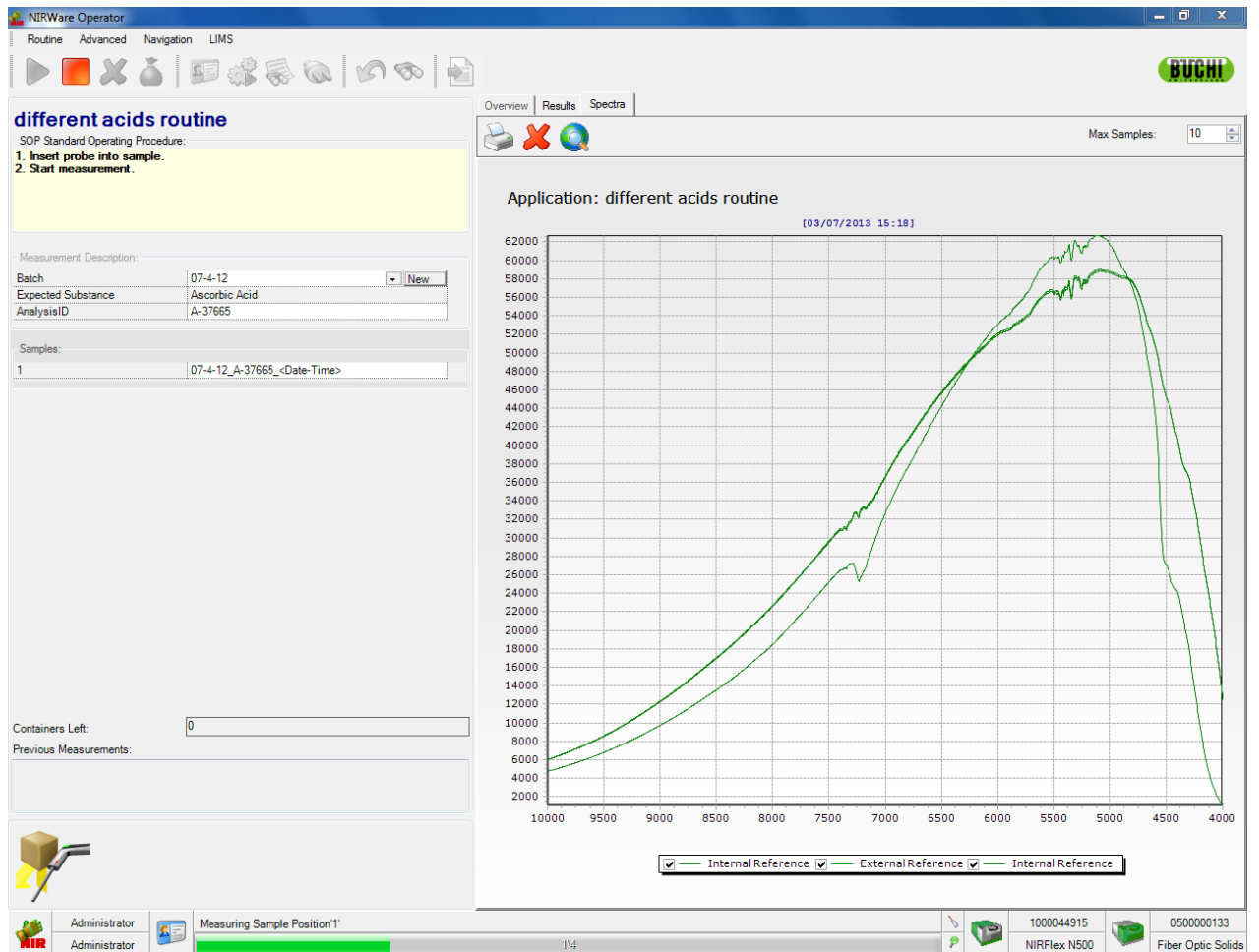




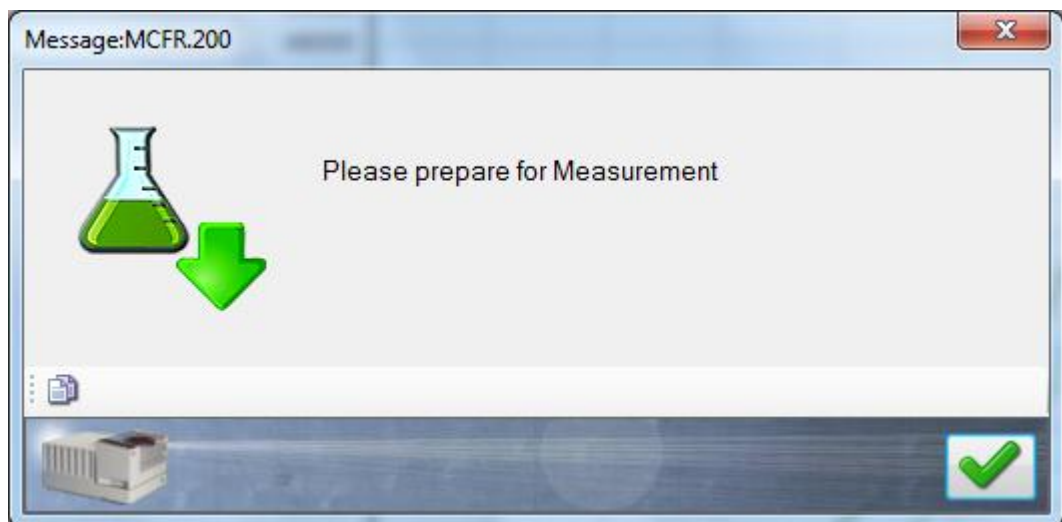
- If the system determines that a new external reference needs to be collected, the external reference scan will begin automatically. As long as the user has placed the reference cap on the probe he does not need to take any action other than waiting for the scan to finish (as indicated by the progress bar at the bottom of the screen). If the reference cap is not in place, a warning prompt will appear, advising the user to place the reference cap on the probe. Once the scan is finished, it will be displayed on the right side of the screen.



- If the system determines that a new internal reference needs to be collected, that measurement will automatically be collected. No special action is required of the user other than waiting for the scan to finish.



- A message will appear saying "Please Prepare for measurement".



- Now the reference cap is removed and the probe window is brought in good contact with the sample. The user now clicks the green check mark or the button on the probe to initiate the scan. During the scan, the progress bar will be moving on the bottom of the screen.
- Once the measurement is complete, the result report will appear on the right side of the screen. Two report formats are available (but only one will be presented to the user).
- If the "Detail" report is activated in the application "Report" adjustment:

The screenshot displays the NIRWare Operator software interface. The main window is titled "different acids routine" and shows a Standard Operating Procedure (SOP) with two steps: "1. Fill in the field below" and "2. Insert probe into sample". The interface includes a "Main Report" section with the following data:

Sample: 07-4-12_A- 37665_2013-03-07_16-33-51

Identity: ok
Expected substance: Ascorbic Acid
Expected substance ID: 100020
Found substance: ok Ascorbic Acid
Distance: ok 0.004275 **Max. distance:** 0.070337
Spectrum residual: ok 0.005148 **Max. allowed residual:** 0.020481

Hitlist

Hit	Substance	Distance allowed	Distance
1	Ascorbic Acid	0.070337	0.004275 ok
2	Ascorbic Acid	0.070363	0.004608 ok
3	Ascorbic Acid	0.070284	0.004619 ok

Calibration

Calibration name:	6 acids	Version:	6
GUID:	(7F7C9F1C-7005-4399-B354-D41302B8A896)	Method:	Cluster
Properties:	Stearic Acid Salicylic Acid Ascorbic Acid Citric Acid Tartaric Acid		

The interface also shows a "Containers Left" field set to 0 and a "Previous Measurements" table with one entry: 03/07/2013 16:33:51 07-4-12_A- 37665_2013-03-07_16-33-51. The bottom status bar indicates "Current Page No.: 1", "Total Page No.: 1", and "Zoom Factor: 110%".

- If the "Batch Overview" is activated in the application "Report" adjustment and the "Number of Container" is also activated:

NIRWare Operator

Routine Advanced Navigation LIMS

different acids routine
 SOP Standard Operating Procedure:
 1. Fill in the field below
 2. Insert probe into sample
 2. Start measurement

Measurement Description:
 Batch: AA-2
 Expected Substance: Ascorbic Acid
 NumberOfContainers: 3
 AnalysisID:

Samples:
 1

Containers Left: 0

Previous Measurements:
 03/07/2013 16:43:18 AA-2_323_2013-03-07_16-43-18
 03/07/2013 16:42:04 AA-2_322_2013-03-07_16-42-04
 03/07/2013 16:40:25 AA-2_321_2013-03-07_16-40-25

Overview Results Spectra

Main Report

Summary
 Expected substance: **Ascorbic Acid**
 Expected substance ID: 100020

Sample	Found substance	Residual	Distance	Identity
AA-2_321_2013-03-07_16-40-25	ok Ascorbic Acid	ok	ok	ok
AA-2_322_2013-03-07_16-42-04	ok Ascorbic Acid	ok	ok	ok
AA-2_323_2013-03-07_16-43-18	ok Ascorbic Acid	ok	ok	ok

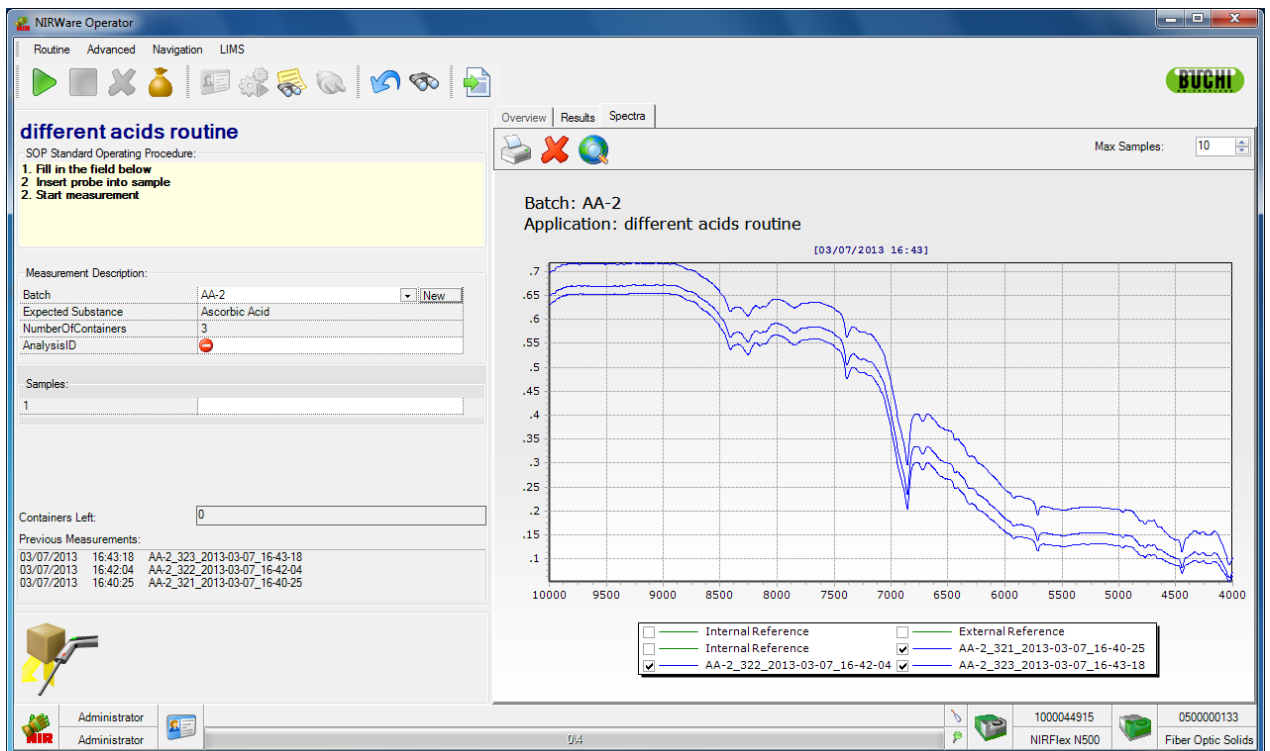
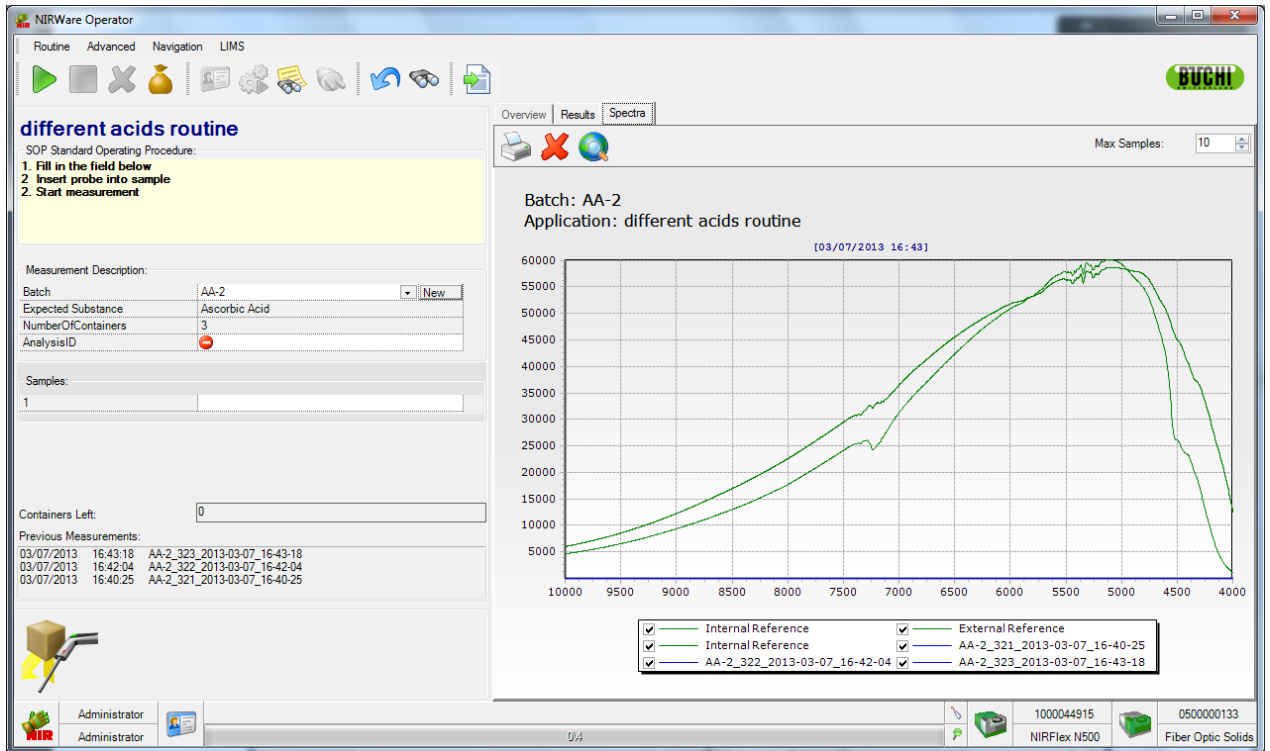
Identity ok: 3
 Identity not ok: 0
 Total: 3

Calibration
 Calibration name: 5 acids
 GUID: (7F7C8F1C-7005-4399-B354-D41302B8A886)
 Properties: Salicylic Acid, Ascorbic Acid, Citric Acid, Tartaric Acid
 Version: 6
 Method: Cluster

Current Page No.: 1 Total Page No.: 1 Zoom Factor: 110%

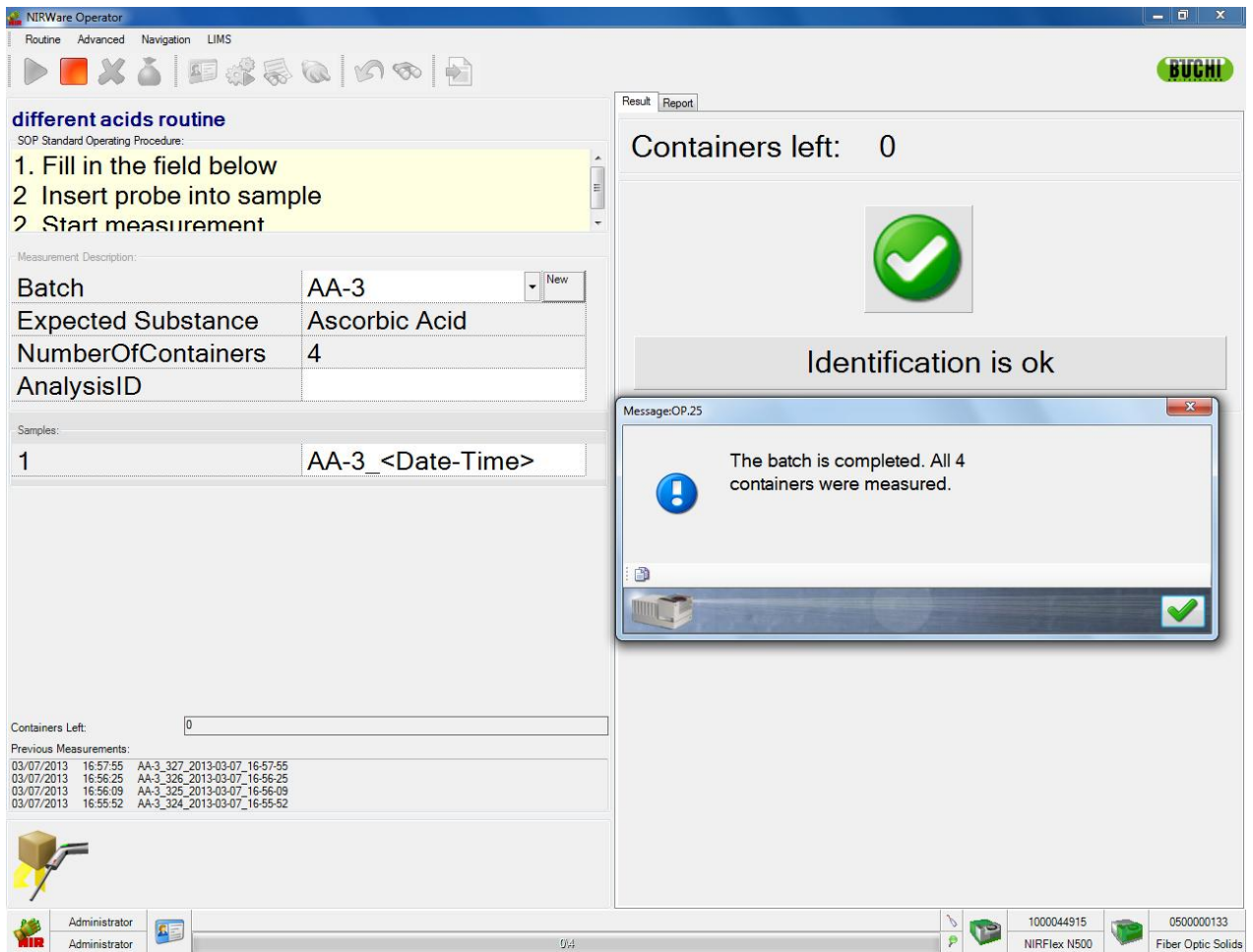
Administrator Administrator 100044915 0500000133
 NIRFlex N500 Fiber Optic Solids

- For both report formats, for a material to be successfully identified, a green “OK” should appear next to the Name, Distance, and Spectral Residual in the area of the report corresponding to the calibration that identifies the material just scanned. If one of the 3 criteria is not fulfilled, the substance is not identified. Only if Distance and Residual are OK, there is a substance name in the "Found substance" field. Reports may be printed by clicking the print icon above the report.
- In order to view the spectrum of the material just scanned, the user clicks the “spectra” tab on the right side of the screen. If reference scans are being displayed, it will be necessary to “uncheck” these scans under the plots to allow the y-axis to scale appropriately.



- Additional samples are measured accordingly.

For identification, the "Atline View" can be activated. In this case the user has only the symbol green check: ID OK or red cross: ID NOT OK will be visible.



- The user can see only the report, no spectra are available.

different acids routine
SOP Standard Operating Procedure:
1. Fill in the field below
2. Insert probe into sample
2. Start measurement

Measurement Description:

Batch	AA-3	New
Expected Substance	Ascorbic Acid	
NumberOfContainers	4	
AnalysisID		

Samples:

1	AA-3_<Date-Time
---	-----------------

Containers Left: 0

Previous Measurements:

03/07/2013	16:57:55	AA-3_327_2013-03-07_16:57:55
03/07/2013	16:56:25	AA-3_326_2013-03-07_16:56:25
03/07/2013	16:56:09	AA-3_325_2013-03-07_16:56:09
03/07/2013	16:55:52	AA-3_324_2013-03-07_16:55:52

Main Report

Summary

Expected substance:	Ascorbic Acid			
Expected substance ID:	100020			
Sample	Found substance	Residual	Distance	Identity
AA-3_324_2013-03-07_16:55:52	ck Ascorbic Acid	ck	ck	ok
AA-3_325_2013-03-07_16:56:09	ck Ascorbic Acid	ck	ck	ok
AA-3_326_2013-03-07_16:56:25	ck Ascorbic Acid	ck	ck	ok
AA-3_327_2013-03-07_16:57:55	ck Ascorbic Acid	ck	ck	ok
Identity ok	4			
Identity not ok	0			
Total	4			

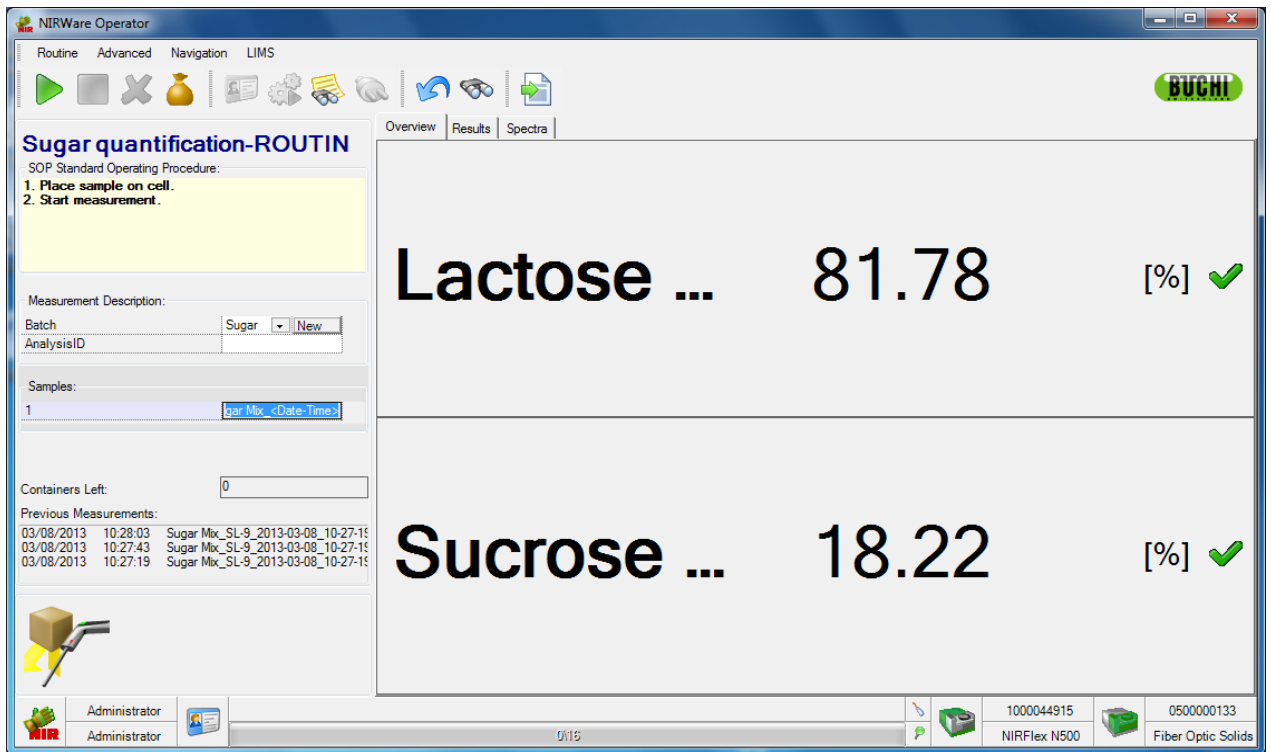
Calibration

Calibration name:	5 acids	Version:	6
GUID:	(7F7C8F1C-7005-4399-8354-D4130288A896)	Method:	Cluster
Properties:	Stearic Acid Salicylic Acid Ascorbic Acid Citric Acid Tartaric Acid		

Current Page No.: 1 Total Page No.: 1 Zoom Factor: 100%

Administrator Administrator 1000044915 0500000133
NIRFlex N500 Fiber Optic Solids

For quantitative measurements for measurement option for only ONE sample, the "Overview" always shows the average of the already measured sample results (here the average of 3 repeated measurements of the same sample).



By "Results" the 3 single results and the average is available, if the Report type "Detail" is activated.

1		Value		Residual		
Sugar						
Mix_SL-9_2013-03-08_10-27-1						
9						
	1	81.30	%	ok	0.000263	ok
	2	81.65	%	ok	0.000262	ok
	3	82.40	%	ok	0.000263	ok
Lactose Gehalt		81.78	%	ok		ok
	1	18.70	%	ok		ok
	2	18.35	%	ok		ok
	3	17.60	%	ok		ok
Sucrose content		18.22	%	ok		ok

Calibration			
Lactose Gehalt	Calibration name:	Lactose QN-02-13	Version: 2
	Calibration range:	0.00 - 100.00 [%]	Method: PCR
	Action range:	0.00 - 100.00 [%]	SEP: 2.552099
	Warning range:	0.00 - 100.00 [%]	Bias: 0.000000
	Max. Residual:	0.000361	Slope: 1.000000
	GUID:	(28AEE4E6-70F2-4F9A-8CFB-36C96E63122F)	
Sucrose content	Calibration name:	CalculatedValue = 100-ApProperty ['Lactose Gehalt'].Value;	Version:
	Calibration range:		Method: Calculated
	Action range:	0.00 - 100.00 [%]	SEP:
	Warning range:	0.00 - 100.00 [%]	Bias: 0.000000
	Max. Residual:		Slope: 1.000000
	GUID:		

There are 4 report types available, please choose the best suitable for your application (in "MC: Application Designer"). By "Spectra" the measured spectra are visible.

5.12. Extended Wavelength Range

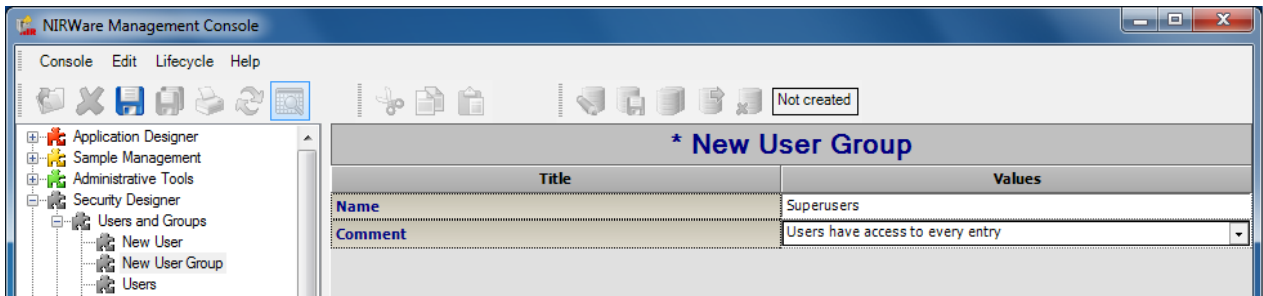
Commonly the NIR spectral range is defined from 780 – 2'500 nm (appr. 12'800 – 4'000 cm⁻¹). The accessible default range for NIRFlex N-500 is 1'000 – 2'500 nm or 10'000 – 4'000 cm⁻¹ for all measurement cells except Solids Transmittance. Solids Transmittance has a default range of 870 – 1660 nm (11'520 – 6000 cm⁻¹).

In both cases, the range can be expanded up to 820 nm (12200 cm⁻¹), although there is usually no benefit from using the extended wavelength range for normal applications. However for some applications (coloured samples, thick samples) there can be advantages, and it might be worthwhile to test the extended range for such samples, if no reasonable calibration could be developed using the default range of the NIRFlex N-500.

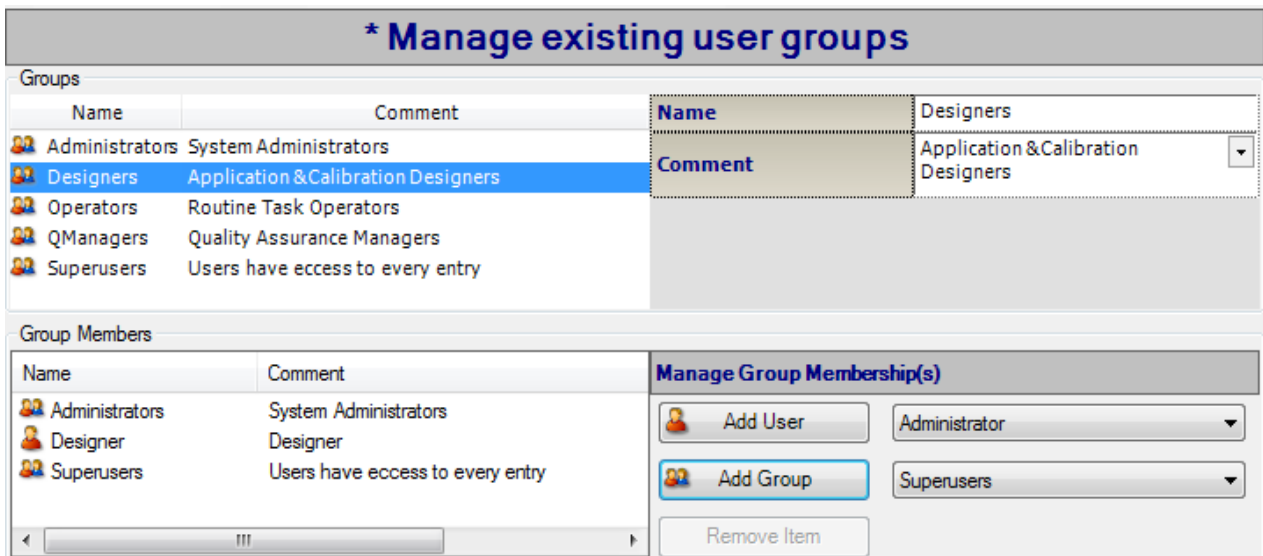
5.12.1. How to Setup NIRWare for the Extended Range

Please create a new usergroup e.g. "Superusers" first.

Select: **Security Designer => Users and Groups => New User group** and create the new group.



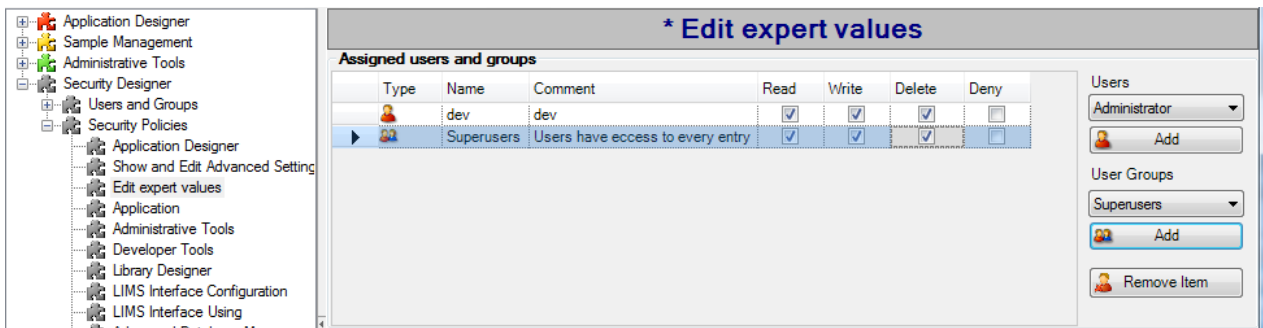
Go to **Security Designer => Users and Groups => User Groups** and add the group of Superusers i.e. to the group of Designers:



Now you need to assign some privileges to the group of Superusers.

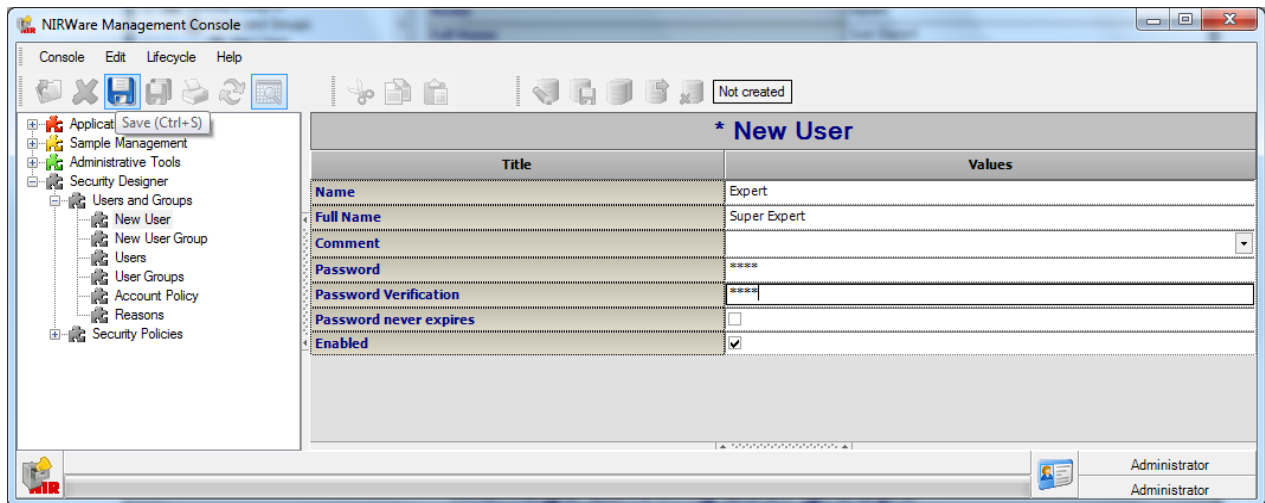
Go to **Security Designer => Security Policy => Edit expert values** and add the User Groups "Superusers" to the "Assigned users and groups".

Tick the entries "read", "write", and "delete" as you can see in the figure below:

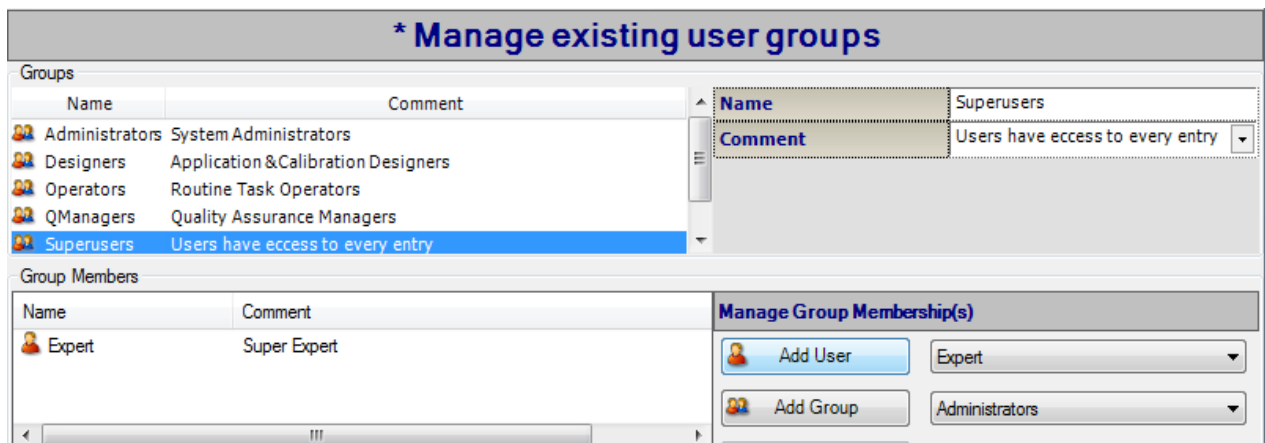


If you now create a new user and assign her/him to the group of "Superusers" she/he will have access to the "Application Designer" and "Sample Manager" like any designer but will also be able to change all the instrument settings in every application.

Go to **Security Designer => Users and Groups => New user** and create the new user.

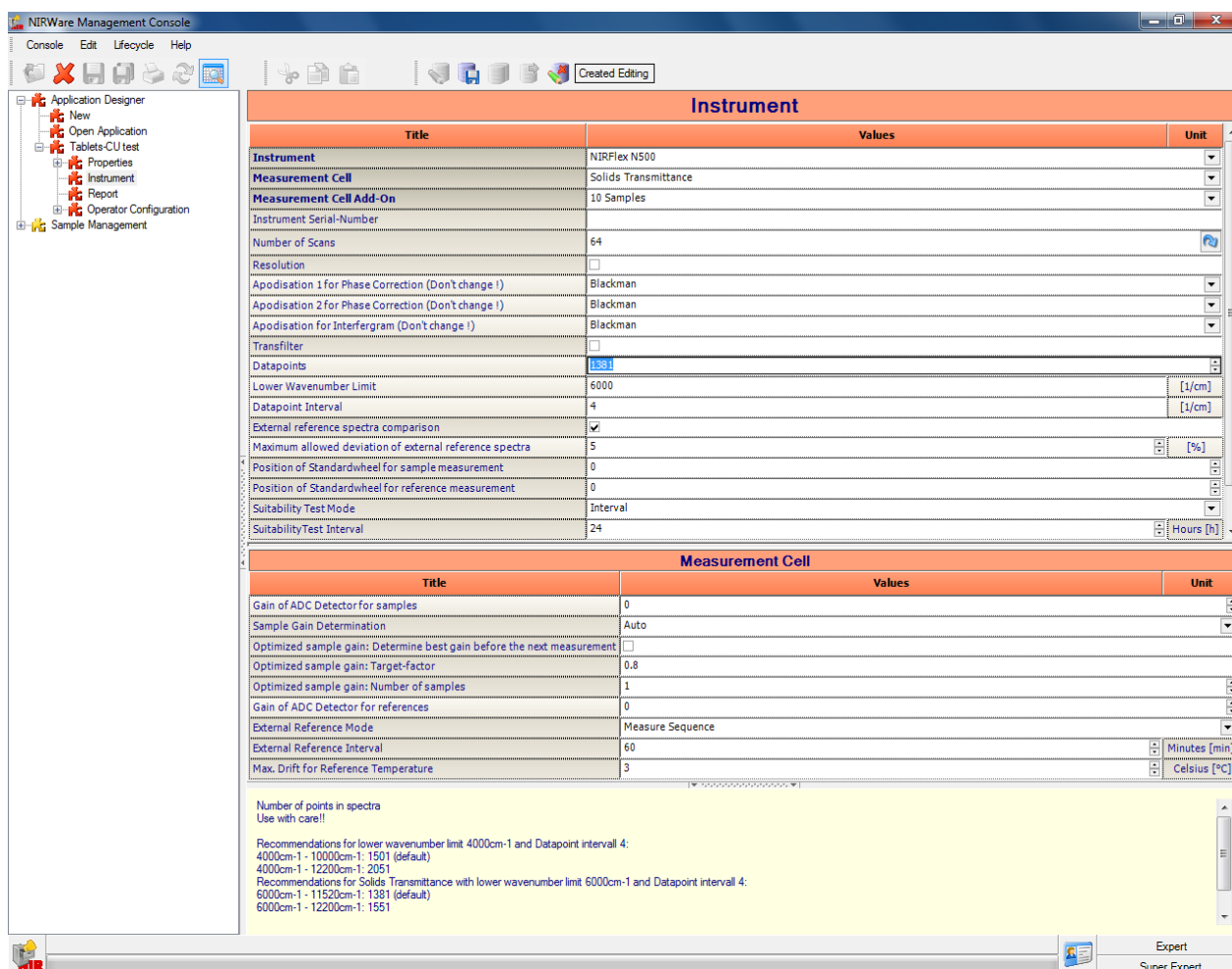


Go to **Security Designer => Users and Groups => User Groups** and assign her/him to the group of “Superusers”.



The next time this user logs in with this account she/he will be able to change the settings in applications. (Instead of the group “Designers” you may also use the group of “Administrators”).

The Application Designer for this user will now look as shown below:



In order to change the wavenumber range first changes the number of datapoints. Using an interval of 4 cm^{-1} and starting at 4,000 cm^{-1} the upper limit will be reached at 10,000 cm^{-1} using 1,501 datapoints (default) and at 12,200 cm^{-1} using 2051 datapoints.

For Solids Transmittance an interval of 4 cm^{-1} and starting wavenumber at 6,000 cm^{-1} is used. The default number of datapoints is 1,381 (11,520-6,000 cm^{-1}). The upper limit will be reached with 1,551 datapoints (12,200-6,000 cm^{-1}).

It is also possible to change the lower wavenumber limit. However the intensity will drop dramatically below 4,000 cm^{-1} (6,000 cm^{-1} for Solids Transmittance). Therefore we do not recommend doing so.

5.12.2. Limitations, Risks and Warnings

- The NIRFlex N-500 has been designed for a spectral range of 10.000 – 4.000 cm^{-1} . Therefore all optical components are laid out according to this specification. The overall performance of the NIRFlex N-500 is decreasing for shorter wavelengths. Source, detector coatings and interferometer all contribute to this effect.
- The lower limit is defined by the cut-off of the extended range InGaAs detector and the intensity drops very much below 4.000 cm^{-1} . Therefore the reproducibility will decrease in this range.
- Therefore in the extended range the NIRFlex N-500 will not be as stable as it is in the specified range and data transfer will be more problematic, because each individual system may behave differently in that range.

- The noise increases considerably above 12.000 cm⁻¹ and the baseline is less stable.

These limitations are caused by physics and they are not specific for the NIRFlex N-500 but can be observed for every FT-NIR spectrometer regardless of the manufacturer.

WARNING

Spectra recorded in the extended range will have a different number of datapoints than spectra measured in the default range. Mixing up these types of spectra in the same database can cause problems. Please consider: only spectra measured with the same wave number range are compatible.

There is no way to use both types of spectra in one NIRCal calibration. NIRCal will reject incompatible spectra from import. If the wave range is not matching, the Spectra Converter can help (see NIRCal Manual).

Problems may occur using the Library Designer. Mixing spectra with different number of datapoints is not prevented by design and can cause the software to crash.

Applications configured for a certain wavelength range will crash if a calibration is assigned that have been developed with spectra of a different wavelength range.


6. NIRWare Suite

6.1. NIRWare Management Console

6.1.1. Management Console

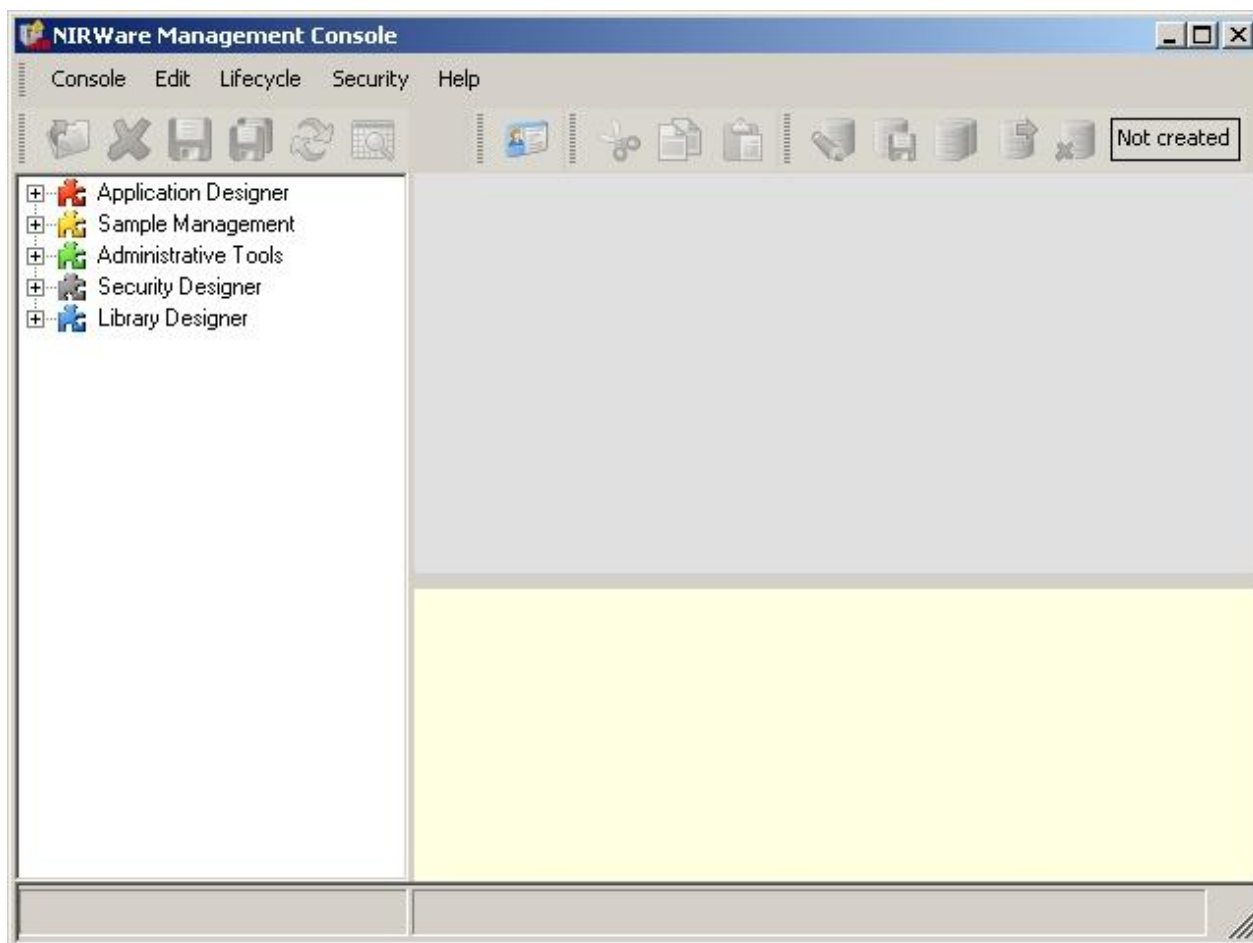
The NIRWare Management Console is structured similar to the Microsoft Management Console (MMC). It hosts all SnapIn Modules of the NIRWare Suite except NIRWare Operator and NIRCal 5.

To open the NIRWare Management Console, click on the **Start** button in your task bar and select **All Programs / BUCHI / NIRSolutions / Management Console** or click the corresponding icon on your

desktop, if applicable. .

Then log on with your user name and password and confirm by clicking the green arrow.

The **NIRWare Management Console** opens:



The Management Console is divided into three sections:











- On the left side is a tree view for navigation through all available SnapIn Modules.
- The right side is horizontally divided into two areas. The upper area displays the parameters, which can be modified.
- The lower area displays an advanced help for each value selected in the upper area.

Menus and icons


Console

New	No function in current software version
Save As...	Save the currently set Snap In view to an xml-file which is then used as default setting each time the Management Console is opened
Print	Send the opened document to the default printer
Page Setup	Opens the default printer adjustment
Snap-Ins...	Opens the dialog to display further available Snap In Modules (see below)
Exit	Closes the Management Console






Database related icons (represent the same functions as contained in the Edit menu):

	Open	Open an existing data set
	Remove	Remove an existing data set from the file tree view
	Save	Save a modified data set
	Print	Send the opened document to the default printer
	Save All	Save all modified data set
	Refresh	Refresh the current data set
	Show Advanced Settings	Toggles between Basic and Advanced Settings. The icon is only active in the Application Designer.
	Cut	Cut a data set and copy it to the clipboard
	Copy	Copy a data set into the clipboard
	Paste	Paste a data set from the clipboard into the application

User related icon (represents the same function as contained in the Security menu):

	Logon	Open the Logon dialog and log on as a different user
---	-------	--

Lifecycle related icons (represent the same functions as contained in the Lifecycle menu):

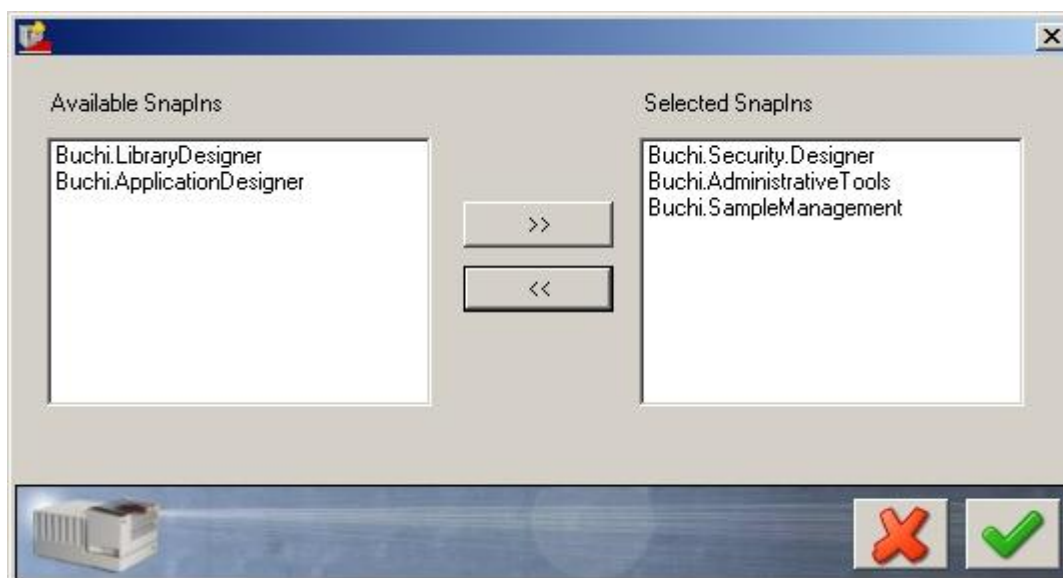
	Edit	Change data of an application which is already implemented in the database
	Save	Save data into the database
	Copy	Copy data from one data set into another
	Next	Put data set into the next stage
	Delete	Delete data set

Help

Help NIRWare ...	Open the NIRWare HTML Help
Software Registration ...	Open the registration form to registrate your software version
About	Open a dialog giving information on the current software version installed

Snap In Modules

To load further Snap-In Modules into your Management Console, select **Console > Snap-Ins....** The following dialog opens:



In the left window under "Available Snap Ins" all NIRWare Snap Ins are listed which are accessible through the license activated on the PC and which are not already displayed within the tree view of the Management Console.

In the right window "Selected Snap Ins" all Snap Ins are listed that are currently displayed within the tree view of the Management Console.

To move a Snap In from one side to the other, click it so that it is highlighted and press the corresponding arrow button. Then click save button to confirm your settings.

NOTE

Generally all entries within the Module windows of the Management Console have to be saved by means of the Save icon. When new settings in an active window have not been saved, yet, this can be seen from an asterisk next to the window header.

6.1.2. Filter

In the tables of Application Designer, Sample Management and Administrative Tools and Security Designer, three different filter functions are provided to determine which applications, samples, reports, etc. should be displayed.

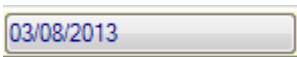
The filter row is always placed directly under the columns header row.

Samples									
Name	Application	Version	Batch	Time Stamp	No. Referencevalues	Analysis ID	Comment	Customer Fields	
▶ Sugar Mix_SL-9	Sugar quantification	2	Sugar Mix	03/08/2013 10:27:19	0	SL-9			
AA-3_327_201	different acids routin	4	AA-3	03/07/2013 16:57:55	0	327			
AA-3_326_201	different acids routin	4	AA-3	03/07/2013 16:56:25	0	326			
AA-3_325_201	different acids routin	4	AA-3	03/07/2013 16:56:09	0	325			
AA-3_324_201	different acids routin	4	AA-3	03/07/2013 16:55:52	0	324			
AA-2_323_201	different acids routin	4	AA-2	03/07/2013 16:43:18	0	323			
AA-2_322_201	different acids routin	4	AA-2	03/07/2013 16:42:04	0	322			
AA-2_321_201	different acids routin	4	AA-2	03/07/2013 16:40:25	0	321			
07-4-12_A-376	different acids routin	4	07-4-12	03/07/2013 16:33:51	0	A-37665			
07-4-12_A-376	different acids routin	4	07-4-12	03/07/2013 15:19:13	0	A-37665			
Mixed rice_216	Whole Rice- Nov.20	3	Mixed rice	03/05/2013 15:05:24	0	21645			

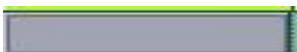
Time related filter

The time related filter enables to determine the time interval the data to be displayed have been generated.

Two different default settings are possible:

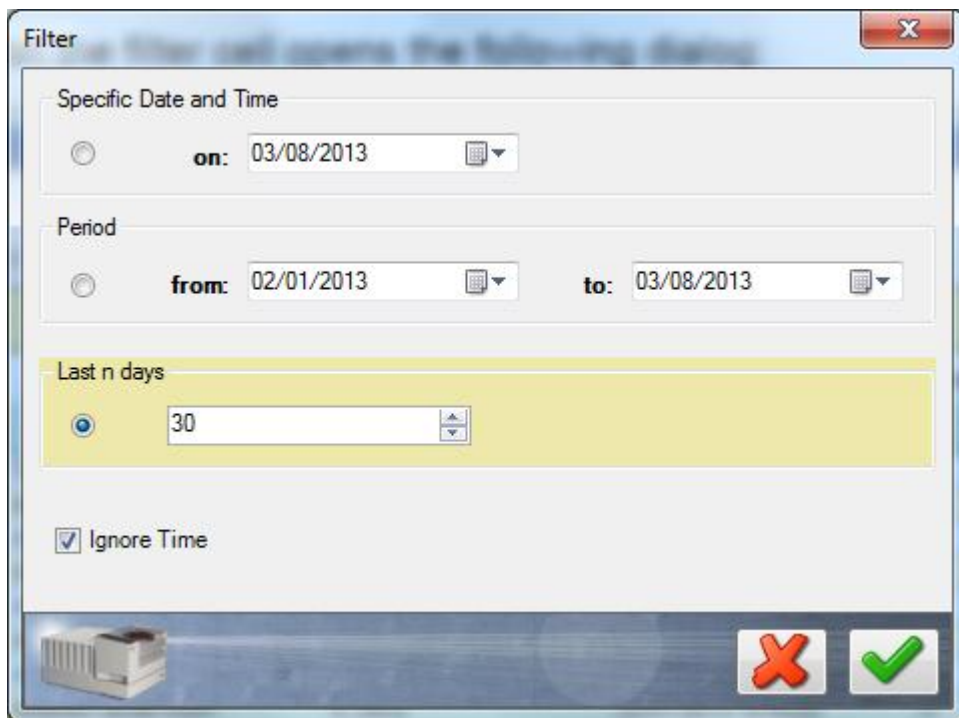


By default, only the data from the present day will be displayed.



All entries will be displayed. A right mouse click on the filter cell will reset the filter to "show all entries".

Left mouse click on the filter cell opens the following dialog:



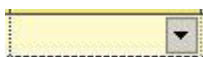
Entries can be searched according different time definitions:

Specific Date and Time	If checked, only samples measured on the selected day will be available in the selection list.
Period	Alternative to a specific date/time; if checked only samples measured within the selected time interval will be available in the selection list.
Last n days	Alternative to period or specific date/time; if checked the samples measured in the last n days, specified in the field below, will be available in the selection list.
Ignore Time	If not checked, time (additional to date) can be used as additional filter criterion.

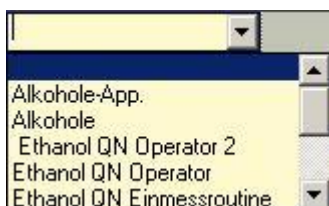
Confirmation of the set entries will narrow down the displayed entries according to the set criteria.

Drop Down filter

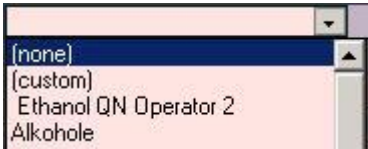
The second filter is a drop down filter.



Two different variations are used in the tables.

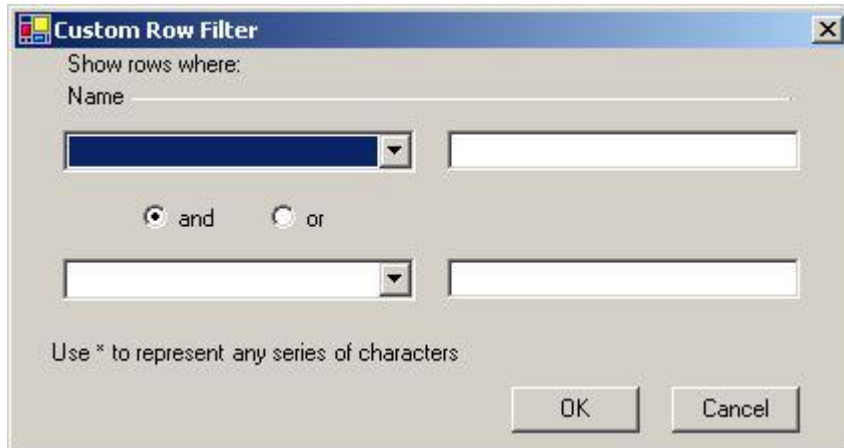


The first drop down filter shows a list of all available entries. Search the entry of choice by scrolling down and click on the entry or type in the first letters to narrow down the list.



With the second variant of drop down filter, you can select the entry from the list or activate a special Custom Row Filter.

Selecting (custom) opens the **Custom Row Filter**:



Here you can specify the cell content by which you want to filter the table. Fill in the fields and click **OK** to apply the filter.

Search string filter

The third filter option is the possibility to search by entering a search string in the filter cell:



Enter a search string to narrow down your search and press **Enter** :

"%" = show all results for this column

"**su**cr" = show all results for this column starting with this string.

"%**v**ial" = show all results for this column that contain this string at any position.

For columns with numbers only, the search can be narrowed down with:

">" =bigger than....

"<" =smaller than....

To reset applied filters, so that all available entries are displayed, delete the content of the filter field followed by **Enter** or click the **Reset Filters** button.

Filter Templates

By default, filter settings and column widths changed by the user remain in the system for each table. Entering the dialog again, all settings from the last session will be loaded.

It is possible to define and save filter templates with used defined settings.

Double Click on the the left upper corner of a table. The following dialog opens:



	Create new template.
	Activate selected template.
	Save existing template.
	Delete selected template.
	<p>Reset all user specific filter settings, excluding the templates.</p> <p>Templates: Enter a new template name or search for existing templates from the drop down menu.</p> <p>Persist column widths and filter strings can be deactivated.</p> <p>To create a new template, first configure the filter settings in the table. Then open the above shown dialog. Under "Templates" enter a template name. Click on the "Create new template" button.</p>

6.2. Application Designer

6.2.1. Introduction Application Designer

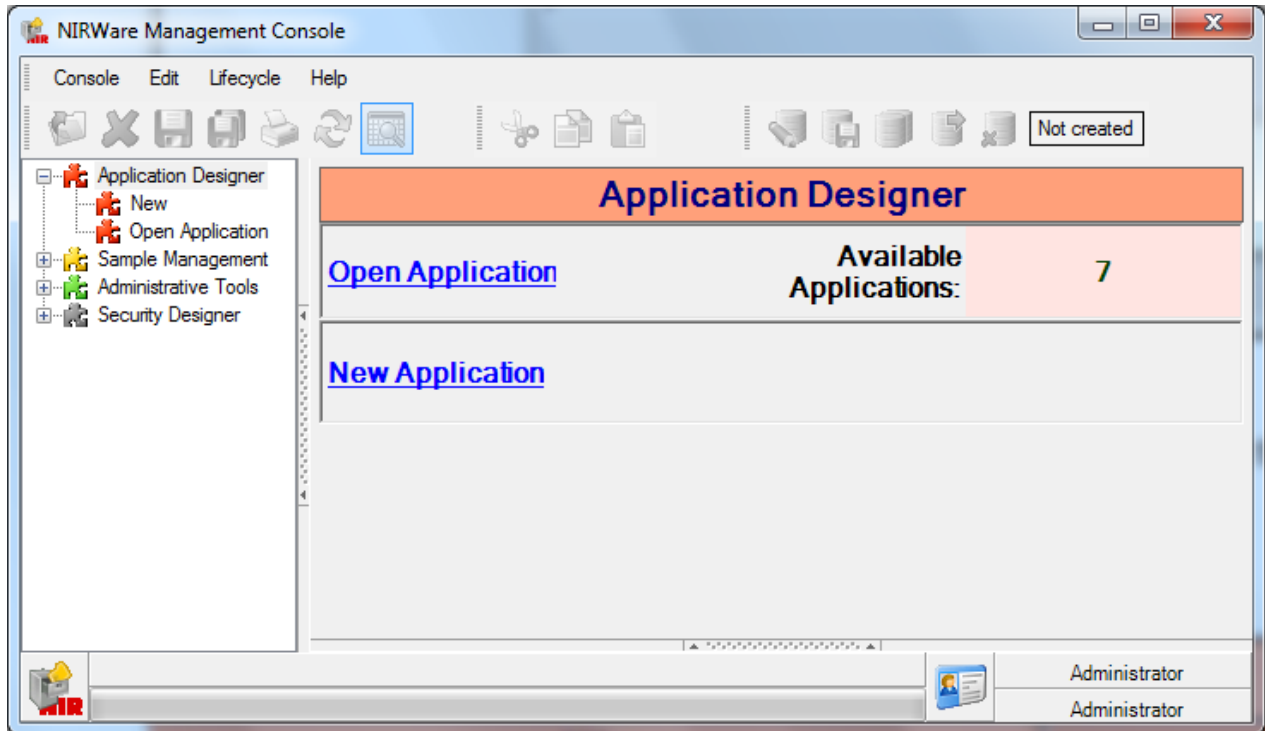
The main function of the Application Designer is to provide an easy to use configuration tool to **create new or modify existing applications**. The design of an application mainly defines how the end user (operator) has to perform a specific analysis. It includes the definition of the required inputs, the calibrations to be used with their properties, the SOP displayed in order to guide the operator, and finally the requested batch entries and the definition of the report displayed.

To make the work with the Application Designer as easy as possible, the basic mode can be used where only a few parameters need to be edited.

For expert users an advanced mode can be activated by a mouse-click. All advanced parameters have a default value and can be edited, if needed.

To open the Application Designer proceed as follows:

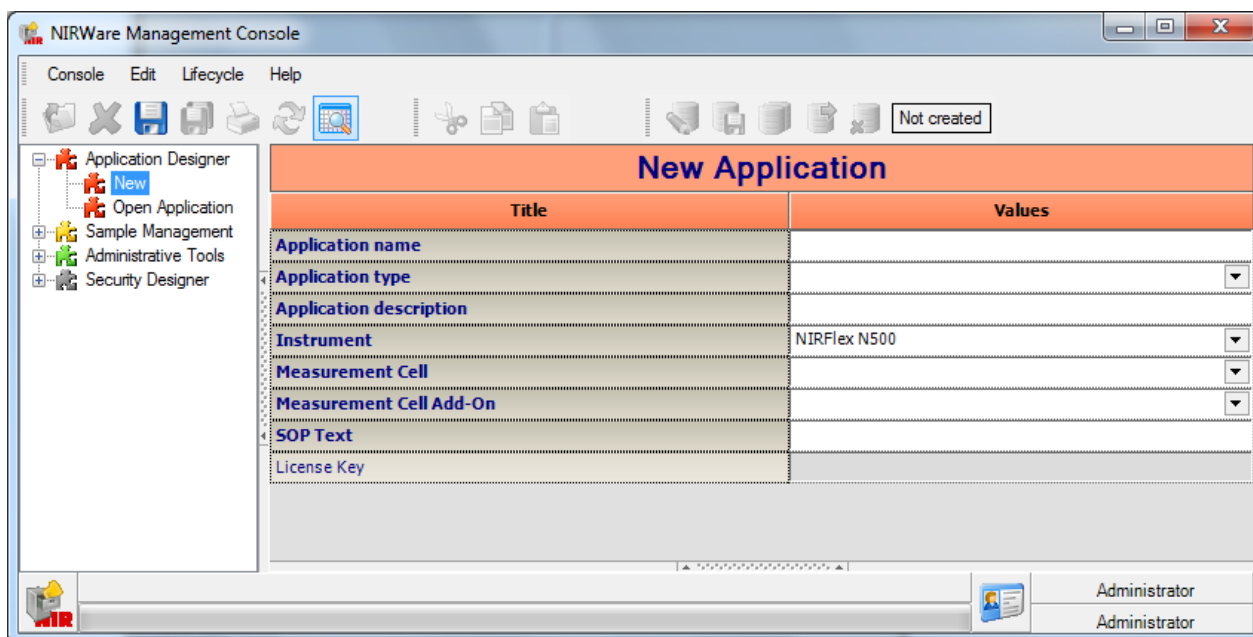
In the file tree on the left side of the **NIRWare Management Console** select **Application Designer**. The following dialog opens:



Creating a new application

To create a new application open the submenu by clicking on **"New"** in the file tree or on **"New Application"** in the center of the Application Designer window.

The following window opens:



By default, only the basic settings are visible.

To show and hide the advanced settings again, click the corresponding icon .

Parameter Name	Description
Application name	Entry for application name
Application type	Select: "Quantification" or "Identification".
Application description	Entry for an application description (optional).
Instrument	Select: "NIRFlexN500".
Measurement Cell	Select used measurement cell: 1. NIRMaster 2. Fiber Optic SMA (for continuous measurement) 3. CheckMaster Transmittance 4. Solids Transmittance 5. Fiber Optic Liquids 6. Fiber Optic Solids 7. Liquids 8. Solids
Measurement Cell Add-on	Select used measurement cell add-on. The dialog offers different choices depending on the selected measurement cell type: 1. No Option 2. No Option 3. No Option 4. 10 Samples 30 Samples USP Testkit for Solid Transmittance (only for BUCHI internal use) Reference Samples (only for BUCHI internal use) 5. No Option

	6. No Option Transflection Head 7. No Option (Cuvette) 8. Vial Petri USP Testkit (only for BUCHI internal use) Tablet XL
License Key*	Application of a license protection to this application

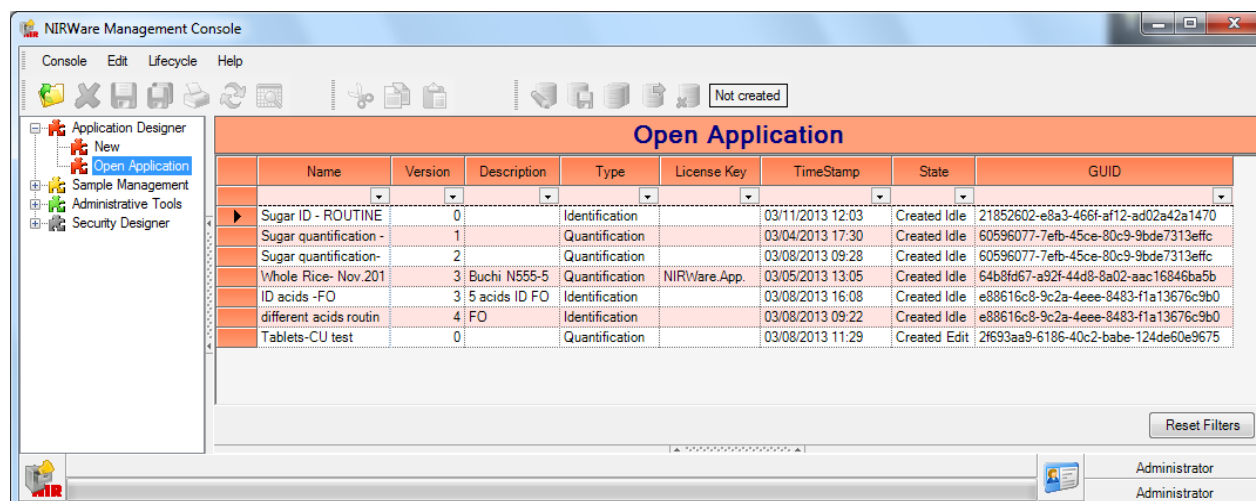
* non bold parameters are advanced settings.

Some basic parameters are mandatory, i.e. the corresponding fields have to be filled in. If you try to save your settings with some mandatory fields still empty, an error message is displayed and the fields to be filled in are marked with a red frame.

Opening and editing existing applications



To open and edit an existing application open the submenu by clicking on "Open" in the file tree or on "Open Application" in the center of the Application Designer window.

The following dialog opens:

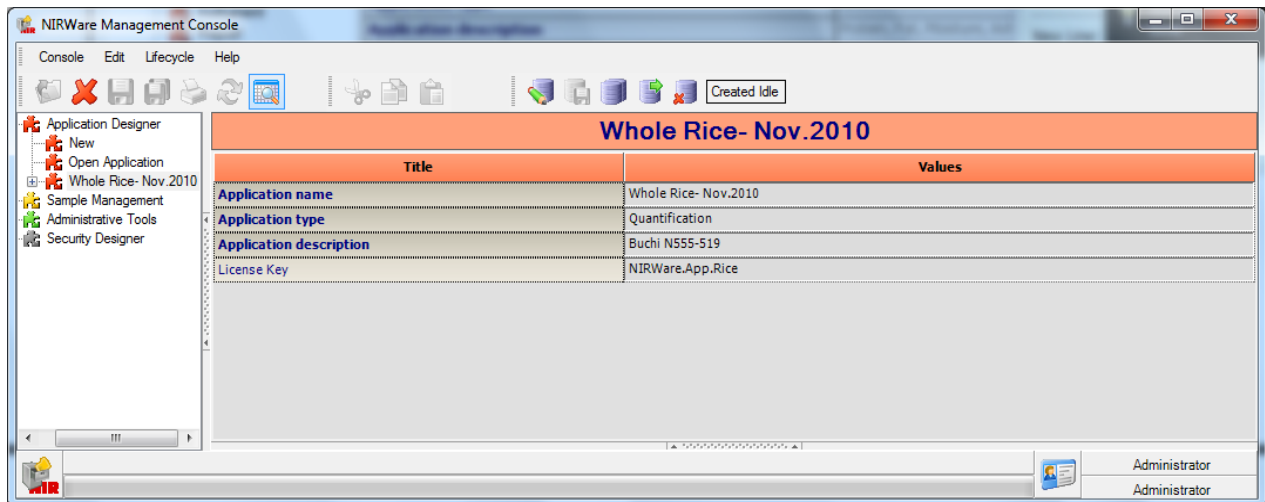


From the provided list, select an application. Use the filter functions to narrow down the displayed results.

Name	Application name
Version	Copy number in the course of the lifecycle
Description	Optional information entered during application design
Type	Application type (Identification or Quantification)
License Key	License protection code for this application
Time stamp	Time of the last modification
State	Lifecycle state
GUID	Global Unique Identification


Select an application and open it by clicking on the "Open existing DataSet" button  or with double click on the corresponding row indicator .

The following dialog opens:



Parameter Name	Description
Application name	Entry for application name
Application type	"Quantification" or "Identification".
Application description	Entry for an application description (optional).
License Key	Application of a license protection to this application
Max. Size of the result hitlist (only for identification)	Defines the hitlist size shown for qualitative results min: 1 max: 15 default: 3
Content Uniformity Test Type according to (only for CU test)	Individual Monograph General Procedure (European and United States Pharmacopeia) General Procedure (Japanese Pharmacopeia) Disabled (default)
CUT Procedure Name (only for CU test)	Name of CUT procedure (if selected above)

By default, only the basic settings are visible.

To show and hide the advanced settings again, click the corresponding icon .

Modifying parameters



Click the "Edit" icon and change the application name, the application description and for qualitative applications the hitlist size.

The application parameters are grouped in 4 different categories.

- [Properties](#)
- [Instrument](#)
- [Report](#)
- [Operator Configuration](#)

Each of this categories contain basic and advanced settings which can be modified.

6.2.2. Comparing external reference spectra and defining the tolerance limit

(De)activating the test

The test can be activated or deactivated for each individual application (default: active). This is done in the **Management Console – Application Designer - <YourApplication> - Instrument: External Reference Spectra Comparison**.

The screenshot shows the NIRWare Management Console interface. The left sidebar contains a tree view with categories like Application Designer, Sample Management, and Security Designer. The main window displays the 'Instrument' configuration table for 'NIRFlex N500'.

Title	Values	Unit
Instrument	NIRFlex N500	
Measurement Cell	Solids	
Measurement Cell Add-On	Vial	
Instrument Serial-Number		
Number of Scans	8	
Resolution	<input checked="" type="checkbox"/>	
Apodisation 1 for Phase Correction (Don't change !)	Blackman	
Apodisation 2 for Phase Correction (Don't change !)	Blackman	
Apodisation for Interferogram (Don't change !)	Blackman	
Transfilter	<input type="checkbox"/>	
Datapoints	1501	
Lower Wavenumber Limit	4000	[1/cm]
Datapoint Interval	4	[1/cm]
External reference spectra comparison	<input checked="" type="checkbox"/>	
Maximum allowed deviation of external reference spectra	5	[%]

Changing the tolerance limit – Who is allowed to?

The tolerance limit of the test is found under **Management Console – Application Designer - <YourApplication> - Instrument: Maximum allowed deviation of external reference spectra [%]**, and the default value is 5%. It is recommended not to change this value, and therefore even administrators

cannot change it by default. If you really need to, you have to log in as a user with the right to 'Edit expert values' (Management Console – Security Designer – Security Policies).

6.2.3. Parameter list

Properties: Assigning a property or several properties to an application


This menu is used for assigning calibrations to the application. The calibration properties will be used for prediction during the routine use.

NOTE:

Leave the property field empty for applications used for spectra collection. The properties can be added to the spectra, which are stored in the Database with the "Sample Manager" later.

6.2.4. Assigning a property

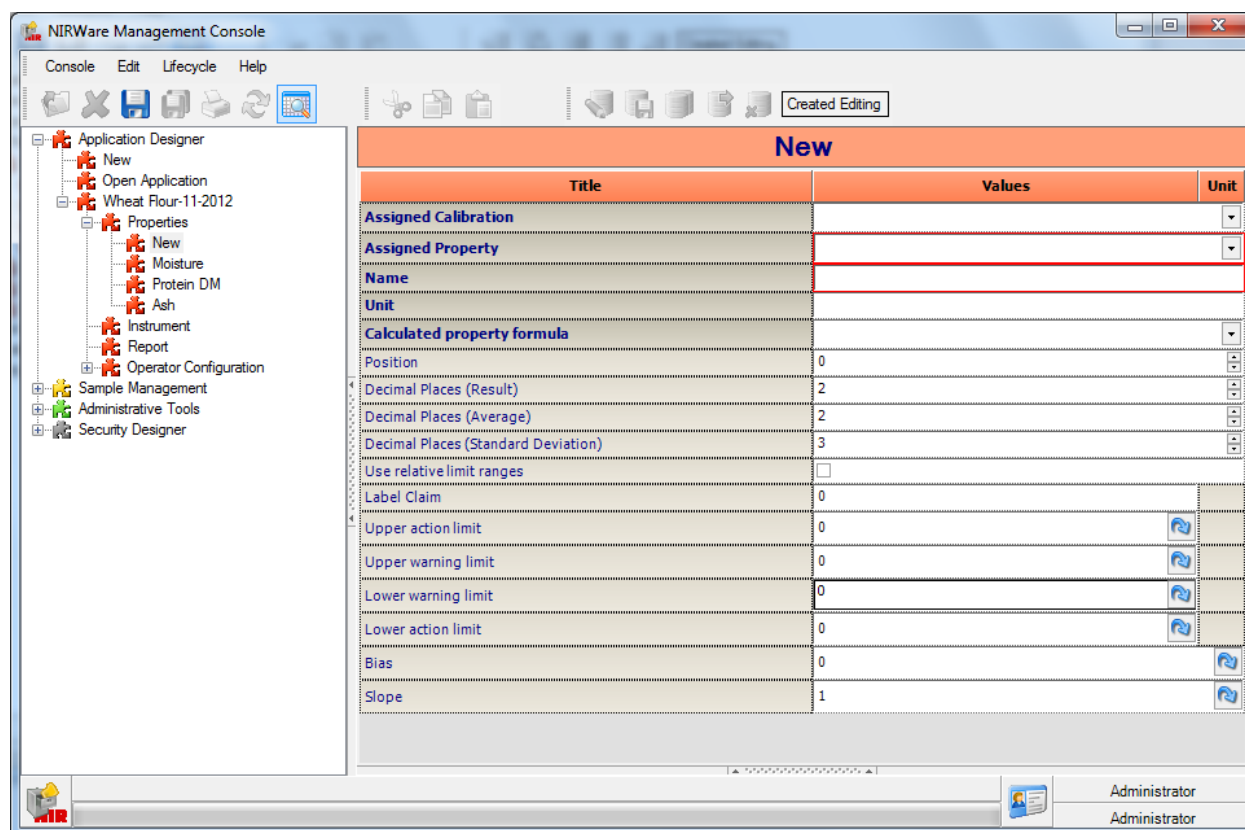
To get the access to the Properties, click on the entry "Properties" and open with the Lifecycle / Edit

symbol. 

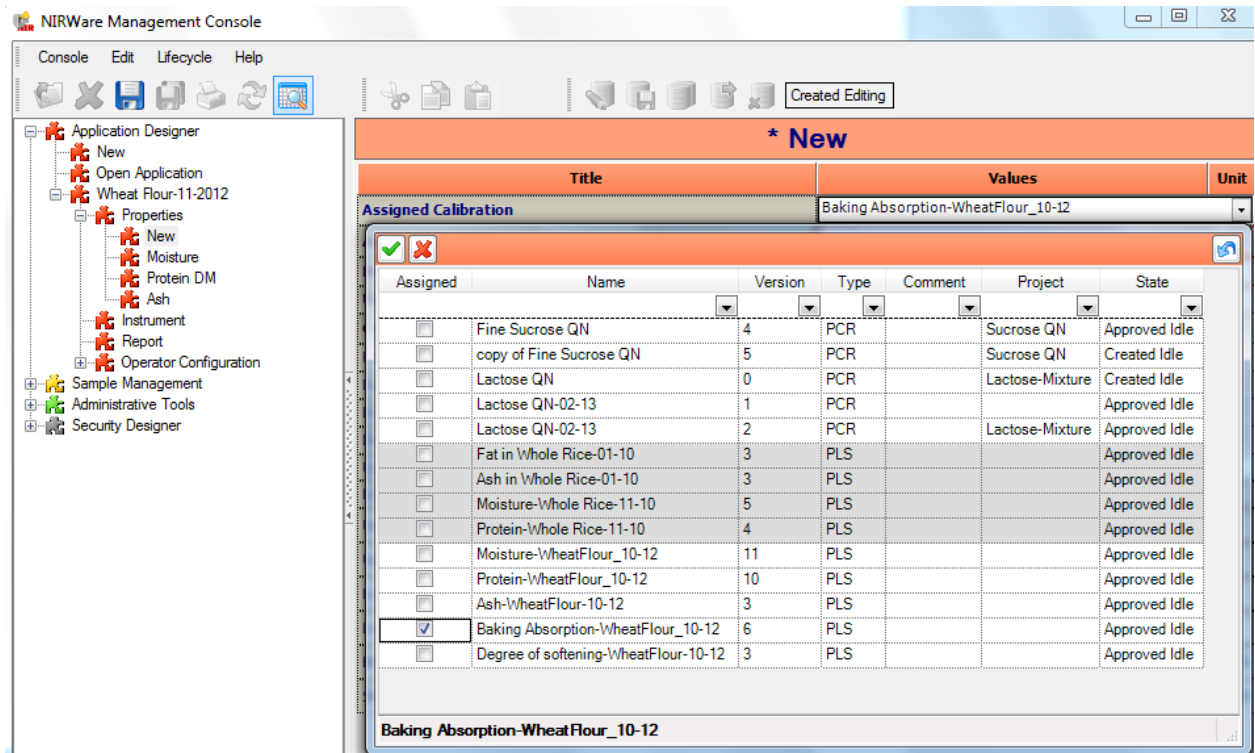
NOTE:

Only application in Lifecycle "Created" can be editable. Application in Lifecycle "Approved" or "Checked" cannot be edited, only after creating a copy.

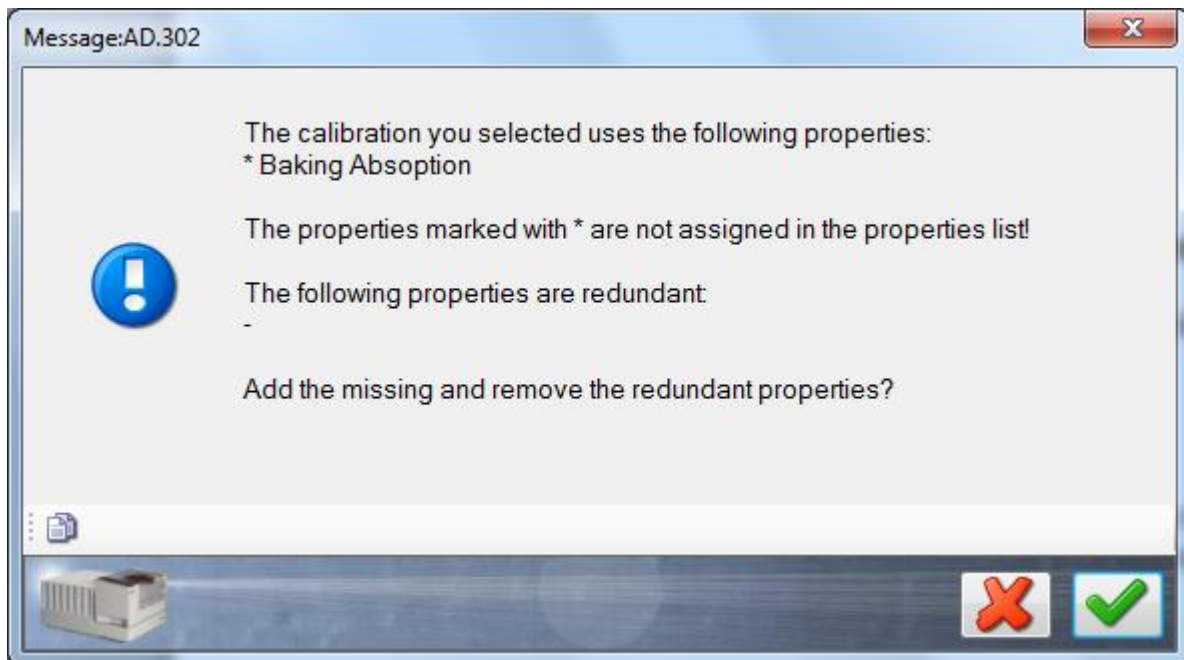
Select "New" for a new parameter:



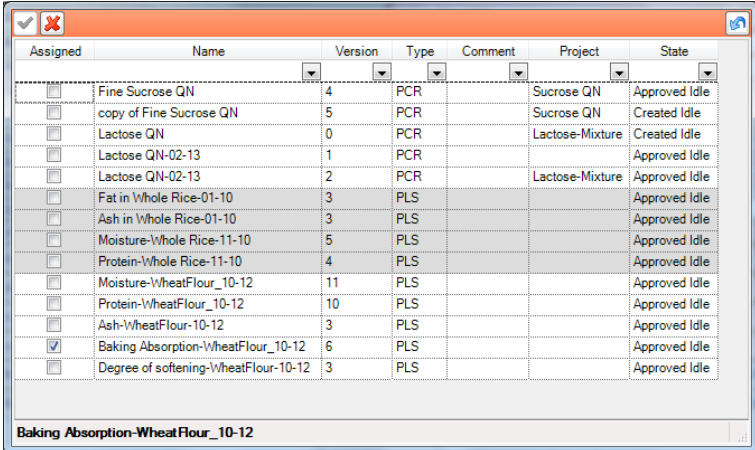
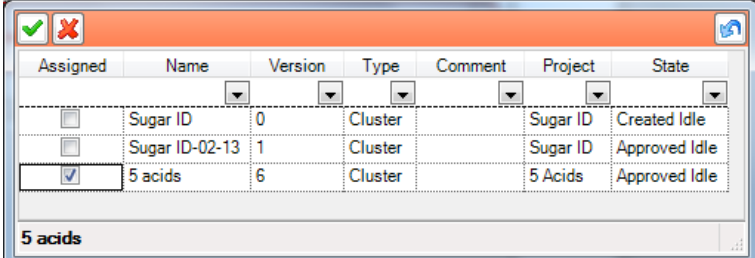
First select the calibration desired to use by the “**Assigned Calibration**”. Confirm this with the green check:



The name of the Assigned Property, Name and Unit will be automatically filled in accepting the following message:



The following list of parameters is available:

Parameter Name	Description
Assigned Calibration	<p>Name of the calibration which has been calculated in NIRCaI. Only assigned calibration allows prediction of a measurement result.</p> <p>Quantitative: Select the corresponding quantitative calibration model for the property.</p>  <p>Identification: Select the corresponding qualitative calibration model:</p> 
Assigned Property	<p>Do not choose the properties; this field will be automatically filled in after the calibration is chosen.</p> <p>Quantitative: Name of the quantitative property in the database which is calculated in the selected calibration.</p> <p>Identification: Name of the qualitative property (SIMCA) or all qualitative properties in the calibration (CLUSTER).</p>
Name	<p>Quantitative: Language specific name can be entered here or keep the name of quantitative property in the database.</p> <p>Identification: Name of the substance group should enter.</p>
Unit	<p>Use this field only for quantitative property.</p> <p>Quantitative:</p>

	<p>Unit of the quantitative property in the database (e.g. % or ppm or g/kg, please edit it by creating the property).</p> <p>Identification: Leave this field empty.</p>
Position	<p>Quantitative: Position of the parameter to be displayed in NIRWare Operator and all printed documents. Only needed if more than one property is added to the application for predicted.</p> <p>Identification: The position of a calibration has no influence on the prediction.</p>

6.2.5. Calculated property

Only for **quantitative property** there are following parameters:

Calculated property formula	This is new in NIRWare 1.5 and enables the user to define properties which are calculated from other properties, e.g. Dry matter =100-Moisture
-----------------------------	---

A calculated property is defined as a normal property, but without assigning a calibration and property. Pressing on the drop down in the right side brings up the formula editor.

ApProperty	Value	Residual	TargetValue	UpperAction	UpperWarning	LowerWarning
Moisture	0	0	0	16.7	16.7	9
Fat	0	0	0	3	3	0.1
Protein	0	0	0	12.3	12.3	5.03
Ash	0	0	0	1.58	1.58	0.26

The formula editor consists of the editor windows (green) and the property window (red). In the editor the formula is written and one can evaluate the formula using the Check button (upper right). The formula is evaluated using the values in the property window. Sample dependent values (value and residual) are editable; the remaining values are given by the calibration and application and cannot be edited, but can be used in the formula.

ApProperty	Value	Residual	TargetValue	UpperAction	UpperWarning	LowerWarning
Moisture	0	0	0	100	100	-100
Fat	0	0	0	100	100	-100

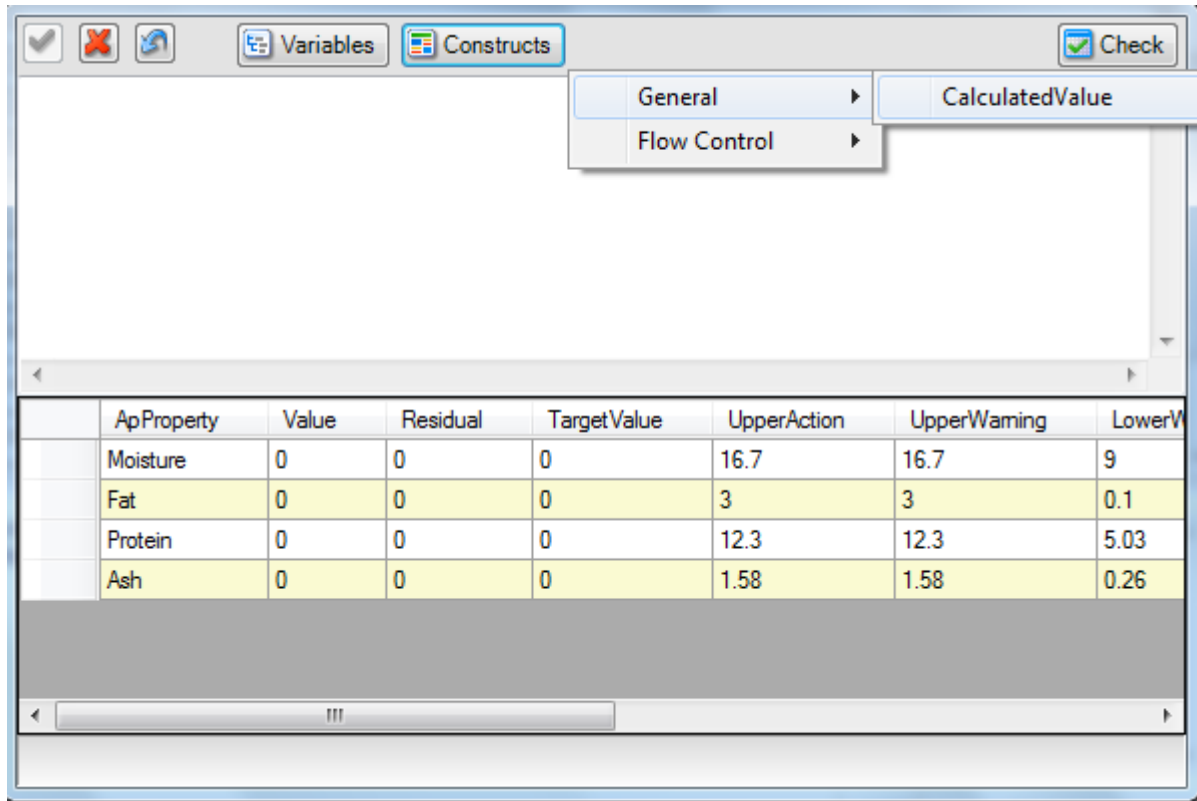
Formulas are written as C# code (read: C-sharp), and can use most of the constructs for flow control which are available in C#

In the following a number of examples illustrate how calculated properties can be used.

The examples can be copy/pasted directly to the formula editor for tests.

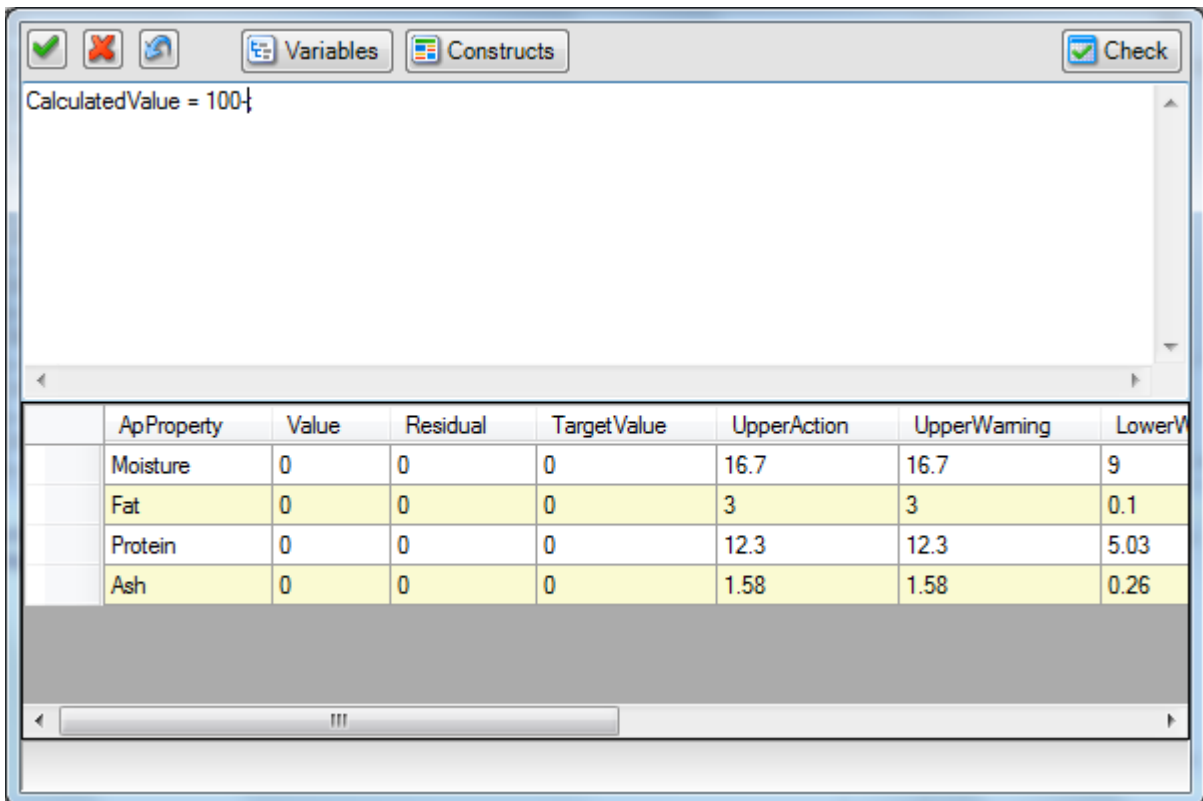
DM is expressed in % and calculated as 100 minus the moisture content.

Select: Constructs / General / CalculatedValue

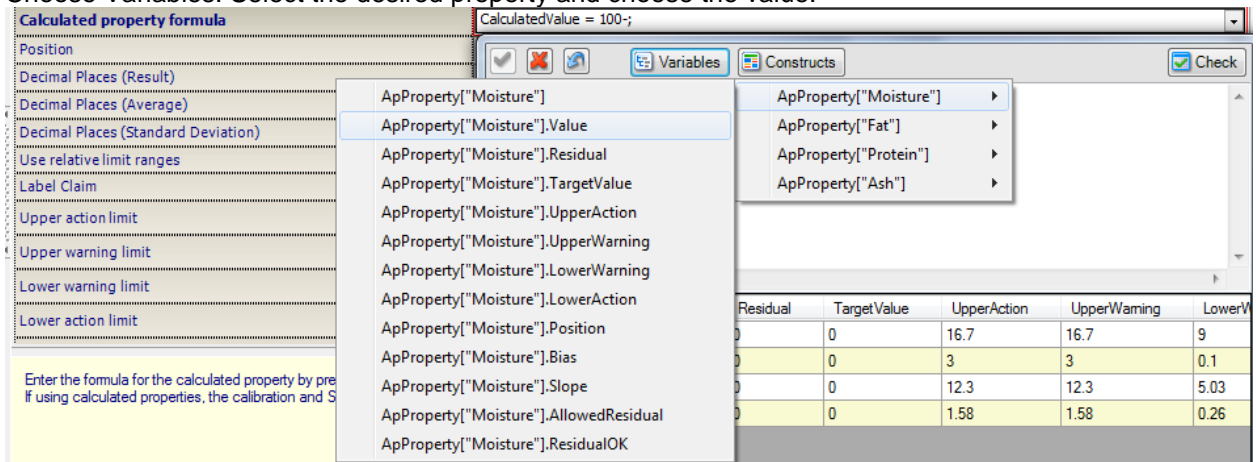


ApProperty	Value	Residual	TargetValue	UpperAction	UpperWarning	LowerWarning
Moisture	0	0	0	16.7	16.7	9
Fat	0	0	0	3	3	0.1
Protein	0	0	0	12.3	12.3	5.03
Ash	0	0	0	1.58	1.58	0.26

Replace the <formula > with "100-"



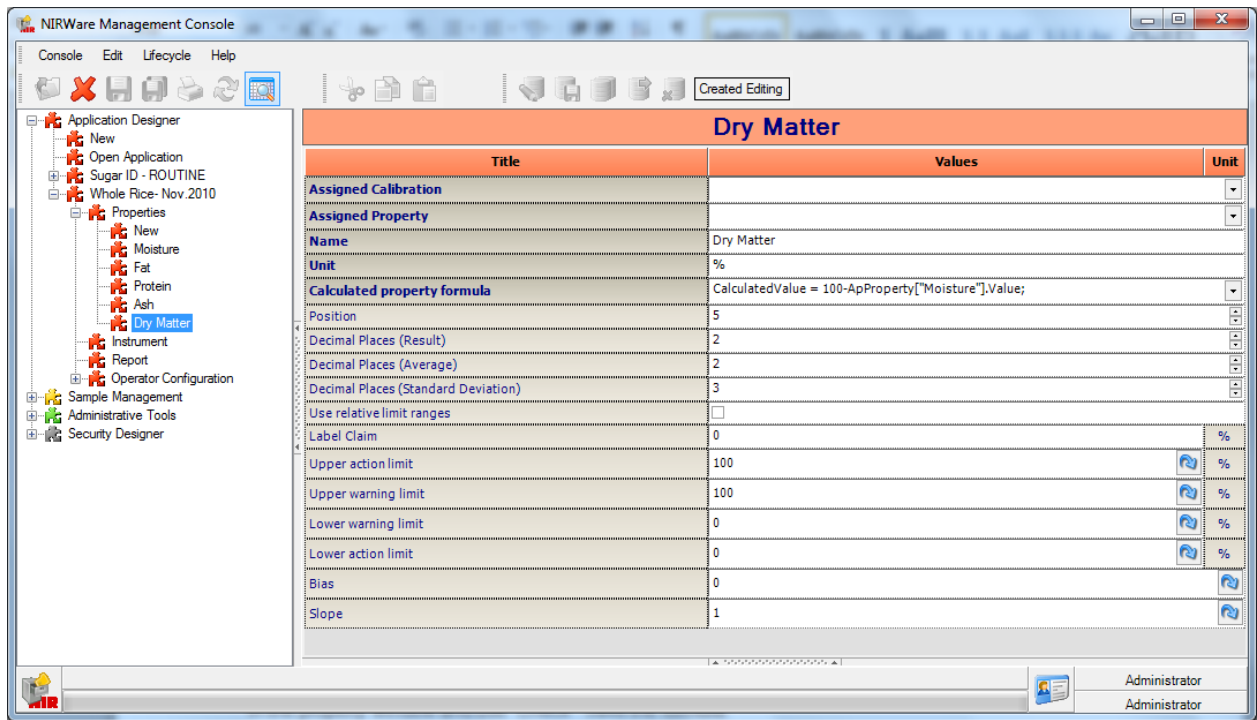
Choose Variables. Select the desired property and choose the value:



```
CalculatedValue = 100 - ApProperty["Moisture"].Value;
```

Take care, that the semicolon is at the end. The calculated property can be controlled with editing values in the property window and use "Check". Save the formula.

Edit the name of the property, the unit and if possible the upper and lower action and warning limits.



Save the new property and change the position if necessary:

Properties					
	Position	Name	Unit	Calibrations assigned	Calculated Property
1	1	Moisture	%	<input checked="" type="checkbox"/>	<input type="checkbox"/>
2	2	Dry Matter	%	<input type="checkbox"/>	<input checked="" type="checkbox"/>
3	3	Fat	%	<input checked="" type="checkbox"/>	<input type="checkbox"/>
4	4	Protein	%	<input checked="" type="checkbox"/>	<input type="checkbox"/>
5	5	Ash	%	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Example 1: Dry Matter

Add conditionality based on the residual:

```

if(ApProperty["Moisture"].ResidualOK)
{
    CalculatedValue = 100 - ApProperty["Moisture"].Value;
}

```

If *CalculatedValue* is not defined in the formula the value will be set to a very high or low number which one might want to avoid. In this case it is advised to define *CalculatedValue* to a value which the user will interpret as not valid, e.g. -999.

In this example *CalculatedValue* is defined as -999 and only if the residual of the moisture is OK, is the DM calculated.

```

CalculatedValue = -999;

```

```

if(ApProperty["Moisture"].ResidualOK)
{
    CalculatedValue = 100 - ApProperty["Moisture"].Value;
}

```

In the report this measurement then appears as -999 and can easily be interpreted as an invalid measurement.

In case frequent error due to too high residuals occurs, the limits can be extended. Here the residual limit is compared to the residual and the limit is multiplied with 1.20 to add 20% higher tolerance limit.

```

CalculatedValue = -999;

if(ApProperty["Moisture"].Residual < ApProperty["Moisture"].AllowedResidual*1.2)
{
    CalculatedValue = 100 - ApProperty["Moisture"].Value;
}

```

Example 2: Nested conditions

In this example nested conditions i.e. conditions within conditions are used. First check if the residual is OK, if it is fulfilled, test if the predicted value is less than 0. If it is lower as 0, set the output to 0 (no negative content), otherwise the output is set to the predicted value.

In this example comments are also use. Comments are text after `"/"` and is shown in green. Comments are not evaluated.

```

CalculatedValue = -999; //Initialise to avoid problems in the Operator reports

//if the residual is less than the allowed residual (we could also have used the field
ResidualOK
if(ApProperty["Moisture"].Residual < ApProperty["Moisture"].AllowedResidual)
{
    //If a negative value is predicted then set the CalculatedValue to 0
    if(ApProperty["Moisture"].Value < 0)
    {
        CalculatedValue = 0;
    }
    //Otherwise use the predicted value
    else
    {
        CalculatedValue = ApProperty["Moisture"].Value;
    }
}

```

The above example can be expand to test also if the value is above 100 and report 100 in case the predicted value is above 100%.

```

CalculatedValue = -999; //Initialise to avoid problems in the Operator reports

//if the residual is less than the allowed residual (we could also have used the field
ResidualOK
if(ApProperty["Moisture"].Residual < ApProperty["Moisture"].AllowedResidual)
{
    //If a negative value is predicted then set the CalculatedValue to 0
    if(ApProperty["Moisture"].Value < 0)
    {
        CalculatedValue = 0;
    }
}

```

```

//Otherwise if a value larger than 100 is predicted then set the
calculatedValue to 100
else if(ApProperty["Moisture"].Value > 100)
{
    CalculatedValue = 100;
}
//Otherwise use the predicted value
else
{
    CalculatedValue = ApProperty["Moisture"].Value;
}
}

```

Example 3: Two properties and local variables

The results from two or more properties can be combined. Here a result present if the residuals of both Fat and Moisture are OK.

```

CalculatedValue = -999;

if(ApProperty["Moisture"].ResidualOK && ApProperty["Fat"].ResidualOK)
{
    CalculatedValue = 100 - ApProperty["Moisture"].Value;
}

```

Adding to the complexity local variables can be defined which can be used to store intermediate results. The following example reports the fat content at a different moisture level than what is measured. E.g. if there is 20% fat at 50% moisture then the *fat of the dry matter* (0% moisture) or any other %moisture can be calculated.

The variable m is used to define the reported moisture level, here 0%.

```

Double m = 0; //The reported moisture level
Double dm = 0; // Fat content at 0% moisture

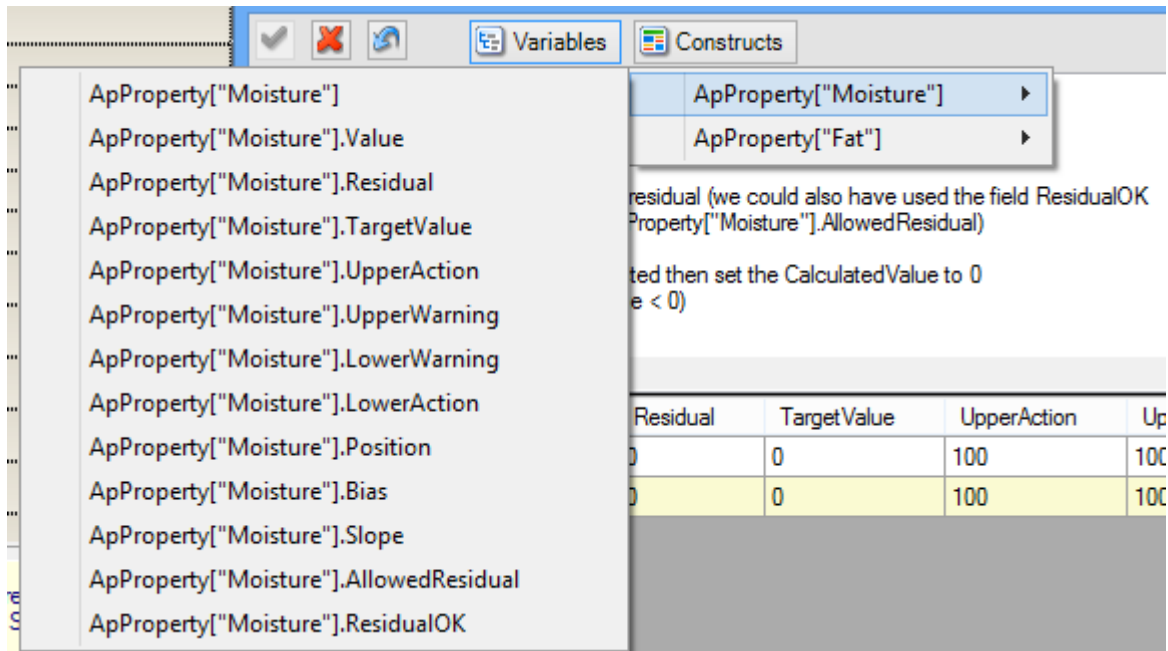
// Calculate the %Fat at 0% moisture
dm = (100*ApProperty["Fat"].Value) / (100-ApProperty["Moisture"].Value);

// Calculate the %Fat at m% moisture
CalculatedValue = (100-m)/100*dm;

```

Using other application properties

In the previous examples the application properties were used: Value, Residual, ResidualOK and AllowedResidual. A complete list of available properties is found by pressing Variables (see below)



Tips and tricks

- The notation used is C# notation. Refer to C# reference documentation for more detailed description of the notation. Not all C# functions and constructs are available.
- Terminate lines with semicolon “;”
- Set the action and warning limits manually for calculated properties. Action limits can be set to catch the value used to indicate an error, e.g. -1000 in the examples above.
- Comments can be written as “//” in front of a line, or after the code in a line.
- One calculated property cannot use another calculated property. Instead one can include the code from the first calculated property in the second.
- Take care of the Bias and slope correction values, if applied for the calculated property.

6.2.6. Property settings

Only for quantitative property there are following parameters:

Decimal Places (Result)	Define, how many positions after the decimal point will be displayed for the prediction result. Default: 2
----------------------------	---

To get access to the property parameter list, click on the entry "**Properties**" and then on "**New**" in the file tree list on the left to create a new property entry.

In case more than one property is created in the application already, it will be possible to adjust the position (order) of the properties how they will be shown in the operator and in reports. To do so, edit the position number for each property.

Properties			
	Name	Unit	Position
1	Moisture	%	1
2	Protein	%	2
3	Fat	%	3
4	Phosphorus	%	4
5	Ash	%	5
6	Fibre	%	6

To edit already created property entries, click on the corresponding entry in the file tree list.

* Moisture			
Title	Values	Unit	
Assigned Calibration	Moisture in Whole Rice-09-07		
Assigned Property	Moisture		
Name	Moisture		
Unit	%		
Position	0		
Decimal Places (Result)	2		
Decimal Places (Average)	2		
Decimal Places (Standard Deviation)	3		
Use relative limit ranges	<input type="checkbox"/>		
Label Claim	0	%	
Upper action limit	15.8	%	
Upper warning limit	15.8	%	
Lower warning limit	9	%	
Lower action limit	9	%	
Bias	0		
Slope	1		

The following list of parameters is available:

Parameter Name	Description
Name	<p>Quantitative: Name of the quantitative property (e.g. Name = grassi / assigned property = fat) to be displayed in the Operator Interface.</p> <p>Identification: Name of the qualitative property (e.g. sucrose for SIMCA) or property group (e.g. white powders for libraries and CLUSTER calibrations).</p>
Unit	<p>Quantitative: Unit of the corresponding quantitative reference data (e.g. % or ppm or g/kg).</p> <p>Identification: No entry for qualitative data.</p>
Assigned Property	<p>Quantitative: Name of the quantitative property (e.g. Name = grassi / assigned property = fat) in the database which corresponds with your selected property name. Select the correct quantitative property from the drop down menu:</p>

Assigned	Name	PropertyType	Unit
<input type="checkbox"/>	Sucrose	eQuantification	
<input type="checkbox"/>	sucrose	eQuantification	
<input type="checkbox"/>	Fat	eQuantification	%
<input checked="" type="checkbox"/>	Moisture	eQuantification	%
<input type="checkbox"/>	Protein	eQuantification	%
<input type="checkbox"/>	Ash	eQuantification	%
<input type="checkbox"/>	Fibre	eQuantification	%

Identification:

Name of the qualitative property (SIMCA) or all qualitative properties in the property group (CLUSTER).

Select the correct qualitative property/properties from the drop down menu:

Assigned	Name	PropertyType
<input checked="" type="checkbox"/>	Lactose	elidentification
<input checked="" type="checkbox"/>	Fructose	elidentification
<input checked="" type="checkbox"/>	Sucrose	elidentification
<input type="checkbox"/>	Methanol	elidentification

For Libraries, no entry should be done.

Assigned Calibration

Name of the calibration which has been calculated in NIRCal. Only an assigned calibration allows prediction of a measurement result.

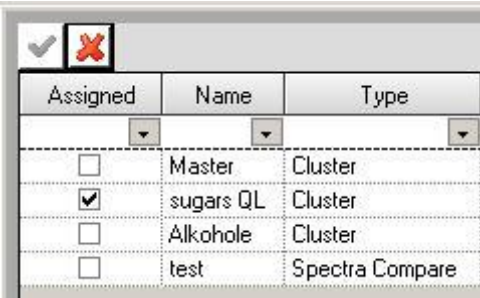



Quantitative:


Select the corresponding quantitative calibration model for the property.

Assigned	Name	Type
<input type="checkbox"/>	Master	PLS
<input type="checkbox"/>	sucrose QN	PLS
<input type="checkbox"/>	DB1, 4-10, F:5	PLS
<input type="checkbox"/>	copy of DB1, 4-10, F:5	PCR
<input type="checkbox"/>	Fat in Chicken_Update	PLS
<input type="checkbox"/>	Moisture in Chicken_Update	PLS
<input type="checkbox"/>	Protein in Chicken_Update	PLS
<input checked="" type="checkbox"/>	Moisture in Feed_Update	PLS

Identification:

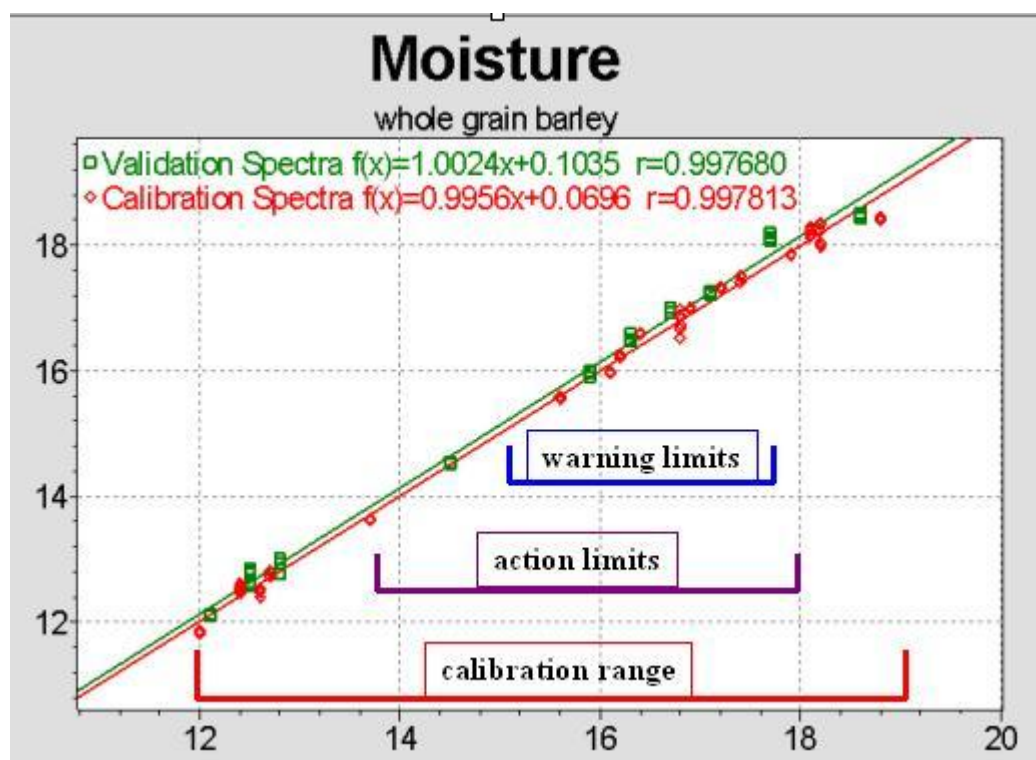
Select the corresponding qualitative calibration model:

	
Position	<p>Quantitative and Identification: Position of the parameter to be displayed in NIRWare Operator and all printing documents.</p> <p>Only needed if more than one property / property group is added to the application. predicted.</p>
Decimal Places (Result)	<p>Quantitative: Define, how many positions after decimal point will be displayed for the prediction result. Default: 2</p>
Decimal Places (Average)	<p>Quantitative: Define, how many positions after decimal point will be displayed for the result average. Default: 2</p>
Decimal Places (Std Dev)	<p>Quantitative: Define, how many positions after decimal point will be displayed for the standard deviation. Default: 3</p>
Upper action limit	<p>Entry for the upper action limit. "Action Limits" define the limits, which if exceeded or under-run, indicate that results are outside of acceptable tolerance. See also "Definition of calibration range, warning and action limits". Default: upper limit of calibration range To set back the default value for the action limit, click on this button </p>
Upper warning limit	<p>Entry for the upper warning limit. "Warning Limits" define the range around an acceptable result (e.g. production optimum). See also "Definition of calibration range, warning and action limits". Default: upper limit of the calibration range To set back the default value for the warning limit, click on this button </p>
Lower warning limit	<p>Entry for the lower warning limit. "Warning Limits" define the range around an acceptable result (e.g. production optimum). See also "Definition of calibration range, warning and action limits". Default: lower limit of calibration range To set back the default value for the warning limit, click on this button </p>
Lower action limit	<p>Entry for the lower action limit. "Action Limits" define the limits, which if exceeded or under-run, indicate that results are outside of acceptable tolerance.</p>

	See also "Definition of calibration range, warning and action limits". Default: lower limit of calibration range To set back the default value for the action limit, click on this button 
Bias	Linear correction of a predicted result using bias function. Correction will be displayed in report. Default: 0
Slope	Linear correction of a predicted result using slope function. Correction will be displayed in report Default: 1
Label Claim (CUT)	Content of active pharmaceutical ingredient per sample
L1 (CUT)	Maximum allowed acceptance value
L2 (CUT)	Maximum allowed range for deviation of each dosage unit tested from the calculated value of M.
T (CUT)	Target test sample amount at time of manufacture.

* non bold parameters are advanced parameters.


6.2.7. Definition of calibration range, warning and action limits





The **calibration range** of a quantitative calibration is defined by the data (minimum and maximum values in calibration set) used for calibration development. By default the related warning and action limits are set to their maximum range which is identical to the calibration range.



It will be possible to define warning and action limits within the calibration range by entering the corresponding values in the parameter list.


"Warning Limits" define the range around an acceptable result (e.g. production optimum).

 indicates, that the predicted result is within the acceptable tolerance limits (warning limits)

 or  indicates an under- or overshooting of these defined limits (but within the defined action limits).

"Action Limits" define the limits, which if exceeded or under-run, indicate that results are outside of acceptable tolerance. Action needs to be taken e.g. to bring the measured production parameter back to the optimal value.

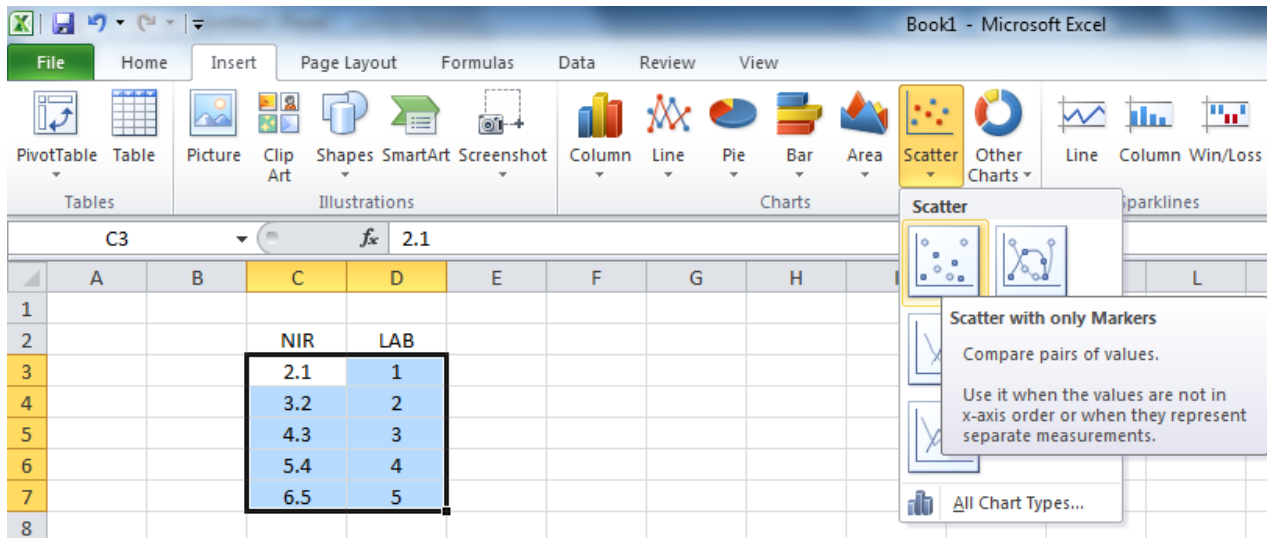
 or  indicates an under- or overshooting of the action limits (but within the calibration range).

 indicates, that the predicted value is outside of the limits given by the calibration range.

6.2.8. Bias and Slope calculation

For the calculation of Bias and Slope the predicted NIR values and the laboratory values should be copied into an **Excel** table:

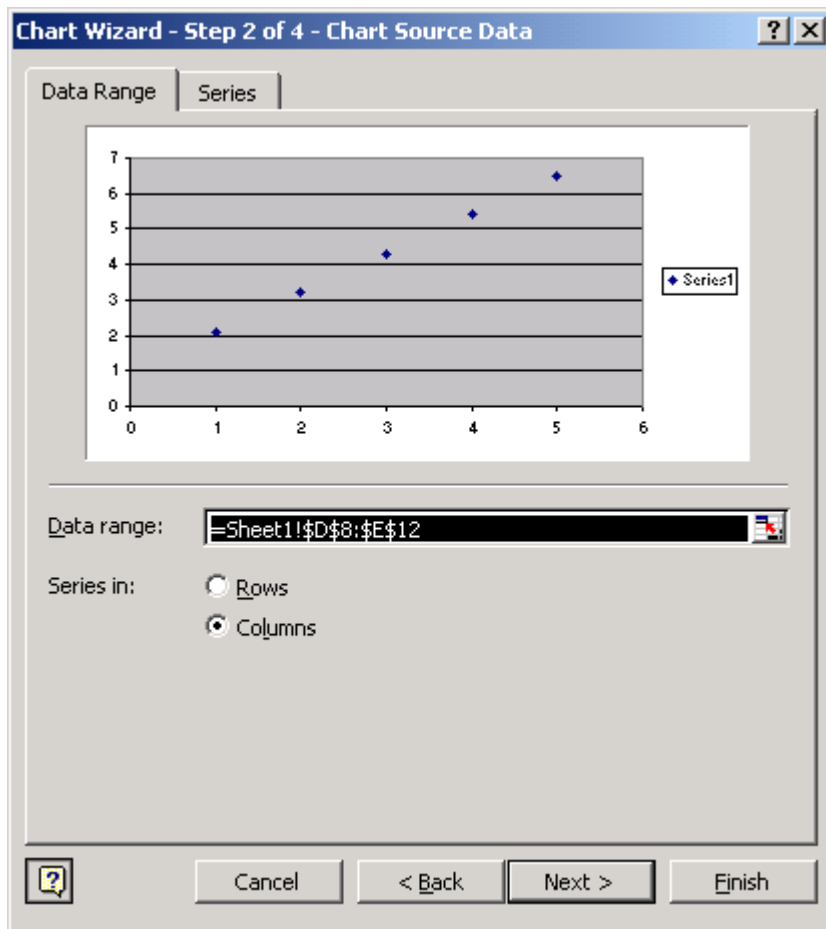
Create a correlation between these values using the **Chart Wizard**:



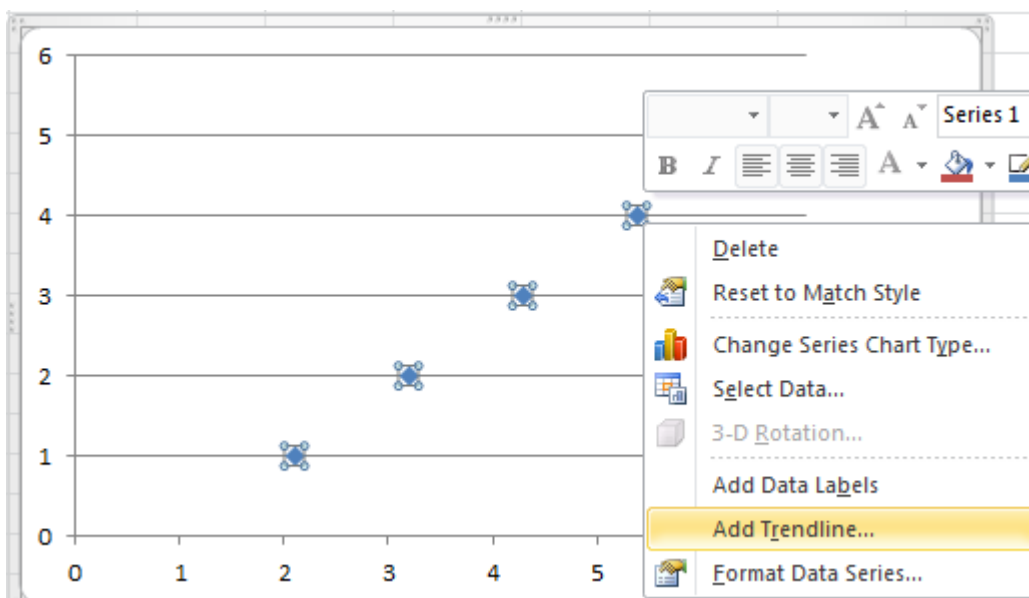
The screenshot shows Microsoft Excel with a data table and the Chart Wizard interface. The data table is as follows:

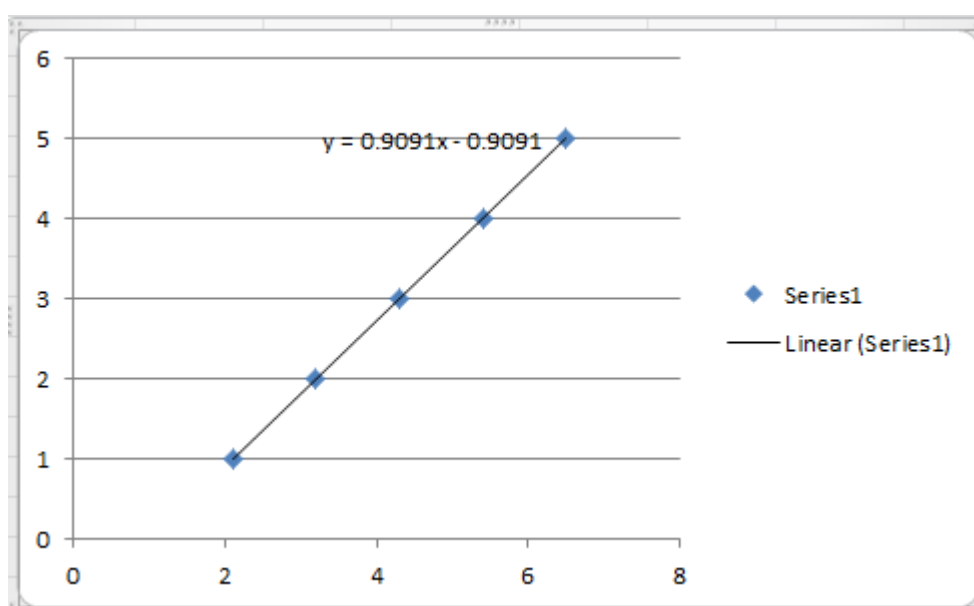
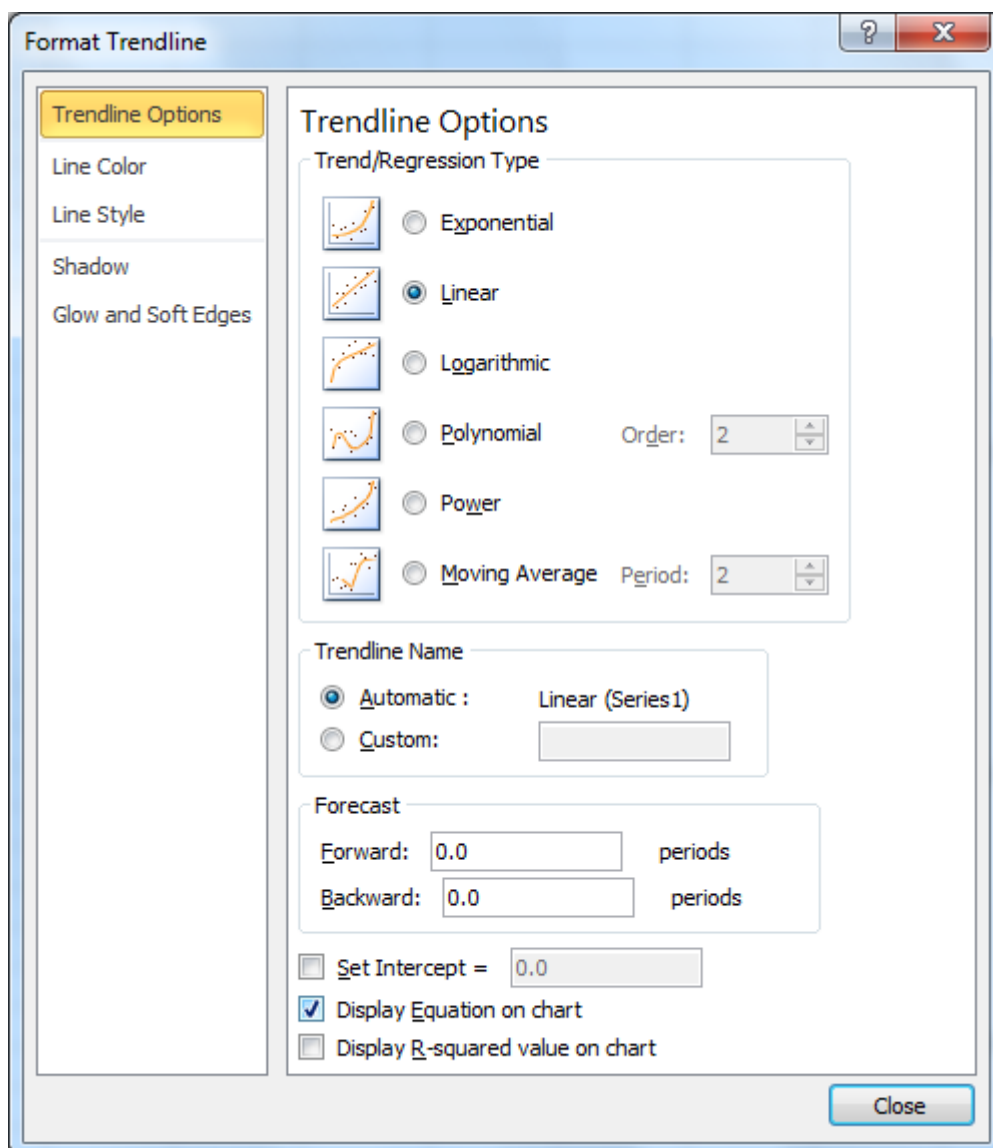
	A	B	C	D	E	F	G	H	I	J	K	L
1												
2			NIR	LAB								
3			2.1	1								
4			3.2	2								
5			4.3	3								
6			5.4	4								
7			6.5	5								
8												

The Chart Wizard interface is open, showing the 'Scatter' chart type selected. The 'Scatter with only Markers' option is chosen, with the following description: 'Compare pairs of values. Use it when the values are not in x-axis order or when they represent separate measurements.'



Select the points and click the right mouse button to get the **Add Trendline**:





The regression coefficient is visible:








$$y=0.9091*x-0.9091$$

To get the original laboratory values, the **correction** is:

- **Bias = -0.9091,**
- **Slope = 0.9091**

6.2.9. Instrument parameters

To get access to the instrument parameter list, click on the entry "Instrument" in the file tree list on the left.

Instrument		
Title	Values	Unit
Instrument	NIRFlex N500	
Measurement Cell	Solids	
Measurement Cell Add-On	Petri	
Instrument Serial-Number		
Number of Scans	32	
Resolution	<input checked="" type="checkbox"/>	
Apodisation 1 for Phase Correction (Don't change !)	Blackman	
Apodisation 2 for Phase Correction (Don't change !)	Blackman	
Apodisation for Interferogram (Don't change !)	Blackman	
Transfilter	<input type="checkbox"/>	
Datapoints	1501	
Lower Wavenumber Limit	4000	[1/cm]
Datapoint Interval	4	[1/cm]
External reference spectra comparison	<input checked="" type="checkbox"/>	
Maximum allowed deviation of external reference spectra	5	[%]
Position of Standardwheel for sample measurement	0	
Position of Standardwheel for reference measurement	0	
Suitability Test Mode	Interval	
SuitabilityTest Interval	12	 Hours [h]
Successful Suitability Test is required for measurement	<input checked="" type="checkbox"/>	
Save Spectra Interferogram	<input type="checkbox"/>	
Measurement Cell		
Title	Values	Unit
Gain of ADC Detector for references	3	
Gain of ADC Detector for samples	3	
External Reference Mode	Interval	
External Reference Interval	60	 Minutes [min]
Internal Reference Mode	Interval	
Internal Reference Interval	10	 Minutes [min]
Max. Drift for Reference Temperature	3	 Celsius [°C]
Sampleholder Rotation for Petri Dish	<input checked="" type="checkbox"/>	


By default, only the basic settings are visible.



To show and hide the advanced settings again, click the corresponding icon.

The following list of parameters is available:

Parameter Name	Description								
Instrument	Type of NIR Instrument to be implemented in this specific application: NIRFlex N500								
Measurement Cell	Selected measurement cell: 1. NIRMaster 2. Fiber Optic SMA (for continuous measurement) 3. CheckMaster Transmittance 4. Solids Transmittance 5. Fiber Optic Liquids 6. Fiber Optic Solids 7. Liquids 8. Solids								
Measurement Cell Add-On	Selected measurement cell add-on. The dialog offers different choices depending on the selected measurement cell type: 1. No Option 2. No Option 3. No Option 4. 10 Samples 30 Samples USP Testkit for Solid Transmittance (only for BUCHI internal use) Reference Samples (only for BUCHI internal use) 5. No Option 6. No Option Transflection Head 7. No Option (Cuvette) 8. Vial Petri USP Testkit (only for BUCHI internal use) Tablet XL								
Instrument Serial-Number	Enter the serial number of the instrument to be used only with this application. Without restriction the application can be used with any instrument. Example: 0500000003.								
Number of Scans	Entry for the number of scans per measurement. Depending on the used measurement cell, used add-on and application type (Quantification, Identification), different default values are set as default: <table border="1" data-bbox="539 1720 1461 2022"> <tbody> <tr> <td>1. NIRMaster</td> <td>8 scans (Qualitative) 32 scans (Quantitative)</td> </tr> <tr> <td>2. Fiber Optic SMA (for continuous measurement)</td> <td>8 scans (Qualitative) 32 scans (Quantitative)</td> </tr> <tr> <td>3. CheckMaster Transmittance</td> <td>64 scans</td> </tr> <tr> <td>4. Solids Transmittance</td> <td>64 scans</td> </tr> </tbody> </table>	1. NIRMaster	8 scans (Qualitative) 32 scans (Quantitative)	2. Fiber Optic SMA (for continuous measurement)	8 scans (Qualitative) 32 scans (Quantitative)	3. CheckMaster Transmittance	64 scans	4. Solids Transmittance	64 scans
1. NIRMaster	8 scans (Qualitative) 32 scans (Quantitative)								
2. Fiber Optic SMA (for continuous measurement)	8 scans (Qualitative) 32 scans (Quantitative)								
3. CheckMaster Transmittance	64 scans								
4. Solids Transmittance	64 scans								

	<table border="1"> <tr> <td>5. Fiber Optic Liquids</td> <td>8 scans (Qualitative) 16 scans (Quantitative)</td> </tr> <tr> <td>6. Fiber Optic Solids</td> <td>8 scans (Qualitative) 32 scans (Quantitative)</td> </tr> <tr> <td>7. Liquids</td> <td>8 scans (Qualitative) 16 scans (Quantitative)</td> </tr> <tr> <td>8. Solids with Vial Add-On</td> <td>8 scans (Qualitative) 32 scans (Quantitative)</td> </tr> <tr> <td>8. Solids with XL Add-On</td> <td>8 scans (Qualitative) 32 scans (Quantitative)</td> </tr> <tr> <td>8. Solids with Petri Add-On</td> <td>8 scans (Qualitative) 32 scans (Quantitative)</td> </tr> <tr> <td>8. Solids with Tablet Add-On</td> <td>8 scans (Qualitative) 32 scans (Quantitative)</td> </tr> </table> <p>It is possible to enter a different number of scans optimized to the task. To set back the default value for the instrument configuration, click on this button .</p>	5. Fiber Optic Liquids	8 scans (Qualitative) 16 scans (Quantitative)	6. Fiber Optic Solids	8 scans (Qualitative) 32 scans (Quantitative)	7. Liquids	8 scans (Qualitative) 16 scans (Quantitative)	8. Solids with Vial Add-On	8 scans (Qualitative) 32 scans (Quantitative)	8. Solids with XL Add-On	8 scans (Qualitative) 32 scans (Quantitative)	8. Solids with Petri Add-On	8 scans (Qualitative) 32 scans (Quantitative)	8. Solids with Tablet Add-On	8 scans (Qualitative) 32 scans (Quantitative)
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8. Solids with Vial Add-On	8 scans (Qualitative) 32 scans (Quantitative)														
8. Solids with XL Add-On	8 scans (Qualitative) 32 scans (Quantitative)														
8. Solids with Petri Add-On	8 scans (Qualitative) 32 scans (Quantitative)														
8. Solids with Tablet Add-On	8 scans (Qualitative) 32 scans (Quantitative)														
Resolution	<p>Select check box:</p> <ul style="list-style-type: none"> • Checked = full instrument resolution 8cm^{-1} with Boxcar (default) • Unchecked = half resolution (16cm^{-1}) with Boxcar (default for Solids Transmittance) <p>The default resolution is recommended.</p>														
Apodisation 1 for Phase Correction (Don't change!)	<p>This parameter is for information only and shows the apodisation function 1 used for phase correction.</p> <p>A different Apodisation function may be available in the future (Default function = Blackman)</p>														
Apodisation 2 for Phase Correction (Don't change!)	<p>This parameter is for information only and shows the apodisation function 2 used for phase correction.</p> <p>A different Apodisation function may be available in the future (Default function = Blackman)</p>														
Apodisation for Interferogram (Don't change!)	<p>This parameter is for information only and shows the apodisation function used for interferogram treatment.</p> <p>A different Apodisation function may be available in the future (Default function = Blackman)</p>														
Transfilter	<p>Don't change!</p> <p>This function is only used during the phase correction.</p> <ul style="list-style-type: none"> • Checked = Transfilter activated • Unchecked = Transfilter deactivated (default) 														
Datapoints	<p>Use with care.</p> <p>Recommendations for lower wavenumber limit 4000cm^{-1} and Datapoint interval 4:</p>														

	<p>10000cm⁻¹ - 4000cm⁻¹ : 1501 (default) 12200cm⁻¹ - 4000cm⁻¹ : 2051 12500cm⁻¹ - 4000 cm⁻¹: 2126 (max. allowed range)</p> <p>Recommendations for Solids Transmittance with lower wavenumber limit 6000 cm⁻¹ and Datapoint interval 4: 11520cm⁻¹ - 6000cm⁻¹ : 1381 (default) 12200cm⁻¹ - 6000cm⁻¹ : 1551 12500cm⁻¹ - 6000cm⁻¹ : 1626 (max. allowed range)</p> <p>To get access to the entry field, the right to "Edit Expert Values" need to be assigned to you in the Security Designer under Security Policies. For further details read more under "Extended Wavenumber Range".</p>
Lower Wavenumber Limit	This parameter is for information only. Lowest wavenumber of the spectra.
Datapoint Interval	This parameter is for information only. Intervall between two datapoints in wavenumbers.
External Reference Comparison	If checked, the new measured external reference spectrum will be compared to the last measured spectrum.
Maximum allowed deviation of the reference spectra	<p>This parameter defines the maximum allowed deviation in percentage. For the calculation of the deviation the following formula is used:</p> $Ra = \text{Max}(\text{Abs}(R1/G1 - R2/G2) / \text{Max}(\text{Abs}(R1/G1)))$ <p>R1 = Previously accepted external reference spectrum vector R2 = Newly measured external reference spectrum vector G1 = Gain factor of R1 G2 = Gain factor of R2</p> <p>Value range: 1...100</p>
Position of Standardwheel for sample measurement	<p>Use with care! The standard wheel contains 5 grey standards, a internal wavenumber standard and an empty position. Define, which position should be in the light beam for sample measurement:</p> <p>0 = empty (Default) 1 = filter 1 (ca. 2%) 2 = filter 2 (ca. 10%) 3 = filter 3 (ca. 29%) 4 = filter 4 (ca. 64%) 5 = filter 5 (ca. 92%) 6 = PMMA 7 = Do not use this setting (causes error)</p>
Position of Standardwheel for reference measurement	<p>Use with care! The standard wheel contains 5 grey standards, a internal wavenumber standard and an empty position. Define, which position should be in the light beam for reference measurement:</p> <p>0 = empty (Default)</p>
Suitability Test Mode	<p>Define the SST Test procedure:</p> <p>Interval = Test will be performed after the below defined time period is exhausted (default) Disabled = No SST Test will be performed automatically.</p>
Suitability Test Interval	Interval for an automatic start of an SST in hours:

	24 (default)																
Successful suitability test is required for measurement	<p>A routine measurement can be started only if the SST was successful.</p> <ul style="list-style-type: none"> • Checked = A routine measurement can be started only with a successful SST. It is suggested to work with this adjustment. • Unchecked = A routine measurement can be started regardless of the SST result (default) 																
Save Spectra Interferogram	<p>Next to the spectral information, the interferogram of each measurement can be stored in the system. Activating this function will increase the use of database space and the further use of the interferogram data is not yet implemented.</p> <ul style="list-style-type: none"> • Checked = save spectra interferogram is activated • Unchecked = save spectra interferogram is deactivated (default) 																
Gain of ADC Detector for samples	<p>This parameter is for information only. The detector has 5 levels of sensitivity. Depending on the measurement cell used, the optimal gain is used automatically.</p>																
Gain of ADC Detector for references	<p>This parameter is for information only. The detector has 5 levels of sensitivity. Depending on the measurement cell used, the optimal gain is used automatically.</p>																
External Reference Mode	<p>Mode to measure the external reference. Choose from the following possibilities:</p> <ul style="list-style-type: none"> • Interval or Temperature Drift = regularly or if the temp. changes • Manual = Manual reference measurement • Measurement Sequence = at each start of a measurement sequence • Once a day = once a day, before the first measurement • Interval = regularly (see interval value below) • Temperature Drift = after a certain temperature drift of the interferometer (see value below) • Batch = once after a new batch has been created • Disabled = No measurement for computing <p>Default:</p> <table> <tr> <td>1. NIRMaste</td> <td>Interval (60 min)</td> </tr> <tr> <td>2. Fiber Optic SMA (for continuous measurement)</td> <td>Manual (60 min)</td> </tr> <tr> <td>3. CheckMaster Transmittance</td> <td>Measure Sequence</td> </tr> <tr> <td>4. Solids Transmittance</td> <td>Measure Sequence</td> </tr> <tr> <td>5. Fiber Optic Liquids</td> <td>Interval (60 min)</td> </tr> <tr> <td>6. Fiber Optic Solids</td> <td>Interval (60 min)</td> </tr> <tr> <td>7. Liquids</td> <td>Measure Sequence</td> </tr> <tr> <td>8. Solids with Vial Add-On</td> <td>Measure Sequence</td> </tr> </table>	1. NIRMaste	Interval (60 min)	2. Fiber Optic SMA (for continuous measurement)	Manual (60 min)	3. CheckMaster Transmittance	Measure Sequence	4. Solids Transmittance	Measure Sequence	5. Fiber Optic Liquids	Interval (60 min)	6. Fiber Optic Solids	Interval (60 min)	7. Liquids	Measure Sequence	8. Solids with Vial Add-On	Measure Sequence
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7. Liquids	Measure Sequence																
8. Solids with Vial Add-On	Measure Sequence																

	<p>8. Solids with XL Add-On Interval (20 min)</p> <p>8. Solids with Petri Add-On Interval (60 min)</p> <p>8. Solids with Tablet Add-On Measure Sequence</p>																						
External Reference Interval	Interval in minutes to measure the external reference, if the mode to measure the external reference was selected as "interval".																						
Internal Reference Mode	<p>Mode to measure the internal reference (not available for Solids Transmittance). Choose from the following possibilities:</p> <ul style="list-style-type: none"> • Disabled = No measurement for computing • Manual = Manual reference measurement • Measurement Sequence = at each start of a measurement sequence • Interval = regularly (see interval value below) • Temperature Drift = after a certain temperature drift of the interferometer (see value below) • Batch = once after a new batch has been created <p>Default:</p> <table> <tr> <td>1. NIRMaster</td> <td>Interval (10 min)</td> </tr> <tr> <td>2. Fiber Optic SMA (for continuous measurement)</td> <td>Interval (10 min)</td> </tr> <tr> <td>3. CheckMaster Transmittance</td> <td>n.a.</td> </tr> <tr> <td>4. Solids Transmittance</td> <td>n.a.</td> </tr> <tr> <td>5. Fiber Optic Liquids</td> <td>Interval (10 min)</td> </tr> <tr> <td>6. Fiber Optic Solids</td> <td>Interval (10 min)</td> </tr> <tr> <td>7. Liquids</td> <td>Disabled</td> </tr> <tr> <td>8. Solids with Vial Add-On</td> <td>Disabled</td> </tr> <tr> <td>8. Solids with XL Add-On</td> <td>Disabled</td> </tr> <tr> <td>8. Solids with Petri Add-On</td> <td>Interval (10 min)</td> </tr> <tr> <td>8. Solids with Tablet Add-On</td> <td>Disabled</td> </tr> </table>	1. NIRMaster	Interval (10 min)	2. Fiber Optic SMA (for continuous measurement)	Interval (10 min)	3. CheckMaster Transmittance	n.a.	4. Solids Transmittance	n.a.	5. Fiber Optic Liquids	Interval (10 min)	6. Fiber Optic Solids	Interval (10 min)	7. Liquids	Disabled	8. Solids with Vial Add-On	Disabled	8. Solids with XL Add-On	Disabled	8. Solids with Petri Add-On	Interval (10 min)	8. Solids with Tablet Add-On	Disabled
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8. Solids with Vial Add-On	Disabled																						
8. Solids with XL Add-On	Disabled																						
8. Solids with Petri Add-On	Interval (10 min)																						
8. Solids with Tablet Add-On	Disabled																						
Internal Reference Interval	Interval in minutes to measure the internal reference, if the mode to measure the internal reference was selected as "interval".																						
Max. Drift for Reference Temperature	Maximum allowed drift in °C inside the NIRFlex N-500. If this maximum drift is exceeded, the software will ask to do an SST and to measure external and internal reference.																						
Sample holder rotation for Petri dish	<p>Special parameter for Measurement Cell "NIRMaster" and "Solids with Petri add-on" to turn on or off the rotation.</p> <ul style="list-style-type: none"> • Checked = rotation of petri dish add-on is turned on • Unchecked = rotation of petri dish add-on is turned off 																						
Heater Temperature Nominal	<p>Special parameter for Measurement Cell Liquids. Set temperature in [°C] in cuvette holder for liquid measurements.</p> <p>Default: 35°C Range: ambient temperature (+10°C) to 65°C</p>																						
Sample Gain	Setting for NIRFlex Solids Transmittance.																						

Determination	<p>Definition of the gain determination procedure:</p> <ul style="list-style-type: none"> • Manual: The gain specified in 'Gain of ADC Detector for samples' is used for all sample measurements. • Optimized: The optimum gain is determined when the application is run for the first time by analysing one or more samples. • Auto: The optimum gain is determined automatically for each sample before the measurement.
Determine best gain before the next measurement (Optimized)	<p>Setting for NIRFlex Solids Transmittance.</p> <p>This function is combined with the gain determination setting "Optimized". When it is activated, the amount of samples defined in the line "Number of samples used for optimized gain determination" is scanned prior to each measuring cycle and the resulting average gain is used for the samples measured in the cycle.</p>
Sample intensity scatter limit	<p>Setting for NIRFlex Solids Transmittance.</p> <p>The scatter limit is defined between 0.1 and 1 (default is 0.8) and ensures that the detector is not oversaturated.</p>
Number of samples used for optimized gain determination	<p>Setting for NIRFlex Solids Transmittance.</p> <p>The number defined in this field is used for the Gain Determination eOptimized (see above).</p> <p>Default: 1</p>

* non bold parameters are advanced parameters.

Apodisation function

Function ID	Function
1	Hamming (Hape-Genzel)
2	Hanning (cosine)
3	Blackman-Harris
4	Blackman-Harris 4Term
5	Bartlet (triangle)
6	Blackman
7	Blackman exact
8	Forman

6.2.10. Measurement cell specific settings

Solids Transmittance

External Reference is measured through air. The Gain settings for the reference measurements are set to the value 0 per default. This field can be edited with expert rights.

The light that reaches the detector during measurement strongly depends on the physical nature of the sample (the tablet). Thickness, density, colour and coatings will have an influence on the signal. There are different options to control the **sample gain**.

- **Manual:** The gain specified manually in 'Gain of ADC Detector for samples' is used for all sample measurements. Increasing gain levels: 0,1,2,3,4
- **Auto:** The optimum gain is determined automatically for each sample before the measurement. One scan is performed prior to every sample measurement and the gain is automatically determined afterwards. Individual spectra of one measurement sequence can have different gain settings.
- **Optimized:** With these settings an optimized sample gain for the next measurement sequence is determined. The number of samples used to calculate the optimized level can be set in the field "Optimized sample gain: Number of samples. Additionally, the field "Optimized sample gain: Determine best gain before the next measurement" has to be checked. After the next measurement the checkmark is automatically removed and the gain that had been determined can be seen in the field "Gain of ADC Detector for samples". (For that purpose the application has to be closed and reopened in the Management Console.)

Fiber Optic SMA

The Fiber optic SMA offers some unique settings.

Select between Transmission and Reflection depending on your measurement probe head.

The sample gain determination can be set analogously to the Solids Transmittance measurement cell.

External reference gain determination. Manual, Optimized and Auto are available. Default settings are Manual with a gain value of 1 for Transmission, and a gain value of 4 for Reflection.

Scan Quality Check

While measuring liquid samples in transmission, air bubbles may occur that change the effective pathlength and therefore disturb the interferogram which is used to calculate the spectra. If this field is checked an algorithm is applied that can detect disturbed interferograms via a comparison of the amplitude signals. The amplitude of the distortion is compared to the interferogram peak size. If the relative distortion is bigger than the maximum allowed error, the scan is rejected. The upper limit of "bad" quality scans is set to 80% per default. This is the stop criterion after which a spectrum is rejected. The number of "good" scans that needs to be integrated to give a spectrum is still set in the Number of Scans.

Liquids

Reference Cuvette Slot

The Liquids Measurement Cell offers the possibility to choose one of the six cuvette slots as a reference channel, if a liquid is supposed to be measured for that purpose.

6.2.11. Report parameters

To get access to the report parameter list, click on the entry "**Report**" in the file tree list on the left.

Report	
Title	Value
Reporttype	Detail <input type="button" value="v"/>
Custom report template file name	
Show Calibrations	<input checked="" type="checkbox"/>
Show the address	<input checked="" type="checkbox"/>
Show the instrument part	<input checked="" type="checkbox"/>
Show the Serial Number	<input checked="" type="checkbox"/>

Parameter Name	Description
Report type	<p>Different report templates are available from which you can choose.</p> <ul style="list-style-type: none"> • QL: Detail (detailed result report for each measurement sequence) Batch Overview (summary report over all measurements of a batch) • QN: Detail (detailed result report for each measurement sequence) Overview (summary result for each measurement sequence) Batch Detail (detailed summary report over all measurements of a batch) Batch Overview (summary result over all measurements of a batch) • Default: Detail <p>Additional report types for special applications:</p> <ul style="list-style-type: none"> • Library Search (detail report) • Report for Content Uniformity Test (batch report)
Custom report template file name	<p>A customized report template which can be used. For this an additional template file created by BUCHI with the relevant information has to be saved into the directory C:\Program Files\Buchi\NIRSolutions\Report.</p> <p>Enter the full file name including the extension (e.g. CompanyReport.rpt).</p>
Show Calibrations	<p>Calibration details can be displayed on reports.</p> <ul style="list-style-type: none"> • Checked = Calibration details appear on reports (default) • Unchecked = Calibration details do not appear on reports
Show the address part	<p>Under Administrative Tools-Customer Information the address or customer specific information can be entered. This information will be shown in each report header if activated.</p> <ul style="list-style-type: none"> • Checked = Customer Info will be shown in report (default) • Unchecked = Customer Info will not be shown in report
Show the instrument part	<p>Instrument type and measurement cell type (e.g. NIRFlex N500; Solids) will be shown in report header.</p> <ul style="list-style-type: none"> • Checked = Instrument and measurement cell type shown in report (default) • Unchecked = Instrument and measurement cell type not shown in report

Show the serial number	<p>Instrument and measurement cell serial number will be shown in report header.</p> <ul style="list-style-type: none"> • Checked = Instrument and measurement cell serial number shown in report (default) • Unchecked = Instrument and measurement cell serial number not shown in report
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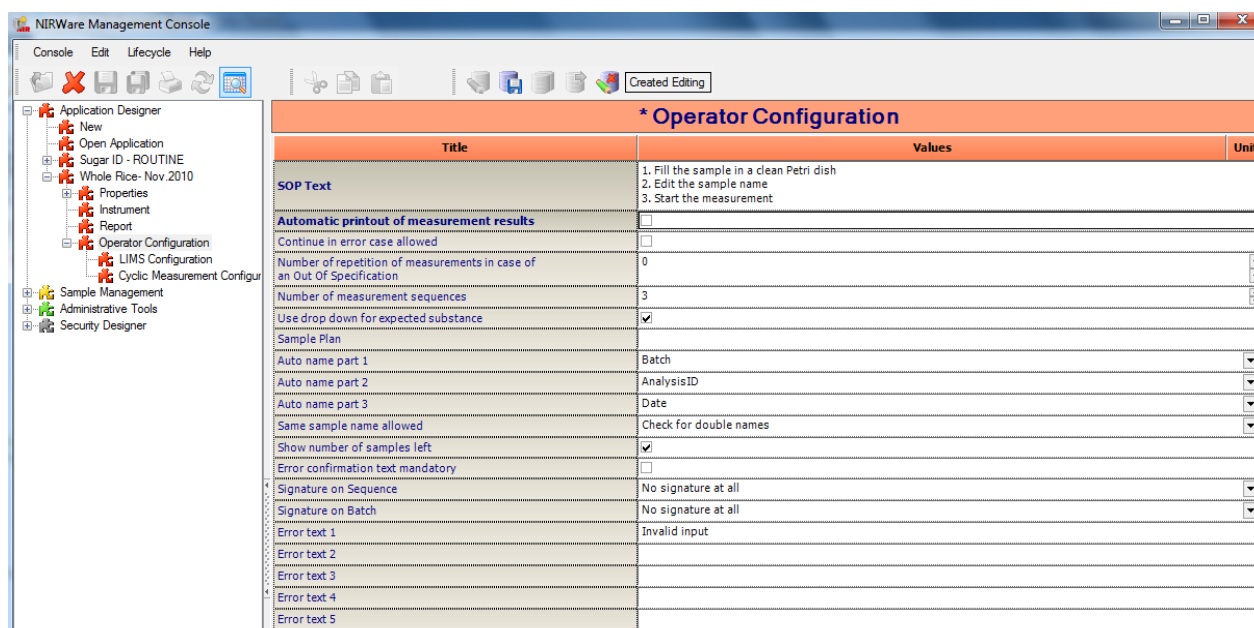
* non bold parameters are advanced parameters.

NOTE:

In case a batch report is selected, make sure that the following parameters are set in the application under Operator Configuration:

- Automatic printout of measurement results: **DISABLED**
- Number of repetition measurements in case of an out of specification (OoS): **0**

6.2.12. Operator configuration parameters



Parameter Name	Description
SOP Text	<p>An SOP text can be generated, which is displayed in the Operator Modules SOP-window</p> <p>Value: "Text"</p>
Automatic printout of measurement results	<p>The measurement results are automatically printed out on the default printer if this function is checked.</p>
Continue in error case allowed	<p>"Checked": If a sample result is not ok, a process continuation without repeating the measurement of this sample is possible (this function is only</p>

	<p>useful in combination with "Number of repetition..." is greater than zero)</p> <p>"Unchecked": No continuation possible</p>
Number of repetition measurements in case of an Out of Specification (OoS)	<p>"0": If a sample result is not ok, no repetition is requested.</p> <p>"1...N": Repetition possible.</p>
Number of measurement sequences	<p>"1...N": A sequence is the max. number of possible measurements without changing the samples: e.g. Fiber Optics => 1 sample, Solids and Liquids => 6 samples. The number of measurement sequences defines the N-fold measurement of the appropriate sequence</p> <p>Suggestion:</p> <ul style="list-style-type: none"> - 3 for spectra collection, - 1 for identification; - 3 for quantitative determination
Use drop down for expected substance	<p>Only ID-testing.</p> <p>"Unchecked": The expected substance name must be selected from a drop down list.</p> <p>"Checked": The expected substance code must be entered by keyboard or barcode (expected substance ID)</p>
Sample Plan	<p>Only for measuring cells having more, than one sample (Liquid, Solid with Vials or Tablet add-on).</p> <p>Enter sample positions and/or position ranges separated by commas.</p> <p>Autonaming will be applied to the selected positions or to all positions if no selection is entered.</p> <p>Example: 1, 3, 5-8</p>
Auto name Part 1	<p>"Drop down list": Nearly every field from the "Sample Description Field" list can be selected. It is suggested to use this adjustment.</p>
Auto name Part 2	<p>"Drop down list": Nearly every field from the "Sample Description Field" list can be selected. It is suggested to use this adjustment.</p>
Auto name Part 3 Note: Allows automatic definition of the sample names. Each combination of all possibilities from the 3 parts are allowed.	<p>"Counter": Defines a counter for all samples belonging to a batch</p> <p>"Date": Corresponds to the date of the first measurement</p> <p>"Blank": Leaves third part blank</p>
Same sample name allowed	<p>Checks current input of sample names for double names.</p> <p>"Double names are not allowed": Double names are prohibited</p> <p>"Check for double names": Only a warning message is displayed</p> <p>"No check": No action defined.</p>
Show number of samples left	<p>"Checked": Displays the number of samples left before each actual sample measurement. Especially important for ID if the Number of Container is activated.</p> <p>"Unchecked": not displayed</p>
Error confirmation text	<p>"Checked": In case of not-ok-measurement, a comment must be entered.</p>

mandatory	"Unchecked": No comment is necessary
Signature on Sequence	For LC "ERES" and selected report type "Detail" : "Electronic signature on report" is set active (signature on batch will be deactivated). For LC "ER" and "Unregulated": "Manual signature on report": Enables manual signature line on the report-type "Detail" "No signatures at all": No signatures
Signature on Batch	For LC "ERES" and selected report type "Batch": "Electronic signature on report" is set active (signature on sequence (detail report) will be deactivated). For LC "ER" and "Unregulated": "Manual signature on report": Enables manual signature line on the report-type "Batch" "No signatures at all": No signatures
Error text 1 - 5	"Text" numbers can be linked to input errors in the SOP-fields. In the Operator Module "Text" will occur as a tooltip in case of error input.

* non bold parameters are advanced parameters.

Sample Description Fields

Configures a series of fields for an exact sample description in the Operator module and the reports. The given data array allows the individual definition of each field.

Example of a quantitative application:

Sample Description Fields								
SOP Fields	Label	Visible	Request Input	Read Only	Error Text	Field Reset	Validation Range	Start reading at barcode position
Batch	Product-Batch	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Campaign	Campaign	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Number of Containers	NumberOfContainers	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Vendor Qualification	VendorQualification	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
AnalysisID	AnalysisID	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::	0
Customer Field 1	CustomerField1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Customer Field 2	CustomerField2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Customer Field 3	CustomerField3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Customer Field 4	CustomerField4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Customer Field 5	CustomerField5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Customer Field 6	CustomerField6	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Comment	Comment	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0
Samples		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0

Example of a qualitative application:

Sample Description Fields									
SOP Fields	Label	Visible	Request Input	Read Only	Error Text	Field Reset	Validation Range	Start reading at barcode position	Length of barcode field
Batch	Batch	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	10	6
Expected Substance	Expected Substance	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	5	5
Campaign	Campaign	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Number of Containers	NumberOfContainers	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Vendor Qualification	VendorQualification	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
AnalysisID	AnalysisID	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::	17	4
Customer Field 1	CustomerField1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 2	CustomerField2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 3	CustomerField3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 4	CustomerField4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 5	CustomerField5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 6	CustomerField6	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Comment	Comment	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Samples	-	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0

Parameter Name	Description
SOP Fields	<p>List of all sample description fields available.</p> <p>Remark: Some of these fields are related to the sample and some are related to the batch information.</p> <p>The examples of a sample report and a batch report with the maximum possible information will demonstrate the difference, so it is possible to generate highly customized Operator templates and depending Reports</p> <p>Example batch report</p> <p>Example sample report</p>
Label	<p>Allows the custom labeling of the SOP fields, as done in the batch field</p> <p>Any SOP field can be labeled as desired, e.g. to the Operator's language or to a company specific naming.</p>
Visible	<p>"Checked": The field is visible in the Operator and Report</p> <p>"Unchecked": The field is not visible in the Operator and Report</p> <p>Note: grey fields cannot be changed.</p>
Request Input	<p>"Checked": Request input is mandatory (should be set if visible is yes)</p> <p>"Unchecked": Request input is not mandatory</p> <p>Note: grey fields cannot be changed.</p>
Read Only	<p>"Checked": Input fields are set to read only</p> <p>Note: grey fields cannot be changed.</p> <p>Remark: In case of „New batch“, all batch related fields are set to write state. In case of selecting an existing batch, the batch related information is set to read only</p>

Error Text	Links the above defined Error Text 1 to 5 to the sample SOP fields in the Operator module
Field Reset	"Checked": The field content is reset after each measurement "Unchecked": The field content is not reset after each measurement Remark: If field reset is set to yes, a keyboard or barcode input is mandatory for every sample measurement.
Validation Range	A lot of constraints for input verification can be set, e.g. batch numbers shall be nine digit numbers. For test purposes the validity of an input can be tested in place (green = valid, red = invalid input) Values: Numeric or alphanumeric
Start reading at barcode position	These two column values trigger the partitioning of a long barcode into several fields during a single barcode reading. The default values 0; 0 mean: each barcode entry will be completely filled in the respective field
Length of barcode field	Values: Numeric (Integer)

6.2.13. Bar code configuration

Introduction

NIRWare is designed to support bar code readers. Bar code readers can be used to replace manual input of measurement relevant data, and thus avoid human error.

Bar code readers are typically connected to the PC via USB, and feed the bar code into the keyboard buffer.

Direct bar code input

The simplest way of using a bar code reader is to directly enter a bar code string into an input field of the software. No configuration at all needs to be done for this type of use, but it .

is only applicable if there is exactly one complete bar code available for each corresponding input field.

Example: If this bar code



is presented to the scanner, this is what is read as input: "810295001169".

The same number can be read by human eye and entered via keyboard - the system will notice no difference.

Bar code fractionation

Alternatively, several code numbers can be concatenated to form one mutual bar code.

Example:

Code0 = '0000' (four leading zeroes)

Code1 = Substance-ID: Integer number with 5 digits

Code2 = Batch-ID: Integer number with 6 digits

Code3 = Container-ID: Integer number with 7 digits

This sums up to one bar code with 4+5+6+7= 22 digits, e.g.

0000111112222223333333

Now one bar code label carries all information- but the system must now be configured so that it can fractionate the bar code into its components. This is done in the NIRWare Management Console.

Configuring an application for bar code fractionation

Each application needs to be configured individually, as it might be that only a part of the existing applications is intended for use with a bar code reader.

The configuration is made under **Application Designer - <YourApplication> - Operator Configuration - Sample Description Fields:**

Sample Description Fields									
SOP Fields	Label	Visible	Request Input	Read Only	Error Text	Field Reset	Validation Range	Start reading at barcode position	Length of barcode field
Batch	Batch	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	10	6
Expected Substance	Expected Substance	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	5	5
Campaign	Campaign	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Number of Containers	NumberOfContainers	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Vendor Qualification	VendorQualification	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
AnalysisID	AnalysisID	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::	16	7
Customer Field 1	CustomerField1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 2	CustomerField2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 3	CustomerField3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 4	CustomerField4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 5	CustomerField5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Customer Field 6	CustomerField6	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Comment	Comment	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0
Samples	-	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::	0	0

The field "start reading at bar code position" specifies the start digit of each fraction, and "length of bar code field" defines how long the cut-out string will be.

Coming back to our example, the configuration will cut our original bar code:

"0000111112222223333333"

into the following parts:

Start @ digit 5, read 5 digits --> "11111" will go into "Expected Substance" field;

Start @ digit 10, read 6 digits --> "222222" will go into "Batch" field;
 Start @ digit 16, read 7 digits --> "3333333" will go into "Analysis ID" field;
 The leading four zeroes ("0000") are used nowhere, and thus be discarded.

NOTE

The bar code must contain information about both, the Batch as well as the Expected Substance. These two fields depend on each other.

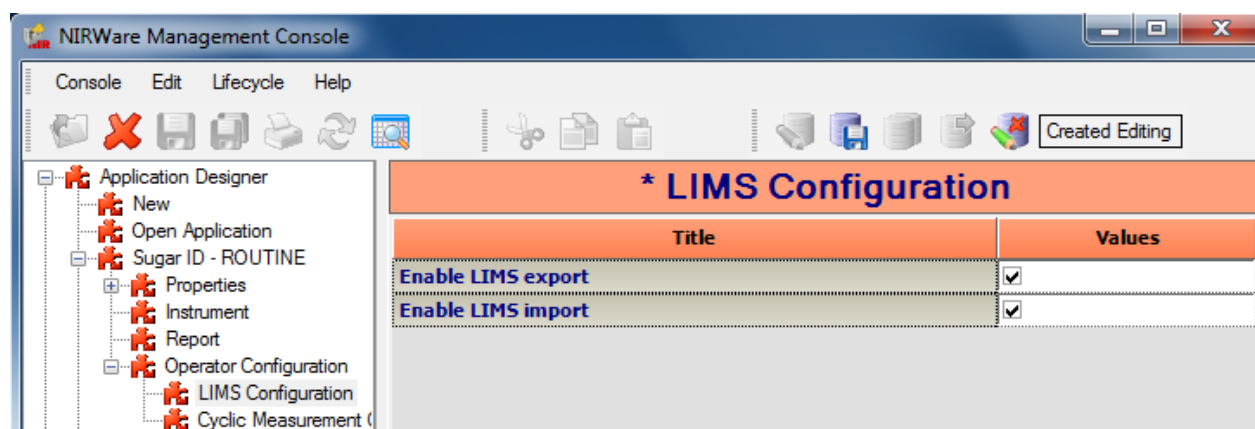
Comment Field:

If activated, you can enter information in the Operator to describe the samples. The Comment Field with its information will be displayed in the Sample Manager under 'Samples' and 'Measurements' at corresponding entries.

In the NIRCal spectra selection filter the Comment Field will be shown for selection and the information is displayed in the comment field of every spectrum related to these measurements.

6.2.14. Settings for LIMS

The use of LIMS Import or Export can be configured application-wise. For this purpose select **Application Designer - <YourApplication> - Operator Configuration - LIMS Configuration**.



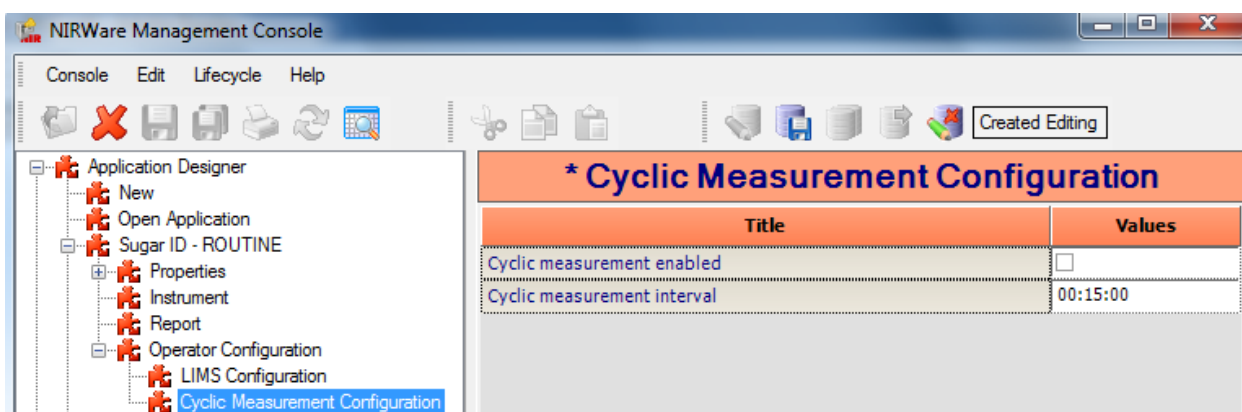
Per default the use of the LIMS export is deactivated. Only if this option is activated, AND the general LIMS-settings are activated, the LIMS-interface will be used.

To ensure a proper functionality of applications with the NIRWare LIMS Interface, the following settings are recommended:

- The applications used with LIMS should be in the "approved" lifecycle state to prevent changes on application parameters that are incompatible with the LIMS Import/Export functions.
- If LIMS Import is in use, all visible fields should be set to "read only" and "field reset" under "Operator Configuration - Sample Description Fields".

Sample Description Fields							
SOP Fields	Label	Visible	Request Input	Read Only	Error Text	Field Reset	Validation
Batch	Batch	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::
Campaign	Campaign	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::
Number of Containers	NumberOfContainers	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::
Vendor Qualification	VendorQualification	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input type="checkbox"/>	::
AnalysisID	AnalysisID	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Customer Field 1	CustomerField1	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Customer Field 2	CustomerField2	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Customer Field 3	CustomerField3	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Customer Field 4	CustomerField4	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Customer Field 5	CustomerField5	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Customer Field 6	CustomerField6	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Comment	Comment	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Invalid input	<input checked="" type="checkbox"/>	::
Samples	-	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Invalid input	<input type="checkbox"/>	::

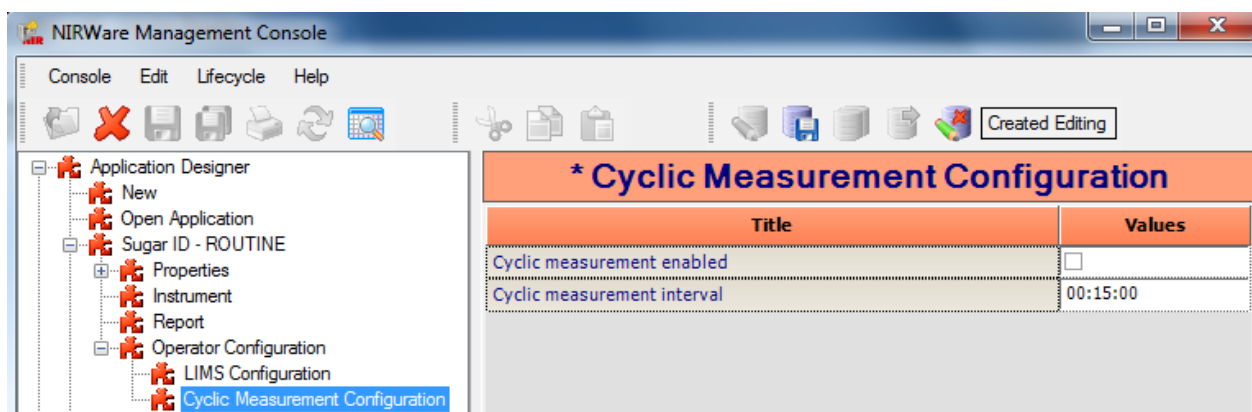
- All defined fields for LIMS Import should be activated in the application as well.
- The "repetition measurements in case of Out of Specification" should be deactivated (value =0) and the "number of measurement sequences" should be set to 1. Multiple measurements of the same sample should be triggered by the LIMS.



6.2.15. Cyclic Measurement configuration

General information

The cyclic measurement function allows performing a series of NIR measurements, which are automatically triggered by the system in a specific frequency.



Prerequisites and limitations

Cyclic measurements are intended to monitor one or more analytes over the course of time.

The repetition mode for applications can be generally used. Nevertheless, extra care should be taken with application design to ensure smooth operation - the system cannot judge if a specific configuration does indeed make sense or not. So please have a look at the 'Tips and Tricks' chapter to avoid some common pitfalls.

Applications for cyclic measurement have one limitation: The "Number of repetition of measurements in case of an Out Of Specification" [result] is automatically set to zero if "Cyclic measurement enabled" is selected.

Manual SST and referencing

Automatic SST- and reference measurements can interfere with the sample measurement cycle.

Therefore, it is advisable to disable the SST. The external reference measurement **must** be switched to 'Manual' shortly before the actual measurement start.

The internal reference measurement can remain on 'Automatic' if slower processes are monitored, where a short delay of a single measurement in the cycle is tolerable.

IMPORTANT!

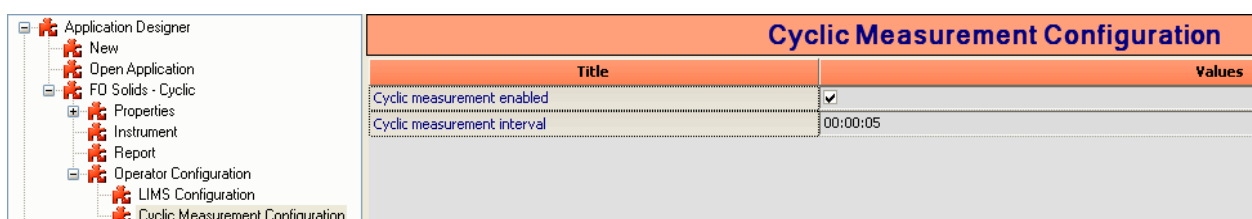
The actual implementation of cyclic measurements is NOT yet intended to be used for process control, but is strictly limited monitoring applications that have no safety demands towards this feature.

Configuring an application for cyclic measurement

To configure an application for cyclic measurements, proceed as follows:

In the NIRWare Management Console select **Application Designer - <YourApplication> - Operator Configuration - Cyclic Measurement Configuration**.

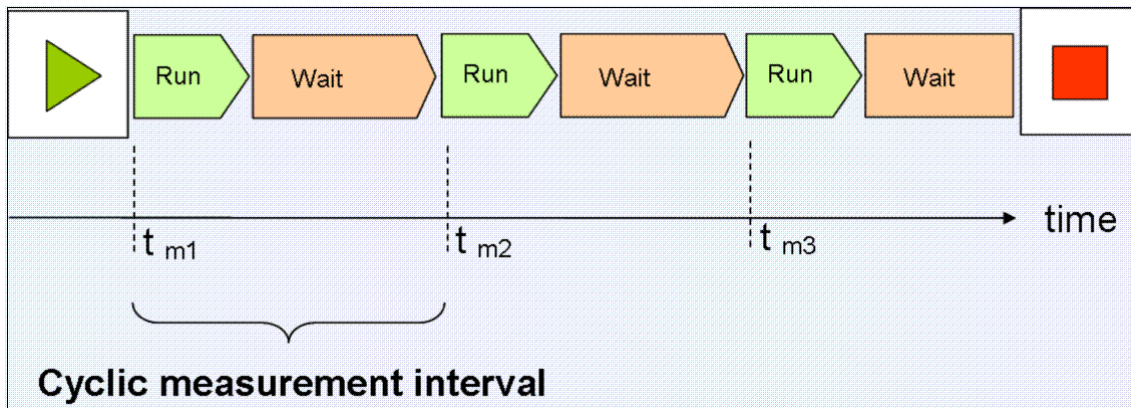
The following dialog opens:



Activate the checkbox "**Cyclic measurement enabled**".

The cyclic measurement is started when the green start button is pressed, and ends when the red stop button is pressed. In the meantime, the system will

1. Trigger a measurement,
2. Wait for the countdown to finish,
3. Start over again with step 1.



The picture shows the order of events during a cyclic measurement run. You can see that the individual measurement times (t_{m1} , t_{m2} , t_{m3}) are spaced at constant times; this is the 'cyclic measurement interval'.

It is important to understand that the interval is defined from start to start; this means that the countdown is already started at the BEGINNING of the measurement, and not at the end!

The countdown duration is specified in the field '**Cyclic measurement interval**' in the format [d.][hh:]mm[:ss]. This means that if only one number is entered, it will be interpreted as minutes.

Example:

Input Time interval

"12" = 12 minutes

"0:01" = 1 second

"1:20:30" = 1 hour, 20 minutes and 30 seconds

"1.00:00:00" = 1 day (allowed max.)

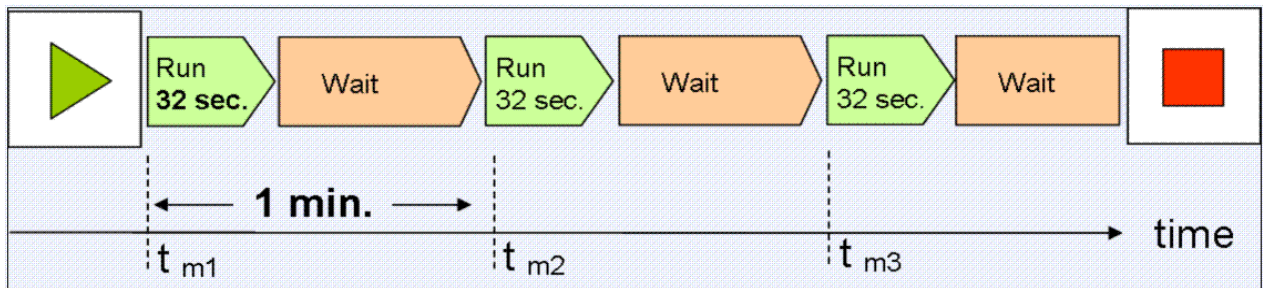
To better understand the implications of this parameter, let's look at two exemplary applications:

Application 1: Interval > Runtime for Measurement

Cyclic Measurement Interval = 1 [min], and

64 scans/ measurement = $64 * 0.5 \text{ sec} / \text{scan} = \text{ca. } 32 \text{ seconds} / \text{measurement}$

will have a new measurement starting every minute:

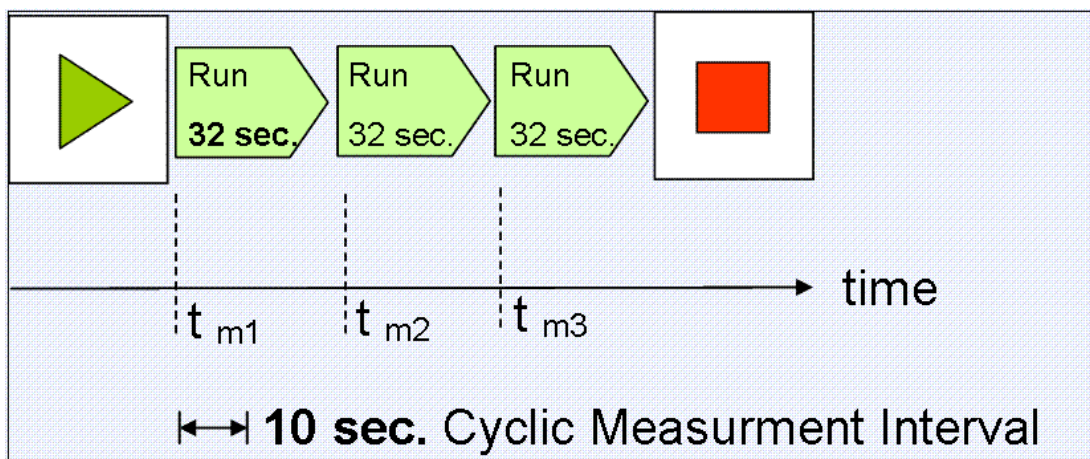


The optimum measurement interval is as long as possible to avoid unnecessary data creation, but short enough to cover changes in the process to be observed.

Application 2: Interval < Runtime for Measurement

Cyclic Measurement Interval = 0:10 [min:sec], and

64 scans/ measurement * 0.5 sec/ scan = ca. 32 seconds / measurement



Here the measurement is taking longer than the specified countdown time (32 sec. > 10 sec.); therefore, the system will measure as fast as possible, even if measurements have a larger time distance than specified.

In general, this situation should be avoided, since it creates an unnecessary amount of data, and the measurement interval is now completely dependent on the measurement speed.

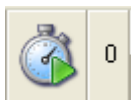
Running an application for cyclic measurement

An application for cyclic measurement is handled in the Operator like any other application.

The only difference is the following stop-watch icon, which symbolizes the countdown and is displayed in the lower-left corner of the Operator window after loading the application:



If the application is started (via the usual green start button), the symbol switches to green:



After the first measurement is done, the number next to the stopwatch-symbol counts down the remaining time before the second measurement is started- and so on.

The measurement cycle is running infinitely until it is manually stopped (via the usual red stop button).

Tips and Tricks

Application name indicating cycle mode

Using a reference to cyclic measurement in the name of the application can be very helpful to differentiate cyclic- from single measurement- applications (e.g. Application 'Water content monitoring – 1min CYCLE'.)

Same Application for single- and cyclic measurement

You can configure an application EITHER for regular (= single measurements) use, OR for cyclic measurements. If you need to use both alternatively, create a copy of one application and just change the setting for '**Cyclic measurement enabled**' –plus changing the name so that you know which is which (see above).

Autoname

Using the Autoname function for giving sample names is a must for cyclic measurements (**Management Console- Application Designer - <YourApplication> - Operator Configuration: Autoname Part 1 / ...2 / ...3.**) Especially '**Date**' for '**Autoname Part 3**' is a highly recommendable setting.

Trade Spectral Noise for Speed

Fast chemical processes require short enough measurement times. Speeding up a single measurement can be achieved by lowering the '**Number of Scans**' in the applications' instrument configuration.

But be aware that spectral noise will increase when doing so ('**Square root of n-law**', meaning that the signal-to-noise ratio is proportional to the square root of the number of scans)! Whether a decrease in spectra quality is tolerable or not is thus strictly dependent on the actual application and needs to be carefully validated!

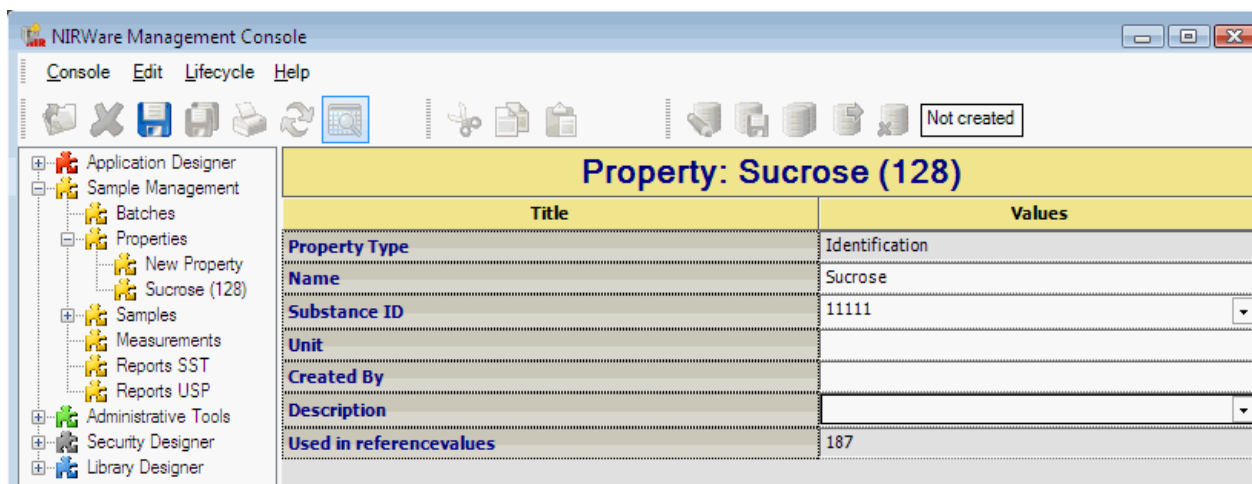
Countdown time seems to change randomly

The runtime of a measurement includes calculation and storage procedures which are influenced by the current performance of the PC. This can result in small fluctuations in the duration of a measurement. Therefore, a measurement might take a few seconds longer than the previous, so that the remaining countdown time is getting shorter, since the time from one measurement to the next must remain constant.

Configuring the PropertyID for Expected Substance recognition

So far, the "Expected Substance" is entered as a number - but how can we make the system recognize the corresponding property?

Let's assume that "11111" is the material code for "Sucrose", then we simply go to the Sample Manager and tell this fact to NIRWare:



Additionally, we configure the application so that it will expect the Substance-ID to define the “Expected Substance”- simply by deactivating “Use drop down for expected substance” (found under **Application Designer - <YourApplication> - Operator Configuration**, see the application example above).

Tips and Tricks

Property-IDs must be UNIQUE

Each property must have its own, unique PropertyID! Otherwise you lose the traceability of a substance-code to the corresponding substance.

Do not use suppliers' codes as Property-IDs

Two suppliers might use the same code for different things – therefore create your own, unique Property-IDs!

Remember using Autaname

Use Autaname to copy parts of the input fields into the sample name field.

Use a bar code reader that can read your bar code

Before you buy a bar code reader, make sure that it can read the type of bar code used on your specific labels - maybe you are using some advanced holographic bar codes in your company not every reader model is compatible with.

Expected Substance search

In the NIRWare Operator the entered expected substance is searched in properties that are used in the application in the following order:

1. Property Name
2. SubstanceIDs (aka Alias) in the semicolon separated list.

The first found is used.

This is done independent of the "use drop down for expected substance" setting.

The string comparison is done with removed leading- and trailing-spaces, case sensitive over the full length.

NOTE

Make sure that inside an application the Property Names and the SubstanceIDs are unique. The software will not check this!

NOTE

The start position for the first character is 1.

For not using bar code fractionation set positions to 0.

6.3. Sample Management

6.3.1. Introduction Sample Manager

The Sample Manager is designed to check and review previous measurement results and system reports and to enter reference values.

During data acquisition in the Operator, measurement sequences will be recorded. Depending on the used measurement cell and add-on, a measurement sequence contains 1 sample (NIRMaster, NIRCheckMaster, Fiber Optic SMA, Fiber Optic Solids, Fiber Optic Liquids, Solids with XL or Petri) or several samples (Liquids (up to 6), Solids, Vial (up to 6), Tablet (up to 10) and Solid Transmittance).

Each sample contains out of 1 or more spectra depending on the used application setting (Application Designer - Operator Configuration - Number of Measurement Sequences).

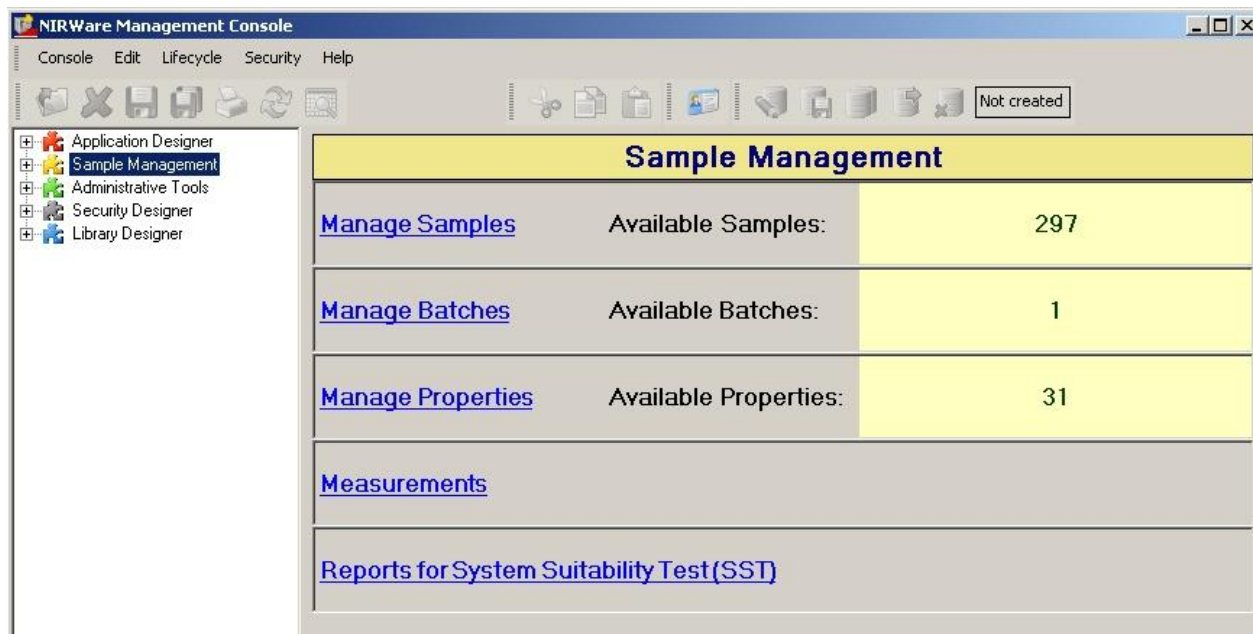
One spectrum is an average of 1 or more scans. A scan records the whole spectral information. The number of scans used for averaging the spectra depends on the used application setting (Application Designer - Instrument - Number of Scans).

The following actions are possible in the sample manager:

- enter property information (e.g. sucrose or fat [%])
- assign properties and reference values to samples
- review and print-out of sample reports from routine measurements
- review and print-out of system suitability (SST) reports
- review and print-out of USP test reports
- change sample names
- delete unused samples
- disable not important routine results (measurement sequences)
- electronic signature on batches
- verification of signed routine results
- electronic signature on results (measurement sequences)

To open the Sample Manager proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Sample Management**. The following dialog opens:



You can now open a submenu by clicking on their names in the file tree or in the center of the Sample Management window.

The Sample Manager comprises the following menus:

[Manage Samples](#)

In this menu property information can be linked to sample information and reference values can be entered. In addition sample names can be edited (in case of mistyping during data acquisition).

[Manage Batches](#)

This menu offers an overview of all batches.

[Manage Properties](#)

This menu offers an overview of existing property information. New properties for identification (e.g. sucrose) with substance ID or quantitative property information (e.g. Fat [%]) can be entered.

[Measurements](#)

This menu gives access to all measurement sequences. Measurement sequences and corresponding samples can be deleted (recorded with applications not used in routine) or hidden (recorded with routine applications). Reports of measurement sequences can be reviewed, verified and printed out.

Electronic Signatures on reports (sequence or batch) are applied here.

[Reports for System Suitability Test \(SST\)](#)

Overview over SST test results. SST reports can be reviewed and printed out.

Reports for USP

Overview over USP test results. USP reports can be reviewed and printed out (visible only with valid license).

6.3.2. Batches

Batches

In the file tree on the left side of the **NIRWare Management Console** select **Sample Management - Batches**.

The following dialog opens:

Batches								
Name	Version	Application	Campaign	Supplier	NoContainer	Used In Samples	State	GUID
▶ Sucrose-Lactose Mix	0	Sugar quantification -REFERENCE			0	2	Created Idle	86c7761e-53d6-4eae-b791-f40962fd3562
Mixture	0	Sugar quantification-ROUTINE USE			0	1	Created Idle	09f60d61-26b7-4d4e-8ec4-a08da4dd412d
Sugar Mixture	0	Sugar quantification-ROUTINE USE			0	4	Created Idle	2e34d16f-ba71-47c6-8887-05a7a402554a
Mixed rice	0	Whole Rice- Nov.2010			0	1	Created Idle	3977358a-975e-4a3e-9f63-b2a1c952013e
Ascorbic Acid-03-13	0	different acids routine			0	0	Created Idle	57cab399-ddec-404b-a536-43d295b3a617
Ascorbic Acid-2955	0	different acids routine			0	0	Created Idle	5c43daea-17ae-42d3-b0af-16a0aee5b457
07-4-12	0	different acids routine			0	3	Created Idle	3d3de235-e1f6-46d1-bd92-6d95795796d4
AA-2	0	different acids routine			3	3	Created Idle	7f7139f8-5a55-41d8-b3cb-1d71990882ae
AA-3	0	different acids routine			4	5	Created Idle	928c3990-cf2c-4d62-a4cd-618de5e3c216
AA-5	0	different acids routine			2	2	Created Idle	58aeb35d-ac18-49f5-8f25-ecdf47b96ea4
Sugar Mix	0	Sugar quantification-ROUTINE USE			0	1	Created Idle	7fa663cf-fb75-4ca3-9d3f-949fca05f976
Crotamiton	0	Test-Liquids			0	2	Created Idle	1e912563-f5cc-49fc-a360-d9f1735bf9b2
luft	0	HELLMA 1.0			0	1	Created Idle	2a64b0af-04fb-4709-a78e-8f7527c73757
Wasser	0	HELLMA 1.0			0	1	Created Idle	00b124b3-687b-46cf-8fe7-80a72fc5dfab

If necessary, narrow down the information displayed in the table, using appropriate [filter settings](#).

Table columns

The table consists of the following columns:



Name	batch name
Version	Copy number in the course of the lifecycle
Application	Name of the used application
Campaign	Campaign name (data entry not yet implemented)
Supplier	Supplier information (data entry not yet implemented)
NoContainers	Defined number of containers (if activated in Application Designer - Operator Configuration) 0 = function not activated
Used In Samples	Number of samples connected to this batch
State	Lifecycle State
GUID	Global Unique Identifier

NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

Closing a batch and batch verification with electronic signature

Narrow down the information displayed in the table, using appropriate filter settings.

Select a batch and open it by clicking on the "Open existing DataSet" button  or with double click on the corresponding row indicator .

The following window opens:

Batch: 1234	
Name	1234
Campaign	
Supplier Qualification	
Numer of Containers	0
Used in Samples	1

Detailed Information of the selected batch will be displayed.

Name: batch name
Campaign: Entry field for campaign name (not yet supported)
Supplier: Entry field for supplier qualification information (not yet supported)


Qualification

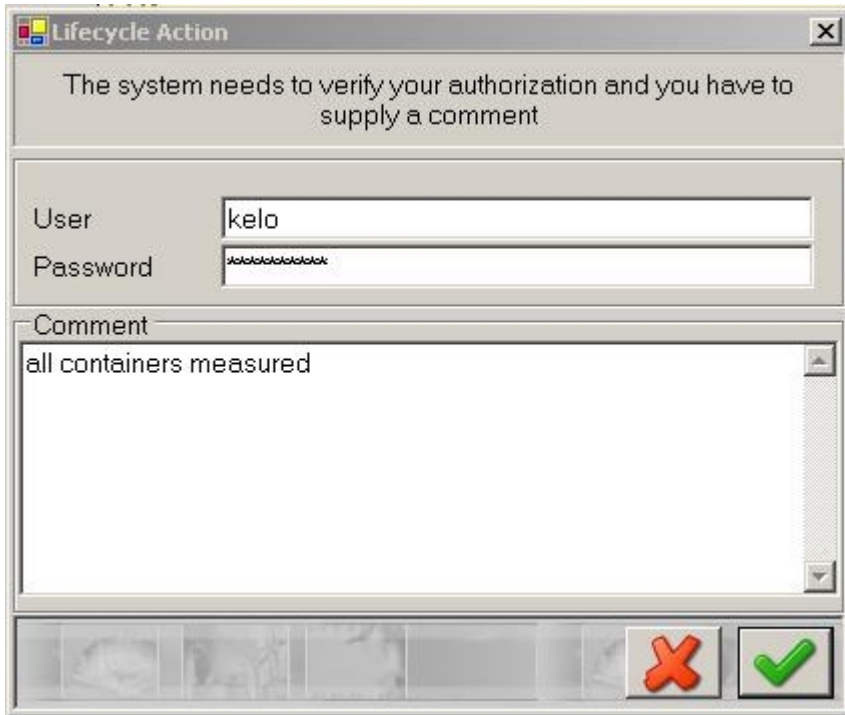
NoContainers: Defined number of containers (if activated in Application Designer – Operator Configuration)
0 = function not activated

Used In: Number of samples connected to this batch Samples

A batch can be closed and signed electronically using the Lifecycle functions



Click on  in the menu bar. The following window opens:



Closing a batch and batch verification with electronic signature

Enter User, Password and a Comment or reason. Confirm your entry.

The Lifecycle state of the batch changes from created to checked (if Lifecycle template "High" is selected in the Management Console).

Note:

The same action (closing a batch) can be done in the Operator directly by clicking on the corresponding button.

To verify the batch information with an electronic signature, click on in the menu bar again. The following window opens:



The Lifecycle state of the batch changes from checked to approved (if Lifecycle template "High" is selected in the Management Console).

Note:

With the electronic signature on batch, all individual measurement sequence reports related to this batch will be signed automatically.

6.3.3. Properties

Properties

In the file tree on the left side of the **NIRWare Management Console** select **Sample Management - Properties**.

The following dialog opens:

Properties							
	Name	Type	Unit	Description	Created By	Substance ID	Used
	▼	▼	▼	▼	▼	▼	▼
▶	Lactose	Identification			Holger Keller		41
	Fructose	Identification			Holger Keller		42
	Sucrose	Identification			Holger Keller		39
	Sucrose	Quantification			Holger Keller		23
	sucrose	Quantification		Autogenerated			0
	Fat	Quantification	%				0
	Moisture	Quantification	%				0
	Protein	Quantification	%				0
	Ash	Quantification	%				0
	Fibre	Quantification	%				0
	Phosphorus	Quantification	%				0
	Salt	Quantification	%				0
	Particle Size	Quantification	%				0

If necessary, narrow down the information displayed in the table, using appropriate [filter settings](#).

Table columns

The table consists of the following columns:

Name	Property name
Type	Property type (Identification or Quantification)
Unit	Unit of quantitative reference data (e.g. %, mg/kg,.....)
Description	Description entered during property creation
Created By	Creator name entered during property creation
Substance ID	<p>Substance ID code for identification properties entered during property creation.</p> <p>Please remember that your application needs to be configured correctly in order to use Substance IDs for the specification of the 'expected substance'. This is done in the Application Designer - <YourApplication> - Operator Configuration: Deselect 'Use drop down for expected substance'. If a 'new batch' is to be specified in the operator, the user can enter the Substance ID code now (instead of selecting it from a list).</p> <p>If several substance ID are available, separate them with semicolon ";"</p>
Used	Number of samples the property is assigned to

NOTE

You can sort alphabetically and inverse the order of the individual column entries by clicking the corresponding column header.

Narrow down the information displayed in the table, using appropriate filter settings.

Create a new Property entry

To create a new property entry, go to the file tree on the left side of the **NIRWare Management Console**, select **Sample Management - Properties - New Property**.

The following dialog opens:

New Property	
Title	Values
Property Type	Identification <input type="text"/>
Name	
Substance ID	
Unit	
Created By	
Description	
Used in referencevalues	0

Property Type	Select from the drop down menu the property type: Identification or Quantification
Name	Enter the property name or for identification the substance name
Substance ID	Substance ID code for identification properties entered during property creation. Leave this field empty for quantitative property.
Unit	For Quantification Properties, the unit of quantitative reference data (e.g. %, mg/kg,...) can be entered. Optional entry
Created By	Name of the creator of the property can be entered. Optional entry
Description	Additional information to describe the property can be entered. Optional entry
Used in referencevalues	Display of number of samples the property is assigned to.

Example for a qualitative property:

* New Property*	
Title	Values
Property Type	Identification <input type="text"/>
Name	Lactose
Substance ID	54357
Unit	
Created By	SCHC
Description	
Used in referencevalues	0

Example for a quantitative property:

Property: Moisture (2)	
Title	Values
Property Type	Quantification
Name	Moisture
Substance ID	
Unit	%
Created By	SCHC
Description	
Used in referencevalues	0

Multiple Substance IDs

Introduction

In ID-tests (=qualitative analyses) a substance-specific code can be used to identify the substance to be tested; this is the so-called 'Substance ID', which can be very helpful if a bar code reader is used.

In many companies the same material is received from different vendors, therefore one material can have n code numbers for the n suppliers of this material. This allows traceability of deliveries back to the source.

Thus, it is now possible to specify several Substance ID codes per property.

Prerequisites and Limitations

Substance ID codes must be unique! Otherwise the Substance ID codes cannot identify the respective material unambiguously.

How to specify several Substance IDs

The Substance ID is specified in the NIRWare Management Console by opening the following menu tree node and clicking on the 'arrow-down' button at the end of the 'Substance ID'-line:

A window pops up where it is now possible to enter several ID codes, **separated by a semicolon and without blank**:

Clicking the green check-mark button confirms the entries made as Substance ID s, and copies them into the Substance ID's value field; clicking the red X-button, however, will just close the pop up window without making any change to the Substance ID's value field.

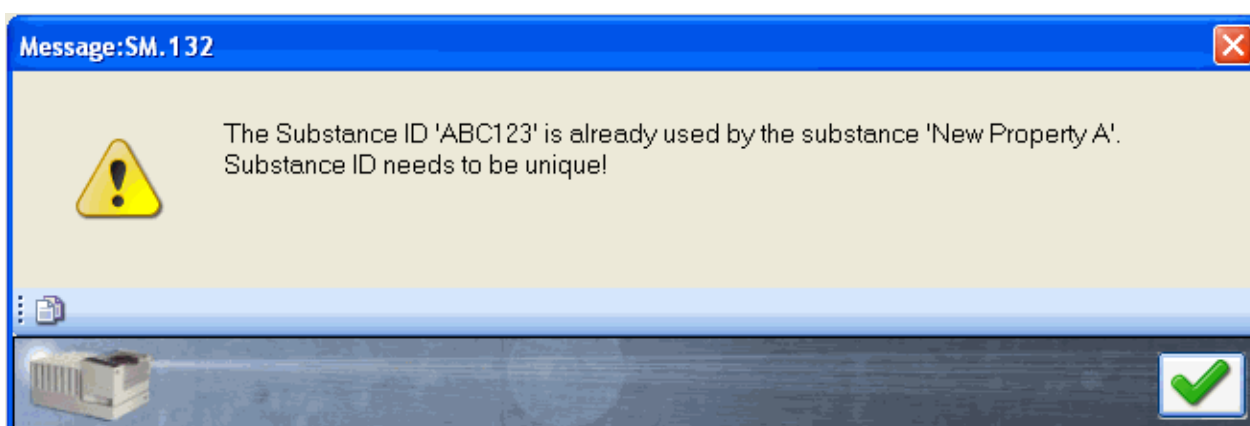
NOTE:

You can specify any string as Substance ID, no matter what length or symbols you use: any number (0...9), character (a...z, A...Z), or symbol (!/+...) can be used – except for the semicolon, which serves as separator.*

Tips and Tricks

Use your own material codes – and not the supplier's codes

Two suppliers might use the same code for two different materials. Therefore you need to create your own, unique substance codes. But do not worry: the software will tell you if a Substance ID is not unique:



Configuring an application for Substance IDs

Please remember that your application needs to be configured correctly in order to use Substance IDs for the specification of the 'expected substance'. This is done in the **Application Designer - <YourApplication> - Operator Configuration**: Deselect 'Use drop down for expected substance'. If a 'new batch' is to be specified in the operator, the user can enter the Substance ID code now (instead of selecting it from a list).

6.3.4. Samples

Sample Management

In the file tree on the left side of the **NIRWare Management Console** select **Sample Management - Samples**.

The following dialog opens:

Samples							
	Name	Application	Version	Batch	Time Stamp	No. Referencevalues	Analysis ID
▶	123	Sugar Quant	1	test1	01/04/2007 17:23:58	0	
	60				11/21/2006 13:54:02	1	
	60				11/21/2006 13:53:38	1	
	55				11/21/2006 13:53:16	1	
	55				11/21/2006 13:52:52	1	
	50				11/21/2006 13:52:30	1	
	50				11/21/2006 13:52:06	1	
	45				11/21/2006 13:51:44	1	
	45				11/21/2006 13:51:20	1	

Reset Filters

Table columns

The table consists of the following columns:

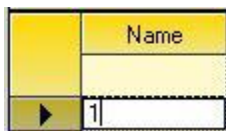
Name	Sample name
Application	Name of the related application
Version	Copy number in the course of the lifecycle
Batch	Batch information
Time Stamp	Date and time
No. Reference values	Number of assigned reference values
Analysis ID	ID of analysis
Comment	Optional information entered during measurements in the comment field
Customer fields	Optional information of the customer

If necessary, narrow down the information displayed in the table, using appropriate [filter settings](#).

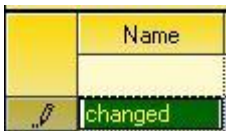
NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

Change sample name



In the row Name, click on the cell where you wish to change the sample name.



Change the sample name information and click "Enter" on the keyboard to accept the change (or "ESC" to leave without change).

	Name
	changed

The sample name is now changed.

Sample names can be changed as long as the corresponding samples are not part of an approved measurement result or approved calibration.

Assign qualitative property information (identification) to samples

To assign qualitative property information (identification) to samples, select all samples you wish to edit (multi selection). If necessary, narrow down the information displayed in the table, using appropriate filter settings.

Open the selected samples by clicking on the "Open existing DataSet" button  or with double click on the last corresponding row indicator .

Samples				
	Name	Application	Version	No. Referencevalues
	Sucrose 09		0 1	
	Sucrose 08		0 1	
	Sucrose 07		0 1	
	Sucrose 06		0 1	
	Sucrose 05		0 1	
	Sucrose 04		0 1	
	Sucrose 03		0 1	
	Sucrose 02		0 1	
▶	Sucrose 01		0 1	
	Sucrose12		0 1	

The following dialog opens in case the samples were recorded with an application to which no calibration was assigned to (e.g. application for data acquisition to build up a calibration).

Samples	
Samples	
	Name
▶	Sucrose 08
	Sucrose 07
	Sucrose 06
	Sucrose 05
	Sucrose 04
	Sucrose 03
	Sucrose 02
	Sucrose 01

Here a property needs to be assigned to the samples first, before the classification information can be entered.

The following dialog opens, if the samples were recorded with an routine application to which one ore more qualitative calibrations are assigned to:

Samples				
	Name	sugars/Lactose	sugars/Fructose	sugars/Sucrose
▶	Fru 1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	Fru 2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	Fru 3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	Fru 4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	Fru 5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	Fru 6	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

All samples have the properties related to the application assigned automatically. The labeled name contains as information the property group name and the name of the assigned property.

To assign a property to the samples, select from the shown **"Other Available Properties"** window the correct property:

Other Available Properties				
	Name	Type	Unit	Description
		Identificati		
	Fructose	Identification		
▶	Sucrose	Identification		
	Lactose	Identification		

Table content:

Name	Property name
Type	Property type (Identification or Quantification)
Unit	Unit of quantitative reference data (e.g. %, mg/kg,....)
Description	Description entered during property creation
Created By	Creator name entered during property creation
Substance ID	Substance ID code for identification properties entered during property creation.


If necessary, narrow down the information displayed in the table, using appropriate filter settings.



Click on  to add the selected property to the **"Other Assigned"** window. Repeat action if additional properties should be assigned to the samples.

Other Assigned Properties			
	Name	Type	Unit
▶	Sucrose	elidentification	


The property is now added to the samples and the classification information can be entered directly by clicking on the check box or use "Enter" and the arrow down button to fill in the information.

Samples		
	Name	Sucrose
	Sucrose 08	<input checked="" type="checkbox"/>
	Sucrose 07	<input checked="" type="checkbox"/>
	Sucrose 06	<input checked="" type="checkbox"/>
	Sucrose 05	<input checked="" type="checkbox"/>
	Sucrose 04	<input type="checkbox"/>
	Sucrose 03	<input type="checkbox"/>
	Sucrose 02	<input type="checkbox"/>
	Sucrose 01	<input type="checkbox"/>

After all entries are made, click on  to save changes to the database.

With two exceptions, properties can also be removed from samples.

To remove a property, select the corresponding entry in "**Other Assigned Properties**" and click


on . The entered reference values will be lost.


In case the sample is used in a calibration the property and the reference values can not be deleted. The following message appears:



Only properties added to the sample manually can be removed. Properties related to the routine application can not be removed.


The colour of the row indicator shows the type of property:

 Property from routine application. This property will be assigned automatically to samples measured with a routine application. These properties can not be removed from samples.

 Property assigned by user. This property can be removed from samples as long as the corresponding samples are not used in a calibration.

Assign quantitative property information to samples

To assign quantitative property information to samples, select all samples you wish to edit (multi selection). If necessary, narrow down the information displayed in the table, using appropriate filter settings.

Open the selected samples by clicking on the "Open existing DataSet" button  or with double click on the last corresponding row indicator .

Samples				
	Name	Application	Version	No. Referencevalues
	10		0	1
	9		0	1
	8		0	0
	7		0	0
	6		0	0
	5		0	0
	4		0	0
	3		0	0
	2		0	0
▶	1		0	0

NOTE

Imported samples show no entries under 'Application'. Only samples measured collected with the current database show the corresponding 'Application' information.

The following dialog opens in case the samples were recorded with an application to which no calibration was assigned to (e.g. application for data acquisition to build up a calibration).

Samples	
	Name ▲
▶	1
	2
	3
	4
	5
	6
	7
	8

Here a property needs to be assigned to the samples first, before reference values can be entered.

The following dialog opens, if the samples were recorded with an routine application to which one ore more calibrations are assigned to:

Samples References		
Samples		
	Name	Ethanol Content/Ethanol Content
▶	60	
	60	
	60	
	98	
	98	
	98	

All samples have the properties related to the application assigned automatically. The labeled name contains as information the assigned property name and the name used in the operator. The reference value can be entered directly.

To assign a property to the samples, select from the shown **"Other Available Properties"** window the correct property:

Other Available Properties			
	Name	Type	Unit
	Fat	Quantification	%
▶	Moisture	Quantification	%
	Protein	Quantification	%

Table content:

Name	Property name
Type	Property type (Identification or Quantification)
Unit	Unit of quantitative reference data (e.g. %, mg/kg,....)
Description	Description entered during property creation
Created By	Creator name entered during property creation
Substance ID	Substance ID code for identification properties entered during property creation.

If necessary, narrow down the information displayed in the table, using appropriate filter settings.



Click on  to add the selected property to the **"Other Assigned"** window. Repeat action if additional properties should be assigned to the samples.

Other Assigned Properties			
	Name	Type	Unit
▶	Moisture	eQuantification	%


The property is now added to the samples and reference values can be entered. The reference values for each sample can be entered manually or with copy/paste (Ctrl + C / Ctrl + V) from Windows Excel or other office programs.

Samples		
Samples		
	Name ▲	Moisture
	1	10
	2	12
▶	3	
	4	
	5	
	6	
	7	
	8	

After all entries are made, click on  to save changes to the database.

With two exceptions, properties can also be removed from samples.

To remove a property, select the corresponding entry in **"Other Assigned Properties"** and click

on . The entered reference values will be lost.


Other Assigned Properties			
	Name	Type	Ur
	Ethanol Content/Ethanol Content	eQuantification	%
▶	Methanol Content	eQuantification	%


In case the sample is used in a calibration the property and the reference values can not be deleted. The following message appears:



Only properties added to the sample manually can be removed. Properties related to the routine application can not be removed.

The colour of the row indicator shows the type of property:

 Property from routine application. This property will be assigned automatically to samples measured with a routine application. These properties can not be removed from samples.

 Property assigned by user. This property can be removed from samples as long as the corresponding samples are not used in a calibration.

Deleting individual samples

Individual samples can be deleted under certain circumstances:

- not connected to routine measurements to which reports are available
- not used for calibration development

Information about this can be found by selecting a single or group of samples in the bottom window in case the deletion was not possible:

1. Filter the samples (Application, Version,...)
2. Select the samples for which you want to enter reference values
3. Choose Open

or edit sample names at your desire

Name = '60', SampleID = 281, Deletion DENIED

Used Calibrations: "Difen, 0.7685, 1-4./5, 8500-10600.(0)"

NOTE

Delete only individual samples from a sequence in case you wish not to delete the whole sequence or imported samples (from data conversion or import without application) under "Samples". Delete complete measurement sequences under "[Measurements](#)".

6.3.5. Measurements

Measurements

In the tree view on the left side of the **NIRWare Management Console** select **Sample Management - Measurements**.

The following dialog opens:

Make the desired selection							
	Application	Version	Batch	StartTime	EndTime	Type	State
							<> N'Disabled'
▶	sugars vial	1	123	12/16/2005 17:05	12/16/2005 17:06	Identification	Created Idle
	sucrose QN	2	345	12/16/2005 17:30	12/16/2005 17:33	Quantification	Created Idle
	sucrose QN 2	3	456	12/16/2005 17:34	12/16/2005 17:36	Quantification	Created Idle
	sucrose QN 2	3	456	12/16/2005 17:37	12/16/2005 17:39	Quantification	Created Idle
	Ethanol QN Operator	1	Test neu	12/21/2005 13:59	12/21/2005 14:05	Quantification	Approved Idle
	Ethanol QN Operator 2	2	Test neu	12/21/2005 14:11	12/21/2005 14:22	Quantification	Checked Idle
	Ethanol QN Operator 2	2	Test neu	12/21/2005 14:24	12/21/2005 14:31	Quantification	Checked Idle
	Alkohole-App.	1	21-12	12/21/2005 15:18	12/21/2005 15:26	Identification	Checked Idle

Table columns

The table consists of the following columns:

Application	Name of the related application
Version	Copy number in the course of the lifecycle
Batch	Batch information
Batch Lifecycle state	Lifecycle state of the batch
Start Time	Date and time
End Time	Date and time
Sample Names	Name of the sample
Type	Type of measurement (Identification or Quantification)
Report Type	Type of report
Sequence Lifecycle State	Lifecycle state of the sequence
Prediction	Type of measurement sequence (0= sequence without prediction result; 1=sequence with prediction result) Default: 1
Result OK	Result status (0= one ore more results of the sequence are not OK; 1= all sequence results are OK) Default: 1
Sequence	State of the sequence: Closed: sequence is closed and, if activated, signed electronically by the operator Not Closed: sequence is open in Operator and measurements are still in progress
Description	Optional information
CUT	Result for Content Uniformity Test
Analysis ID	Entered analysis ID information
Customer Fields	Optional information of the customer entered during analysis (content of Customer Fields 1-6 is summarized here)
Comment	Optional information entered during measurements in the comment field
Workstation	PC or workstation name
Container No	Number of containers
Instrument	Instrument type
Measure Cell	Type of measurement cell used
Cell Option	Type of measurement cell add-on used


If necessary, narrow down the information displayed in the table, using appropriate filter settings.

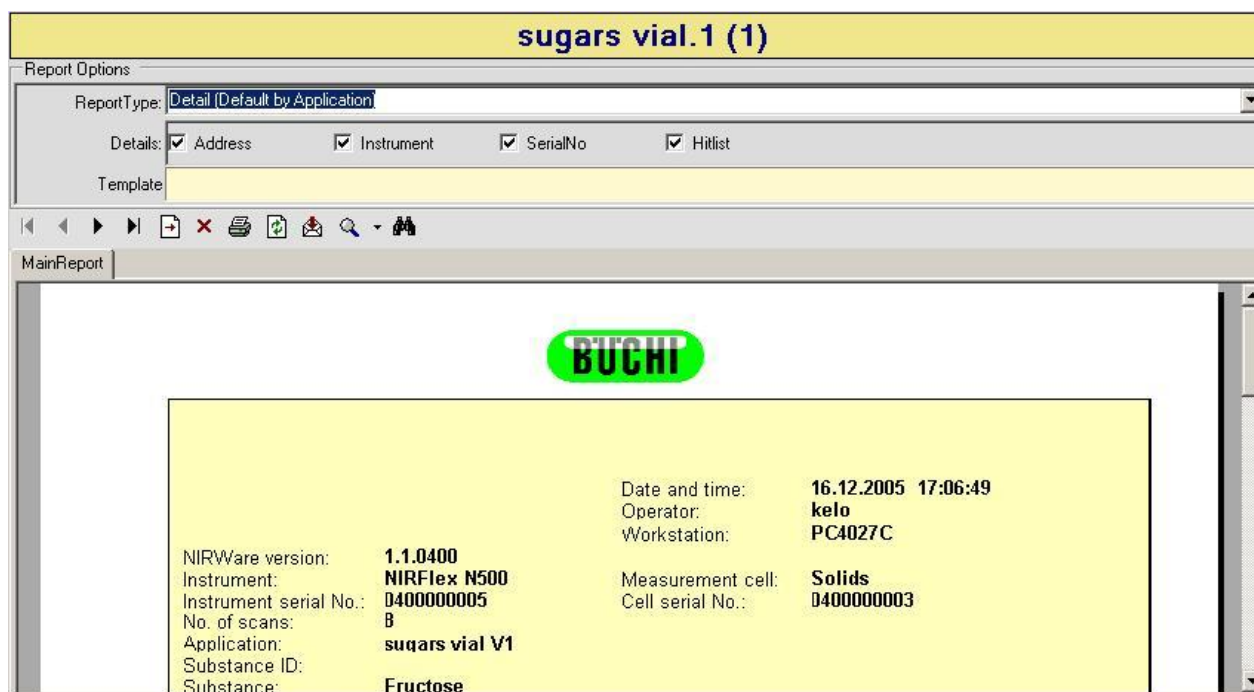
NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

View and Print Reports

To open a report, proceed as follows:

1. Use [filters](#) to specify the table content or reset your filter settings listed in the area below the table by clicking the corresponding button.
2. To select the measurement from the list of which you want to see the report, click the corresponding row.
3. The row shows the measurement sequence. A sequence can contain one or more samples. The detailed information of number of samples and sample names can be found at the end of the overview table.
4. To open the report click the icon  or select **Edit > Open**. The report appears as additional link in the file tree on the left and is displayed in the window on the right.



By default the report type defined in the application will be displayed. Additional report views are available to show the results.

For **Identification** you can choose between a 'Detail' report and a 'Batch Overview' report.

Certain details of the report can be activated or deactivated in the report preview:


- Calibration details
- Address (if information is entered under **Administrative Tools - Customer Info**)
- Instrument and Measurement cell Type
- Serial Number of instrument and measurement cell

- Hitlist (for Identification results)

For **Quantification** you can choose between 'Detail' report, 'Overview' report, 'Batch Detail' report and 'Batch Overview' report.












Certain details of the report can be activated or deactivated in the report preview:

- Calibration details
- Address (if information is entered under **Administrative Tools - Customer Info**)
- Instrument and Measurement cell Type
- Serial Number of instrument and measurement cell

After changing displayed detail information in the report preview, you need to click on  for the change to take action.

If available a customized report template can be displayed.

There are some additional functions available via the report icon bar. Use the icons in the icon bar to navigate within the report and to process it:

	Go to first page icon
	Go to previous page icon
	Go to next page icon
	Go to last page icon
	Go to page icon: When you click here, a dialog opens, where you can specify the page number of the page you want to go to. Click OK afterwards.
	Close report icon.
	Print Report icon. Click here to print the report on the connected printer. A print dialog opens, where you can define different print settings. After that, click OK .
	Refresh icon: Click here to refresh the report and to get back to the default display.
	Export Report icon: Click here to export the report.
	Zoom icon: Click the arrow. A drop-down menu opens, where you can select the size in which the report is displayed by clicking on the corresponding percentage.
	Search Text icon: Click here to search for text within the report. A dialog opens, where you can enter the text to be searched for. After that click Find Next .

Depending on the type of report, i.e. whether it is a Cluster or SIMCA or a Library report or quantitative reports, the layout is different.

Some examples are shown here: [Cluster and SIMCA reports](#) and [Library reports](#)

From the preview, reports can be printed out or exported in different file formats.

NOTE

A report preview is only available for individual measurement sequences.

With multi selection of several measurement sequences (e.g. selection of all sequences of one batch)

only a direct print-out is possible. All sequence reports will be printed out as individual reports (as defined in the application).



Electronic Signature on Reports

Using the LC model "ERES", electronic signatures have to be applied to the reports. Only report types defined in the application can be signed electronically.


The first electronic signature is applied directly in the Operator for:

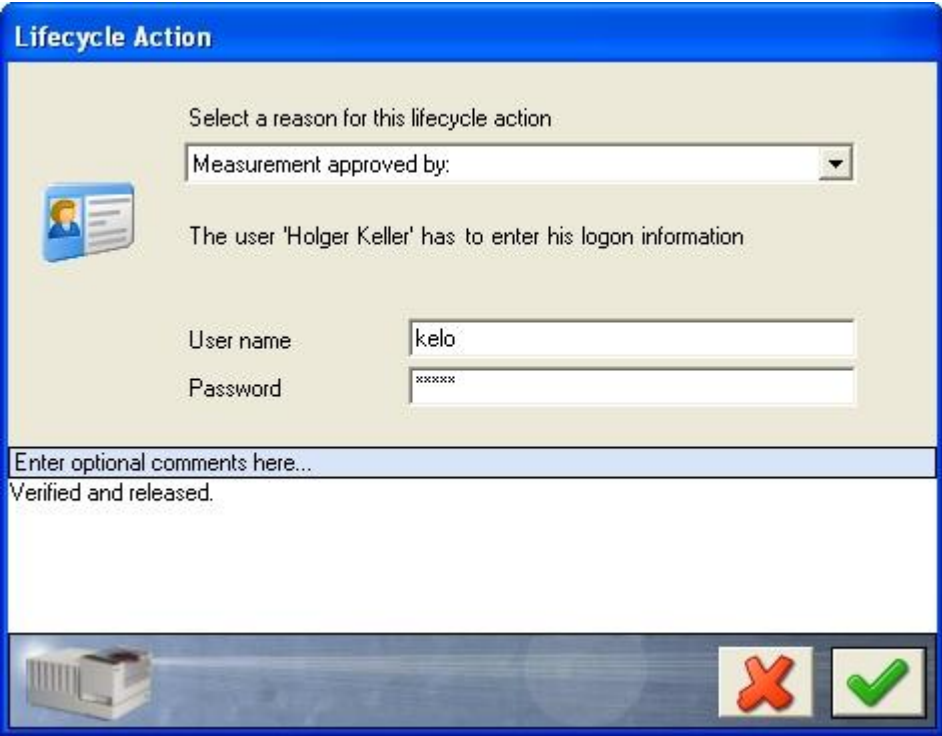
- each Detail report after measurement (in case detail report is selected in the application)
- the Batch report after actively closing the batch

For the second electronic signature narrow down the information displayed in the table, using appropriate filter settings.

Select a measurement sequence with prediction results and open it by clicking on the **"Open existing DataSet"** button  or with double click on the corresponding row indicator .

The report preview window opens.


To verify the result of this individual measurement sequence click on the "Next" button  in the Life Cycle bar. The following window appears:



Lifecycle Action

Select a reason for this lifecycle action

Measurement approved by:




 The user 'Holger Keller' has to enter his logon information

User name



Password

Enter optional comments here...


Verified and released.

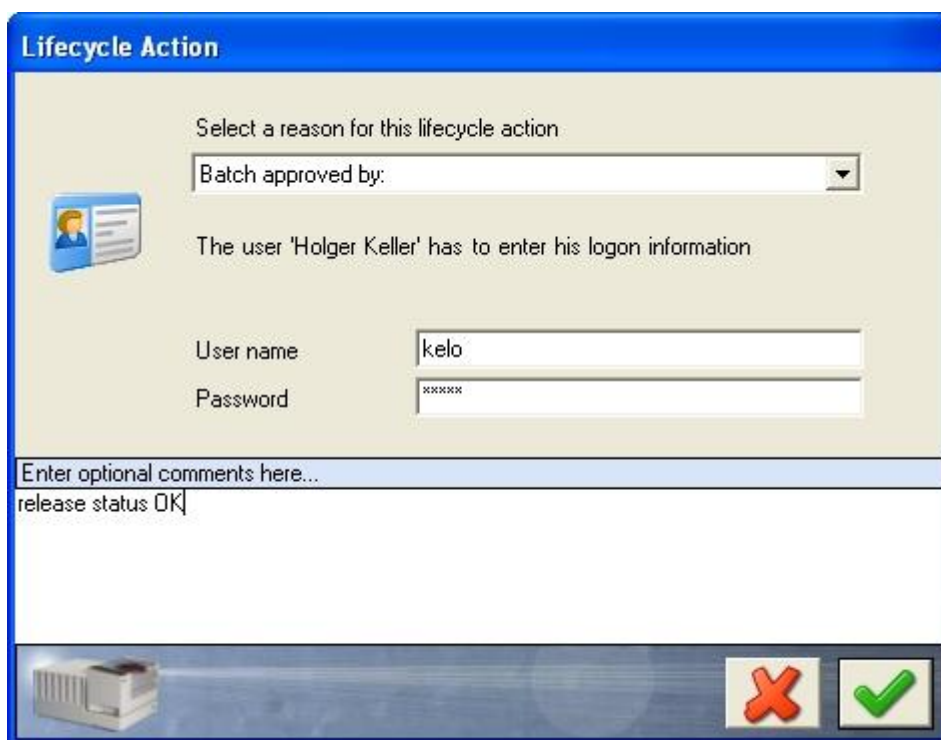
  

For electronic signature on a detail report (measurement sequence), select the corresponding reason, enter User, Password and an optional Comment to verify the measurement sequence.

In case "Batch report" is defined in the application, select a corresponding measurement sequence with prediction results and open it by clicking on the "Open existing DataSet" button  or with double click on the corresponding row indicator .

The batch report preview window opens.

To verify the result of this batch click on the "Next" button  in the Life Cycle bar. The following window appears:



Lifecycle Action

Select a reason for this lifecycle action
Batch approved by: [v]

The user 'Holger Keller' has to enter his logon information

User name: kelo
Password: xxxxxx

Enter optional comments here...
release status OK

For electronic signature on a batch report, select the corresponding reason, enter User, Password and an optional Comment to verify the measurement sequence.

NOTE

Using electronic signature on detail reports the corresponding measurement sequence can be deleted unless the second electronic signature is applied. Only an approved measurement sequence can not be deleted anymore.

Using electronic signature on batch, the corresponding measurement sequences can not be deleted anymore, once the batch has been closed.

Delete or Disable Measurement Sequences

Deleting Measurement sequences without prediction results

Measurement sequences without prediction result (sequence type filter setting 0 in selection table) can be deleted permanently if the corresponding samples are not used in any calibrations.


Information about this can be found by selecting a single or group of measurement sequences in the bottom window:

1. Filter the samples (Application, Version,...)
2. Select the samples for which you want to enter reference values
3. Choose Open

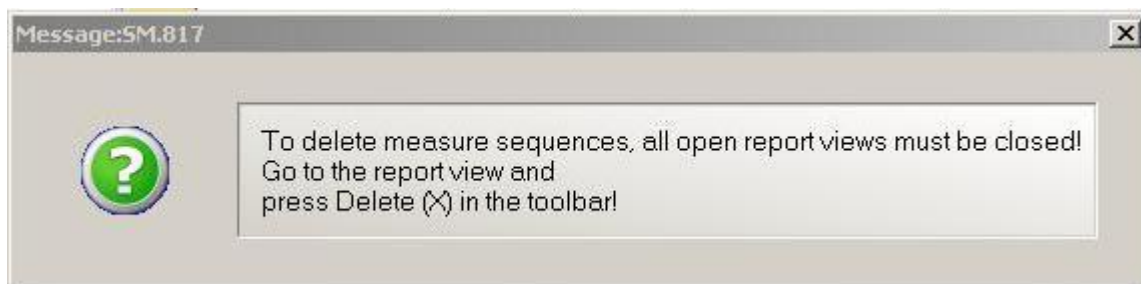
or edit sample names at your desire

Name = '60', SampleID = 281, Deletion DENIED

Used Calibrations: "Olfen, 0.7685, 1-4./5, 8500-10600.(0)"

Select one or more measurement sequences and click on  in the menu bar.

In case some report entries are listed in the file tree on the left, the following message appears:



Close all entries in the file tree list before continue deleting measurement sequences without prediction results by selecting each entry individually and click on the red cross button.

Delete and disable Measurement sequences with prediction results

Measurement sequences with prediction results (sequence type filter setting 1 in selection table) can be deleted as long as they are in the life cycle state created or checked. Only measurement sequences which are put in the life cycle state approved can not be deleted.

Once a measurement sequence is in the life cycle state 'Approved', it will be possible to hide the measurement sequences by putting them in the Life Cycle state "Disabled". The results remain in the database but samples and measurement sequences will not be visible in the tables any more.

In case samples of a particular measurement sequence are used in a calibration, the sequence can not be deleted or disabled.

Information about this can be found by selecting a single or group of measurement sequences in the bottom window:

1. Filter the samples (Application, Version,...)
2. Select the samples for which you want to enter reference values
3. Choose Open

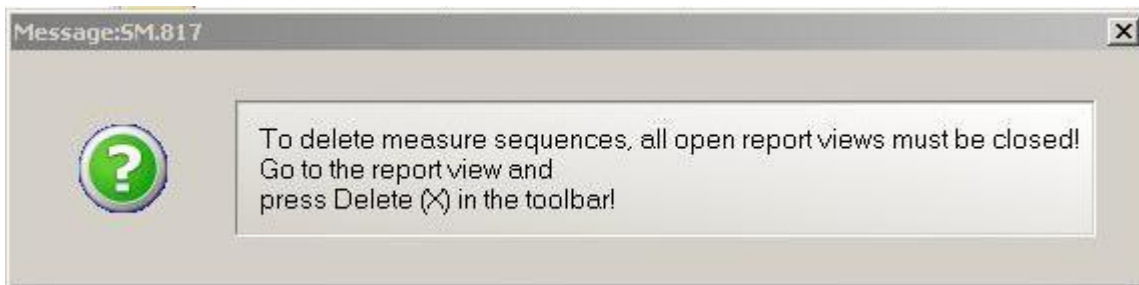
or edit sample names at your desire

Name = '60', SampleID = 281, Deletion DENIED

Used Calibrations: "Olfen, 0.7685, 1-4./5, 8500-10600.(0)"

Select one or more measurement sequences and click on the red cross button in the menu bar.

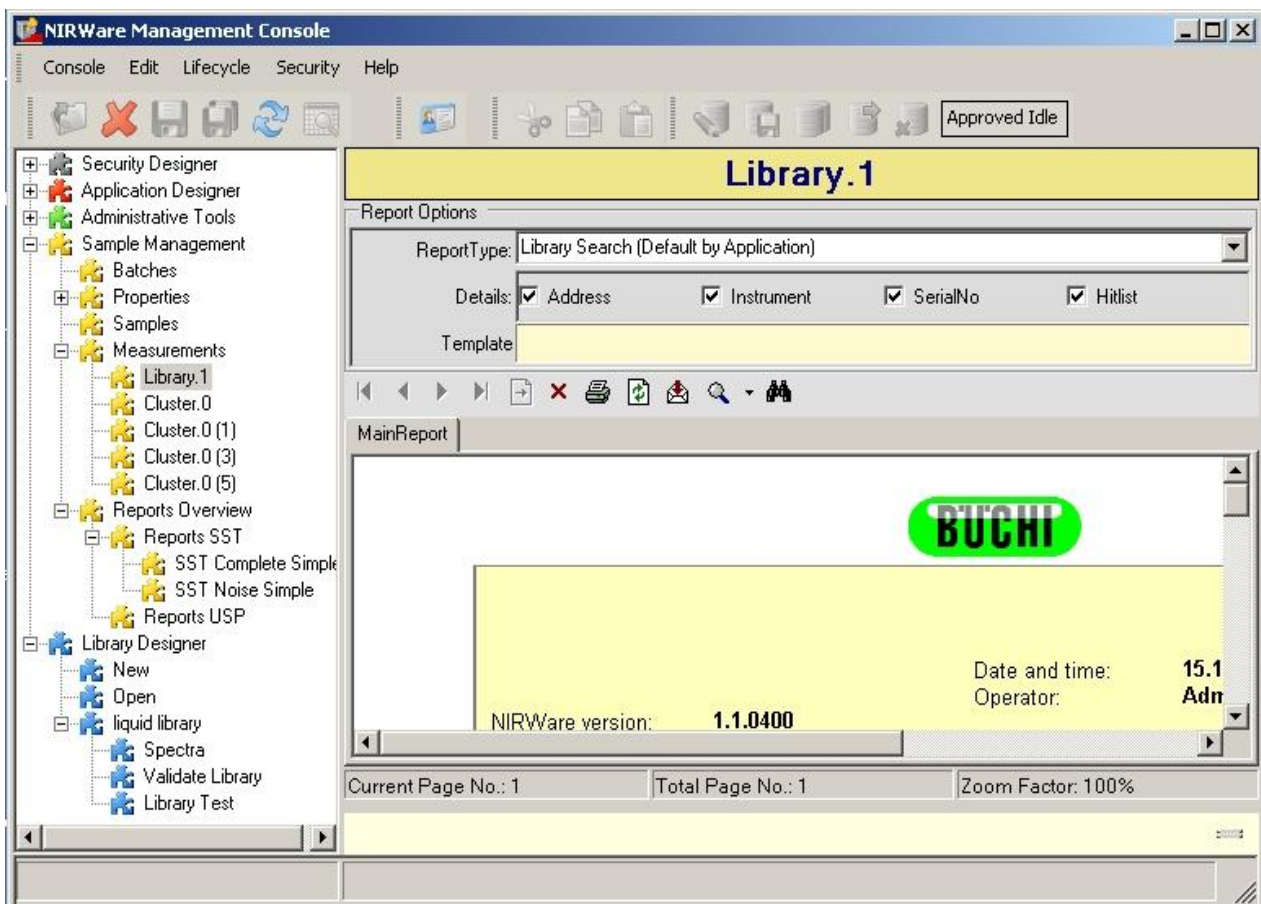
In case some report entries are listed in the file tree on the left, the following message appears:



Close all entries in the file tree list before continue deleting measurement sequences without prediction results by selecting each entry individually and click on the red cross button.

Library reports


When a library report is opened, the following window appears:



Under **Report Options** you can determine another **Report Type** by clicking the arrow and highlight another one from the drop-down list.

Under **Details** you can define whether the Address, the Instrument, the SerialNo and the Hitlist are indicated on the report by activating the corresponding check box.

Under **Template**, ...

To refresh the report so that it displays possible modified settings of the report options, click the refresh icon .

The report is divided in three parts:

Header	Contains all information for traceability of the measured samples. A customer address, instrument and measurement data can be indicated.
Results	The results are shown as a hitlist of the most similar spectra in the library.
Calibration details	The calibration name and used method are indicated. A GUID is included according to regulation requirements.

NIRWare version:	1.1.0400	Date and time:	15.12.2005 12:52:48
Instrument:	NIRFlex N500	Operator:	Administrator
Instrument serial No.:	0400000019	Measurement cell:	Fiber Optic Liquids
No. of scans:	500	Cell serial No.:	0500000102
Application:	Library V1		
Substance:	Isopropanol		
Batchososososososos:	einmessen isopropanol		

Result		
Container:	2005-12-15 12-43-51 einmessen isopropanol	
Expected Substance:	Isopropanol	
Found substance:	✘ Ethanol	
Max allowed distance:	0.010000	
Distance:	0.000026	
Hit	Substance	Distance
0	Ethanol	0.000026 ok
1	Isopropanol	0.027192 ✘

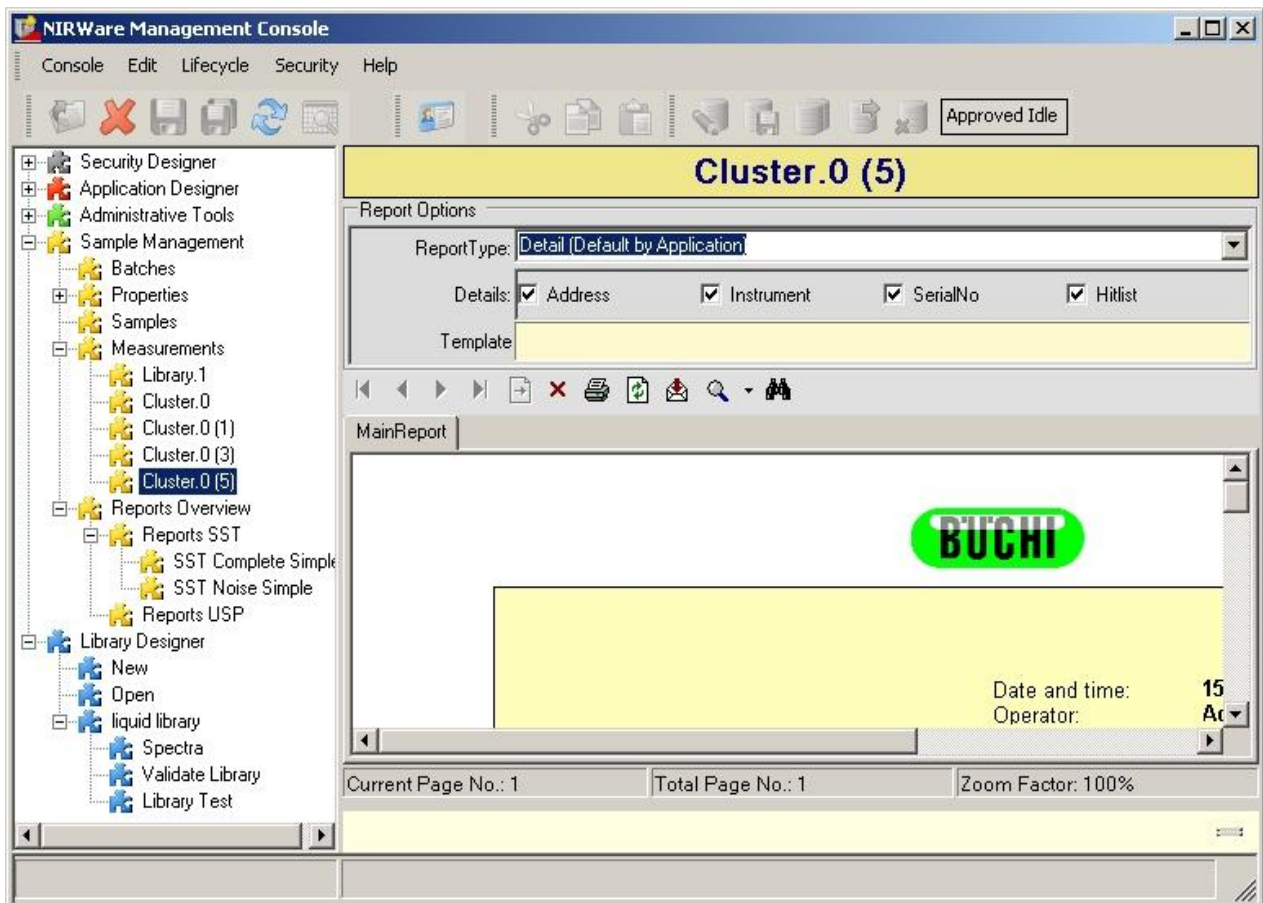
Result		
Container:	2005-12-15 12-43-51 einmessen isopropanol	
Expected Substance:	Isopropanol	
Found substance:	ok Isopropanol	
Max allowed distance:	0.010000	
Distance:	0.000065	
Hit Substance		Distance
0 Isopropanol		0.000065 ok
1 Ethanol		0.026942 x
Calibration Details		
Calibration Name:	liquid library	
GUID / Version:	{56E7EA82-4F2D-42FD-BEB4-16D8FC37C4F5}	0
Methode:	Squared Difference of Derivative	

Done by:

Signature: _____
Administrator


Cluster and SIMCA reports

When a cluster or SIMCA report is opened, the following window appears:



Under **Report Options** you can determine another **Report Type** by clicking the arrow and highlight another one from the drop-down list.

Under **Details** you can define whether the Address, the Instrument, the SerialNo and the Hitlist are indicated on the report by activating the corresponding check box.

To refresh the report so that it displays possible modified settings of the report options, click the refresh icon .

The report is divided in three parts:

Header	Contains all information for traceability of the measured samples. A customer address, instrument and measurement data can be indicated.
Sample details	The results are shown as a hitlist of the most similar spectra in the library.
Calibration details	The calibration name and used method are indicated. A GUID is included according to regulation requirements.

NIRWare version:	1.1.0400	Date and time:	15.12.2005 08:25:41
Instrument:	NIRFlex N500	Operator:	Administrator
Instrument serial No.:	D400000019	Workstation:	PC4027C
No. of scans:	16	Measurement cell:	Fiber Optic Liquids
Application:	Cluster V0	Cell serial No.:	D500000102
Substance ID:			
Substance:	Ethanol		
Batchososososososos:	routine2		

Sample: 2005-12-15 08-25-23Isoprop		Measurement No.: 1	
Identity:	not ok		
Expected substance:	Ethanol		
Found substance:	x Isopropanol		
Distance:	ok 0.000191	Max. distance:	0.142600
Spectrum residual:	ok 0.000260	Max. allowed residual:	0.001087
Hitlist			
Hit	Substance	Distance allowed	Distance
1	Isopropanol	0.142600	0.000191 ok
2	Isopropanol	0.142600	0.000257 ok
3	Isopropanol	0.142600	0.000471 ok

Sample: 2005-12-15_08-25-23Isoprop				Measurement No.: 2	
Identity:		not ok			
Expected substance:		Ethanol			
Found substance:	x	Isopropanol			
Distance:	ok	0.000189	Max. distance:	0.142600	
Spectrum residual:	ok	0.000332	Max. allowed residual:	0.001087	
Hitlist					
Hit	Substance		Distance allowed	Distance	
1	Isopropanol		0.142600	0.000189	ok
2	Isopropanol		0.142600	0.000254	ok
3	Isopropanol		0.142600	0.000468	ok
Calibration					
Calibration name:	Isopropanol, Ethanol, 0.9834, 1./3, 4000-10000.			Version:	0
GUID:	{1EB56CCE-F604-478F-B948-3B3BA259EEA5}			Method:	Cluster
Properties:	Isopropanol Ethanol				

6.3.6. Reports overview

SST report

In the file tree on the left side of the **NIRWare Management Console** select **Sample Management - Reports SST**.

The following dialog opens:

Reports SST

Choose an SST type

SST Complete

Make the desired selection

	Type	TimeStamp	Info	Success	Aborted	Instrument	M
▶	Complete SST	12/29/2005 15:30		<input checked="" type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/28/2005 10:34		<input checked="" type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/28/2005 09:43	Noise SST:	<input type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/28/2005 09:36	Noise SST:	<input type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/27/2005 09:33		<input checked="" type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/27/2005 09:27	Noise SST:	<input type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/20/2005 15:56		<input checked="" type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/19/2005 14:59		<input checked="" type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	12/13/2005 10:39		<input checked="" type="checkbox"/>	<input type="checkbox"/>		
	Complete SST	09/09/2005 11:47		<input checked="" type="checkbox"/>	<input type="checkbox"/>		

Reset Filters

Report Options

Details Select All

The complete SST test contains out of four test categories. From the drop down list select the part of the SST test that should be displayed in the selection window:

- SST Complete (all test results will be displayed)
- SST Wavenumber Accuracy (results from wavenumber test will be displayed)
- SST Noise (results from noise test will be displayed)
- SST Linearity (Linearity test results will be displayed)
- SST Temperature (Temperature test results will be displayed)

The reports list contains the following columns according to which it can be filtered:


Type	Type of selected SST test result
TimeStamp	Date and time
Info	additional test information such as reason for "not passed result"
Success	SST passed (no check mark = not passed; check mark = passed results)
Aborted	SST test aborted (no check mark = not aborted; check mark = aborted tests)
Instrument	Instrument type
MeasureCell	cell type

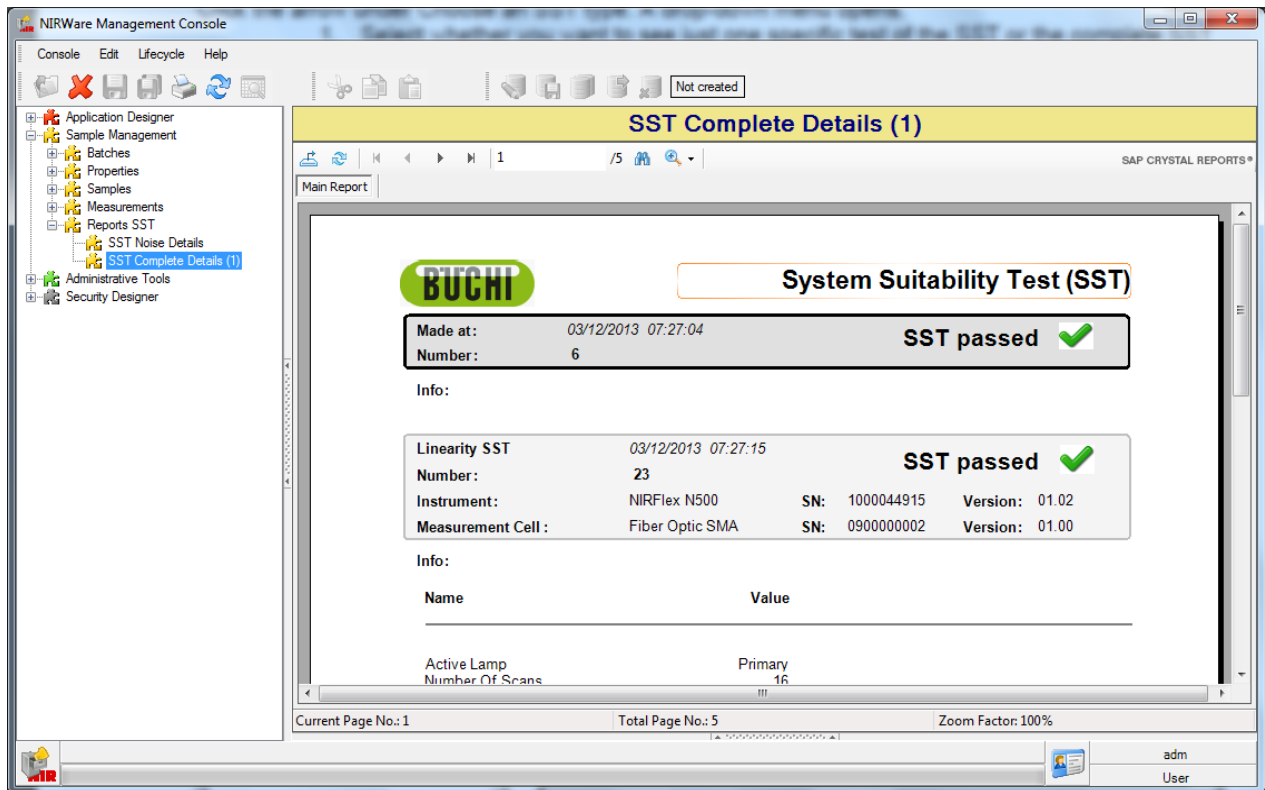
To define the content of the report, you can show or hide test details:

- "Details" checked: detailed results will be shown in report
 "Details" not checked: only result overview will be shown in report

To open a SST report, proceed as follows:

Click the arrow under Choose an SST type. A drop-down menu opens.

1. Select whether you want to see just one specific test of the SST or the complete SST by clicking on it. The corresponding selection is displayed in the table below.
2. You can now use [filters](#) to specify the table content or reset your filter settings listed in the area below the table by clicking the corresponding button.
3. Under Report Options you can specify whether the report(s) should be displayed with details () or not by checking the corresponding checkbox.
4. To select one or several reports from the list, click the corresponding row(s), to select all reports listed in the table above, click **Select All**.
5. To open the selected reports click the icon  or select **Edit > Open**. The report is now generated. It appears as additional link in the file tree on the left and is displayed in the window on the right.



There are some additional functions available via the report icon bar. Use the icons in the icon bar to navigate within the report and to process it.

USP report

In the file tree on the left side of the **NIRWare Management Console** select **Sample Management - Reports USP**.

The following dialog opens:


Reports USP								
Make the desired selection								
Type	Timestamp	Success	Aborted	Info	User	ValidUp	Installed at	
	10/19/2005-01/19/2006							
Installation	12/16/2005 17:46:52	<input checked="" type="checkbox"/>	<input type="checkbox"/>		kelo	10/18/2007	12/16/2005	
Regular	12/16/2005 17:47:05	<input checked="" type="checkbox"/>	<input type="checkbox"/>		Service	10/18/2007		
Regular	12/16/2005 17:55:48	<input checked="" type="checkbox"/>	<input type="checkbox"/>		kelo	10/18/2007		
Regular	12/22/2005 12:06:37	<input checked="" type="checkbox"/>	<input type="checkbox"/>		kelo	10/18/2007		

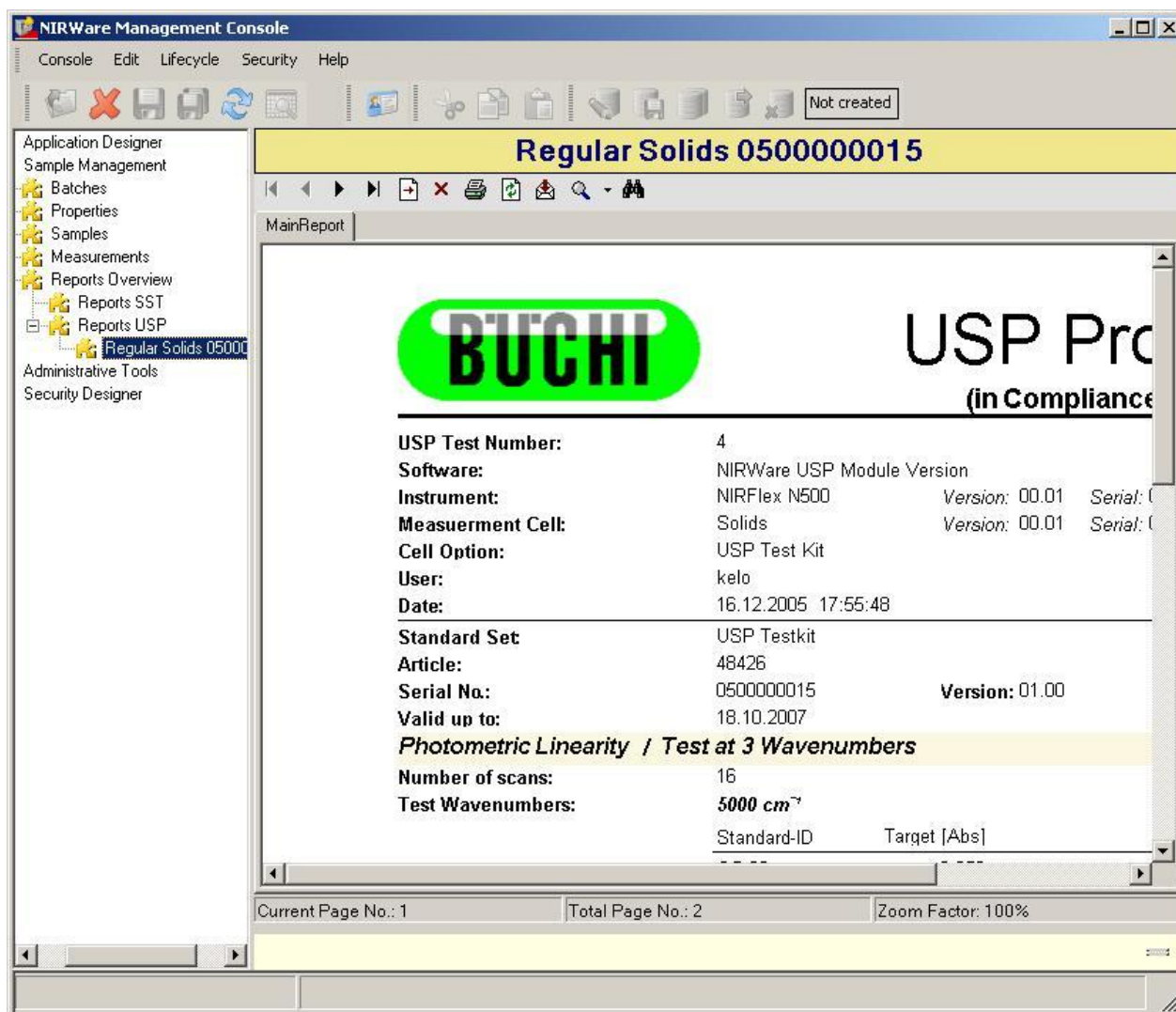
The reports list contains the following columns according to which it can be filtered:

Type	Report type: Installation: Report documenting the installation of the USP Test Kit Regular: USP Test report
TimeStamp	Date and time
Success	SST passed (0= not passed; 1= passed results)
Aborted	SST test aborted (0= not aborted; 1= aborted tests)

Info	additional test information such as reason for "not passed result"
User	User login account
ValidUp	date up to which the USP Test is valid
Installed at	Installation date
Installed by	full name who has performed installation
Standard	standard type
Std. Serial	serial number of standard wheel
Std. Version	version of standard wheel
Instrument	Instrument type
Instr. Serial	serial number of instrument
Cell	cell type
Cell Serial	serial number of measurement cell

To open a USP report, proceed as follows:

1. Use [filters](#) to specify the table content or reset your filter settings listed in the area below the table by clicking the corresponding button.
2. Select a report and click the icon  or select **Edit > Open**. The report opens. It appears as additional link in the file tree on the left and is displayed in the window on the right.



There are some additional functions available via the report icon bar. Use the icons in the icon bar to navigate within the report and to process it.

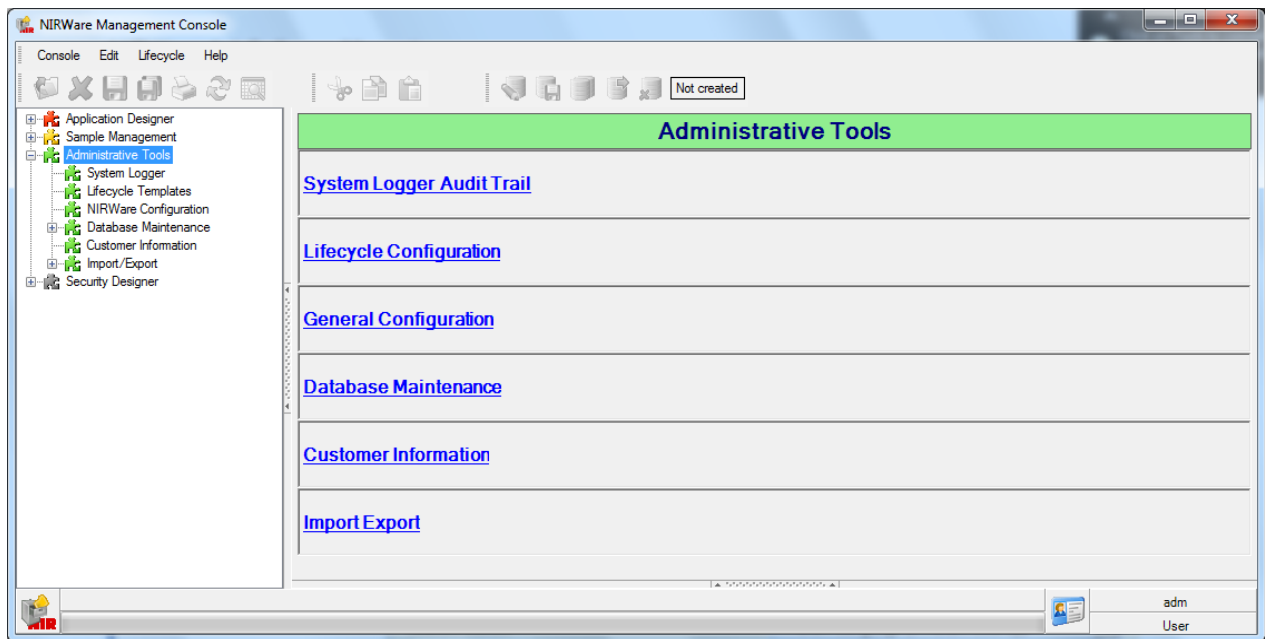
6.4. Administrative Tools

6.4.1. Introduction Administrative Tools

The Administrative Tools enable to make general administrative settings within the software package. They comprise logging functions, lifecycle settings, system configuration, maintenance and import / export options.

To open the Administrative Tools proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools**. The following dialog opens:



You can now open a submenu by clicking on their names in the file tree or in the center of the Administrative Tools window.

6.4.2. System Logger

The system logger is the logbook for all events taking place during operation of the software package.

To open it, in the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - System Logger** or click **System Logger Audit trail** in the submenu list in the center.

The following dialog opens:

Logger					
	MessageType	TimeStamp	ApplicationContextType	User	Message
		02/14/2007			
1	Audit Trail	02/14/2007 11:57:50	eContextManagementConsole	Holger	Deletion of sample DENIED, because the sam
2	Audit Trail	02/14/2007 11:54:43	eContextManagementConsole	Holger	Sample name changed, old Name Template sp
3	Audit Trail	02/14/2007 11:54:39	eContextManagementConsole	Holger	Sample name changed, old Name Fine Sucros
4	Audit Trail	02/14/2007 11:39:01	eContextManagementConsole	Holger	Account policy was saved
5	Audit Trail	02/14/2007 11:38:48	eContextManagementConsole	Holger	New 'Application Lifecycle' created
6	Error	02/14/2007 11:38:41	eContextManagementConsole	Holger	There are missing mandatory or incorrect value
7	Incident	02/14/2007 11:13:35	eContextManagementConsole	Holger	The last backup of your database has been pe
8	Incident	02/14/2007 10:43:45	eContextControl		Could not connect to device at address `10.10.
9	Incident	02/14/2007 10:43:37	eContextControl		Could not connect to device at address `10.10.
10	Incident	02/14/2007 10:43:30	eContextControl		Could not connect to device at address `10.10.
11	Incident	02/14/2007 10:43:24	eContextControl		Could not connect to device at address `10.10.

Max displayed rows 1000

The System Logger consists of a table in the upper part, listing all events in chronological order, an area in the center, giving source string information about the filter currently applied in the table above, and an area at the bottom, concisely listing the information of the line currently highlighted in the table above.

Table columns

The table in the upper part comprises different columns:





Header	Description
Message Type	Type of message; Audit Trail, Trace, Error, Incident, Info
Time Stamp	Date and time when the message was logged
Application Context	Software module, in which the message was produced
User	User log in name of the current user at that time
Message	Content of main message
Nested Message	Additional Message: Detailed driver information or comments on actions
InstrumentUnit	Instrument and measuring cell number
SubsystemID	Software component, which produced the message (relevant in developer context)
ID	Unique Error Number with Subsystem ID displayed
Workstation	Name of the computer, where the message was produced
UTC TimeShift	Deviation from the "Universal Time Coordinated"

NOTE

You can inverse the order of the individual column entries by clicking the corresponding column header. Use the [filter](#) functions to narrow down the content of the table.

Buttons

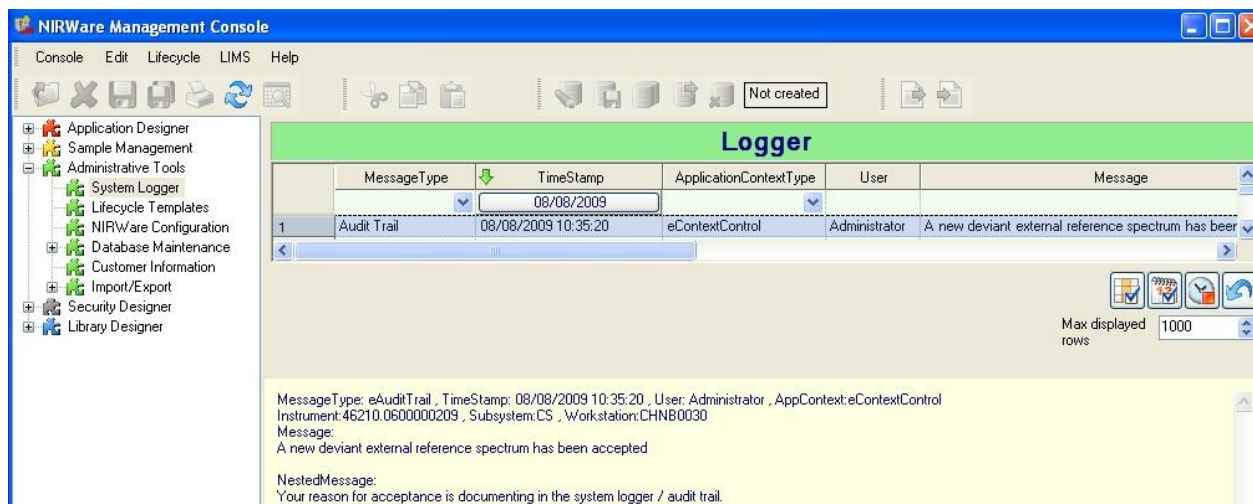
By means of the three buttons in the right center, you can change the information displayed in the table above. By clicking the buttons

	Each event is displayed by default as a single line. This function increases the line and column width to show the whole content of the messages.
	Only the events logged on the current day are displayed.
	The display is automatically refreshed.
	All set filters are reset, so that the table is displayed empty now and you can choose new filter settings.

In the field **Max displayed rows** the amount of entries displayed in the table can be limited. The list of data can be very big. For performance issues, a limitation is necessary.

Documentation of a deviating external reference spectrum

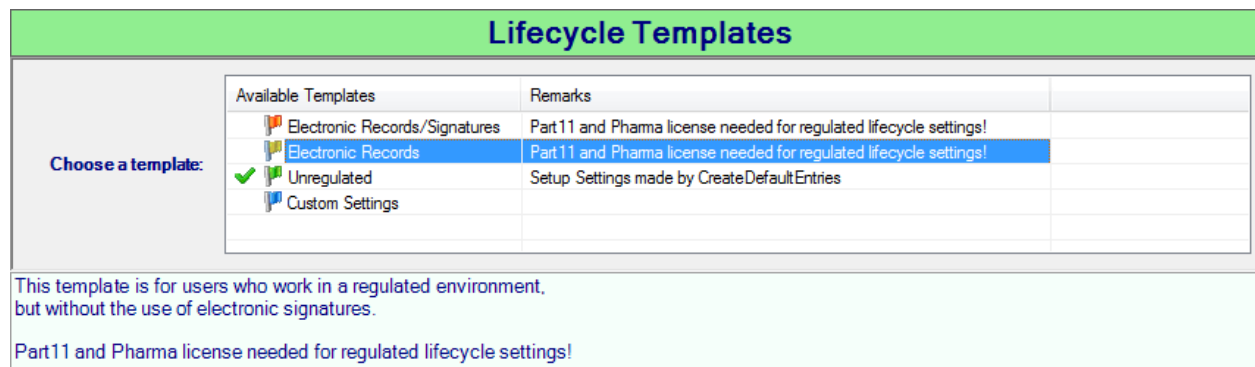
The acceptance of a deviating external reference spectrum has a direct effect on subsequent sample spectra. Therefore, an entry in the Audit Trail documents who has made the decision, when and why.



6.4.3. Lifecycle Templates

The selected lifecycle template determines certain operational procedures within NIRCAl and the Application Designer. To view or change the corresponding settings, in the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Lifecycle Templates** or click **Lifecycle Configuration** in the submenu list in the center.

The following dialog opens:



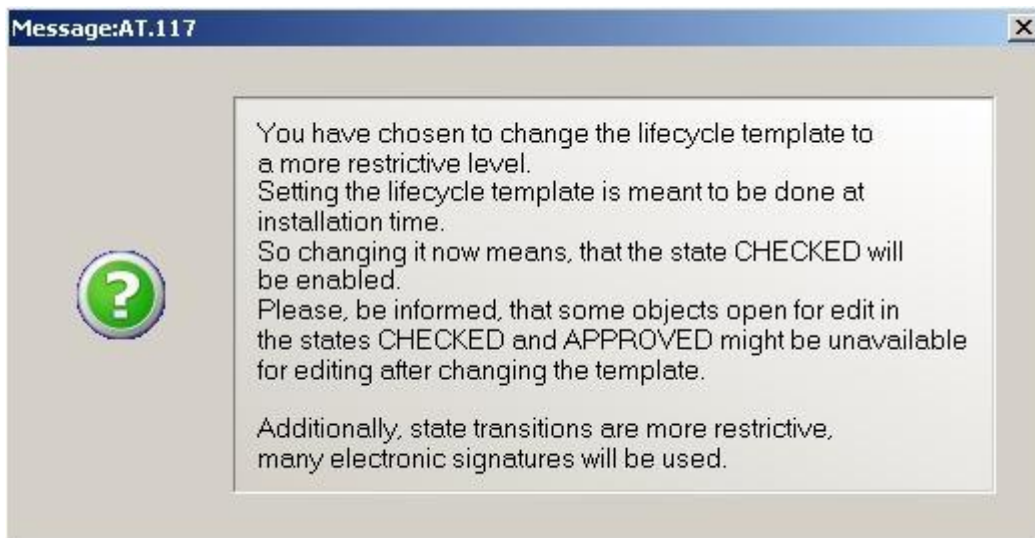
Four different template types are provided:

- **Electronic Records/Signatures:** Covering all requirements of 21 CFR Part 11 (relevant for pharmaceutical applications)
This template is only available together with the NIRWare Advanced License or with the additional NIRWare Regulatory Kit License. It is designed for user in a regulated environment who work with electronic signatures and records.
- **Electronic Records:** For user in a regulated environment, who do not work with electronic signatures but with electronic records. This template is only available together with the NIRWare Advanced License or with the additional NIRWare Regulatory Kit License.
- **Unregulated:** For users in unregulated environments, who do not work with electronic signatures and records.
- **Custom Settings:** Customer specific settings, which are generated on request by BUCHI Labortechnik AG (for information on how to import a corresponding template, see [Lifecycle Configuration](#))

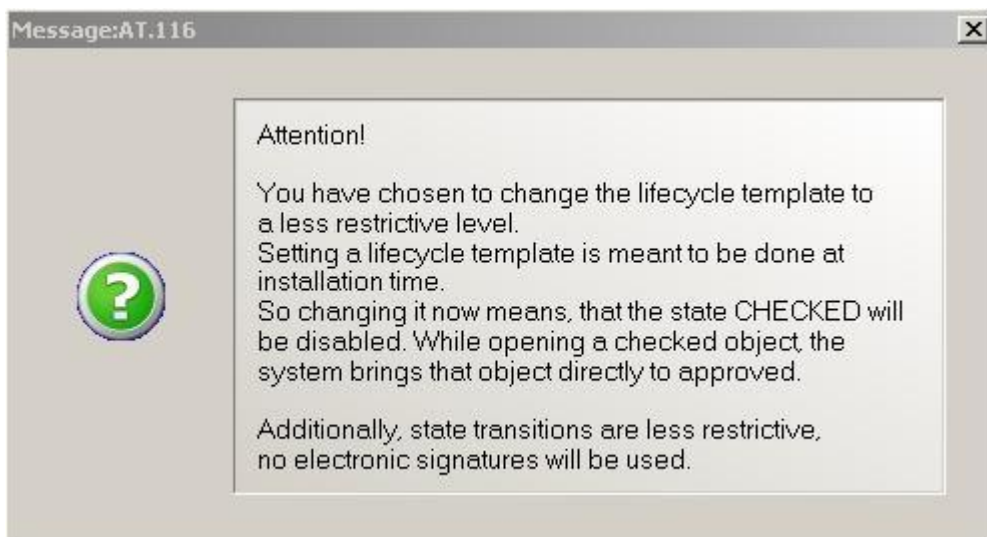
If you highlight a template type, a detailed explanation of its characteristics is displayed in the area below. To change the lifecycle template, highlight the desired template and click the Save button or double-click the desired template.

The dialog "Authorize with your signature" opens. Type in your user name and password and click the Okay button (green arrow).

When changing the lifecycle template to a more restrictive one, the following message appears



When changing the lifecycle template to a less restrictive one, the following message appears:



Confirm the corresponding message by clicking the Okay button.

A second message is displayed:



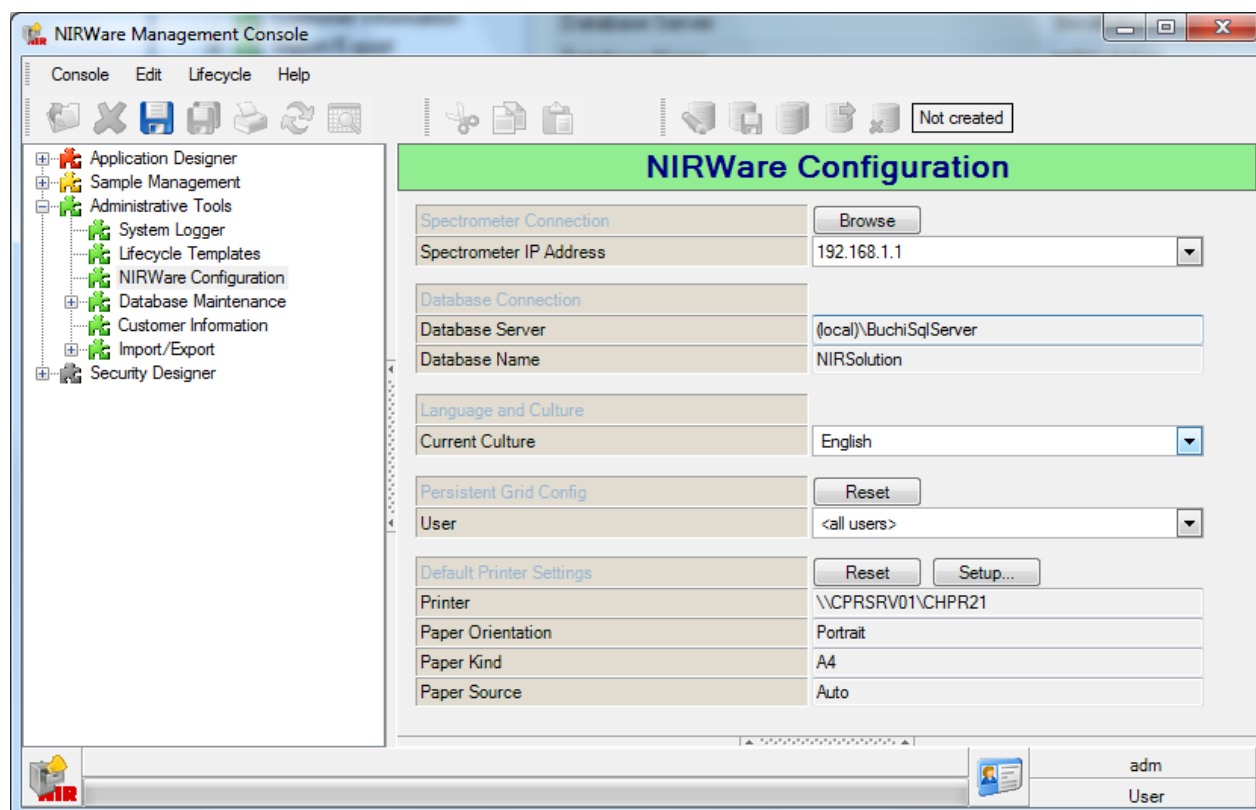
Confirm it again with the Ok button.

For further information on the lifecycle philosophy and templates, see [Templates](#).

6.4.4. NIRWare Configuration

The NIRWare Configuration dialog serves to set certain instrument parameters. To open it, in the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - NIRWare Config**.

The following dialog opens:



The dialog consists of five areas:

Spectrometer Connection

The IP address on which the software should search for the NIRFlex N-500 instrument to establish the communication can be selected from the drop-down list. Alternatively, you can click the **Browse** button to create a selection list of all available NIRFlex N-500 spectrometers that are accessible on the network.

IMPORTANT NOTE

The browsing function can only find spectrometers if

- the spectrometer is switched on and connected to the network
- the spectrometer's IP-address is within the same subnet as the PC that tries to connect
- no firewall interferes with the communication

When all this prerequisites are fulfilled, click Browse. After the searching procedure is finished, you can select the IP Address of a spectrometer from the corresponding drop-down list.

Database Connection

In the fields **Database Server** the path of the database server running the database which the software package accesses is indicated. The field **Database Name** shows the name of the corresponding database.

Language and Culture

NIRWare Management Console and NIRWare Operator are multi-language capable. In order to switch to a different language a language package needs to be installed additionally. From the drop-down menu select the language in which the software should be displayed. In case the localization for your selected language is not applicable yet, English will be used as default language.

Press the Save button to save the modification.

Persistent Grid Config

When you have established some user dependent filter settings for the table content in the Application Designer, the Sample Management or the Administrative Tools, you are able to reset these settings here by clicking **Reset**. Otherwise your filter settings will be applied again each time you log in with your user name and password again.

Press the Save button to save the modification.

Default Printer Settings

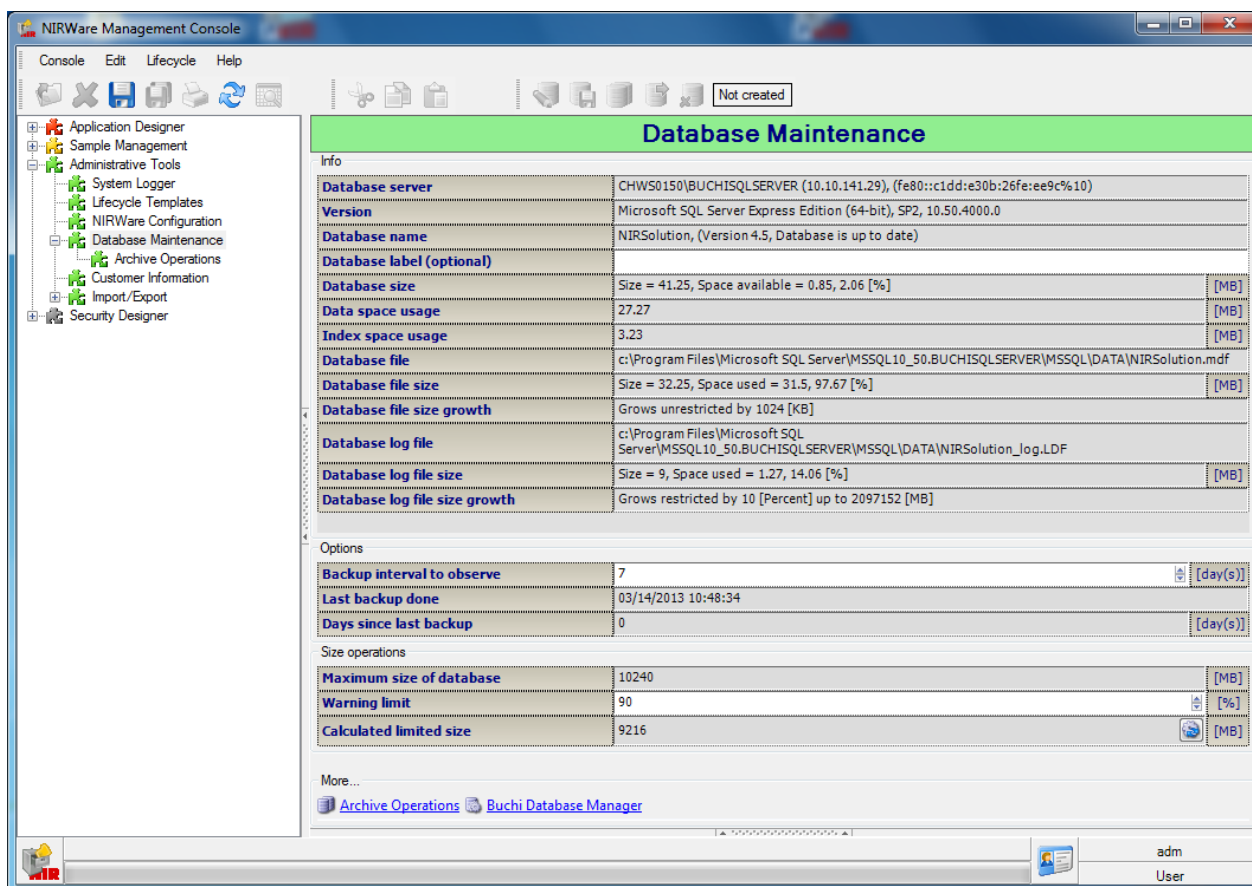
Here the printer settings for the used printer are indicated. To setup these settings, click the **Setup...** button. The Paper Setup dialog opens, where you can define the paper size and source, the orientation, the margins and the used printer. To get back to the default printer configuration of your operating system, click the **Reset** button.

6.4.5. Database Maintenance

Database Maintenance

The Database Maintenance dialog gives an overview of the database properties. To open it, select in the file tree on the left side of the **NIRWare Management Console** the entry **Administrative Tools - Database Maintenance**.

The following dialog opens:



Via the **Database Maintenance** dialog one additional functions are accessible: **Archive Operations** and the access to Buchi Database Management (BDM). In BDM the regular database backup can be performed.

The archiving process allows you to transfer only part of the database into a new one, thus enabling you to get rid of outdated data to accelerate your current working routine.

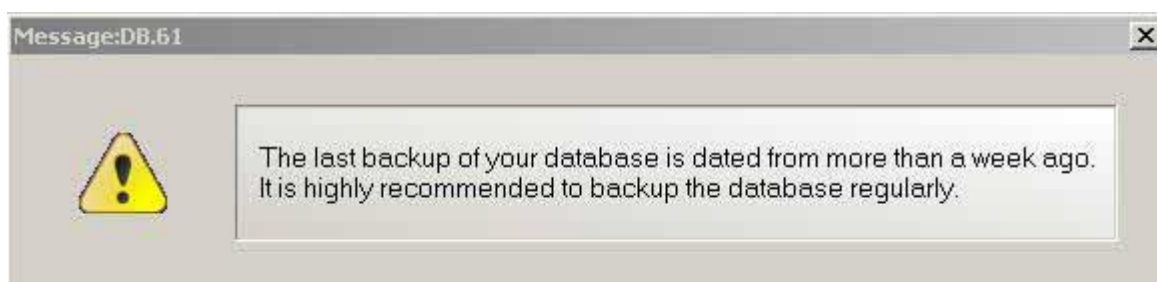
The **Warning limit** for the database size can be configured.

Backup and Restore

The backup and restore function enables to backup the current NIRWare database and restore it later on.

Use BUCHI Database Manager (BDM) for backups and restores. Refer to the Operation Manual of BDM: Start > All programs > Buchi > Operation Manual

Database Backup Reminder



Every week the above reminder dialog recommends to backup the database. Click OK to close the dialog and create a backup as desired.

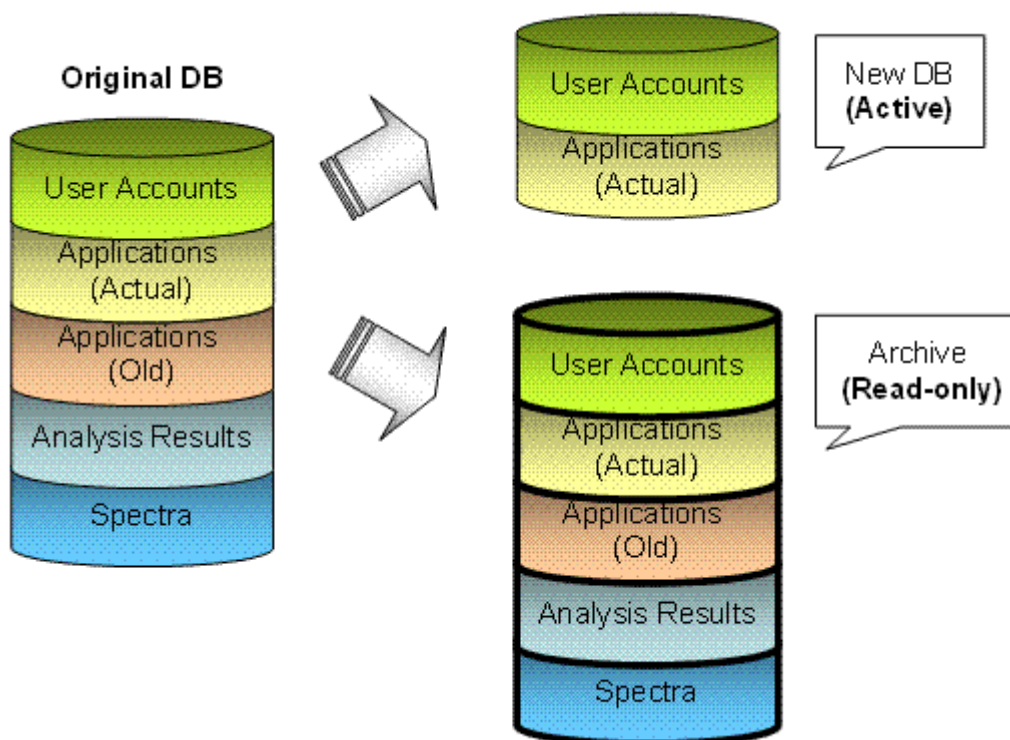
Archive Operations

General information

The archiving function allows to store outdated data in a separate 'container' called archive, and to continue seamlessly with only those (reduced) data which are relevant for your current work.

In the archive all data from the original database are stored, i.e. the archive is in fact the original database, it has just a different status.

The new, slim production database contains a copy of only some part of the original database:



Creating an archive

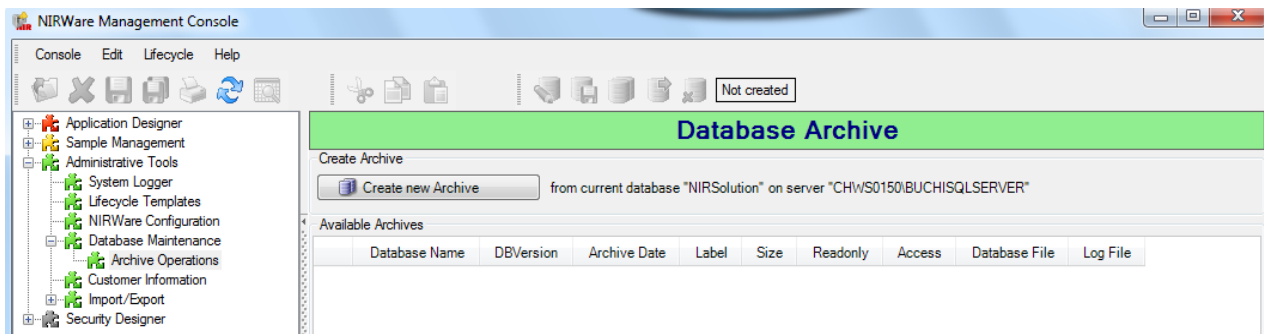
NOTE:

The archiving process requires a definite database status, so that no changes to the database are allowed during archiving.

For this purpose stop all programs and processes accessing the database prior to archiving - including the NIRWare Operator and the Control System Service.

To start the archiving process, proceed as follows:

Select **Administrative Tools - Database Maintenance - Archive Operations** and click on the button "Create new Archive".

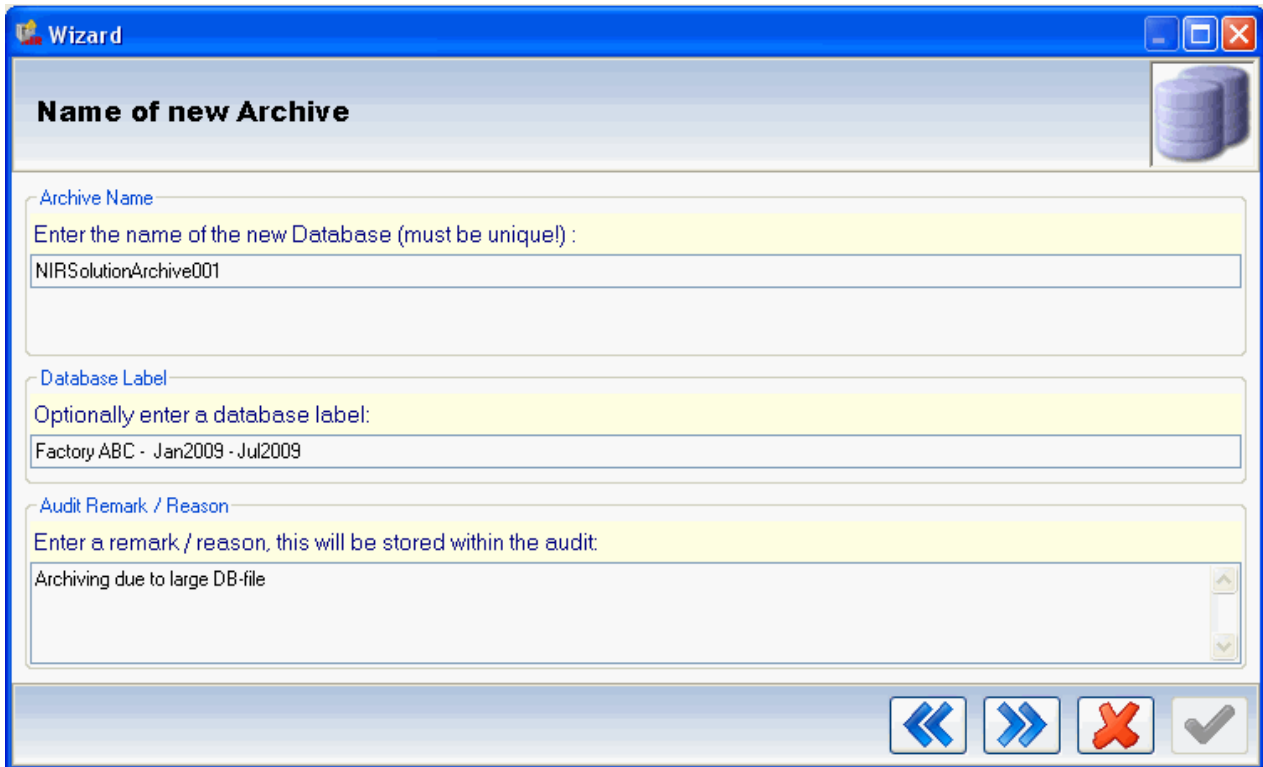


A Wizard window appears and guides you through the archiving process:



You can use the double arrow buttons to switch back and forth between dialog windows or click on the red cross button to abort.

To continue click the right double arrow button.

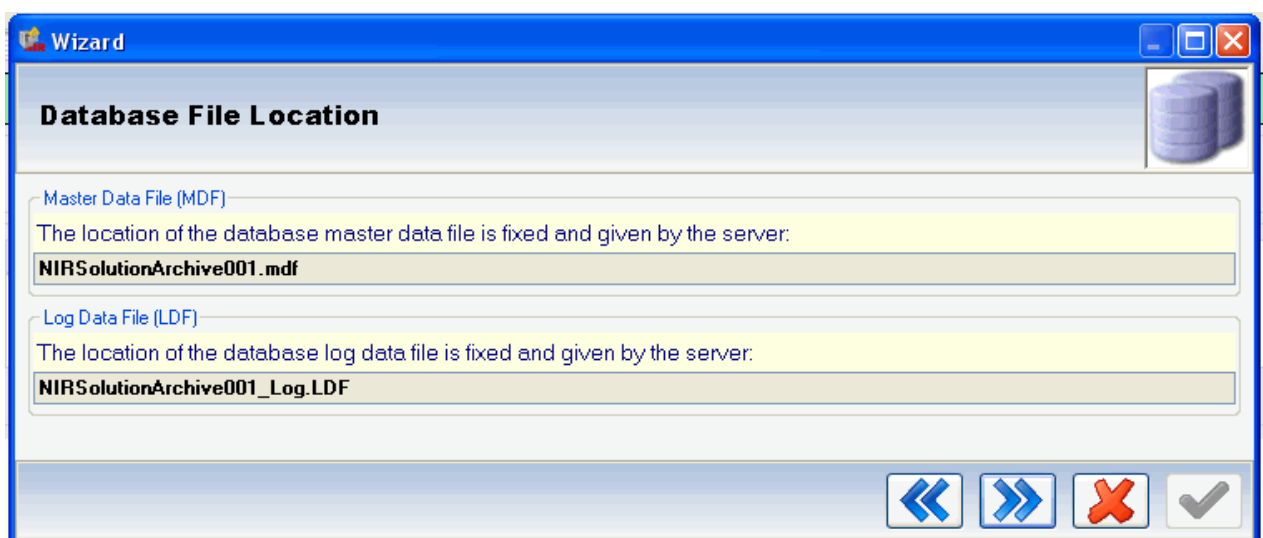


Under **Archive Name** enter a name for your new production database.

NOTE:

We recommend to add a speaking database label, e.g. indicating the local plant and time period.

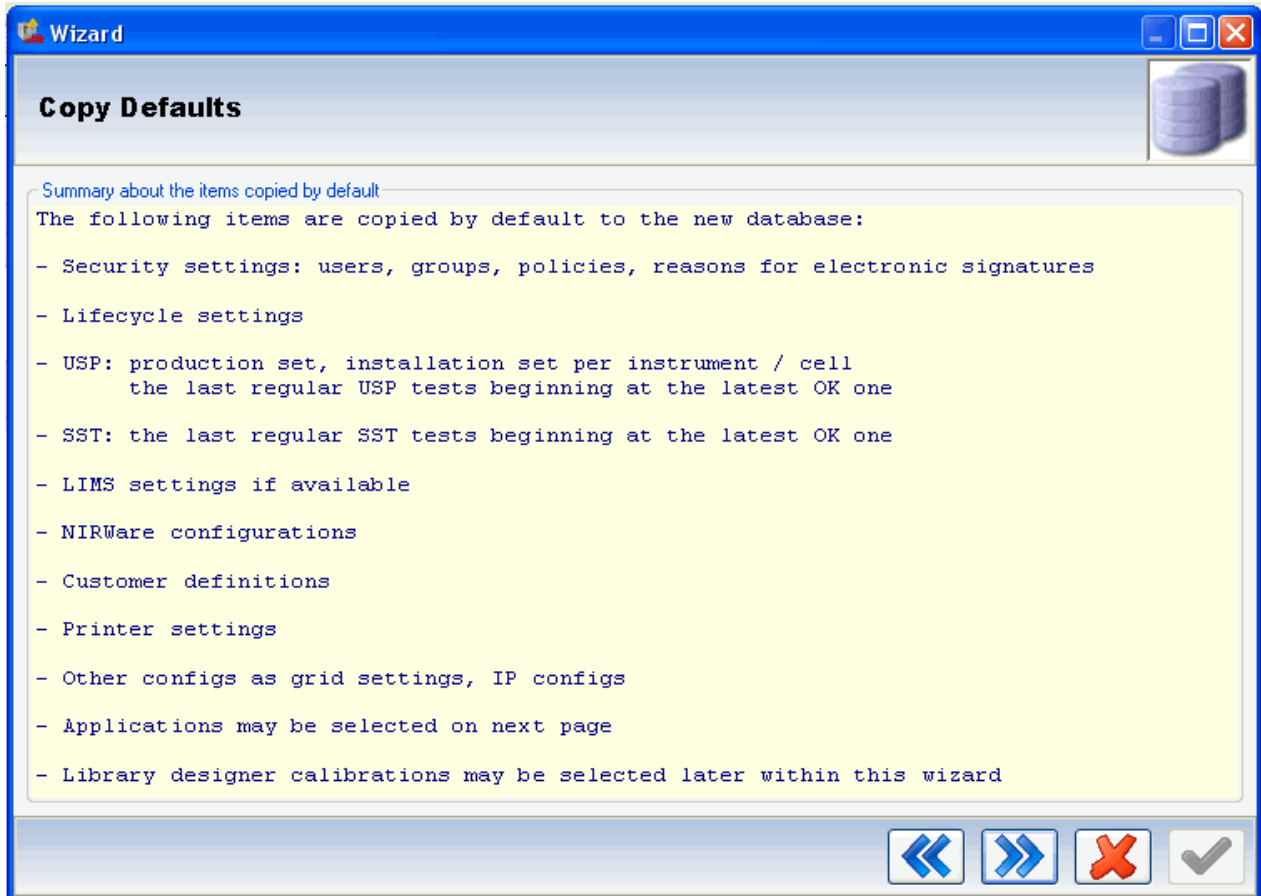
The date and the name of the database creator will always be documented in the audit trail automatically. To continue click the right double arrow button.



The master and log data file (.MDF and .LDF) are controlled by the SQL server and are thus shown for information purposes only.

To continue click the right double arrow button.

To ensure seamless continuation of operation, part of the database content is transferred automatically and listed in the appearing screen:



NOTE

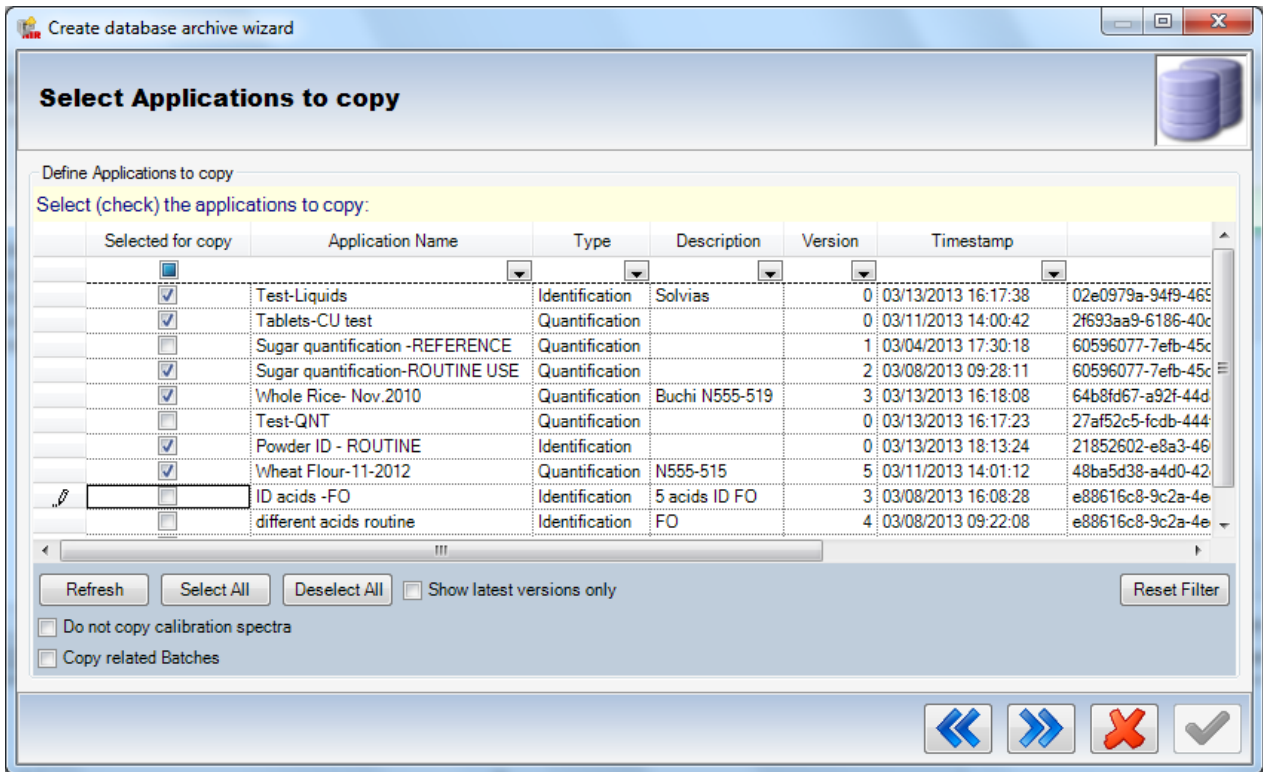
Batches are not copied to the new database.

NIRCal projects and spectra that are not assigned to any calibration are not copied to the new database. This can be done via the export function

Administrative Tools => Import/Export => Export NIRCal Project

Administrative Tools => Import/Export => Export Application (AsCsR)

To continue click the right double arrow button.

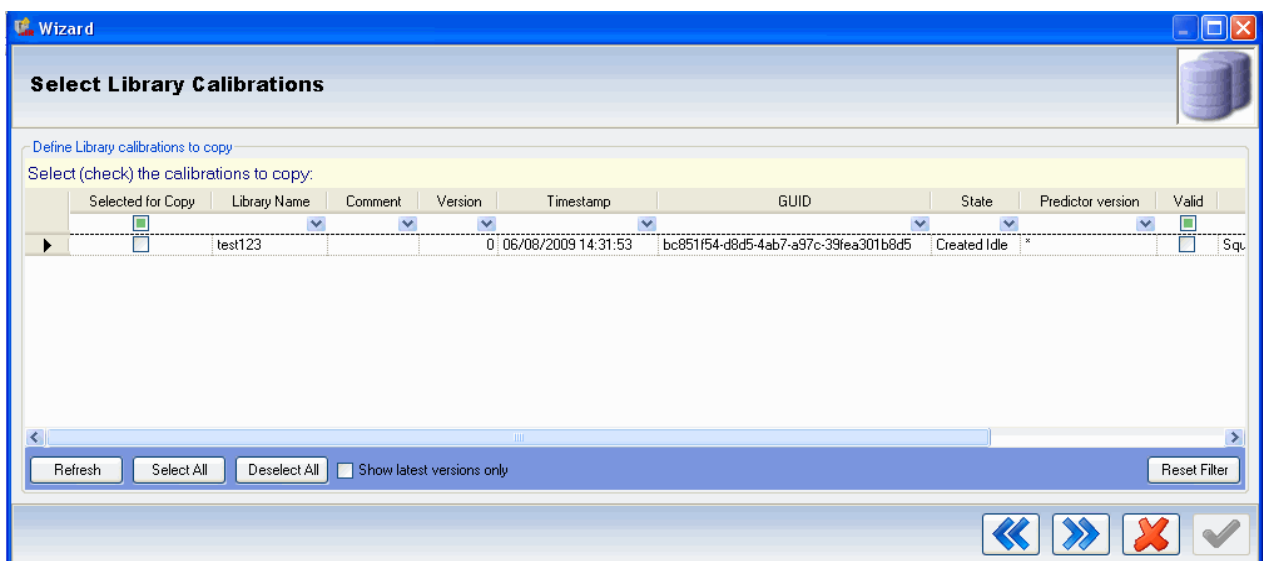


You can now select the applications to be copied into your new database. For this purpose activate the checkbox in the first column of the corresponding line. If nearly all applications should be copied, click **Select All** and then deselect the ones you do not need.

The checkbox "**Show latest versions only**" will hide all older versions of a calibration. The checkbox "**Do not copy calibration spectra**" will copy the calibrations without spectra. The checkbox "**Copy related Batch**", the measured batches are also copied.

Filters can be used to reduce the list to relevant entries. For this purpose select an entry from the drop-down lists or type part of a GUID in the corresponding field. To reset your filter settings, click **Reset Filter**.

To continue click the right double arrow button.

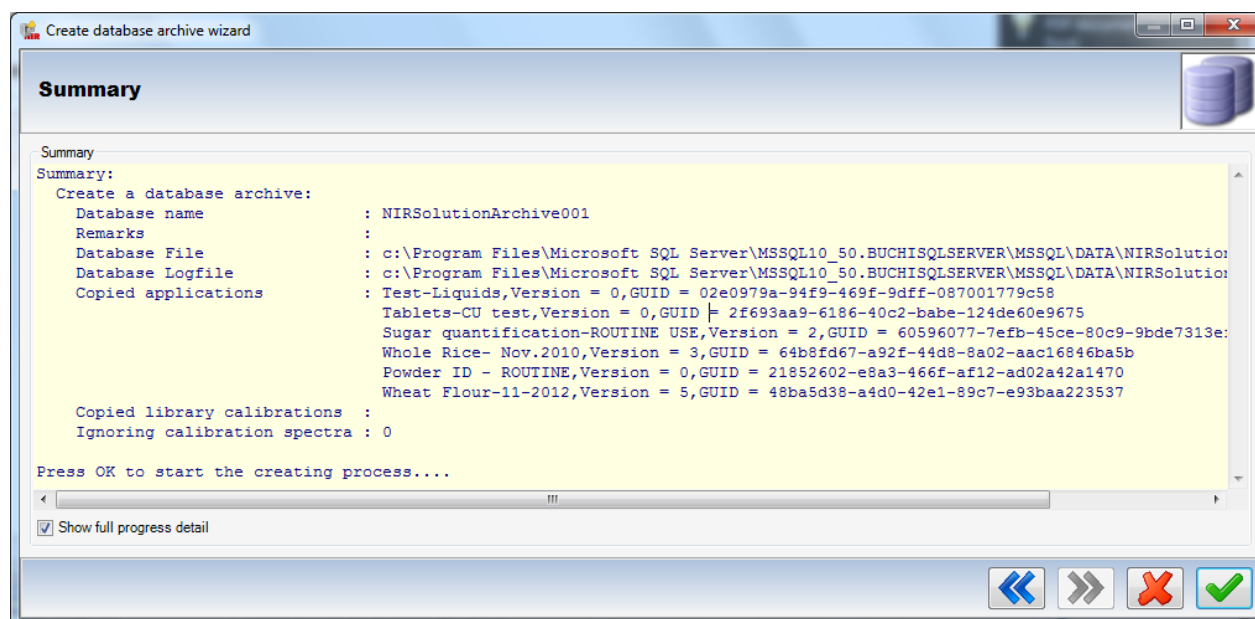


You can now select the libraries to be copied into your new database. For this purpose activate the checkbox in the first column of the corresponding line. If nearly all libraries should be copied, click Select All and then deselect the ones you do not need.

The checkbox "**Show latest versions only**" will hide all older versions of a calibration.

Filters can be used to reduce the list to relevant entries...

To continue click the right double arrow button. A summary will appear, where you can review your settings before the actual archiving process is started:



To start the archiving process, click the green checkmark button.

After the data transfer the new database becomes the active one and the old one is labelled as archive.

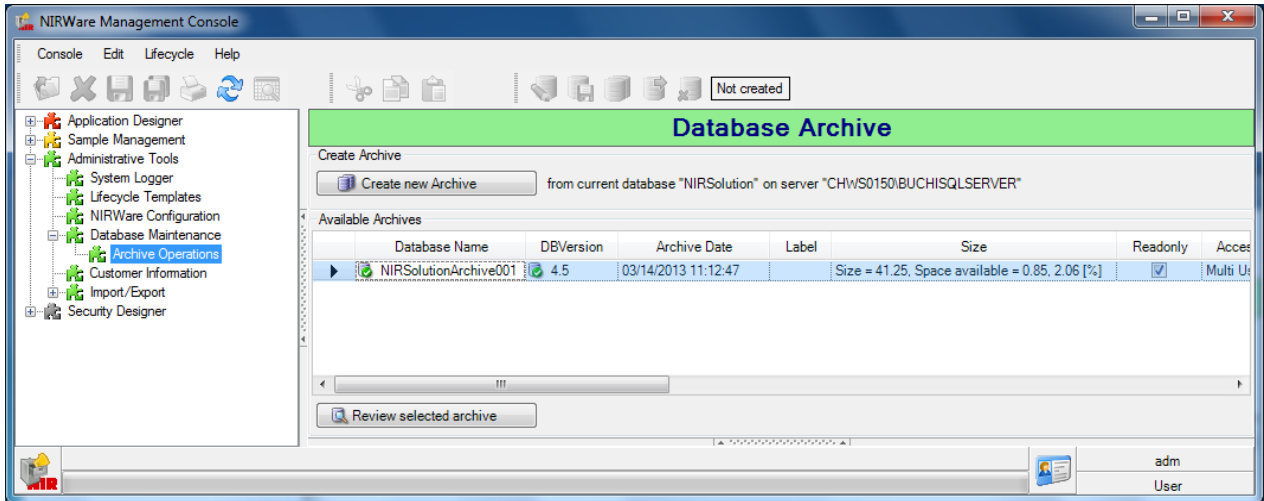
NOTE:

The names of archive and new database are automatically changed when the status is changing. The new database inherits the name of the original database, while the archive is labelled as previously specified by the user.

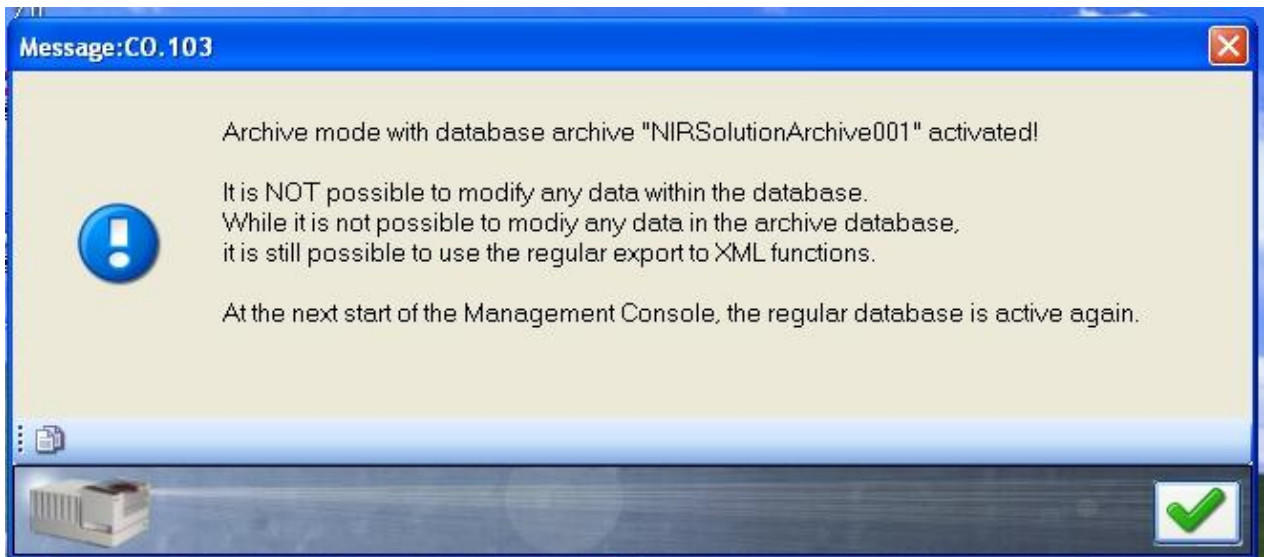
The old and new archives are interlinked by entries in their respective audit trails. Therefore it is always clear where an archive is originated from, and what archive has been created from the current database.

Reaccessing an archive

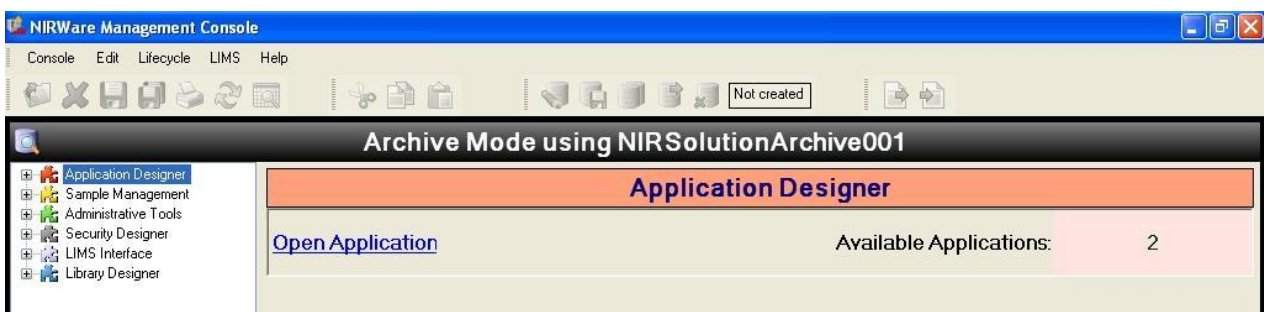
Archives cannot be modified anymore but they can be accessed in read-only mode from the NIRWare Management Console to view old measurements. For this purpose select **Administrative Tools - Database Maintenance - Archive Operations**.



Now select an archive from the list and click "**Review selected archive**". This will initiate a process that will restart the management console in archive-mode. You have to log in again and will see the following message:



Now click the green checkmark button to have read-only access to the selected archive. The archive mode is indicated by a black frame around the window and an additional header:



NOTE:

The productive (new) database contains an audit trail entry with the following content:

- *Time stamp, User, PC name, name of archive*
- *Names and files for productive and archive database*
- *List of copied applications, version, GUID*
- *List of copied library designer calibrations*
- *Remarks*

Tips and tricks

No interference during backup- or archiving activities

IMPORTANT RECOMMENDATION:

Never switch off the computer or interfere in any other way with a running backup- or archiving process! Even though NIRWare is using integrated safety measures (e.g. transactions) to prevent data loss, it is important to not disturb any sensitive system processes.

'Speaking names' for database and archive labels

The label of an object should carry helpful information, especially concerning location and timeframe. 'Archive2' for example is not giving any indication about where and when the data therein have been created, while 'NIRArchive Aug2008-Jun2009 Flawil plant' is telling much more of a story.

Snap-Ins

By accessing the archive functions of the Management Console, the tree-menu is reduced to the Administrative Tools. The other menu items ('snap-ins') must be manually restored after finishing with the archiving tool. This is done via Console – Snap Ins, and adding the entries from the 'Available Snap-Ins'- to the 'Selected Snap-Ins'-list.

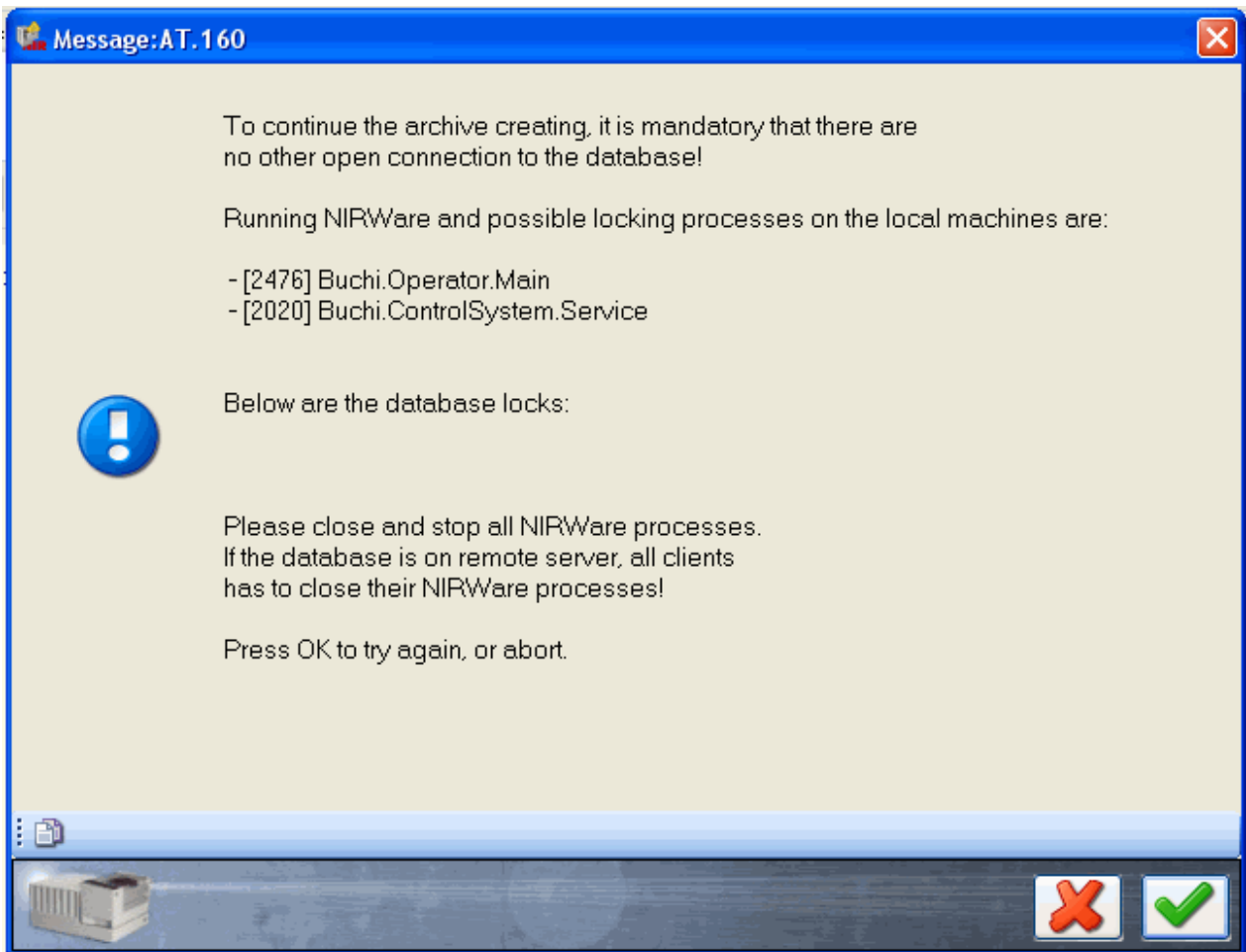
Data Storage

IMPORTANT RECOMMENDATION:

Please regard archives as your 'treasure chests', because they contain your precious data. Therefore make sure the archives are stored away in a safe place (e.g. on streamer backup-tapes in a fireproof safe).

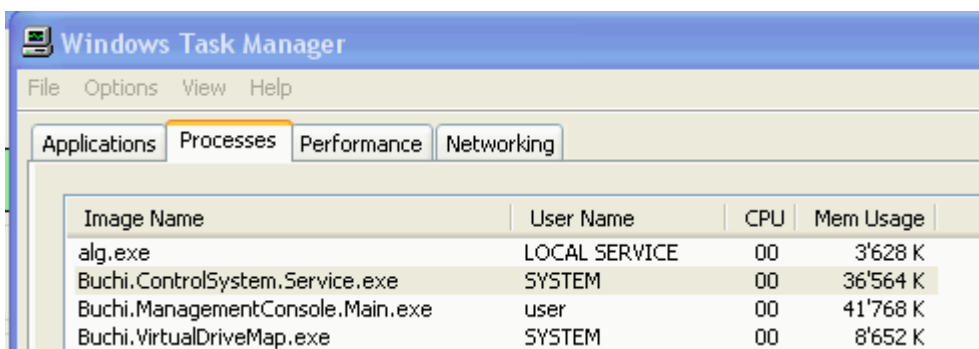
Closing the NIRWare Operator and stopping the Control System Service (CSS)

If the BUCHI.ControlSystem.Service was not stopped before archiving or the NIRWare Operator is still open, the following message appears:



If the NIRWare Operator is still open, close it now.

If the Control System Service is still running, you can stop it via the Windows Task Manager:



For this purpose, right-click it in the list and select "**Stop Service**".

6.4.6. Customer Information Configuration

The Customer Info Configuration dialog serves to define the customer information displayed in the header of the measuring results report.

To open it, in the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Customer Info**.

The following dialog opens:

Customer Info Configuration	
Company Name	
Address	
Postal Code	
City	

Enter the corresponding information in the provided cells and click the Save icon to save your settings.

NOTE

All customer information is optional. The cells can also be left blank.

6.4.7. Import / Export

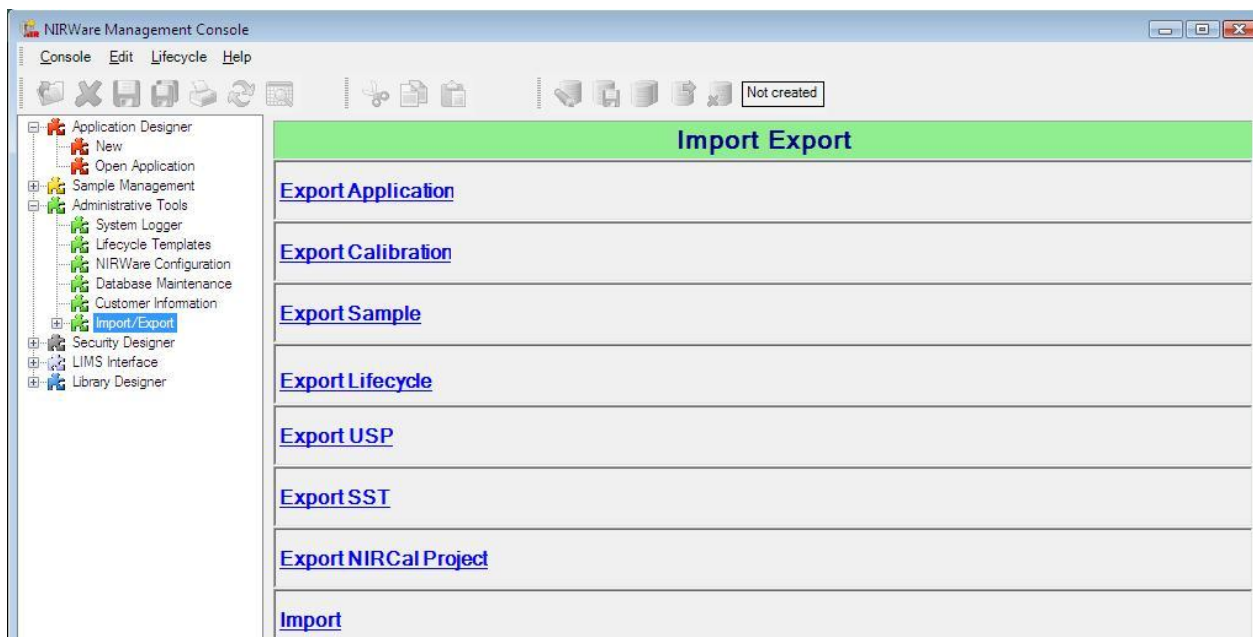
Introduction Import / Export

The Import / Export functions enable to export data from the local database to an *.xml (extensible markup language) file.

It will be possible to export:

- Applications
- Calibrations
- Samples
- Lifecycle
- USP test results
- SST test results
- NIRCAl Projects

Each of the exported files can then be imported to another NIRWare database by means of the import function.



Export Application

With the Function "Export Application" applications including all necessary parameters such as instrument settings, operator configuration, calibrations and property settings will be exported.

Applications can be exported with or without spectra and corresponding reference values.

To export applications proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Import/Export - Export Application**.

The following dialog opens:



The dialog lists all applications available in the software in a table.

Table columns

The table consists of six columns:

Name	Application name
Description	Optional information entered during application design
Version	Copy number in the course of the lifecycle
State	Lifecycle state
Type	Application type (Identification or Quantification)
GUID	Global Unique Identifier

Different possibilities are available to export an application with different attached information.

Select from the shown drop down menu the export type:

- Application and Calibration only (AC)
- Application, Calibrations with Calibration-Samples (ACs)
- Application, Calibrations with Calibration-Samples, all Measured-Samples and all Measurement-Results (AsCsR)

NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

Narrow down the information displayed in the table, using appropriate [filter](#) settings.

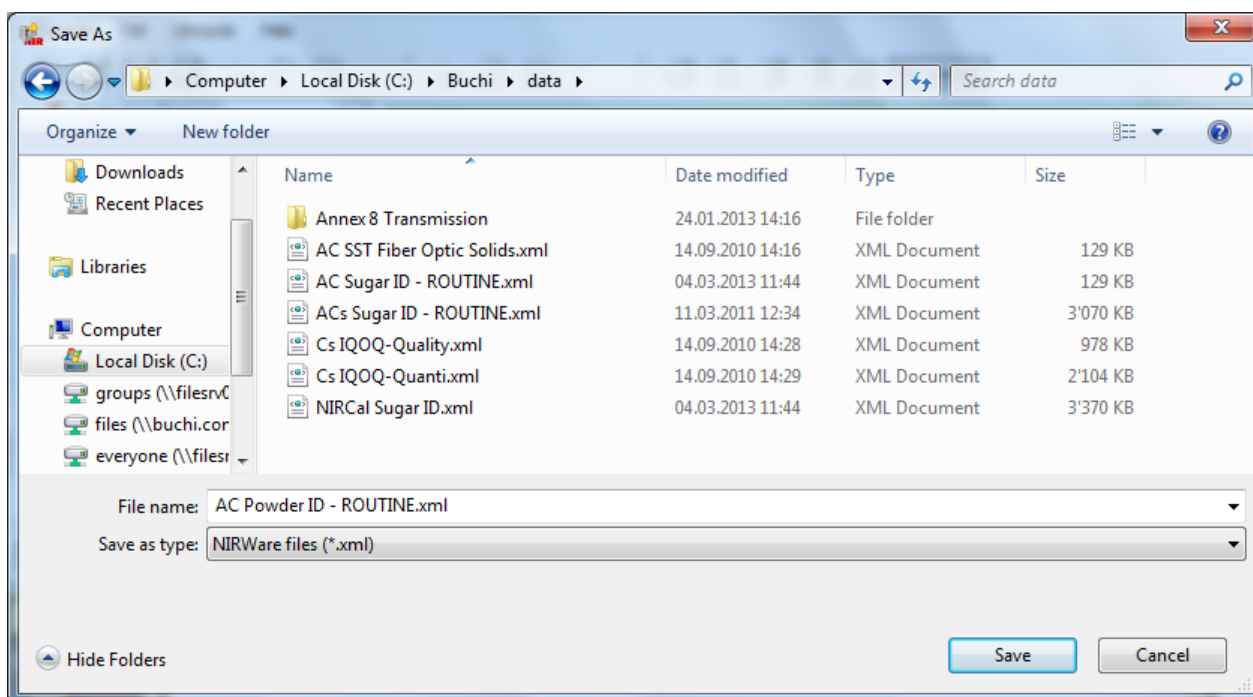
Export

To export an application, highlight the corresponding row in the table and click **Export** or doubleclick the entry.

NOTE

Only one application can be exported at a time.

A dialog opens, where you can select the path and the file name under which the exported application should be saved. Click **Save**.



Export Calibration

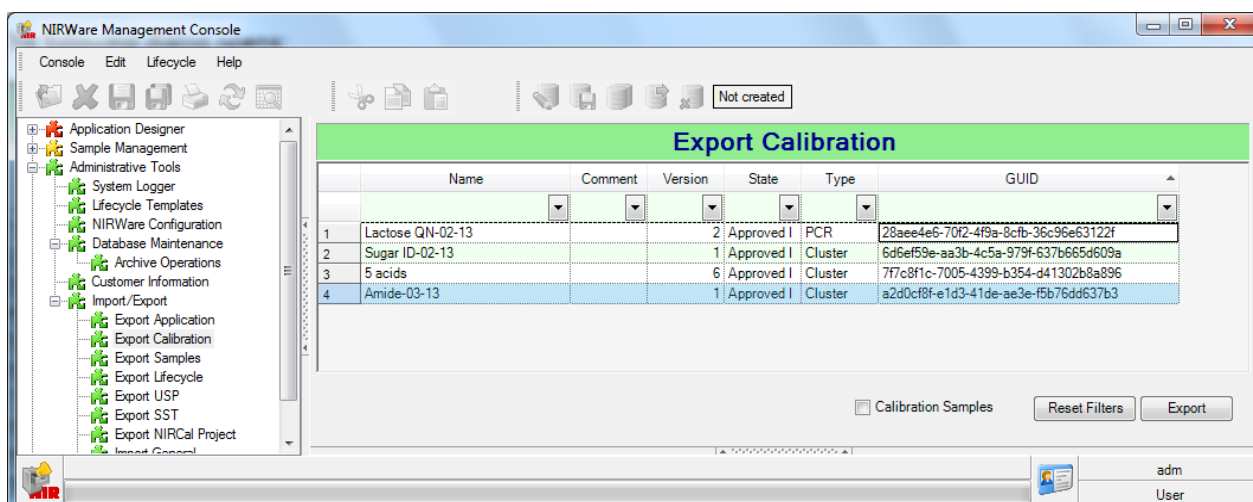
With the Function "**Export Calibration**" calibration models can be exported.

Calibrations can be exported with or without spectra and corresponding reference values.

To export calibrations proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Import/Export - Export Calibration**.

The following dialog opens:



The dialog lists all calibrations available in the software in a table.

Table columns

The table consists of six columns:

Name	calibration name
Comment	Optional information entered
Version	Copy number in the course of the lifecycle
State	Lifecycle state
Type	Calibration type (Cluster, Spectra Compare, SIMCA, PLS, PCR,...)
GUID	Global Unique Identifier

When you activate the check box **Calibration Samples** the calibration will be exported with corresponding spectra and reference values.

When the check box is not activated, the calibration will be exported without corresponding spectra and reference values.

NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

Narrow down the information displayed in the table, using appropriate [filter](#) settings.

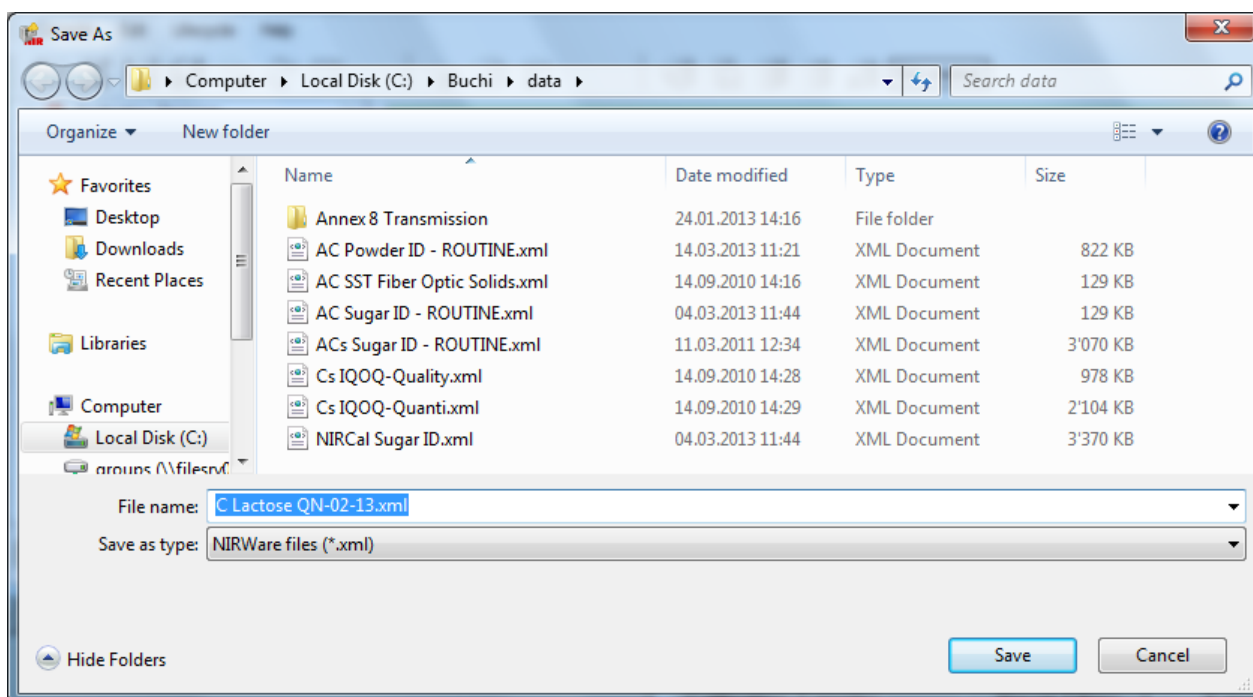
Export

To export a calibration, highlight the corresponding row in the table and click Export or doubleclick the entry.

NOTE

Only one calibration can be exported at a time.

A dialog opens, where you can select the path and the file name under which the exported calibration should be saved. Click **Save**.



Export Samples

With the Function "**Export Samples**" spectra with their corresponding reference values can be exported.

To export samples, proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Import/Export - Export Samples**.

The following dialog opens:

Export Sample							
	Name	Application	Version	Batch	Time Stamp	Customer Fields	No. Reference
1	123	Sugar Quant	1	test1	01/04/2007 17:23		
2	60				11/21/2006 13:54		
3	60				11/21/2006 13:53		
4	55				11/21/2006 13:53		
5	55				11/21/2006 13:52		
6	50				11/21/2006 13:52		
7	50				11/21/2006 13:52		
8	45				11/21/2006 13:51		
9	45				11/21/2006 13:51		
10	40				11/21/2006 13:50		
11	40				11/21/2006 13:50		

Reset Filters Export

NOTE

When you open the *Export Samples* dialog, the table is empty, since the loading procedure when opening

the dialog would take some time (depending on the amount of data). To display samples in the table, use the [filter](#) functions.

Table columns

The table consists of eight columns:

Name	sample name
Application	application name
Version	Copy number in the course of the lifecycle
Batch	Batch name entered during analysis
TimeStamp	Date and time
Customer Fields	Optional information of the customer entered during analysis (content of Customer Fields 1-6 is summarized here)
No. ReferenceValues	Number of assigned properties with reference values
Comment	Optional information entered

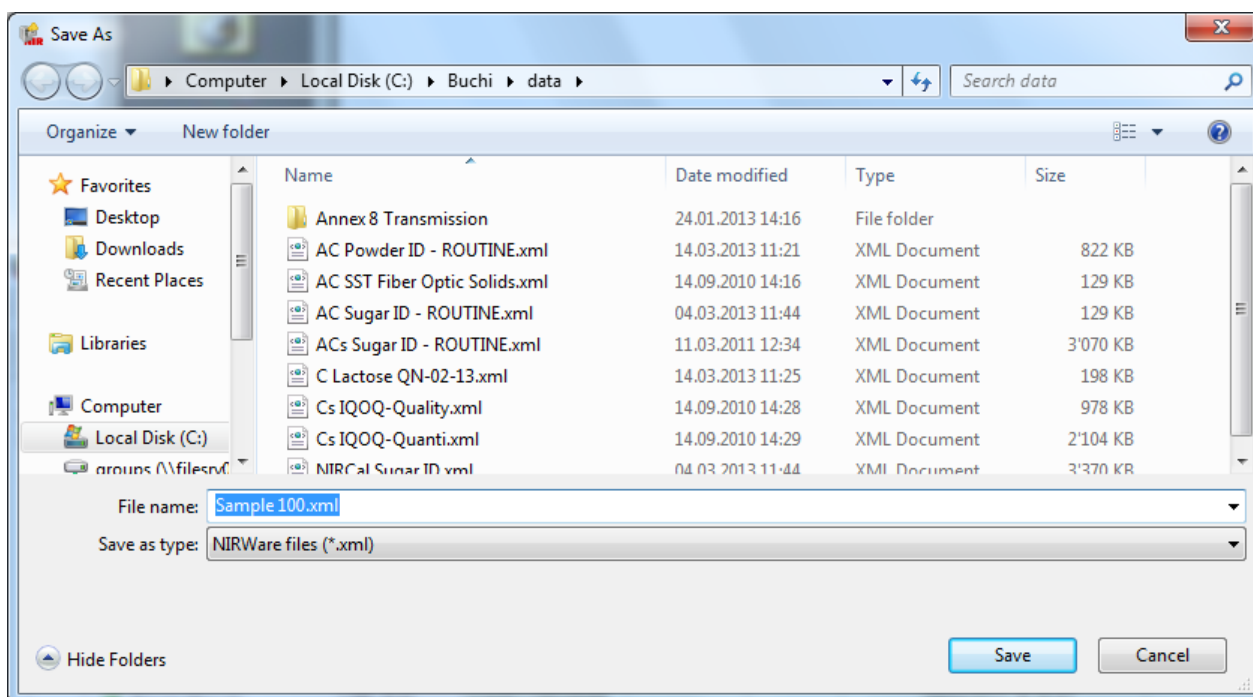
NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

Export

To export a set of samples, highlight the corresponding rows (multiple selection possible) in the table and click **Export** or doubleclick the rows.

A dialog opens, where you can select the path and the file name under which the exported samples should be saved. Click **Save**.

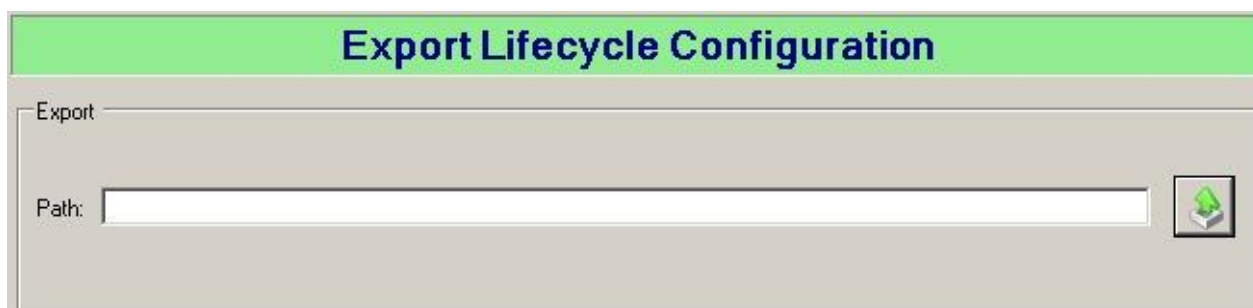


Export Lifecycle

To export a lifecycle template, proceed as follows:


In the file tree on the left side of the **NIRWare Management Console** select **Import/Export - Lifecycle**.

The following dialog opens:



Export



Click the Export icon (). A dialog opens, where you can select the name and path under which the corresponding lifecycle template should be saved. Click **Save**.

Export USP

With the Function "**Export USP**" performed USP reports and the data recorded during test procedure can be exported.

To export USP data, proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Import/Export - Export USP**.

The following dialog opens:



Narrow down the information displayed in the table, using appropriate filter settings.

Table columns

Type	
TimeStamp	Date and time
Success	SST passed (0= not passed; 1= passed results)
Aborted	SST test aborted (0= not aborted; 1= aborted tests)
Info	Additional test information such as reason for "not passed result"
User	User login account
ValidUp	Date up to which the USP Test is valid
Installed at	Installation date
Installed by	Full name who has performed installation
Standard	Standard type
Std. Serial	Serial number of standard
Std. Version	Version of standard
Instrument	Instrument type
Instr. Serial	Serial number of instrument
Cell	Cell type
Cell Serial	Serial number of measurement cell

NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

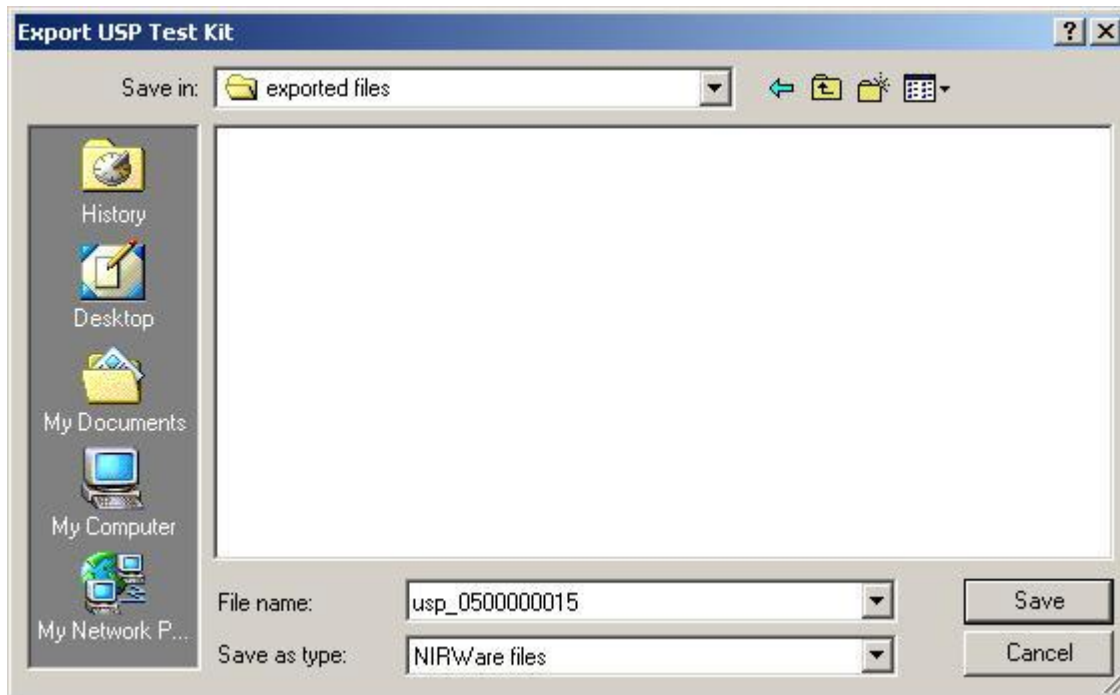
Export

To export a USP result, highlight the corresponding row in the table and click **Export**.

NOTE

Only one USP report can be exported at a time.

A dialog opens, where you can select the path and the file name under which the exported USP result should be saved. Click **Save**.



Export SST

With the Function "**Export SST**" performed SST reports and the data recorded during test procedure can be exported.

To export SST data, proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Import/Export - Export SST**.

The following dialog opens:



Narrow down the information displayed in the table, using appropriate filter settings.

Table columns

TimeStamp	Date and time
Success	SST passed (0= not passed; 1= passed results)
Aborted	SST test aborted (0= not aborted; 1= aborted tests)
Instrument	Instrument type
Cell	cell type
Option	option type
Instrument Serial	serial number of instrument
Cell Serial	serial number of measurement cell
Option Serial	serial number of measurement cell option (add-on)
Instrument Version	version of instrument
Cell Version	version of measurement cell
Option Version	version of measurement cell option (add-on)
Info	additional test information such as reason for "not passed result"
Full User Name	full name of the user

NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

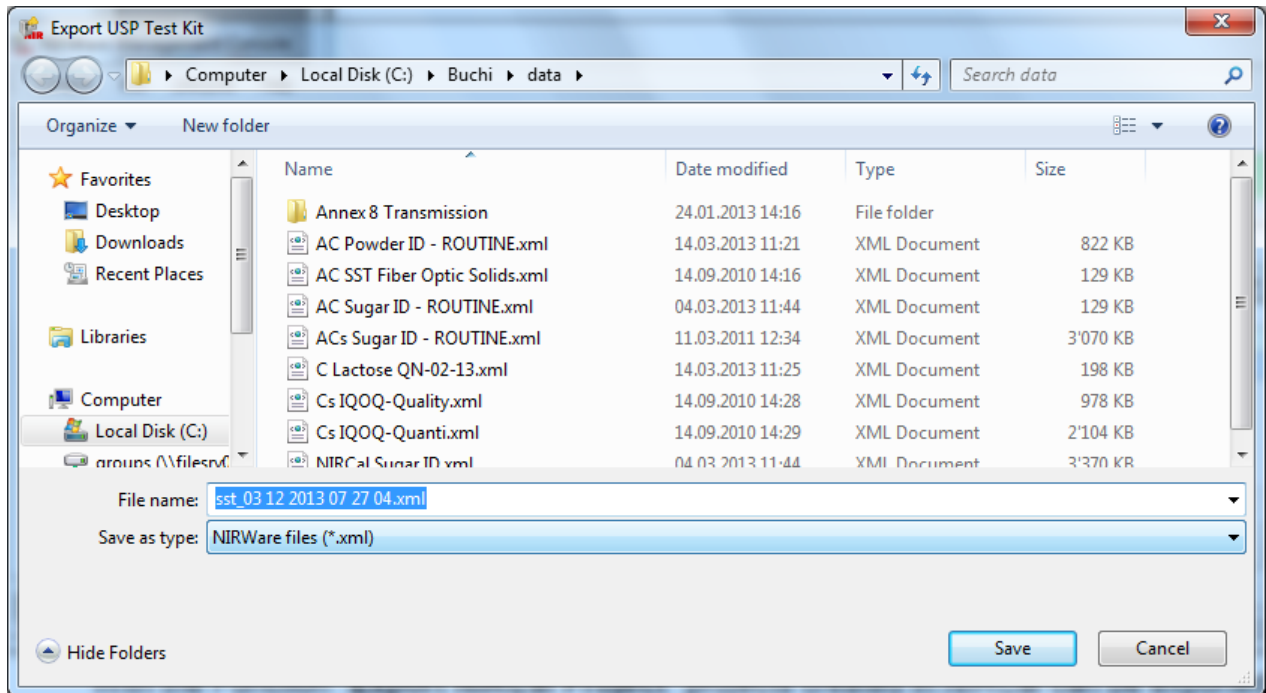
Export

To export a SST result, highlight the corresponding row in the table and click **Export**.

NOTE

Only one SST report can be exported at a time.

A dialog opens, where you can select the path and the file name under which the exported SST result should be saved. Click **Save**.



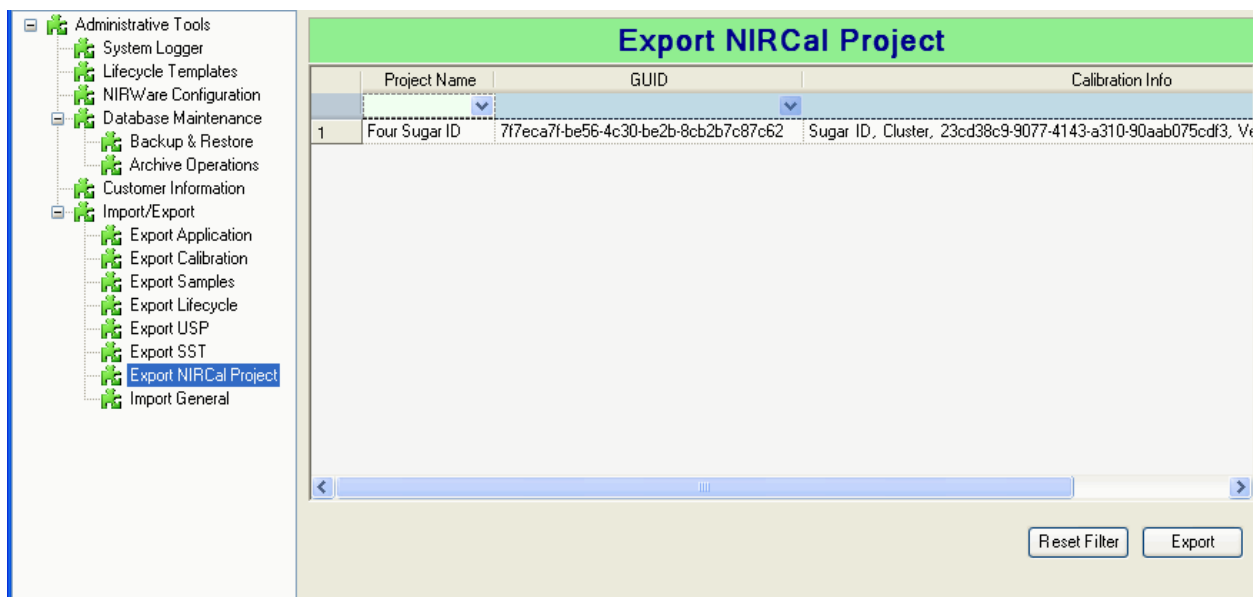
Export NIRCal Project

With the Function "**Export NIRCal Project**" projects created in NIRCal can be exported.

To export calibrations proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Import/Export - Export NIRCal Project**.

The following dialog opens:



The dialog lists all NIRCal Projects available in the software in a table.

Table columns

The table consists of six columns:

Project Name	Name of NIRCal Project
GUID	Global Unique Identifier
Calibration Info	Information describing the contained calibration

NOTE

You can sort alphabetical and inverse the order of the individual column entries by clicking the corresponding column header.

Narrow down the information displayed in the table, using appropriate [filter](#) settings.

Export

To export a NIRCal Project, highlight the corresponding row in the table and click Export or doubleclick the entry.

NOTE

Only one NIRCal Project can be exported at a time.

A dialog opens, where you can select the path and the file name under which the exported NIRCal Project should be saved. Click **Save**.

NOTE

An import into older versions of NIRWare is not possible.

Exporting data from archives

Although archives cannot be modified, it is nevertheless possible to extract information from them. This is done by using the export functions of the Management Console, which are always available in archive mode. For this purpose select **Administrative Tools - Import/Export**.



NOTE:

Importing data to an existing archive is not possible.

Import General

With the function "**Import General**" files, exported from a NIRWare database or customized settings can be imported into a different or new database.

This way it will be possible to import the following files:

- [application].xml with or without spectra
- [calibration].xml with or without spectra
- [sample name].xml
- [SST data].xml
- [USP data].xml
- [Life Cycle Template].xml
- [NIRCal Project].xml (NIRWare version 1.4 and higher)

To import files, proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Administrative Tools - Import/Export - Import General** or click **Import** in the submenu list in the center.

The following dialog opens:



Click the Browse icon .

A dialog opens, where you can select the xml-file with the corresponding information you want to import. Click **Open**.

NOTE

Depending on the file size, the import can take several minutes.

Importing applications, calibrations and sample spectra

During import there are 3 major types of **sample property** related data fields that are compared with already existing values in the database.

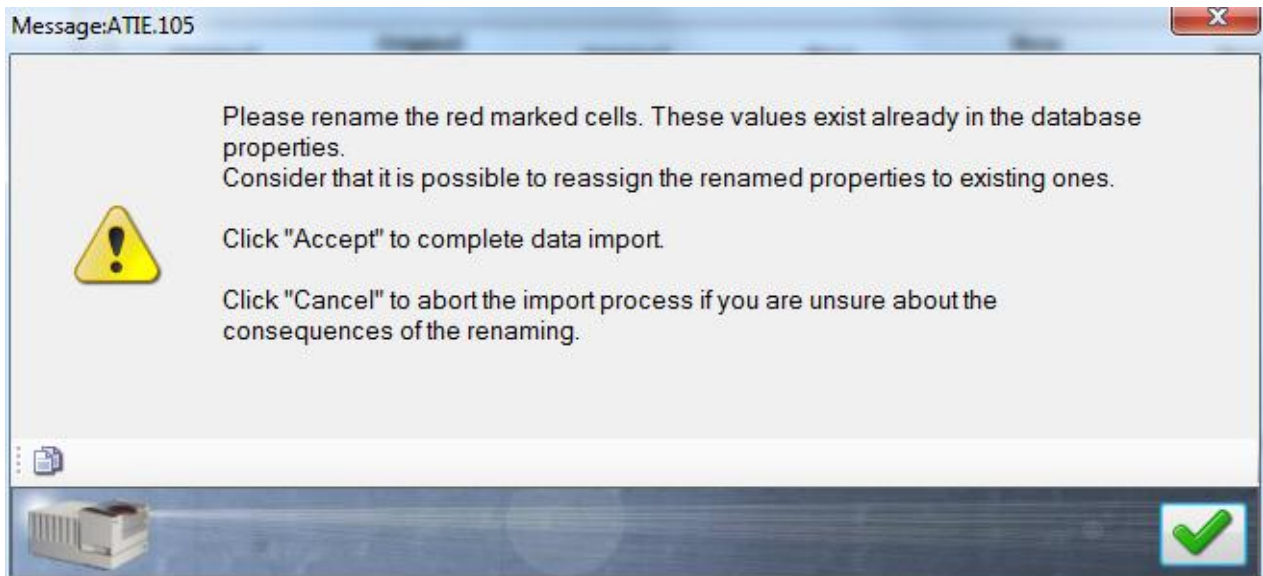
Property GUID, Property Name, Substance ID or unit

Different scenarios will result in different import dialogs.

The table shows the possible cases:.

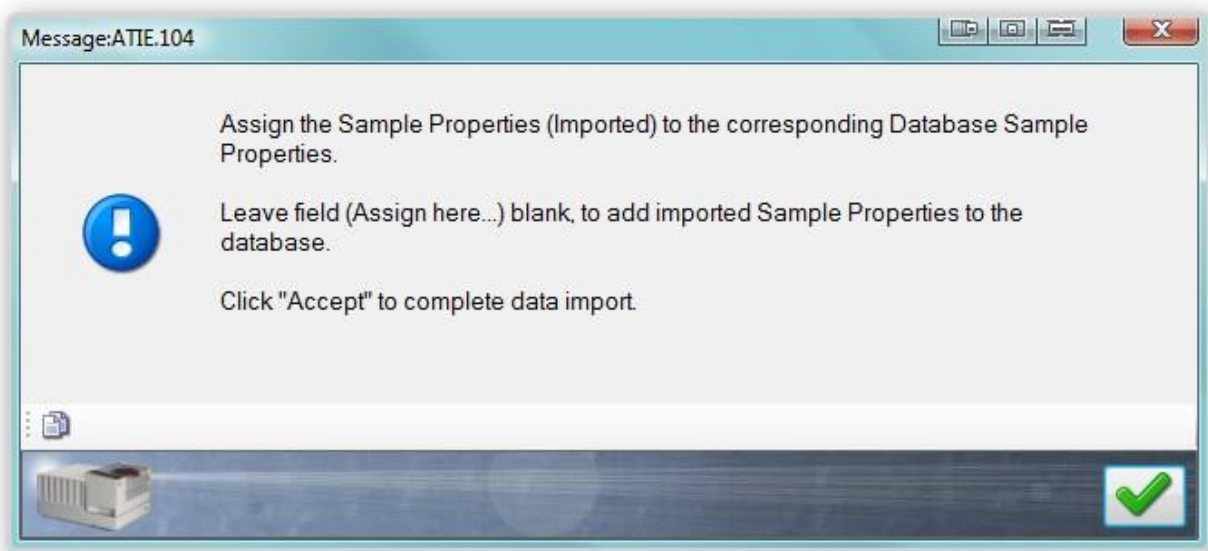
Import Property	Database Property	Behaviour
GUID Name Substance ID or Unit	not existent not existent not existent	Imported without any dialog
GUID Name Substance ID or Unit	identical identical identical	The property will not be imported but is linked to the database property
GUID Name Substance ID or Unit	identical different identical	Rename dialog appears
GUID Name Substance ID or Unit	identical identical different	Rename dialog appears
GUID Name Substance ID or Unit	different identical identical	Rename dialog appears
GUID Name Substance ID or Unit	different different different	Assign dialog appears

The **rename dialog** appears in case of conflicts between name, substance ID, unit and GUID. A renaming has to be done first. In the next step the property can be assigned to existing ones in the database or be imported as a new one.



Original property name	Original property substance ID	Original property unit	New property name	New property substance ID	New property unit
Fructose	Fruchtzucker		Fructose	Fruchtzucker	

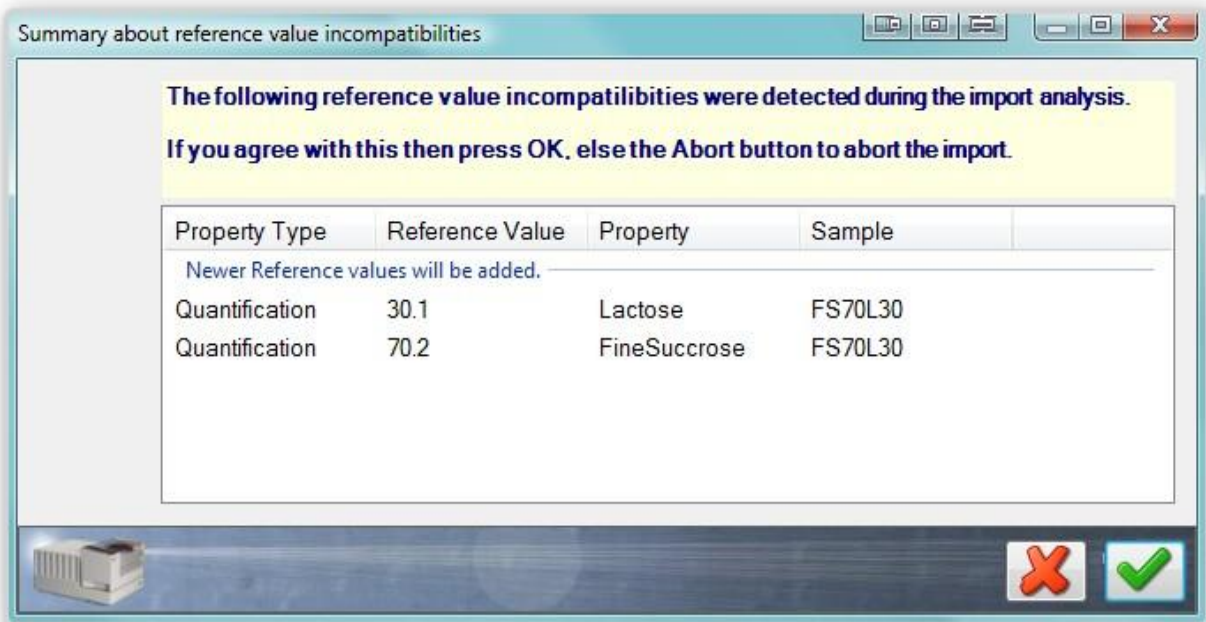
The **assign dialog** allows to link properties that are imported to existing ones in the database.



Reference values

The reference values contain a time stamp.

<p>Reference value (GUID) is already in the database, value is the same</p>	<p>Will not be imported</p>
<p>Reference value (GUID) is already in the database, value is not the same</p>	<div data-bbox="411 504 1433 907" data-label="Image"> </div> <p>Cancel = the reference value in the database will be kept OK = the imported reference value will be taken</p>
<p>Reference value for sample and property exists in the database, times tamp of the data being imported is older</p>	<p>Will not be imported</p>
<p>Reference value for sample and property exists in the database, time stamp of the data being imported is newer and values are not the same</p>	<div data-bbox="391 1458 1444 1861" data-label="Image"> </div> <p>Cancel = the reference value in the database will be kept OK = the imported reference value will be taken</p>



Cancel = import breaks

OK = import continues

6.5. Security Designer

6.5.1. Introduction Security Designer

To open the Security Designer proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Security Designer**. The following dialog opens:



You can now open a submenu by clicking on their names in the file tree or in the center of the Security Designer window.

The Security Designer serves as user administration tool within the NIRWare and NIRCAl software packages. It enables you to realize your own security policy for user access.

The general user management concept within the NIRWare Security Designer provides that every user is part of a user group. For this reason you should have a clear concept of the user groups you need for your work with the NIRFlex N-500.

Related Topic:

[Default user groups](#)

[Default users](#)

6.5.2. Users and Groups

Default users

By default, four users are provided, which can be adapted, completed or disabled.

NOTE:

The default user accounts do not have password protection. It is strongly recommended to enter passwords for the accounts or to disable the accounts after new accounts have been created.

User	Full Name
Administrator	Administrator
Designer	Designer
Operator	Operator
QManager	QManager
Service	Service

Default user groups

Default user groups and default assignments of users to the groups are shown in the following table:

User Groups	Comment	Group Members
Administrators	System Administrators	Administrator (individual user)
Designers	Application & Calibration Designers	Designer (individual user) + Administrators (user group)
Operators	Routine Task Operators	Operator (individual user)

		+ Administrators and Designers (user group)
QManagers	Quality Assurance Managers	QManager (individual user) + Administrators (user group)
Service	Service Technicians	Service (individual user) + Administrators (user group)

NOTE:

Working with user groups helps to reduce administration work for the account policy. All members of a user group have the same rights. That means, it is not needed (but possible) to define for each NIRWare user individual settings (**not recommended**).

NOTE:

The default assignment of user groups to superior user groups results in the fact that by default all members of the Administrators group have access to the applications and functions available to the Designers and Operators group and all members of the Designers group have access to the applications and functions available to the Operators group.

Creating a new user

To create a new user proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Security Designer – Users and Group – New User** or click **create a new user** in the submenu list in the center.

The following dialog opens:

* New User	
Title	Values
Name	James
Full Name	James Pattern
Comment	new user
Password	*****
Password Verification	*****
Password never expires	<input type="checkbox"/>
Enabled	<input checked="" type="checkbox"/>

You can now fill in the fields.

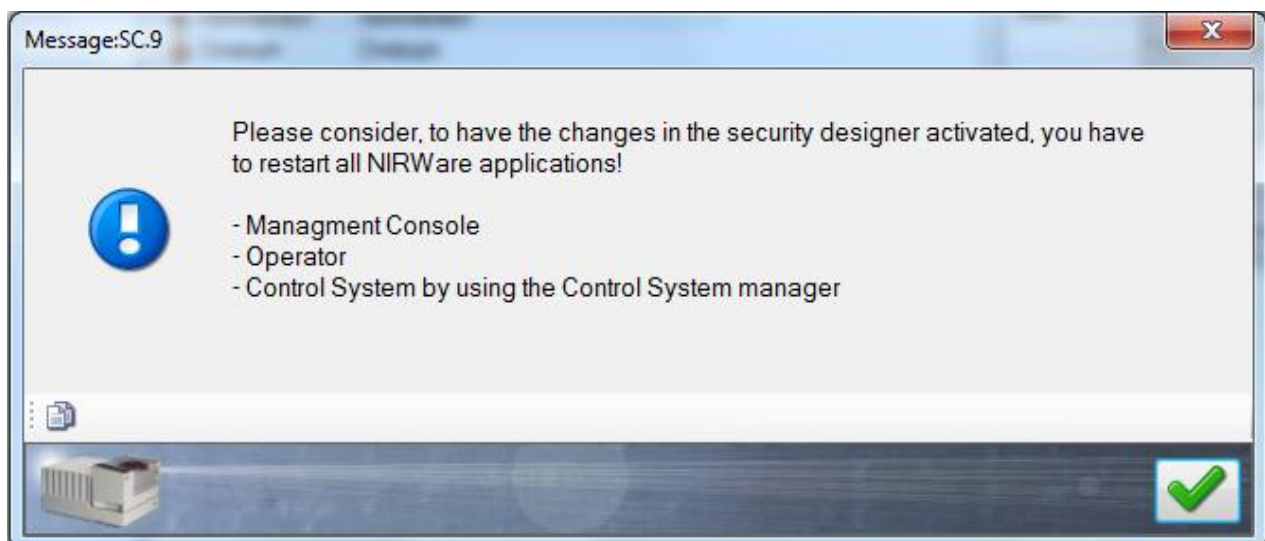
NOTE

The individual settings made for a user always take the priority over the general account policy settings.

Name	Name of the new user to be used for the logon.
	NOTE

	The number of signs required for a user name is set in the Account Policy. The default value is 0. The user name may only consist of one word, spaces are not accepted. To provide more information about the user, enter it in the Full Name field, where spaces are allowed.
Full Name	Full name of the user providing more information.
Comment	Optional comment for the user.
Password	User password
Password Verification	Second entry of the user password as a verification
Blank Password	When this check box is activated, the password fields are switched dim and no password is required for the logon of the user. NOTE For security reasons we recommend to always use a password.
Password never expires:	When this check box is activated the user password always remains active.
Enabled	When this check box is activated, the corresponding user is enabled and has the right to log on. When the checkbox is not activated, the user is disabled and cannot log on anymore.

To save your entries, click the Save icon. The following message appears, that you have to confirm:



A new dialog opens:

Manage existing users						
Name	Full Name	Comment		Category	Property	Value
Administrator	Administrator			User	Name	James
Christoph	Christoph				Full User Name	James Pattern
Designer	Designer				Comment	new user
dev	dev				Enabled	<input checked="" type="checkbox"/>
James	James Patten	new user		Password	Password	*****
Operator	Operator				Password confirmation	*****
QManager	QManager				Change Password At Next Logon	<input type="checkbox"/>
Service	Service				Password Never Expires	<input type="checkbox"/>
test	test	test			Password expired	<input type="checkbox"/>

The upper table in the center lists all users defined in the software with their name and full name and with the comments assigned, i.e. it also contains the user you recently added.

Creating a new user group

The 3 given user groups (Administrators/Designers/Operators) are sufficient for most NIRWare installations.

To create a new user group proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Security Designer – Users and Groups – New User Group** or click **create a new user group** in the submenu list in the center.

The following dialog opens:

* New User Group	
Title	Values
Name	Application Specialist
Comment	
Add a comment to the new user group	
<div style="border: 1px solid gray; padding: 5px;"> ✓ ✗ New user group </div>	

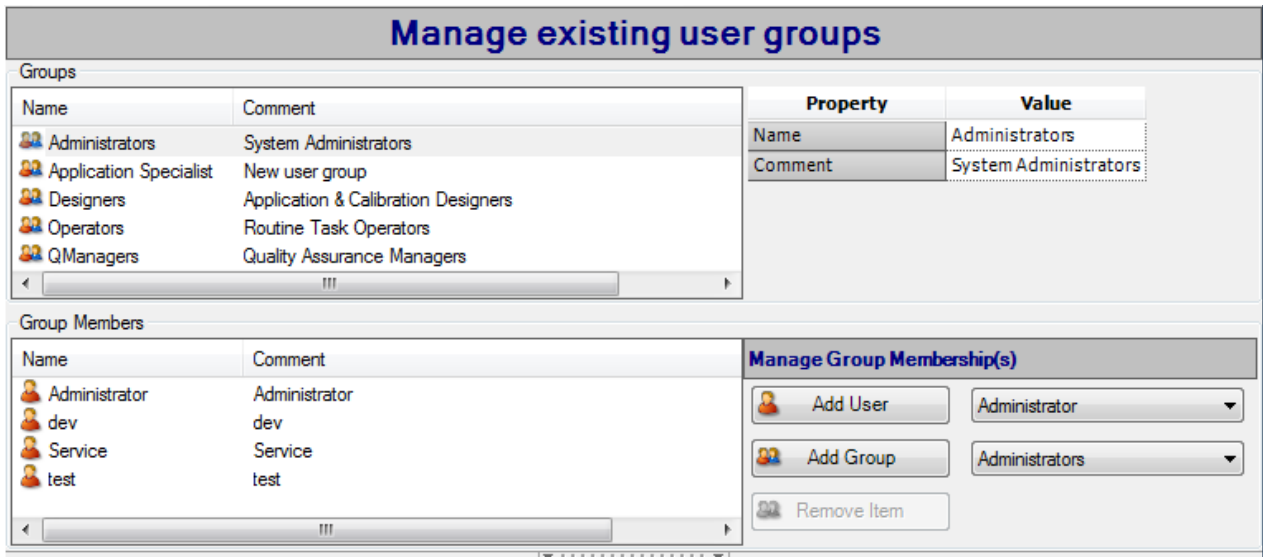
You can now enter a name and an optional comment for the new user group.

NOTE

The number of signs required for a user group name is set in the Account Policy. The default value is 3.

To save your entries, click the Save icon.

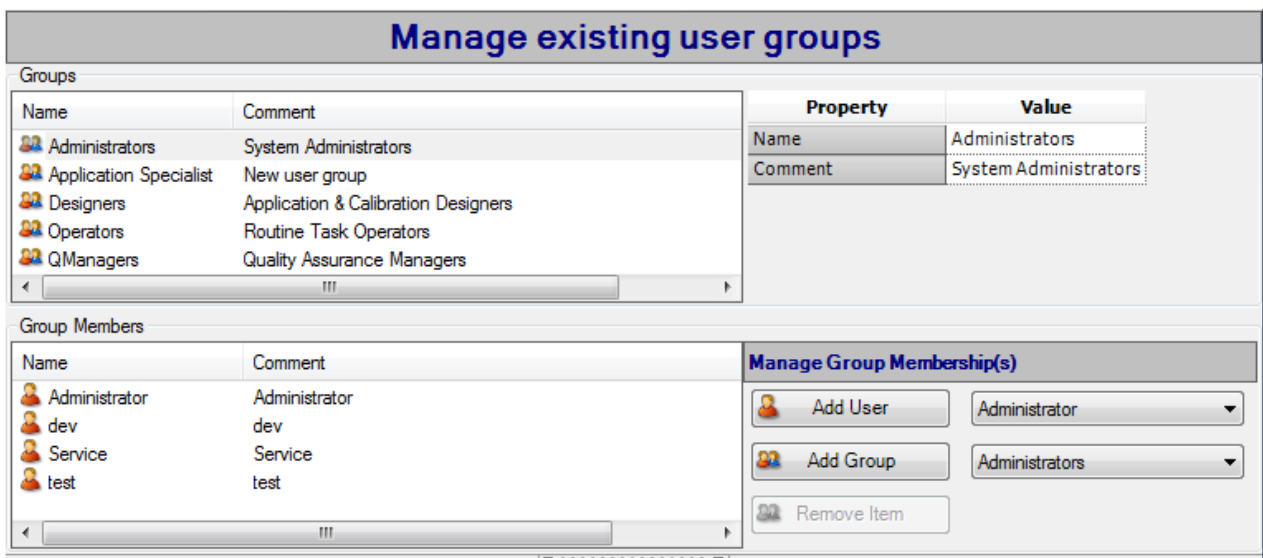
A new dialog opens:



The upper table lists all user groups defined in the software with the comments assigned, i.e. it also contains the user group you recently added.

Assigning a user to a user group

In the file tree on the left side of the **NIRWare Management Console** select **Security Designer – Users and Group – User Groups** or click **manage existing user groups** in the submenu list in the center.



NOTE

After you added a user group you will automatically get to this dialog.

To assign a user to a user group proceed as follows:

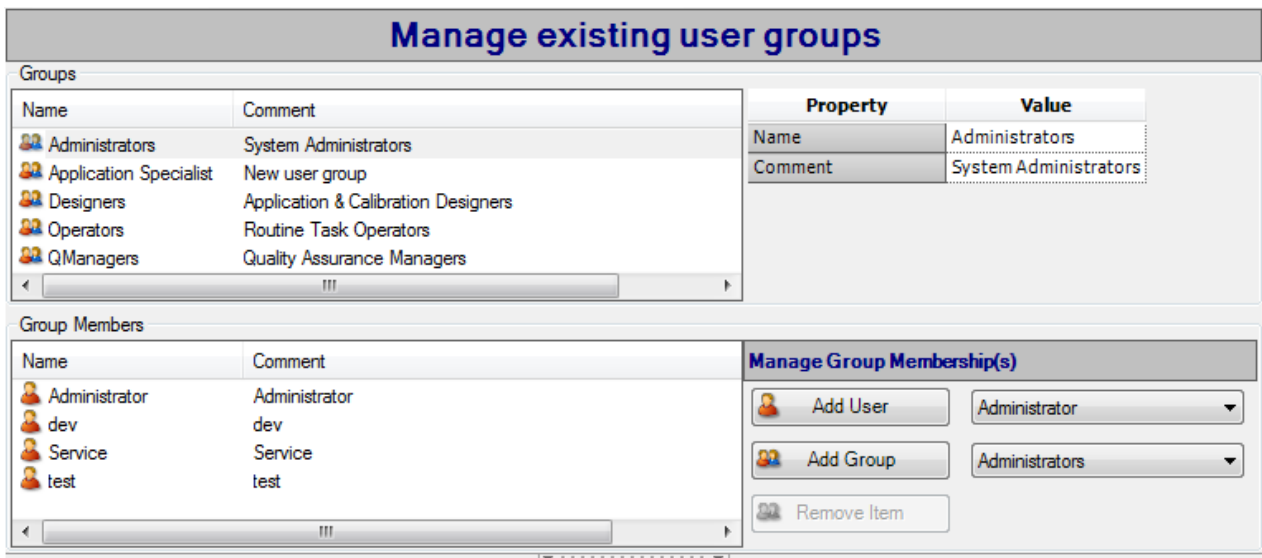
1. In the dialog for user groups (see above) highlight the user group to which you want to add a user in the upper table.
The group members already assigned to this user group are now listed in the table below.
2. Click the arrow next to the upper listbox.
A drop-down list opens, listing all available users.
3. Select the user you want to add by highlighting it and click **Add User**.
The user is now added to the table below.

To save your entries, click the Save icon.

Assigning user groups to a superior user group

The complex administration structure of the Security Designer allows you to add a whole user group to a superior user group.

In the file tree on the left side of the **NIRWare Management Console** select **Security Designer – Users and Group – User Groups** or click **manage existing user groups** in the submenu list in the center.



NOTE

After you added a user group you will automatically get to this dialog.

To assign a user group to a superior user group proceed as follows:

1. In the dialog for user groups (see above) highlight the superior user group to which you want to add a user group in the upper table.
The group members already assigned to this user group are now listed in the table below.
2. Click the arrow next to the lower listbox.
A drop-down list opens, listing all available user groups.

- Select the user group you want to add by highlighting it and click **Add Group**.
The user group is now added to the table below.

To save your entries, click the **Save** icon.

Changing name and comments for existing users

NOTE

Once a user account has been created and has been used, 'Name' or 'Full User Name' should not be changed at any time.

In case the user's family name has changed and the profile needs to be updated, you need to create a new account for this user and disable the existing one.

To change the other possible settings for an existing user, highlight the corresponding user. The current name and comment for this user and his current user account policies are displayed in the table on the right.

Manage existing users						
Name	Full Name	Comment		Category	Property	Value
Administrator	Administrator			User	Name	James
Christoph	Christoph				Full User Name	James Pattern
Designer	Designer				Comment	new user
dev	dev				Enabled	<input checked="" type="checkbox"/>
James	James Pattern	new user		Password	Password	*****
Operator	Operator				Password confirmation	*****
QManager	QManager				Change Password At Next Logon	<input type="checkbox"/>
Service	Service				Password Never Expires	<input type="checkbox"/>
test	test	test			Password expired	<input type="checkbox"/>

NOTE

The individual settings made for a user always take the priority over the general account policy settings.

You can now click in the value lines of the table and change the corresponding value by entering a new text or activating or deactivating a checkbox:

User:

Name	Do not change this entry!
Full User Name	Do not change this entry!
Comment	Optional comment for the user.
Enabled	When this check box is activated, the corresponding user is enabled and has the right to log on. When the checkbox is not activated, the user is disabled and cannot log on anymore.

Password:

Password	This line appears twice and represents the user password and the password verification.
Change Password at next logon	When this check box is activated the user is prompted to change his password during the next logon.
Password never expires	When this check box is activated the user password always remains active.
Password expires	When this check box is activated the user's password expired, so that he cannot log on anymore. To undo this, deactivate the check box.

NOTE

When an administrator assigns a new password to another user, he should check the option "Change Password at next logon" for that user. Any passwords assigned by the administrator will not be recorded and checked in the password history list (if enabled).

To save your entries, click the **Save** icon.

Changing name and comments of existing user groups

To change the settings for an existing user group, highlight the corresponding user group. The current name and comment for this group is displayed in the table on the right.

You can now click in the value lines of the table and change the corresponding value:

Manage existing user groups

Groups

Name	Comment	Property	Value
Administrators	System Administrators	Name	Administrators
Application Specialist	New user group	Comment	System Administrators
Designers	Application & Calibration Designers		
Operators	Routine Task Operators		
QManagers	Quality Assurance Managers		

Group Members

Name	Comment	Manage Group Membership(s)	
Administrator	Administrator	Add User	Administrator ▼
dev	dev	Add Group	Administrators ▼
Service	Service	Remove Item	
test	test		

Name	Name of the user group
Comment	Optional comment for the user group

To save your entries, click the **Save** icon.

Defining the account policy

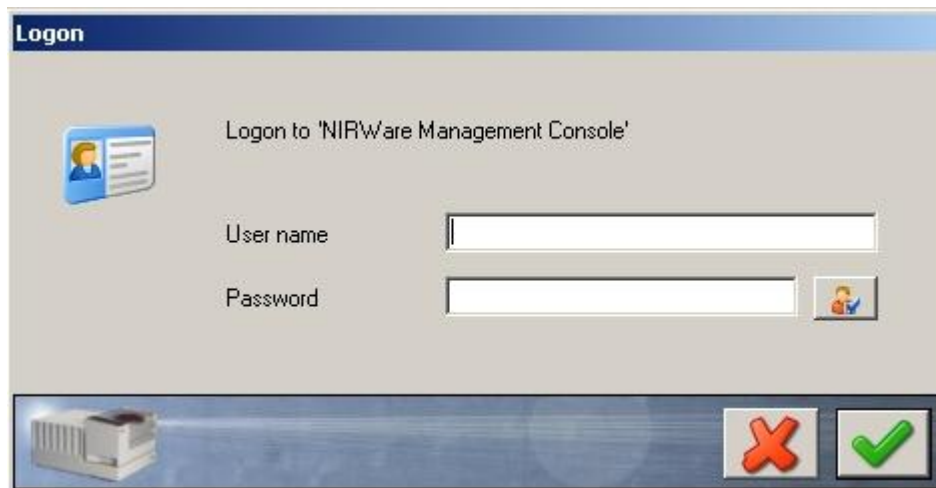
A general account policy is defined in the submenu Account Policy:

Account Policy		
Title	Values	Unit
Minimum User Name Length	3	
Password History Enabled	<input checked="" type="checkbox"/>	
Password History length	10	
Password Expiration Days	90	[Days]
Show Warning Before Expiration (Days)	21	[Days]
Minimum Password Length	0	
Password Complexity Rule Enabled	<input type="checkbox"/>	
Max. Allowed User Inactivity Time	0	[min]

Here you can see the default definition of the account policy. By entering a new value in the value column and activating or deactivating the checkboxes you can change the preset definition. Click the Save icon afterwards.

When the function "Password History Enabled" is activated the number defined in the field "Password History length" defines how many previous passwords are remembered by the program, so that it is not allowed to reuse them.

The "Max. Allowed User Inactivity Time [min]" defines the time interval after which the currently logged in user is logged out when he has not operated the software. The software is now locked for operation and the logon window appears again. The person that was last logged in has to enter his User name and password and click the arrow key to unlock the software. To disable this function, enter the value 0.



NOTE

When the checkbox "Password Complexity Rule Enabled" is activated, consider the password complexity rule described in the field below the table.

Reasons for electronic signature

The electronic signature is required for the lifecycle transition of applications in the Lifecycle model ERES.

To apply the electronic signature you have to state a reason. The lists given in the submenu "Reasons for electronic signature" enable you to define the reasons available for the different user groups:

The screenshot shows a software interface for managing reasons for electronic signature. The main window is titled "Reasons for electronic signature". At the top right, there is a "User group:" dropdown menu currently set to "Administrators". The interface is divided into two main sections. The left section, titled "All reasons", contains a table with 15 rows of reasons. The first row, "Application approved by:", is highlighted with a blue selection bar. Below this table are two buttons: "New" and "Delete". A green arrow button is located between the two tables. The right section, titled "Reasons of selected user group", contains a table with the same 15 reasons as the left section. Below this table is a "Remove" button.

The list on the left shows all reasons currently available.

To create a new reason, click **New**. An empty list field is added at the bottom of the table that you can fill in.

To delete a reason from the list, highlight it by clicking on it and click **Delete**.

To define which reasons shall be available for a certain user group, proceed as follows:

- Select the corresponding user group from the drop down menu on the top of the right side.
- Highlight the reasons on the left side in the list (multiple choice is possible) and click the green arrow. The corresponding reasons are copied to the right.

To remove one or several reasons from the list on the right, highlight it/them and click **Remove**.

NOTE

The Reasons for electronic signature will also be recorded in the system logger.

6.5.3. Security Policies

Default user group access rights

The following table gives an overview of the access rights of the default user groups to individual software modules and actions.

If you create a new users group and add it to one of the existing groups, all rights will automatically be handed down.

If you create a new users group without adding it to an existing group, its access rights have to be configured in the Security Policies.

	Administrators	Designers	Operators	QManagers
Administrative Tools	x			
Application	x	x	x	x
NIRCal		x		x
Operator			x	
Sample Manager		x		x
Acceptance of external references		x		
Security Designer	x			
Library Designer		x		x
Nadia Viewer	x			
Operator Access to applications in development		x		
Operator access to checked applications		x		
Edit Reference Values		x		
Application Designer		x		x
Show and Edit Advanced Settings		x		
Edit expert values				
LIMS Interface Settings		x		x
LIMS Interface Using			x	x
Firmware Update	x			
Advanced Database Manager	x			

NOTE

The option “Operator access to applications in development” makes only sense in combination with “Operator access to checked applications”.

Assigning user rights for applications

By default, all users and user groups have full access to all calibrations and applications created in the software.

To define access rights only for certain users or user groups, on the left side of the **NIRWare Management Console** select **Security Designer – Security Policies – Application**.

NOTE

There are two slightly different types of dialogs on which to assign user rights. One type is used for the security policies of applications, the other type is used for all the other functions.

In the following, the two dialog types are explained by means of an example.

The following dialog opens:

The screenshot shows a software interface for configuring access rights for an application. The window title is '* Application'. It is divided into two main sections.

Select items to configure access rights

Name	Version	State	Assigned Users / Groups
Copy of Meat	7	Created Idle	
Copy of Meat	5	Approved Idle	
Copy of test-lifecycle2	1	Checked Idle	
▶ Meat	6	Approved Idle	1
Meat	4	Approved Idle	
Rice	2	Approved Idle	
test	0	Created Idle	
test2	0	Created Idle	
test-lifecycle	5	Checked Idle	
test-lifecycle2	0	Approved Idle	
test-lifecycle3	0	Approved Idle	
test-lifecycle-new	0	Created Idle	
Yoghurt	2	Approved Idle	
Yoghurt-no Key	1	Approved Idle	

On the right side of this section, there are two buttons: 'Add' and 'Remove'.

Assigned users and groups

Type	Name	Comment	Read	Write	Delete	Deny
▶	James	James Pattern	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

On the right side of this section, there are two sections for adding users and groups:

- Users:** A dropdown menu showing 'James' and an 'Add' button.
- User Groups:** A dropdown menu showing 'Administrators' and an 'Add' button.

In the upper area, select the item for which you want to modify the user rights by highlighting the corresponding line and click **Add**.

The selected item is now added to the Object ID list. The access to all items in the Object ID list is restricted to the users and user groups listed in the lower area.

To assign user rights to an item in the Object ID list, select the corresponding Object ID by clicking the arrow and highlighting it in the appearing drop-down list.

Now select a user or user group you want to assign by clicking the corresponding arrow and highlighting it in the appearing drop-down list. Click **Add**. The selected user or user group is added to the list in the lower area.

You can now define the access rights for the added user or user group by activating or deactivating the corresponding check boxes.

NOTE

To activate the user right, "Read", "Write" and "Delete" need to be checked, "Deny" has to remain unchecked.

To remove an item from the Object ID list, select the corresponding Object ID by clicking the arrow and highlighting it in the appearing drop-down list. Now click **Remove**. The assigned user rights for this item are automatically removed as well.

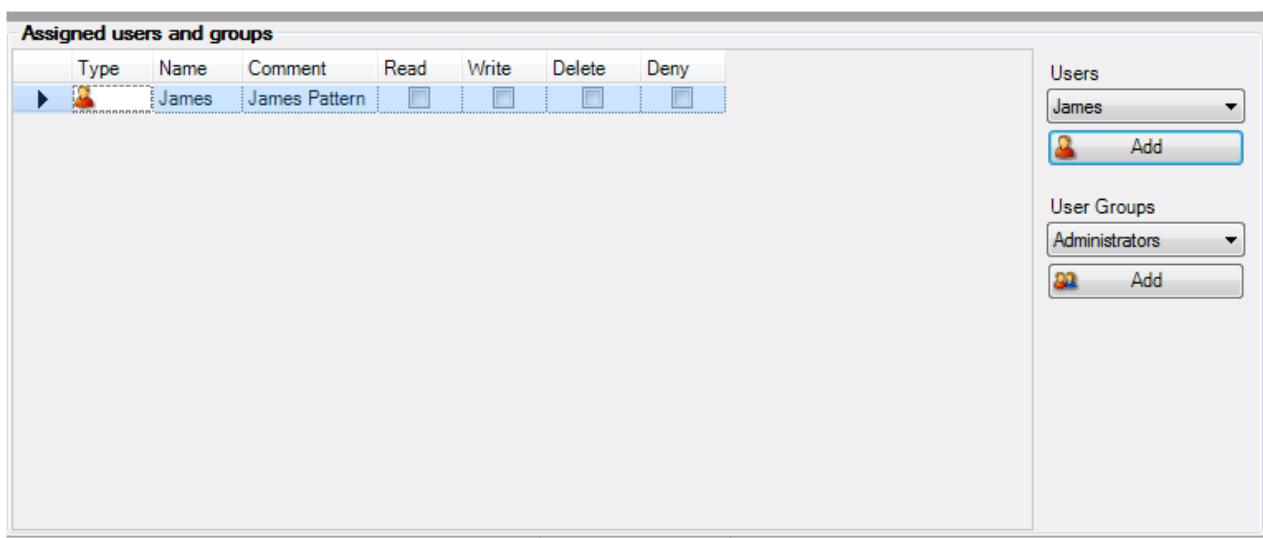
Assigning user rights for all remaining functions

By default certain access rights are assigned to the predefined users and user groups in the software package.

The procedure how to adapt them is explained in the following, considering the NIRCal software as example:

To complete, restrict or remove the default rights for NIRCal from certain users or user groups, on the left side of the **NIRWare Management Console** select **Security Designer – Security Policies – NIRCal**.

The following dialog opens:



Only the users and user groups listed in the center of the dialog have defined access rights to the software or function. All other have no access rights.

To add a user or user group to this list, click the corresponding arrow, highlight a user or user group from the appearing drop-down list and click **Add**.

The selected user or user group is added to the list in the center.

You can now define the access rights for the added user or user group by activating or deactivating the corresponding check boxes.

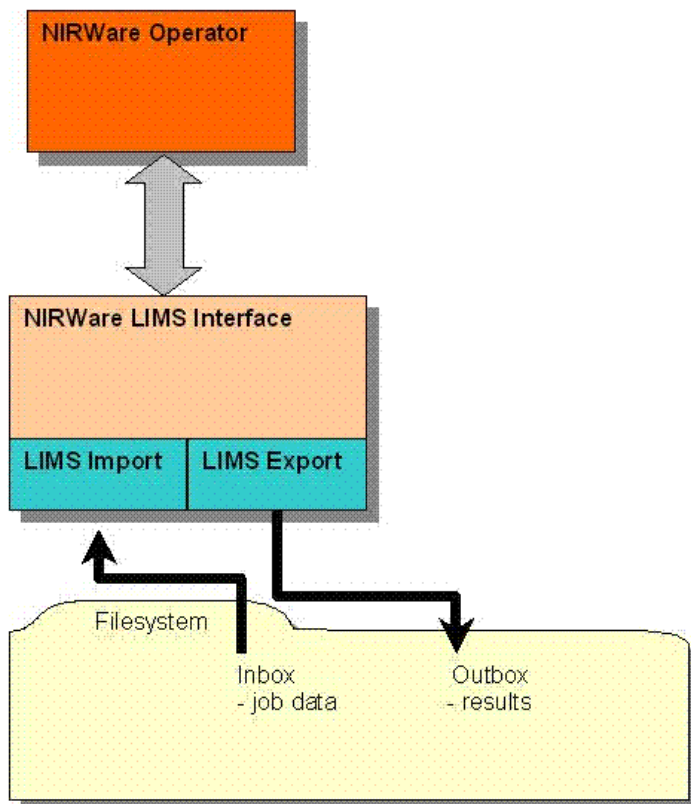
NOTE

The right to delete within the function includes the right to read and write. The right to write within the function includes the right to read.

6.6. LIMS Interface

6.6.1. Introduction LIMS Interface

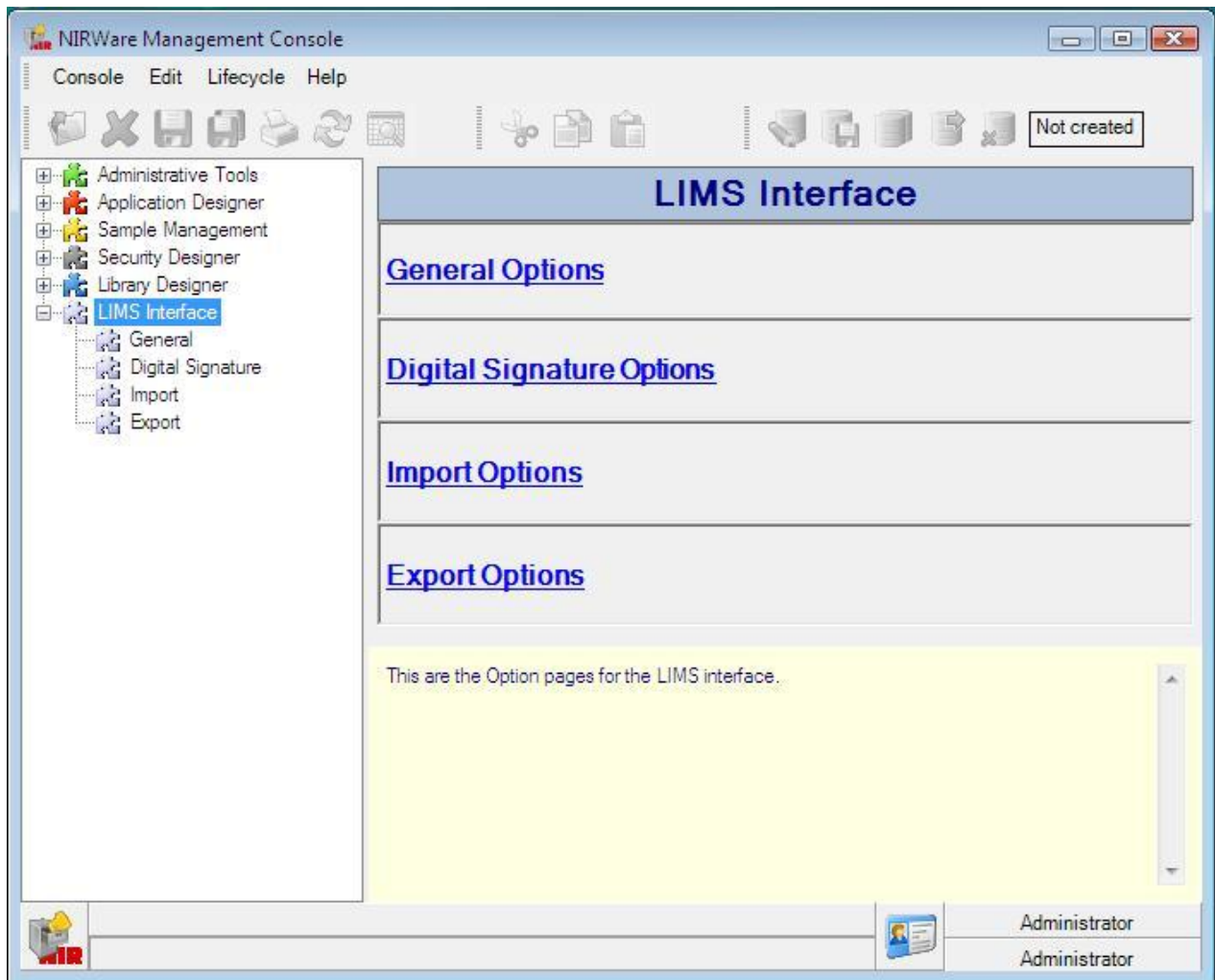
NIRWare LIMS Interface offers the possibility to link the NIRWare Software Suite to a LIMS. With this interface, job data from a LIMS can be transferred directly to the NIRWare Operator and measurement results are passed over to the LIMS.



Job data with all necessary information (application name, batch information, sample description, ...) will be written into a file by the LIMS and stored in the Inbox. In the NIRWare Operator, the user selects LIMS Import from the LIMS menu to import the job data. All input fields will be filled out automatically according to the job file generated by the LIMS. The measurement results will be exported into a file which is stored in the Outbox. From there the LIMS can acquire the result for further data processing.

To open the Application Designer proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **LIMS Interface**. The following dialog opens:

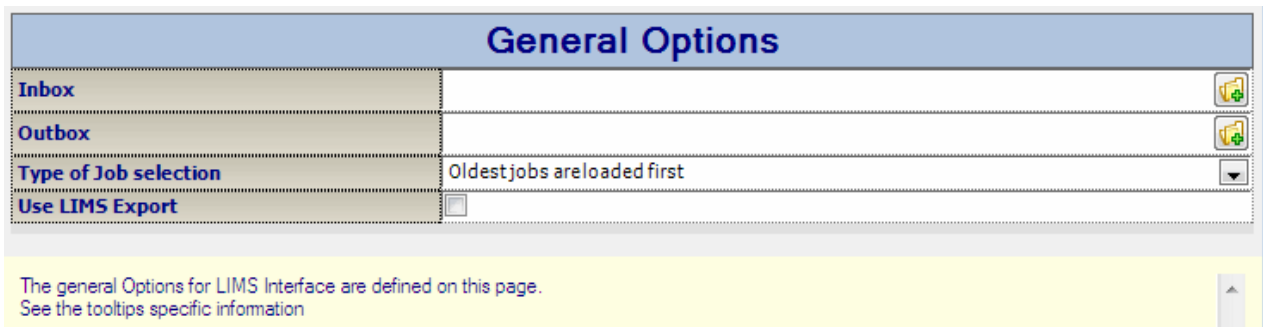


NOTE

The LIMS settings will be saved per PC, so that all settings will be reset to default when the PC name is changed.

6.6.2. General Options

Here, general output options are listed. To open it, in the file tree on the left side of the **NIRWare Management Console** select **LIMS Interface - General** or click **General Options** in the submenu list in the center.



Parameter Name	Description
Inbox	Path for the input files. The Operator receives the LIMS jobs from this folder
Outbox	Path for the output files (result files)
Type of Job selection	Selection mode of the LIMS jobs: <ul style="list-style-type: none"> • Oldest first • Newest first • Manual file selection
Use LIMS Export	Activate the export function (per default this function is deactivated). Only with this general option activated AND with the respective application configured to use LIMS export, measurement results will be written into a LIMS-file.

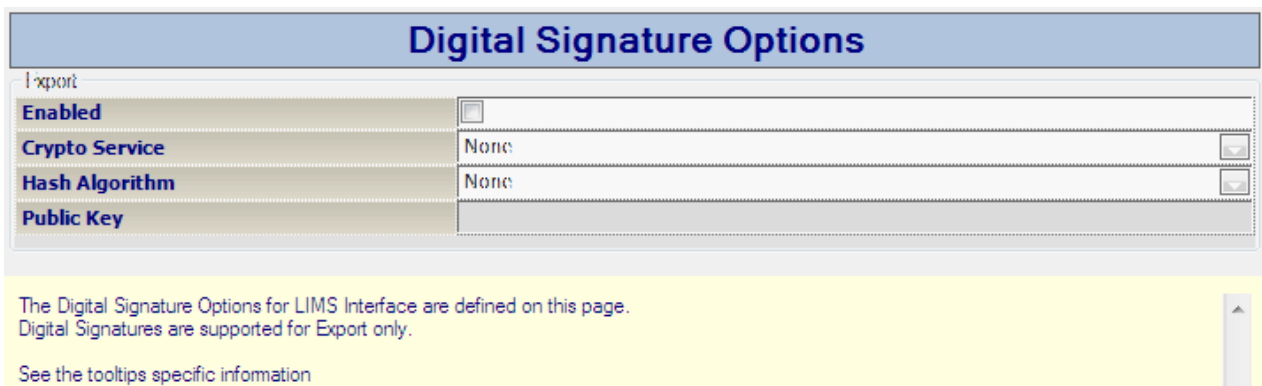
NOTE:

If the configuration in the LIMS Interface is changed, the Operator and the Control System Service have to be restarted.

6.6.3. Digital Signature Options

Only the result files can be signed digitally. Here the algorithms to be used can be defined.

To open it, in the file tree on the left side of the **NIRWare Management Console** select **LIMS Interface - Digital Signature** or click **Digital Signature Options** in the submenu list in the center.



Parameter Name	Description
Enabled	Enabled digital signature
Crypto Service	Type of Crypto Service used
Hash Algorithm	Type of Hash Algorithm used
Public Key	The public key if for the recipient. It is needed to check if the digital signature is un-changed.

The following combinations are possible (the combination marked with yellow is recommended):

Parameter Name	Hash Algorithm		
None	-	-	-
RSA	MD5	SHA-1	-
DSA	SHA-1	-	-

NOTE:

If the configuration in the LIMS Interface is changed, the Operator and the Control System Service have to be restarted.

6.6.4. Import Options

To specify the import, in the file tree on the left side of the **NIRWare Management Console** select **LIMS Interface - Import** or click **Import Options** in the submenu list in the center.

XML file import

Import Options *			
Format			
Format	XML		
File Extension	xml		
Ignore redundant lines in input file	<input type="checkbox"/>		
Use Unicode	<input checked="" type="checkbox"/>		
Field Assignment			
	NIRWare Field	Used	Description
1	Name	<input checked="" type="checkbox"/>	Name of the sample
2	Application	<input checked="" type="checkbox"/>	Application name
3	Batch	<input checked="" type="checkbox"/>	Batch name
4	Expected Substance	<input type="checkbox"/>	Expected substance (Used for Identification/Qualification)
5	Substance ID	<input type="checkbox"/>	Substance ID (Used for Identification/Qualification)
6	Campaign	<input checked="" type="checkbox"/>	Campaign
7	Number of Containers	<input checked="" type="checkbox"/>	Number of containers
8	Vendor Qualification	<input type="checkbox"/>	Vendor Qualification
9	AnalysisID	<input type="checkbox"/>	AnalysisID
10	Customer Field 1	<input type="checkbox"/>	A field defined by the customer, free usable
11	Customer Field 2	<input type="checkbox"/>	A field defined by the customer, free usable
12	Customer Field 3	<input type="checkbox"/>	A field defined by the customer, free usable
13	Customer Field 4	<input type="checkbox"/>	A field defined by the customer, free usable
14	Customer Field 5	<input type="checkbox"/>	A field defined by the customer, free usable
15	Customer Field 6	<input type="checkbox"/>	A field defined by the customer, free usable
16	Comment	<input type="checkbox"/>	A Comment

Parameter Name	Description
Format	Defines the file format used (XML and CSV)
File extension	Defines the extension of the import file
Ignore redundant lines in input file	In case the maximum number of samples in import file exceeds the number of samples possible for the application/instrument configuration (redundant lines): checked = redundant information is ignored for import unchecked = redundant information results in a warning message and the import is canceled
Use Unicode	Defines whether the import file is coded for Unicode. For XML this is standard. Unicode is necessary for all languages that have an expanded character set (e.g. Asian languages)
NIRWare Field	Available fields for import
Used	Defines whether the field is used. Blue marked fields are mandatory
Description	Field description

NOTE:

Blue marked fields (Name, Application, Batch) are mandatory and have to be checked. For identification either "Expected substance" or "Substance ID" has to be selected depending on the procedure used in applications.

Example:

```
<?xml version = "1.0"?>
<DatasetImport xmlns = "http://tempuri.org/DatasetImport.xsd">
  <Job>
    <Application>Quant Test SECOM</Application>
    <Batch>protest4</Batch>
    <ExpectedSubstance/>
    <AnalysisID>11087</AnalysisID>
    <CustomerField1>Administrator</CustomerField1>
    <Comment/>
    <Sample>
      <SampleName>BUCHI_3_SACCHAROSE_protest4_1_01</SampleName>
    </Sample>
    <Sample>
      <SampleName>BUCHI_3_SACCHAROSE_protest4_1_02</SampleName>
    </Sample>
    <Sample>
      <SampleName>BUCHI_3_SACCHAROSE_protest4_1_03</SampleName>
    </Sample>
  </Job>
</DatasetImport>
```

NOTE:

If the configuration in the LIMS Interface is changed, the Operator and the Control System Service have to be restarted.

Import XML schema

The XML schemas of import and export are located on the NIR Software Suite CD in the folder 'fscommand\Operation_Manuals\LIMS Schema'.

CSV file import

Import Options *				
Format				
Format	CSV			
File Extension	CSV			
Separator	;			
Ignore redundant lines in input file	<input type="checkbox"/>			
Use Unicode	<input checked="" type="checkbox"/>			
Field values are "Quoted"	<input type="checkbox"/>			
Field Assignment				
	NIRWare Field	Position	Used	Description
1	Name	1	<input checked="" type="checkbox"/>	Name of the sample
2	Application	2	<input checked="" type="checkbox"/>	Application name
3	Batch	3	<input checked="" type="checkbox"/>	Batch name
4	Expected Substance	0	<input type="checkbox"/>	Expected substance (Used for Identification/Qualification)
5	Substance ID	0	<input type="checkbox"/>	Substance ID (Used for Identification/Qualification)
6	Campaign	4	<input checked="" type="checkbox"/>	Campaign
7	Number of Containers	5	<input checked="" type="checkbox"/>	Number of containers
8	Vendor Qualification	0	<input type="checkbox"/>	Vendor Qualification
9	AnalysisID	0	<input type="checkbox"/>	AnalysisID
10	Customer Field 1	0	<input type="checkbox"/>	A field defined by the customer, free usable
11	Customer Field 2	0	<input type="checkbox"/>	A field defined by the customer, free usable
12	Customer Field 3	0	<input type="checkbox"/>	A field defined by the customer, free usable
13	Customer Field 4	0	<input type="checkbox"/>	A field defined by the customer, free usable
14	Customer Field 5	0	<input type="checkbox"/>	A field defined by the customer, free usable
15	Customer Field 6	0	<input type="checkbox"/>	A field defined by the customer, free usable
16	Comment	0	<input type="checkbox"/>	A Comment

Parameter Name	Description
Format	Defines the file format used (XML and CSV)
File extension	Defines the extension of the import file
Separator	Separator used
Ignore redundant lines in input file	In case the maximum number of samples in import file exceeds the number of samples possible for the application/instrument configuration (redundant lines): checked = redundant information is ignored for import unchecked = redundant information results in a warning message and the import is canceled
Field values are "Quoted"	Defines whether the field information in the csv file is expected to come with or without quotes (e.g. "samplename" or "sample name")
Use Unicode	Defines whether the import file is coded for Unicode. For XML this is standard. Unicode is necessary for all languages that have an expanded character set (e.g. Asian languages)
NIRWare Field	Available fields for import
Position	Position of the field (as it appears in the import file). All used fields must have a well defined position.
Used	Defines whether the field is used. Blue marked fields are mandatory
Description	Field description

NOTE:

For the csv format the exact position of the fields in the import file must be defined. Blue marked fields (Name, Application, Batch) are mandatory and have to be checked.

For this purpose, a double-click on the sample name field will fill all the other used fields in ascending order.

Field Assignment				
	NIRWare Field	Position	Used	Description
1	Samplename	0	<input checked="" type="checkbox"/>	Name of the sample
2	DateTime	0	<input checked="" type="checkbox"/>	Date Time (UTC formatted)
3	DateTime	0	<input checked="" type="checkbox"/>	Date Time (UTC formatted)
4	Date	0	<input checked="" type="checkbox"/>	Date as defined in the NIRWare Configuration at Culture
5	Time	0	<input checked="" type="checkbox"/>	Time as defined in the NIRWare Configuration at Culture
6	Application	0	<input checked="" type="checkbox"/>	Application name
7	Batch	0	<input checked="" type="checkbox"/>	Batch name
8	AnalysisID	0	<input type="checkbox"/>	AnalysisID
9	ExpectedSubstance	0	<input type="checkbox"/>	Expected substance (Used for Identification/Qualification)
10	SubstanceID	0	<input type="checkbox"/>	Expected Substance ID (Used for Identification/Qualification)

A double-click on the 1. property field will automatically fill all other used fields including their position number.

20	User fullname	0	<input type="checkbox"/>	The fullname of the logged in user who started the measure sequence
21	PropertyName1	4	<input checked="" type="checkbox"/>	Property Name (Used For Quantification)
22	Property		<input type="checkbox"/>	The NIRWare Field.
23	Property		<input type="checkbox"/>	
24	Property		<input type="checkbox"/>	Fields marked with colored background are mandatory!
25	Residue		<input type="checkbox"/>	Use Double Click to automatically fill up the further property fields Used / Position with the 1. property as a reference.

Example (unquoted)

```
LIMS_Lactose_0001;Zucker MeasurementSequence Batch;Z03;Lactose;10;Test1;LIMS Appl
```

Example (quoted)

```
"LIMS_Lactose_0001";Zucker Measure Batch";"Z03";"Lactose";"10";"Test1";"LIMS Appl"
```

NOTE:

If the configuration in the LIMS interface is changed, the Operator and the Control System Service have to be restarted.

6.6.5. Export Options

To specify the export, in the file tree on the left side of the **NIRWare Management Console** select **LIMS Interface - Export** or click **Export Options** in the submenu list in the center.

XML export file

Select the fields that should be shown in the export file.

Export Options			
Format			
Format			XML
File Extension			xml
Use Unicode		<input checked="" type="checkbox"/>	
Field Assignment			
	NIRWare Field	Used	Description
1	Samplename	<input checked="" type="checkbox"/>	Name of the sample
2	DateTime	<input type="checkbox"/>	DateTime (UTC formatted)
3	DateTimeOS	<input type="checkbox"/>	DateTime (formatted as defined in the NIRWare Configuration at Culture)
4	Date	<input type="checkbox"/>	Date (formatted as defined in the NIRWare Configuration at Culture)
5	Time	<input type="checkbox"/>	Time (formatted as defined in the NIRWare Configuration at Culture)
6	Application	<input checked="" type="checkbox"/>	Application name
7	Batch	<input checked="" type="checkbox"/>	Batch name
8	AnalysisID	<input type="checkbox"/>	AnalysisID
9	ExpectedSubstance	<input type="checkbox"/>	Expected substance(Used for Identification/Qualification)
10	SubstanceID	<input type="checkbox"/>	Expected Substance ID (Used for Identification/Qualification)
11	FoundSubstance	<input type="checkbox"/>	Found substance(Used for Identification/Qualification)
12	FoundSubstanceID	<input type="checkbox"/>	Found substance ID(Used for Identification/Qualification)
13	IdentificationOK	<input type="checkbox"/>	Identification OK(Used for Identification/Qualification)
14	Residual	<input type="checkbox"/>	Residual of the prediction result (Used for Identification/Qualification)
15	Distance	<input type="checkbox"/>	Distance of the prediction result (Used for Identification/Qualification)
16	Max. Allowed Residual	<input type="checkbox"/>	max. allowed Residual(Used for Identification/Qualification)
17	Max. Distance	<input type="checkbox"/>	max. distance (Used for Identification/Qualification)
18	Lifecycle state	<input type="checkbox"/>	The lifecycle state of the result
19	User ID	<input type="checkbox"/>	The user ID of the logged in user who started the measure sequence
20	User fullname	<input type="checkbox"/>	The fullname of the logged in user who started the measure sequence
21	PropertyName	<input checked="" type="checkbox"/>	Property Name (Used for Quantification)
22	PropertyPredictedValue	<input type="checkbox"/>	Property Predicted Value (Used for Quantification)
23	PropertyUnit	<input type="checkbox"/>	Property Unit (Used for Quantification)
24	PropertyOK	<input type="checkbox"/>	Property OK (Used for Quantification)
25	Residual	<input type="checkbox"/>	Residual of the prediction result (Used for Quantification)
26	Max. Allowed Residual	<input type="checkbox"/>	max. allowed Residual (Used for Quantification)
27	Decimal places	<input type="checkbox"/>	Number of decimal places defined in the application property (Used for Quantification)

Parameter Name	Description
Format	Defines the file format used (XML and CSV)
File extension	Defines the extension of the export file. Please omit the dot (e.g. xml instead of .xml)
Use Unicode	Defines whether the export file is coded for Unicode. For XML this is standard. Unicode is necessary for all languages that have an expanded character set (e.g. Asian languages)
NIRWare Field	Available fields for export
Used	Defines whether the field is used. Blue marked fields are mandatory
Description	Field description

NOTE:

Blue marked fields (Samplename, Application, Batch, PropertyName) are mandatory and have to be checked.

NOTE:

If the configuration in the LIMS Interface is changed, the Operator and the Control System Service have to be restarted.

Export XML schema

The XML schemas of import and export are located on the NIR Software Suite CD in the folder 'fscommand\Operation_Manuals\LIMS Schema'.

CSV export file

Select the fields that should be shown in the export file.

Export Options *				
Format				
Format	CSV			
File Extension	CSV			
Separator	;			
Use Unicode	<input checked="" type="checkbox"/>			
Field values are "Quoted"	<input type="checkbox"/>			
Result is rounded (AP Property)	<input type="checkbox"/>			
Multiple properties are line separated	<input type="checkbox"/>			
Number of properties	1			
Field Assignment				
	NIRWare Field	Position	Used	Description
1	Samplename	1	<input checked="" type="checkbox"/>	Name of the sample
2	DateTime	0	<input type="checkbox"/>	DateTime (UTC formatted)
3	DateTime05	0	<input type="checkbox"/>	DateTime (formatted as defined in the NIRWare Configuration at Culture)
4	Date	0	<input type="checkbox"/>	Date (formatted as defined in the NIRWare Configuration at Culture)
5	Time	0	<input type="checkbox"/>	Time (formatted as defined in the NIRWare Configuration at Culture)
6	Application	2	<input checked="" type="checkbox"/>	Application name
7	Batch	3	<input checked="" type="checkbox"/>	Batch name
8	AnalysisID	0	<input type="checkbox"/>	AnalysisID
9	ExpectedSubstance	0	<input type="checkbox"/>	Expected substance (Used for Identification/Qualification)
10	SubstanceID	0	<input type="checkbox"/>	Expected Substance ID (Used for Identification/Qualification)
11	FoundSubstance	0	<input type="checkbox"/>	Found substance (Used for Identification/Qualification)
12	FoundSubstanceID	0	<input type="checkbox"/>	Found substance ID (Used for Identification/Qualification)
13	IdentificationOK	0	<input type="checkbox"/>	Identification OK (Used for Identification/Qualification)
14	Residual	0	<input type="checkbox"/>	Residual of the prediction result (Used for Identification/Qualification)
15	Distance	0	<input type="checkbox"/>	Distance of the prediction result (Used for Identification/Qualification)
16	Max. Allowed Residual	0	<input type="checkbox"/>	max. allowed Residual (Used for Identification/Qualification)
17	Max. Distance	0	<input type="checkbox"/>	max. distance (Used for Identification/Qualification)
18	Lifecycle state	0	<input type="checkbox"/>	The lifecycle state of the result
19	User ID	0	<input type="checkbox"/>	The user ID of the logged in user who started the measure sequence
20	User fullname	0	<input type="checkbox"/>	The fullname of the logged in user who started the measure sequence
21	PropertyName1	4	<input checked="" type="checkbox"/>	Property Name (Used for Quantification)
22	PropertyPredictedValue1	0	<input type="checkbox"/>	Property Predicted Value (Used for Quantification)
23	PropertyUnit1	0	<input type="checkbox"/>	Property Unit (Used for Quantification)
24	PropertyOK1	0	<input type="checkbox"/>	Property OK (Used for Quantification)
25	Residual1	0	<input type="checkbox"/>	Residual of the prediction result (Used for Quantification)

Parameter Name	Description
Format	Defines the file format used (XML and CSV)
File extension	Defines the extension of the export file
Separator	Separator used
Use Unicode	Defines whether the export file is coded for Unicode. For XML this is standard. Unicode is necessary for all languages that have an expanded character set (e.g. Asian languages)
Field values are "Quoted"	Defines whether the field information in the csv file is written with or without quotes (e.g. "samplename" or "sample name")
Result is rounded (AP Property)	Prediction result is rounded according to the settings in the used application
Multiple properties	Defines whether the csv file contains all information in one line or has multiple

are line separated	lines (one line for each property)
Number of properties	Number of properties (results) in export file (visible in case the function "Multiple Properties are line separated" is not active)
NIRWare Field	Available fields for export
Position	Position of the field (as it appears in the export file). All used fields must have a well defined position.
Used	Defines whether the field is used. Blue marked fields are mandatory
Description	Field description

NOTE:

For the csv format the exact position of the fields in the export file must be defined. Blue marked fields (Name, Application, Batch) are mandatory and have to be checked.

For this purpose, a double-click on the sample name field will fill all the other used fields in ascending order.

	NIRWare Field	Position	Used	Description
1	Samplename	0	<input checked="" type="checkbox"/>	Name of the sample
2	DateTim	0	<input type="checkbox"/>	Date Time (UTC formatted)
3	DateTim	0	<input type="checkbox"/>	Date Time (UTC formatted)
4	Date	0	<input type="checkbox"/>	Date (as defined in the NIRWare Configuration at Culture)
5	Time	0	<input type="checkbox"/>	Time (as defined in the NIRWare Configuration at Culture)
6	Application	0	<input checked="" type="checkbox"/>	Application name
7	Batch	0	<input checked="" type="checkbox"/>	Batch name
8	AnalysisID	0	<input type="checkbox"/>	AnalysisID
9	ExpectedSubstance	0	<input type="checkbox"/>	Expected substance (Used for Identification/Qualification)
10	SubstanceID	0	<input type="checkbox"/>	Expected Substance ID (Used for Identification/Qualification)

A double-click on the 1. property field will automatically fill all other used fields including their position number.

20	User fullname	0	<input type="checkbox"/>	The fullname of the logged in user who started the measure sequence
21	PropertyName1	4	<input checked="" type="checkbox"/>	Property Name (Used for Quantification)
22	Proper		<input type="checkbox"/>	The NIRWare Field.
23	Proper		<input type="checkbox"/>	
24	Proper		<input type="checkbox"/>	Fields marked with colored background are mandatory!
25	Residu		<input type="checkbox"/>	Use Double Click to automatically fill up the further property fields Used / Position with the 1. property as a reference.

Example 1 Quantification:

```
Sucrose_0006;2007_01_18 14:32:27.800Z;Sugar
Content;Sugar001;10;;;Sucrose;25.5255599200529;%;1
```

Example 2 Quantification:

```
"LIMS_sample234";"30/06/2007";"12:01:45";"Feed";"Batch12";"10-
12";"";"";"";"";"Moisture";6.52;"%";"1";"0.000125"
```

NOTE:

If the configuration in the LIMS Interface is changed, the Operator and the Control System Service have to be restarted.

Description of the export fields

The results of the measurements will be validated according to the calibration and application settings with **OK** if all of the following criteria are fulfilled for Identification (I) and Quantification (Q):

- residual is within the given limits (I, Q)
- prediction result is within the calibration range (Q)
- prediction result is within action and warning limits (Q)
- prediction result is within the given distance limit (I)
- expected substance matches found substance (I)

Identifier	Data Type (Text: ASCII or Unicode)	Application Type (I = Identification, Q = Quantification)	Remarks
Samplename	Text	I, Q	sample name
DateTime	DateTime	I, Q	UTC Time in the format: YYYY-mm-dd HH:MM:SSZ example: 2006-11-02 14:58:41Z
DateTimeOS	DateTime	I, Q	short date in time as defined in the operating system
Date	Date	I, Q	short date as defined in the operating system
Time	Time	I, Q	time as defined in the operating system
Application	Text	I, Q	application name
Batch	Text	I, Q	batch name
AnalysisID	Text	I, Q	analysis ID
ExpectedSubstance	Text	I	expected substance identity
SubstanceID	Text	I	ID code for sample property
FoundSubstance	Text	I	found substance (equals first entry in the hitlist; if no substance was found, the entry remains empty)

Found SubstanceID	Text	I	found substance ID (equals first entry in the hitlist; if no substance ID was found, the entry remains empty)
Identification OK	Integer	I	see description above
Residual	Double	I	residual of prediction result
Distance	Double	I	distance of prediction result
MaxAllowedResidual	Double	I	maximum allowed residual
MaxDistance	Double	I	maximum distance
PropertyName	Text	Q	name of the property
PropertyPredictedValue	Double	Q	prediction result
PropertyUnit	Text	Q	result unit
PropertyOK	Integer	Q	see description above
Residual	Double	Q	residual of prediction result
MaxAllowedResidual	Double	Q	max. allowed residual
Decimal Places	Integer	Q	number of decimal places as defined in the application
PropertyName N	Text	Q	name of the property
PropertyValue N	Double	Q	prediction result
PropertyUnit N	Text	Q	result unit
PropertyOK N	Integer	Q	see description above
Residual N	Double	Q	residual of prediction result
MaxAllowedResidual N	Double	Q	max. allowed residual
Decimal Places N	Integer	Q	number of decimal places as defined in the application

6.7. Library Designer

6.7.1. Introduction Library Designer

For identity control in the warehouse it is not always necessary to work with chemometric calibration methods such as Cluster or SIMCA. When sample identification is needed, often a comparison of spectra leads to good and reliable results, is much easier to handle and requires only little reference analysis.

The NIRWare Library Designer serves to create and administrate spectra libraries for spectra comparison. All spectra within the NIRWare database can be used to define spectra libraries.

To carry out the spectra comparison of measured spectra and spectra within the library, 13 different algorithms are available.

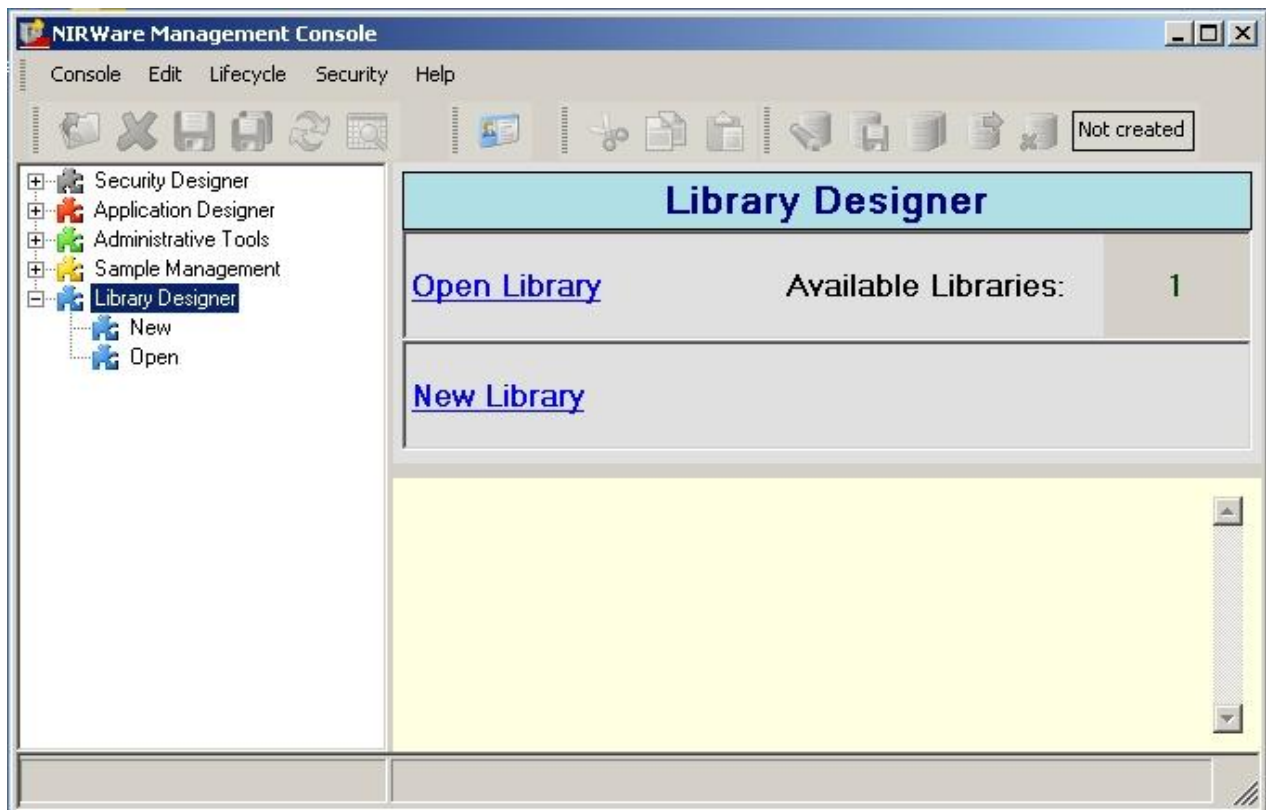
Each library can be validated internally or externally with a test spectra set.

To use the Library Designer, a valid license is necessary. This license is part of the Advanced License Package for NIRWare or can be purchased separately.

To use the Library Designer, the Snap-in has to be added to the ['NIRWare Management Console'](#).

To open the Library Designer proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Library Designer**. The following dialog opens:



You can now open a submenu by clicking on their names in the file tree or in the center of the Library Designer window.

6.7.2. Creating a new library

To create a new library proceed as follows:

In the file tree on the left side of the **NIRWare Management Console** select **Library Designer – New** or click **New Library** in the submenu list in the center.

The following dialog opens:

New Library			
Library name			
Library description			
Library type	Static		
Method formula	Squared Difference of Derivative ▾		
Wavelength selection	4500-10000		
Distance limit	5		
Validation type	External ▾		
Minimum measurement cell temperature			
Measurement temperature maximum			
Template spectrum:			
Sample Name	Property Name	Timestamp	Scans
2005-12-13_11-08-04Ethanol	Ethanol	12/13/2005 11:08:	16
2005-12-13_11-08-28Ethanol	Ethanol	12/13/2005 11:08:	16
2005-12-13_11-08-59Ethanol	Ethanol	12/13/2005 11:08:	16
2005-12-13_11-15-31Ethanol	Ethanol	12/13/2005 11:15:	16
2005-12-13_11-16-12Ethanol	Ethanol	12/13/2005 11:16:	16

If necessary, narrow down the information displayed in the table, using appropriate [filter settings](#).

In case you do not see the samples contained in the database in the lower table, click the grey cell in the Timestamp column with the right mouse button.

The table contains the following columns:

Sample Name: Date and time the sample was measured and name of the sample

Property Name: Name of the property

Time Stamp: Date and time the sample was measured

Scans: Number of scans with which the sample was measured

Resolution: Resolution with which the sample was measured

Comment: Optional comment to the sample

Spectrum ID: ID of the sample spectrum

Now fill in or select the library parameters in the list at the top (a library name is mandatory) and highlight the row with the spectrum you would like to use as template spectrum from the lower table by clicking on it.

The template spectrum determines the measuring conditions for the spectra in the library, all spectra are measured with the same instrument type, cell, cell option, resolution and number of scans and have therefore the same format.

When you have finished your settings for the new library, click the **Save** icon.

The library will now be added to the tree view on the left side under the menu **Open** and three additional submenus are assigned to it: Spectra, Validate Library, Library Test.

NOTE

The library can only be saved when a library name and a template spectrum was defined.

Library parameters:

Library name	Name of the library (mandatory field)
Library description	Optional description of the library
Library type	Type of library, preset to static
Method formula	Select method from the drop-down list: <ul style="list-style-type: none"> • Maximum Distance of 2nd Derivative • Maximum Distance • Wavelength Correlation of 2nd Derivative • Wavelength Correlation • Squared Differences of 2nd Deriv with Smoothing • Squared Differences of Normalisation 0 to 1 • Squared Differences of Vector Normalisation • Correlation Coefficient • Euclidian Distance • Squared Difference of Derivative • Difference of Derivative • Squared Differences • Difference
Wavelength selection	Wavelength range in which the spectra are compared
Distance limit	Limit value defining the maximum allowed distance between a given/measured spectrum and the most similar spectrum within the library. The value depends on the method formula selected for prediction and is defined in the library parameters.
Validation type	Select between internal or external validation from the drop down menu
Minimum measurement cell temperature	Minimum temperature the measuring cell may have (valid only for liquid cells)
Measurement temperature maximum	Maximum temperature the measuring cell may have (valid only for liquid cells)

Method formulas

Maximum Distance of 2nd Derivative	
<p>Maximum Distance</p> <p>NOTE</p> <p>To use this algorithm there must be at least 3 spectra of the same property inside the library.</p>	$d_{uj} = \max \left[\text{Abs} \left(\frac{x_{uj} - \bar{x}_{jp}}{s_{jp}} \right) \right]_{\text{over_all_p}}$ $s_{jp} = \left(1 + \frac{1}{\sqrt{2(n-1)}} \right) \sqrt{\frac{\sum_{i=1}^n (x_{ijp} - \bar{x}_{jp})^2}{n-1}}$ <p><i>u = unknown_spectrum</i> <i>p = wavelength</i> <i>j = product</i> <i>n = number_of_samples</i> <i>x = absorbance_spectrum</i></p>
Wavelength Correlation of 2nd Derivative	
Wavelength Correlation	
Squared Differences of 2nd Deriv with Smoothing	Msq2d= Scale * Sum(Sqr(Magic(s) - Magic(r))) (SecondDerivativeSmoothing)
Squared Differences of Normalisation 0 to 1	Msqn01= Scale * Sum(Sqr(Norm(s) - Norm(r))) Normalization 0 to 1 taking wavelength selection into account
Squared Differences of Vector Normalisation	Msqn= Scale * Sum(Sqr(Norm(s) - Norm(r))) Normalization to Unit Length taking wavelength selection into account
Correlation Coefficient	Meu = Scale * Sqrt(Sum(Sqr(s - r)))
Euclidian Distance	Meu = Scale * Sqrt(Sum(Sqr(s - r)))
Squared Difference of Derivative	Msd = Scale * Sum(Sqr(Deriv(s) - Deriv(r))) (FirstDerivativeSavitzkyGolay9Point)
Difference of Derivative	Mad = Scale * Sum(Abs(Deriv(s) - Deriv(r))) (FirstDerivativeSavitzkyGolay9Point)
Squared Differences	Msq = Scale * Sum(Sqr(s - r))
Difference	Mab = Scale * Sum(Abs(s - r))

Library window

Test library	
Library name	Test library
Library description	
Library type	Static
Method formula	Squared Difference of Derivative
Wavelength selection	4500-10000
Distance limit	5
Validation type	External
Minimum measurement cell temperature	-
Measurement temperature maximum	-
Valid	<input type="checkbox"/>
Number of Substances	0
Number of Spectra	0
Template Spectrum:	
Sample Name	2005-12-13_11-06-11Isoprop
Property Name	Ethanol
Property Type	Identification
Spectrum Type	Transmittance
Comment	
Optical Resolution	8
Datapoint interval	4
Lower wavenumber limit	4000
Datapoints	1501
Time Stamp	12/13/2005 11:06:11

Additional library parameters

As soon as a new library is saved, it can be opened via the tree view on the left of the Management Console and three additional parameters are added to the upper parameter list:

Valid: When this check box is activated the library has been validated

Number of Substances: Number of substances within the library

Number of Spectras: Number of spectra within the library

Spectrum template parameters

Sample Name	Name of the sample
Property Name	Name of the determining parameter, i.e. property (e.g. fat)
Property Type	Type of the property, identification in this case
Spectrum Type	How the spectrum was measured, transmittance in this case
Comment	Optional comment

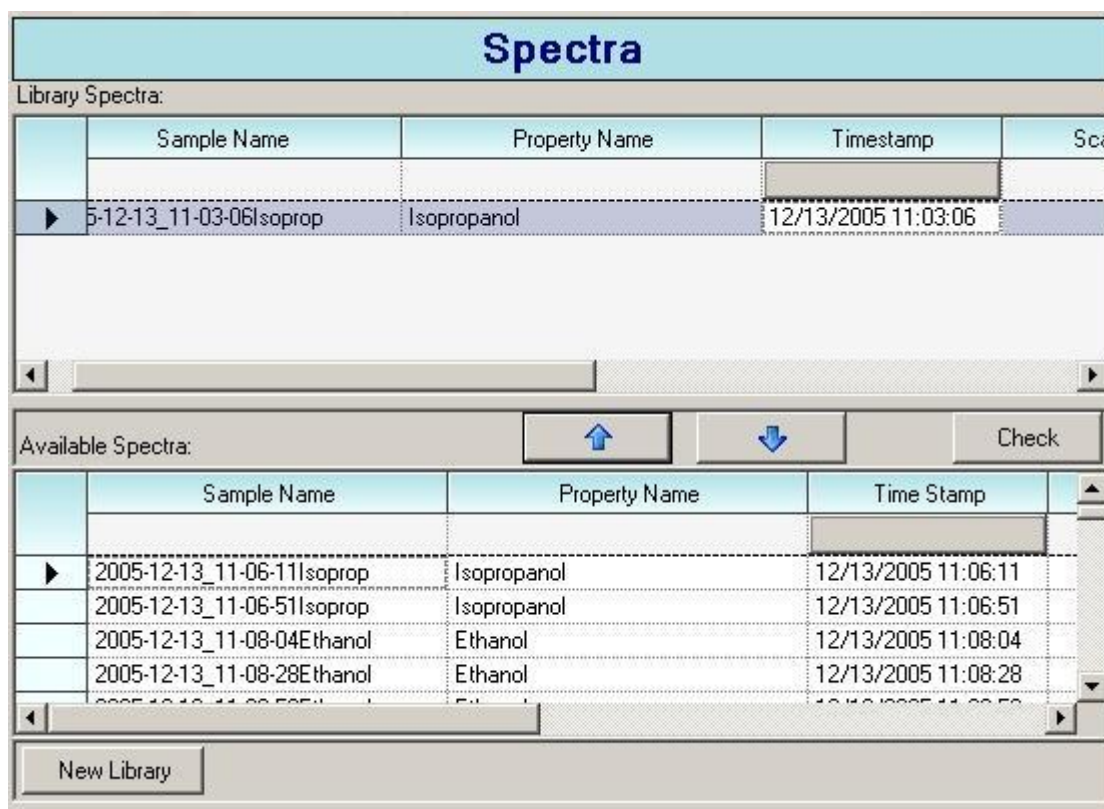
Optical Resolution	Optical resolution of the instrument used for measurement
Datapoint interval	Resolution of datapoints used for the measurement
Lower wavenumber limit	Lower wavenumber limit of the range within the spectrum was measured
Datapoints	Datapoint used for spectrum measurement
Time Stamp	Date and time the spectrum was measured

6.7.3. Spectra

After the library has been initially created, qualitative spectra have to be selected to built up the library.

To open the Spectra window in the file tree on the left side of the **NIRWare Management Console** select **Open**, click on the name of the library for which you want to assign spectra, then select **Spectra**.

The following dialog opens:



The Spectra window contains two tables, the upper for the spectra contained in the selected library, the lower showing all samples contained in the database.

In case the tables or at least the lower table is empty, click the grey cell in the Timestamp column with the right mouse button.

The tables comprise the following columns:

Sample Name: Date and time the sample was measured and name of the sample

Property Name: Name of the property


Time Stamp: Date and time the sample was measured

Scans: Number of scans with which the sample was measured

Resolution: Resolution with which the sample was measured

Comment: Optional comment to the sample

Spectrum ID: ID of the sample spectrum

To be able to assign spectra to your library, you first have to set the corresponding library to the Lifecycle state "Editing". For this purpose, click the Edit DataSet icon . The blue arrow buttons in the center of the window will now become active.

You can now highlight the row of the sample(s) you want to add to the library and click the left arrow button. The sample is moved from the lower to the upper table.

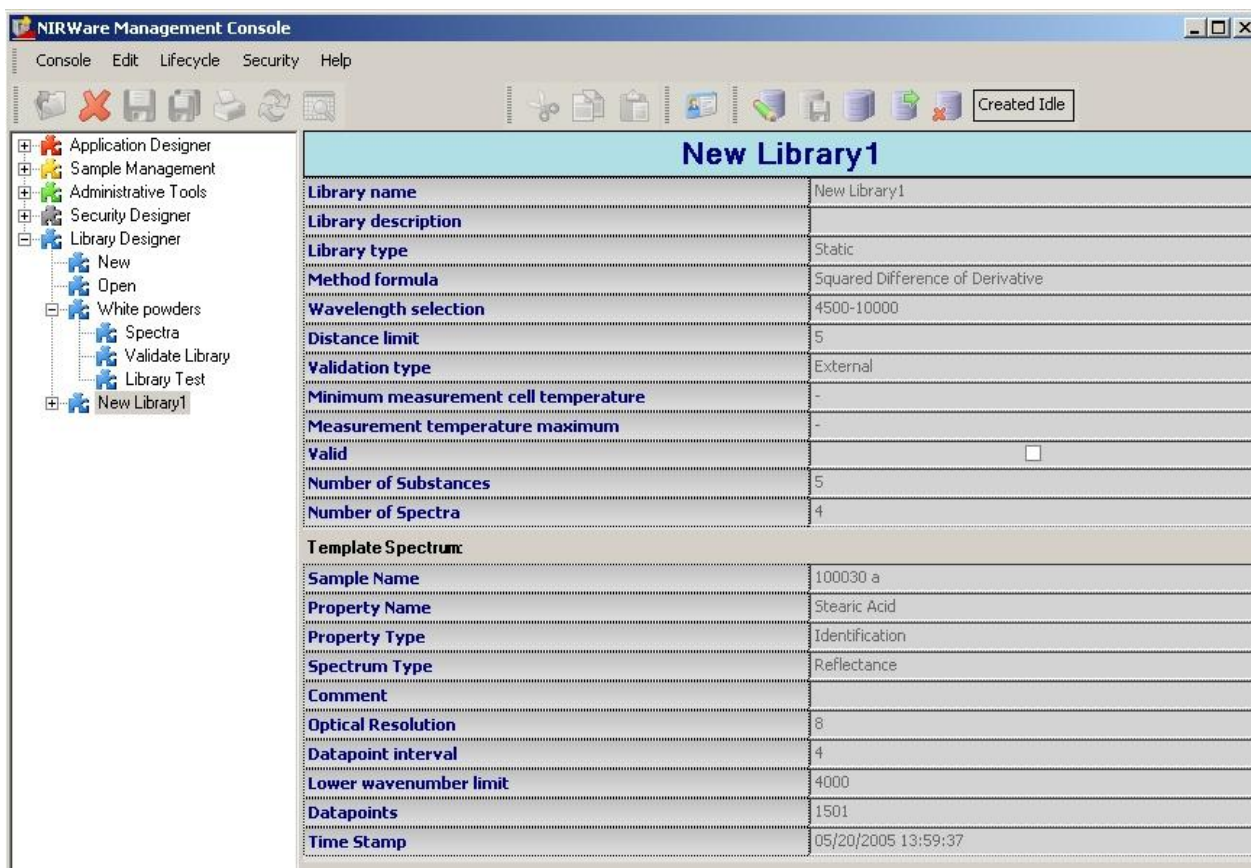
To remove a spectrum from the library again, highlight the corresponding row and click the right arrow button.


To check whether a spectrum assigned to the library meets the requirements defined in the library parameters, click **Check**. The check results, i.e. the Minimum external distance, the Maximum internal distance and the Maximum allowed distance, will be displayed in the lower part of the window.

NOTE:

Make sure, that only spectra are used to built up a library that have the same wavenumber range and number of data points (e.g. 10000cm^{-1} - 4000cm^{-1} ; 1501 data points).

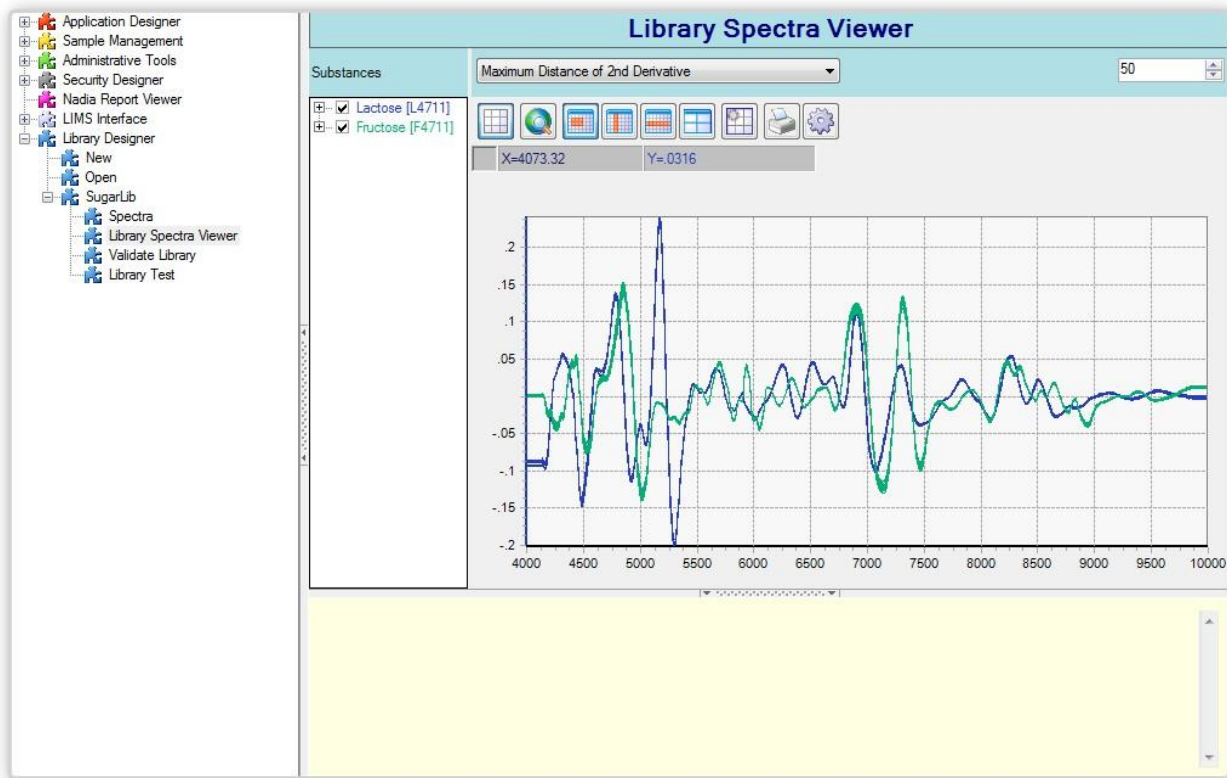
To create a new library from spectra contained in the currently active library, highlight the corresponding spectra in the upper table and click **New Library**. The following window opens:



To be able to change the library parameters, you first have to set the corresponding library to the Lifecycle state "Editing". For this purpose, click the Edit DataSet icon .

6.7.4. Library Spectra Viewer

By means of the Library Spectra Viewer the spectra saved in the library can be displayed.

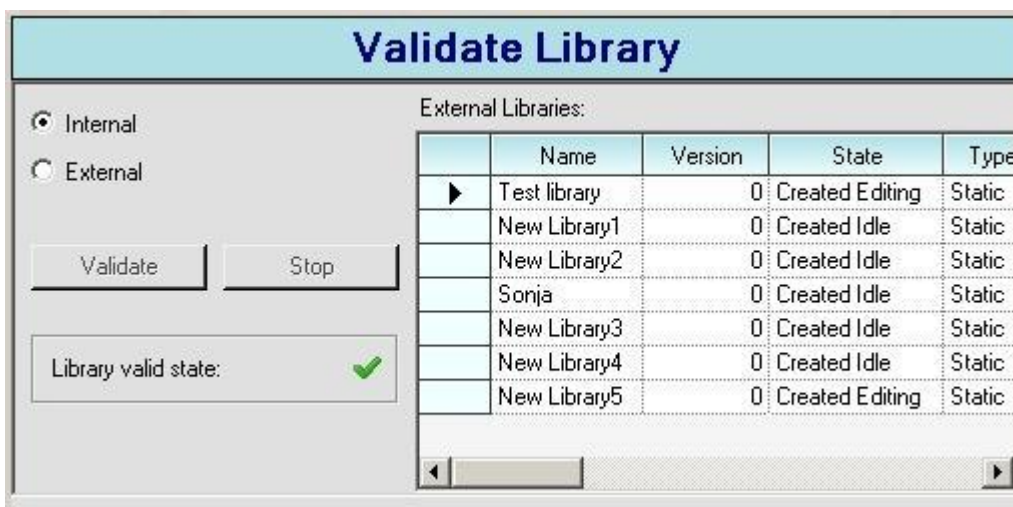


6.7.5. Validate Library

Before the library can be used for routine operation it has to be validated to ensure a clear separation of all samples from each other with the chosen settings (wavenumber selection, Method formula, distance limit).

To open the corresponding window in the file tree on the left side of the **NIRWare Management Console** select **Open**, click on the name of the library which you want to validate, then select **Validate Library**.

The following dialog opens:



The window contains a list of all libraries in the database.

It contains the following columns:

Name: Library name

Version: Library version

State: Lifecycle state of the library


Type: Library type

Method: Method formula used for library validation, testing and routine operation

Validation Type: Type of validation carried out for the library

Wavelength Selection: Wavelength considered within the library

Comment: Optional comment on the library

To be able to validate a library, you first have to set your dataset to the Lifecycle state "Editing". For this purpose, click the Edit DataSet icon . The buttons **Validate** and **Stop** will now become active.

Internal	When this selection button is active, all spectra inside the current library are checked against each other.
External	When this selection button is active, all spectra inside the current library are checked against the spectra within another selectable library.
Validate button	Clicking this button starts the validation procedure.
Stop button	Clicking this button aborts the validation procedure.
Library valid state:	Green tick when the library is valid or red cross when the library is not valid

After the validation has been carried out, the following information is displayed in the lower gray part of the window:

Example:

```
Validation result: ** NOT valid **

Minimum distance between substances: 0.01911797
Maximum allowed dist. for prediction: 0.00955898
Distance limit of the library: 5

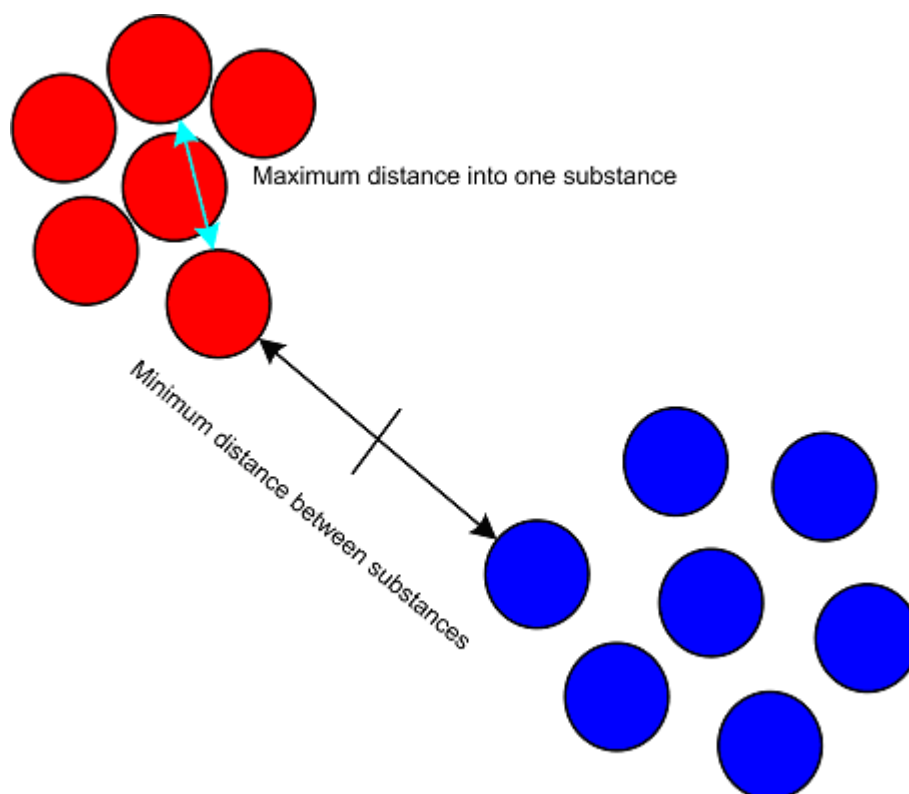
For information
Maximum distance into one substance: 0.00038467
```

Validation result	Valid or not valid.
Minimum distance between substances	Describes the minimum difference between the measuring results of two different substances
Maximum allowed dist. for prediction	Less than half the value of the minimum distance between substances.

Distance limit of the library	Limit value defining the maximum allowed distance between a given/measured spectrum and the most similar spectrum within the library. The value depends on the method formula selected for prediction and is defined in the library parameters.
Maximum distance into one substance	Describes the maximum difference between different measurements of the same substance.

NOTE

The values might be different depending on the method formula selected.

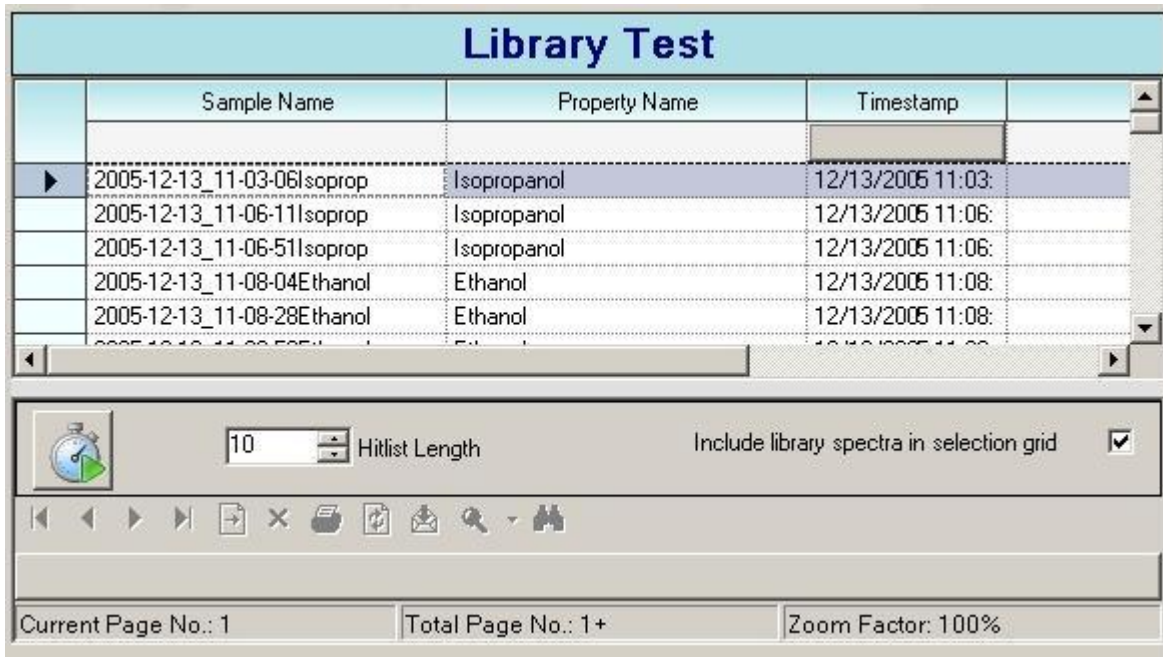


6.7.6. Library Test

After the library was finished and validated, it can be tested, i.e. a spectrum from the database can be predicted by means of the library.

For this purpose in the file tree on the left side of the **NIRWare Management Console** select **Open**, click on the name of the library which you want to test, then select **Library Test**.

The following dialog opens:



The Library test window contains a table listing all samples contained in the database. In case the tables is empty, click the grey cell in the Timestamp column with the right mouse button.

The table comprises the following columns:

Sample Name: Date and time the sample was measured and name of the sample

Property Name: Name of the property

Time Stamp: Date and time the sample was measured


Comment: Optional comment to the sample

Spectrum ID: ID of the sample spectrum


Below the table you can define two parameters influencing the library test:

Hitlist Length: Via the arrows next to the field you can determine the amount of hitlist spectra contained in the test report (if the defined hitlist length exceeds the amount of properties available, the hitlist will be shorter accordingly).

Include library spectra in selection grid: When this check box is activated, the spectra of the currently selected library are also included in the table, so that the case can occur, that a spectrum is predicted by means of itself.

To test the library it must have been saved first by means of the Save DataSet button .

Then select one spectrum or several spectra from the table by highlighting the corresponding row(s) and

click the button Predict selected spectrum .

The test is carried out and the results will be displayed in the center of the window:












Expected substance: Stearic Acid

HitList	Found substance		Distance allowed	Distance	
Stearic Acid	Stearic Acid	ok	5,000000	0,000024	ok
Ascorbic Acid	Stearic Acid	x	5,000000	0,069108	ok
Citric Acid	Stearic Acid	x	5,000000	0,071855	ok
Tartaric Acid	Stearic Acid	x	5,000000	0,073452	ok
Salicylic Acid	Stearic Acid	x	5,000000	0,084407	ok

The column titles have the following meaning:

HitList	Property name (the name of the property with the closest distance to the predicted spectrum is the first in the column)
Found substance	Name of found substance If the name of the found substance in the hitlist matches the name of the expected substance, it will be marked with 'OK' , otherwise a red X is displayed.
Distance allowed	Allowed distance of checked spectrum to the "hitlist" spectrum in the library. The distance depends on the method formula used for prediction and is defined in the library parameters. If the allowed distance is exceeded, the property is marked with a red X, otherwise a 'OK' is displayed.
Distance	Actual distance of checked spectrum to the "hitlist" spectrum in the library. The distance depends on the method formula used for prediction

There are some additional functions available via the report icon bar. Use the icons in the icon bar to navigate within the report and to process it:

	Go to first page icon
	Go to previous page icon
	Go to next page icon
	Go to last page icon
	Go to page icon: When you click here, a dialog opens, where you can specify the page number of the page you want to go to. Click OK afterwards.
	Close report icon.
	Print Report icon. Click here to print the report on the connected printer. A print dialog opens, where you can define different print settings. After that, click OK .
	Refresh icon: Click here to refresh the report and to get back to the default display.
	Export Report icon: Click here to export the report.
	Zoom icon: Click the arrow. A drop-down menu opens, where you can select the size in which the report is displayed by clicking on the corresponding percentage.
	Search Text icon: Click here to search for text within the report. A dialog opens, where you can enter the text to be searched for. After that click Find Next .

6.8. Lifecycle

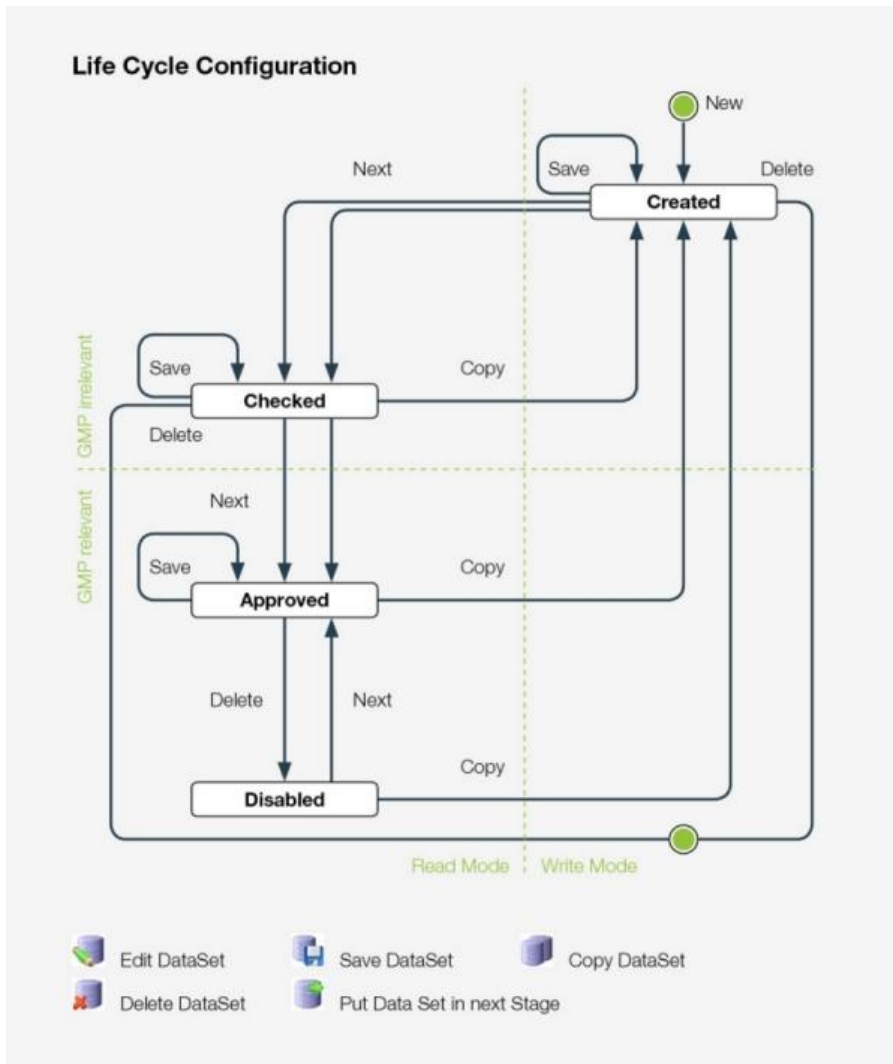
6.8.1. Lifecycle introduction

NIRWare has been designed to comply with 21 CFR Part 11. The Lifecycle model is the core of this compliance.

The Lifecycle approach enables to control the user access to the NIRWare software, transitions from one lifecycle state into the other and to keep a history of actions done (Audit Trail).

The following picture shows the principal lifecycle configuration. There are three relevant modes:

1. Upper right quadrant: this is the part of editing or developing electronic records (calibrations, applications etc.). The electronic records are in an edit state and can be changed. This area is in the write mode and is not GMP relevant.
2. Upper left quadrant: this is the part of testing calibrations or applications. This area is read only but it is not GMP relevant.
3. Lower left quadrant: in this part the electronic records are in routine use, after approval for it. This part is read only and it is GMP relevant.



Electronic records can be transferred into the next phase actively only. The user needs to save the electronic record and put it into the next stage.

6.8.2. Lifecycle states

In the lifecycle model there are four principal states for the data sets.

<ul style="list-style-type: none"> Created 	<p>In this state new data sets are generated and edited or developed, optimized.</p> <p>Two modes need to be differentiated: principally the data set is in the read-only mode. For editing it is necessary to press the Edit icon.</p>
<ul style="list-style-type: none"> Checked 	<p>In this state data sets are tested before they are approved for routine use. (This state is only available with the templates ER and ERES.)</p>
<ul style="list-style-type: none"> Approved 	<p>In this state the data set has been approved for routine use. In all templates the data set is read only.</p>





- Disabled



The data set is no longer in routine use. It is read-only and in a frozen mode.

State		Description
Not Created	No lifecycle data set is defined. Read only mode	
Created	A lifecycle data set is defined. Read only mode	This state allows editing by pressing the Edit icon.
Editing	A lifecycle context is defined Write mode	
Checked	A lifecycle data set is defined. Read only mode in the templates ER and ERES.	This state indicates that the lifecycle is in testing mode, the data is allowed to be used for testing, but not for routine use. Modifications are not possible. (not available with template "Unregulated")
Approved	A lifecycle data set is defined. Read only mode in all templates.	The lifecycle is in routine use mode.
Disabled	A lifecycle data set is defined. Read only mode.	The lifecycle is in a "frozen" mode. It is no longer in routine use. The data set can be reactivated with "Next".

6.8.3. Lifecycle actions

All the lifecycle functionality is managed within the state machine of lifecycle. The state machine holds all the lifecycle states and controls the transitions. In the Created state all electronic records are read-only. In order to edit a data set in the Created state it is necessary to press the Edit icon.

Edit		Edit Data Set Pressing this icon enables to edit the data set.
Save		Save Data Set Pressing this icon saves the data set with lifecycle information.
Copy		Copy Data Set Pressing this icon copies the data set
Next		Put Data Set into Next State

		Pressing this icon puts the data set into the next lifecycle state.
Discard		Discard Pressing this icon discards or aborts the Edit session.
Delete		Delete Data Set Pressing this icon deletes the data set

Action	Condition		Description
New	Created	The data set is the read-only.	Creates a new lifecycle data set.
Edit	Created	Changes to Write mode.	
Save	Created	Changes to read-only mode.	Allows the user to save the data set
Save	Checked Approved	The data set remains unchanged. The read-only mode remains. Used to change the User.	Starting in State Checked and Approved
Delete	In Edit mode	Changes to read only mode.	Aborts the Edit session. Changes are not saved.
Delete	Created Checked	The data set is deleted. The lifecycle context is deleted.	Starting in states Created and Checked:
Delete	Approved	The data set remains unchanged. The lifecycle state changes to Disabled.	Starting in State Approved
Discard	Edit Mode	Discards or aborts the Edit session.	
Copy	Checked Approved Disabled	The original lifecycle data set remains in its state. The new lifecycle data set is read-only.	A new lifecycle data set is created and set to the Created state. This data set has a higher version. Therefore a history (traceability) is given.

6.8.4. Lifecycle transitions

The lifecycle transitions describe the effect of the possible actions on the lifecycle data sets in the different states.

From state Created

To state:	Action	
Created	Save	
Checked	Next State	Audit Trail Log: Ready for testing. LC Condition: Created disabled
Deleted	Delete	Audit Trail Log: Deleted

From state Checked

To state	Action	
Created	Copy	Audit Trail Log: Reason
Checked	Save	Audit Trail Log: User changed
Approved	Next state	Audit Trail Log: ready for routine use LC Condition: Checked disabled
Delete	Delete	Audit Trail Log: Deleted

From state Approved

To state:	Action	
Created	Copy	Audit Trail Log: Copy reason
Approved	Save	User changed
Disabled	Delete	No longer in routine use

From state Disabled

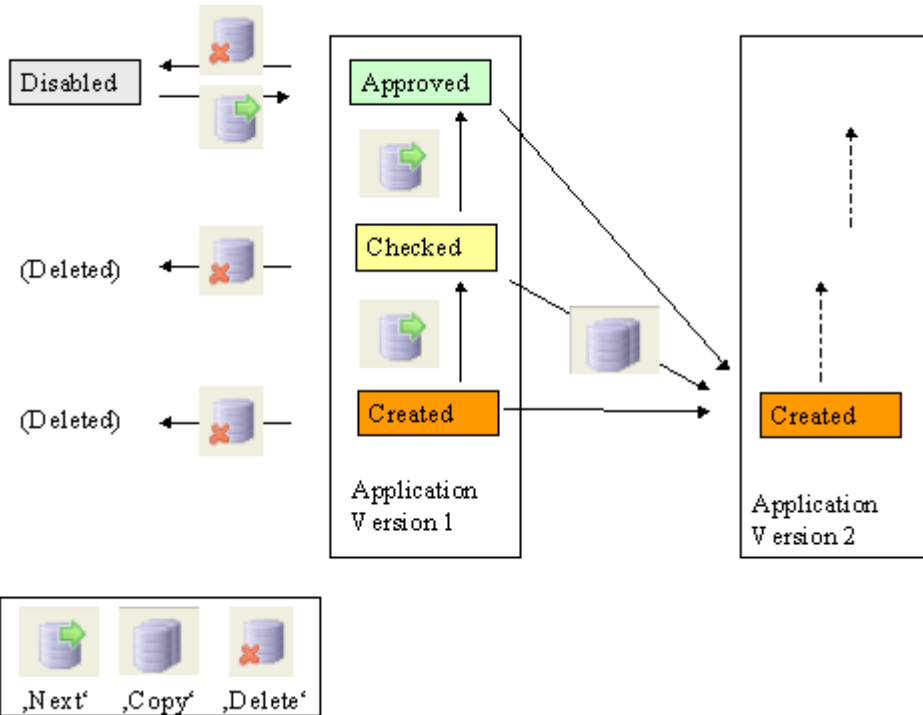
to state:	Action	
Checked	Copy	Reanimate for testing
Approved	Next State	Reanimate for routine use

Example: Lifecycle transitions using Template [ER](#) or [ERES](#).

A newly created Application (Version 1) becomes the state Checked by clicking Next and then Approved by clicking Next a second time. An Approved Application cannot be deleted, only disabled. Disabled Applications can be put back to Approved by clicking Next.

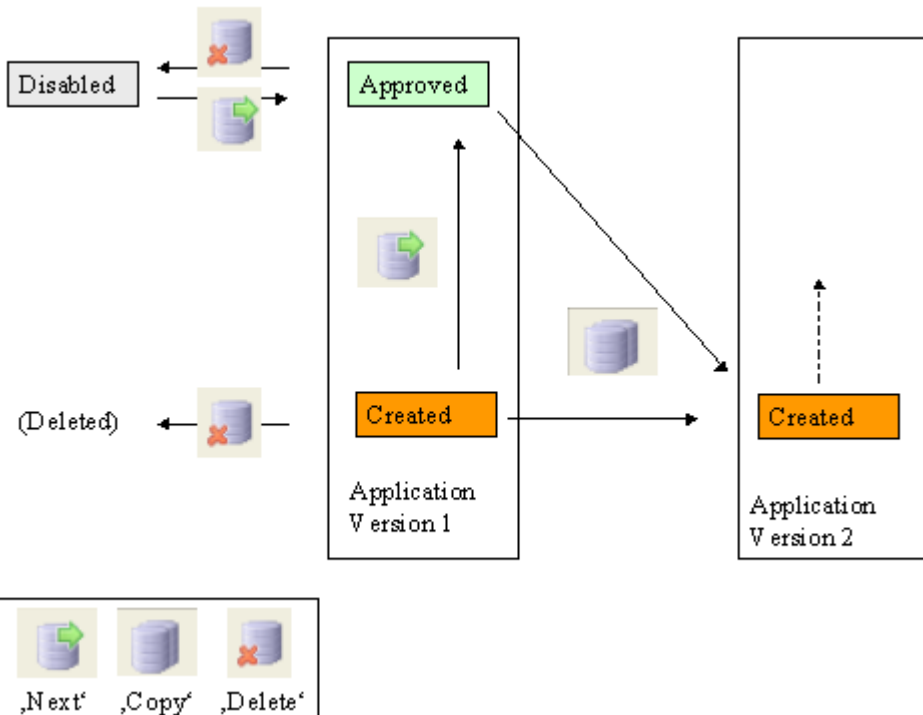
By clicking Copy the Version number of the Application is incremented by one.

Receives Version 2 when clicking copy,



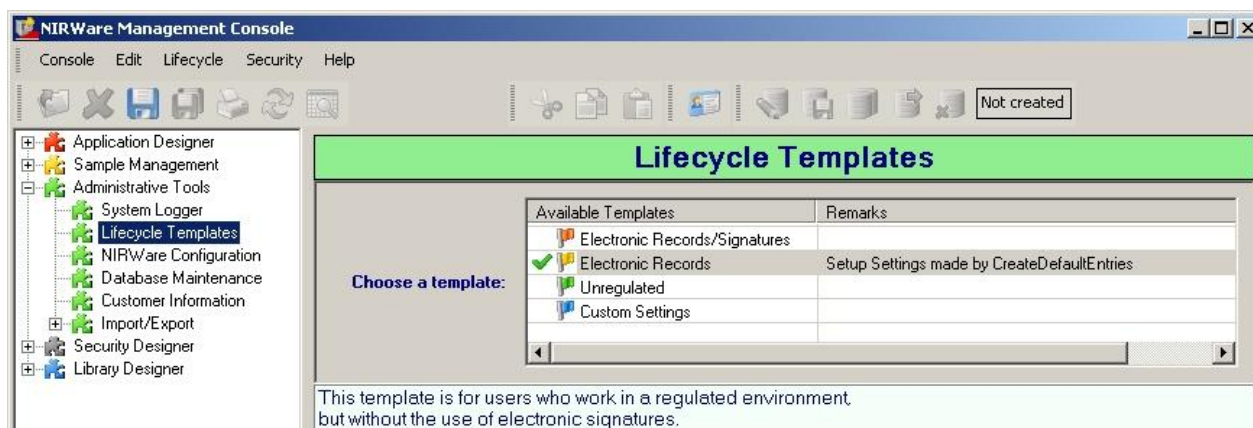
Example: Lifecycle transitions using Template [Unregulated](#).

In Lifecycle Unregulated there is no Checked state, the application is set to Approved by clicking Next instantly.



6.8.5. Lifecycle templates

The requirements for various industries are very different. Only GMP relevant areas of the pharmaceutical industry must comply with all requirements of 21 CFR Part 11. On the other hand there are industries, which are not affected by these requirements at all, e.g. Food&Feed industries. In order to simplify the use of the implemented lifecycle model, there are three pre-defined templates available, which fulfill various requirements.



The following description and tables summarize the settings for the different templates.

Unregulated

This template is for users who do not need to bother with the regulations. The settings are reduced to the minimum. There are no Comments, Audit Trail entries and no electronic signatures needed. From the create state the data sets are directly put into the approved state. With this template it is possible to edit the data sets in the Approved state as well.

Unregulated	Action	Signature	Comment	Audit Trail	Constraint Signature
Create	Copy			<input checked="" type="checkbox"/>	
	Delete			<input checked="" type="checkbox"/>	
	Edit				
	Next			<input checked="" type="checkbox"/>	
Create Edit	Save			<input checked="" type="checkbox"/>	
Approved	Copy			<input checked="" type="checkbox"/>	

	Delete			<input checked="" type="checkbox"/>	
	Edit				
Approved Edit	Save			<input checked="" type="checkbox"/>	
Disabled	Copy			<input checked="" type="checkbox"/>	
	Next			<input checked="" type="checkbox"/>	
Not created	New			<input checked="" type="checkbox"/>	
Deleted	Delete				

Electronic Records

Most transitions do need just a comment and no formal electronic signature. Again the checked state is missed out. There are various Audit Trail entries. However electronic signatures are not needed. With this template it is possible to edit the lifecycle data sets in the Approved state as well.

Electronic Records/Signatures	Action	Signature	Comment	Audit Trail	Constraint Signature
Create	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Delete		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Edit				
	Next		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
Create Edit	Save			<input checked="" type="checkbox"/>	
Checked	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Delete		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Next		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
Approved	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Delete		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	

Disabled	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Next		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	

Electronic Records/Signatures

This template covers all requirements of 21 CFR Part 11. An electronic signature is required for all phase transitions. Going from the checked state into the approved state, the electronic signature must be given by a different person (Constraint Signature). When signing electronically it is mandatory to enter a comment giving the reason for the action. Everything is documented in the Audit Trail. Editing is allowed only in the Create state. Editing the lifecycle data sets is not possible in the Checked and Approved states.

Electronic Records/Signatures	Action	Signature	Comment	Audit Trail	Constraint Signature
Create	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Delete		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Edit				
	Next	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
Create Edit	Save			<input checked="" type="checkbox"/>	
Checked	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Delete	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Next	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Approved	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Delete	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
Disabled	Copy		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
	Next	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	

Custom Settings


If users do have special requests BUCHI can provide a customized template, which will be tailor made to the customers specifications. It can be imported into NIRWare via the import functions.

6.9. Administration

6.9.1. Installshield Update Service

Update over Internet is discontinued with NIRWare 1.4.

6.9.2. BUCHI Control System Service

Menu:	Windows Start / Programs / BUCHI / NIRsolutions / Tools / ControlSystem Service Manager
Icon:	





NOTE

Under Windows 7 Windows administrator rights are required to use the ControlSystem Service Manager.



Only one Operator instance can connect to a Control System at the same time.

If an Operator tries to connect to an already busy Control System a message appears, stating that the Control System is already occupied by another instance of the Operator.

Icon in the SysTray of Windows:

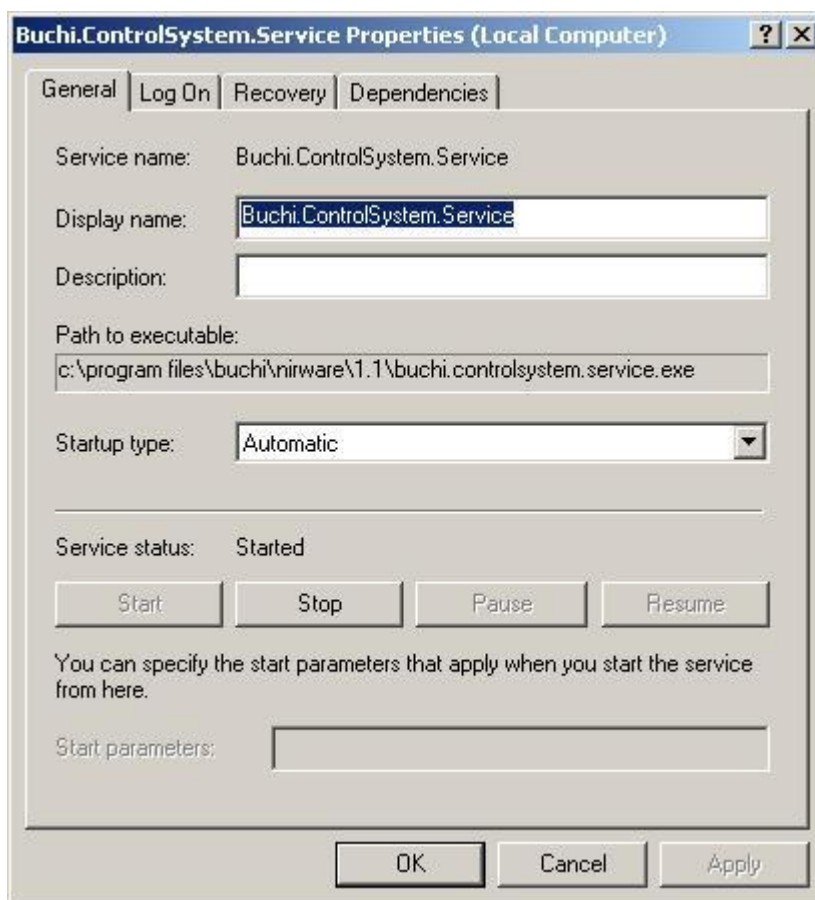
	Icon indicating that the BUCHI Control System is running
	Icon indicating that the BUCHI Control System is stopped

To quit the Control System Service:

- double click the Icon in the SysTray  (e.g. when running)
- Click "Stop the ControlSystem Service"
- Close the User Interface "BUCHI ControlSystem Service"
- Click with the right mouse the Icon in the Systray  and select Quit

Manual Start of the Service

Per default the service automatically starts after booting the operating system and searches for the instrument. It is possible to change this from Automatic to Manual. Open the Microsoft Computer Management Console (e.g. Win2K : Start / Programs / Administrative Tools / Services) and double click the service "BUCHI ControlSystem Service"



Under Startup type it is possible to change from Automatic (default) to Manual.

The Control System is designed to act as a background service in a Microsoft Windows operating system and starts automatically when the operating system is started. The purpose of the Control System Service is to establish the communication between the spectrometer and the PC.

The Control System tries to locate the [configured instrument](#) and establishes a connection.

6.10. System test

6.10.1. SST

The System Suitability Test is an internal system test which is performed regularly to verify the system performance. For this purpose the NIRFlex N-500 is equipped with a standard wheel with the following standards:

- Wavelength standard (PMMA) to check the wavelength accuracy
- Grey standard to check signal to noise ratio (S/N)
- Four different grey standards to check the linearity

The SST consists of four different tests:

Wavenumber Accuracy

Two measurements are performed at two different wavenumbers. Both measurements must be in between a given tolerance of 0.80 cm^{-1} .

The wavenumber accuracy of the system is checked with a standard material which has well defined peaks in the NIR range. This standard material has to be stable and must be traceable to a NIST 1920a standard that is made of a mixture of three Rare Earth Oxide Powders.

Noise

The noise test consists of two methods, the high flux and the low flux test. The SST for noise is passed, when the minimum and the maximum values are below a predefined tolerance.

The high flux noise is measured at approximately 100 % signal level of the instrument using a 99 % reflective white standard (White), the low flux noise is measured at approximately 10 % using a 10 % gray standard.

The spectrum is split into sections of 300 cm^{-1} each. The peak-to-peak noise is measured for each section and used for the calculation of the mean noise and the maximum noise at both high flux and low flux.

Linearity

The system linearity test checks if the response of the spectrometer correlates linearly with a linear signal attenuation.

3 wavenumber positions are used during an SST; $5000 / 6250 / 8330 \text{ cm}^{-1}$

The actual absorbance at each wavenumber position (= measured absorb.) are compared with max. reference values (= Reference Absorb.).

These measurements are done using 5 different gray filters.

The deviation to the reference value as well as the interception are checked.

Temperature

Several temperature sensors are provided within the spectrometer. Temperature is checked at the following positions against reference values: wedge drive, instrument, laser and main board and, depending on the measuring cell, detector, detector board, application board. For every sensor a lower and upper limit value is predefined. The SST for temperatures is passed, when all temperatures are between the lower and the upper value.

The [SST test](#) can be performed manually or configured to be started automatically.

All results of the SST are documented in the [SST report](#).


6.10.2. NADIA

NADIA stands for „NIRWare Automatic Diagnose“ and is a service tool to examine the basic functions of the BUCHI NIRFlex-N500.

It will be used from Service Technicians to evaluate malfunctions of the instrument or to do a performance check of the instrument as part of a service contract.

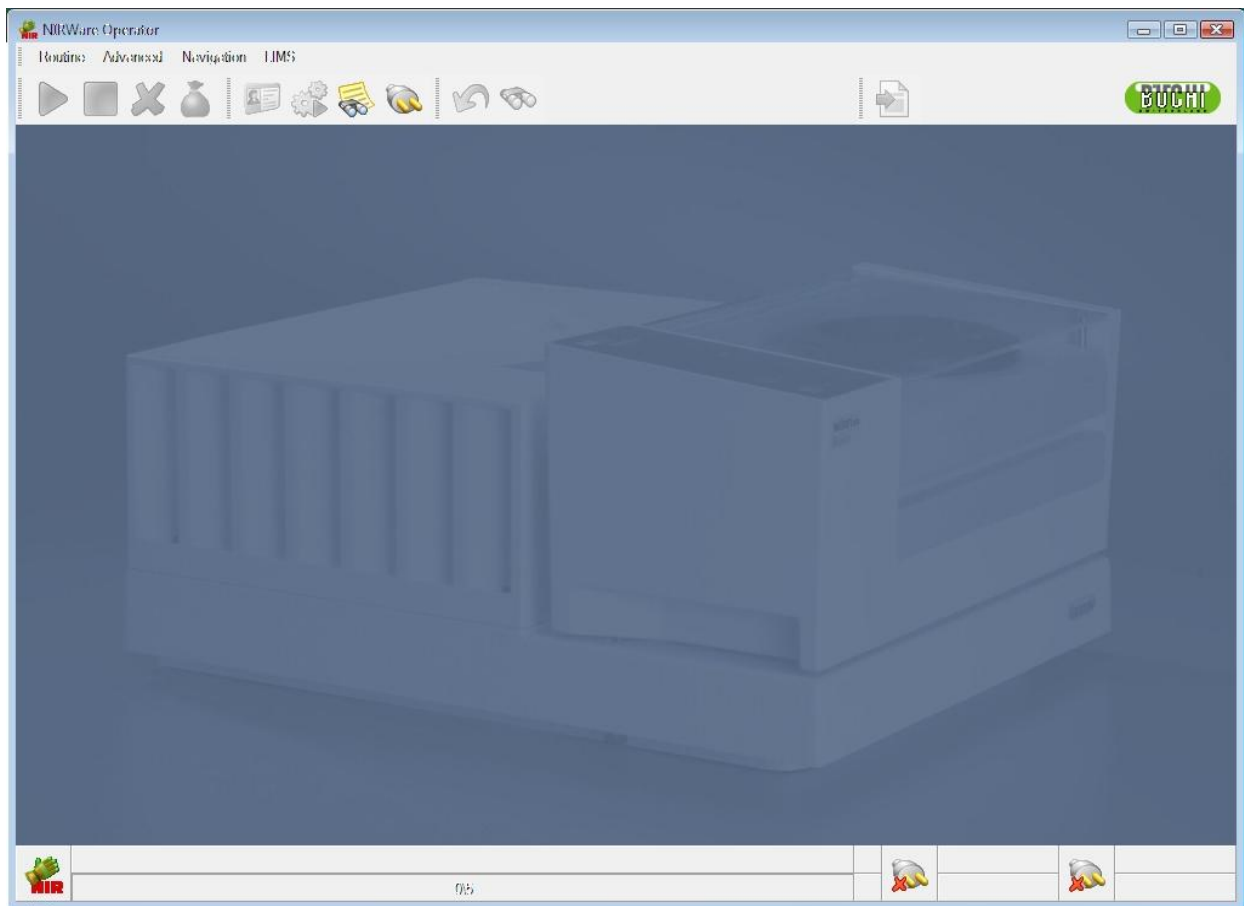
7. NIRWare Operator

7.1. Introduction Operator


Menu:	Windows Start / Programs / BUCHI / NIRsolutions / Operator
Icon:	











Start the application by clicking the Icon for the Operator or using Start Menu.

When prompted type in User and Password into the [Logon](#) dialog.



Icon description:

	Starts a measurement sequence (F2)
---	---

	Stops the current running Operator process (F3)
	Opens the "Delete Samples" menu (only in use with applications for data acquisition (no calibration assigned))
	Close Batch
	Opens the Logon Dialog to change user.
	Service and Maintenance tools (F4)
	Display the the System Logger (F5)
	Connect to NIRFlex N-500 (IP-Address according to configuration) (F6)
	Close Application (F7)
	Opens the dialog to select an application (F8)
	Opens the LIMS Import Options dialog

When everything works properly the status bar looks as follows:

	0400000016		0400000004
	NIRFlex N500		Fiber Optic Solids





green icons indicate that the instrument and the measurement cell are initialized and within specification.

7.2. Tab Overview

For the measurement cells Solids (with Petri and XL Add-On), Fiber Optic Solids and Fiber Optic SMA the so called tab overview is the default screen in the NIRWare Operator.

Parameter	Value	Status
Moisture	11.26	[%] ✓
Protein	11.70	[%] ✓
Baking Absorption	63.13	□ ✓
W	287.98	□ ✓
P	80.53	□ ✓
L	129.37	□ ✓
Falling Number	429.63	□ ✗
Damaged Starch	18.24	[%] ✓
Degree of softening	--	□ ✗
Dough development time	7.14	□ ✓
Stability	21.62	□ ✓

By clicking either on  or  you will find a detailed result window popping up.



The Detailed Result window shows the predicted value for the last measurement (in case the "Number of measurement sequences" is > 1).

When changing from Overview to Results, you will see the results of the individual measurements and the average values.

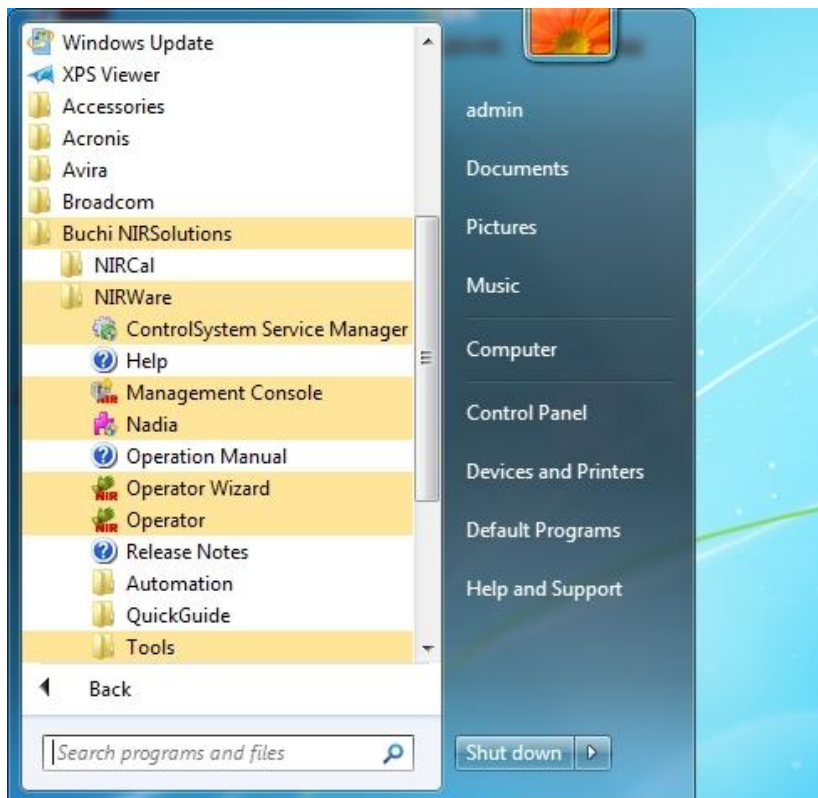


1		Wheat				Value		Residual	
		Flour_2010-10-12_10-51-08							
	1	11.16	%	ok	0.001568	ok			
	2	11.17	%	ok	0.001485	ok			
	3	11.14	%	ok	0.001505	ok			
	4	11.21	%	ok	0.001506	ok			
	Moisture	11.17	%	ok		ok	n:	4	
							StdDev:	0.029	
	1	11.64	%	ok	0.003183	ok			
	2	11.71	%	ok	0.003259	ok			
	3	11.64	%	ok	0.003283	ok			
	4	11.64	%	ok	0.003234	ok			
	Protein	11.66	%	ok		ok	n:	4	
							StdDev:	0.035	

7.3. Operator Wizard

In addition to the standard NIRWare Operator a simplified version is available, where an Operator Wizard will guide you through the process of application selection, batch, sample naming etc. The Operator Wizard is available for the measurement cells Solids (with Petri or XL Add-On), Fiber Optic Solids and Fiber Optic SMA.

The NIRWare Operator can be launched from the Start menu.





In the NIRWare Operator icon bar click the binocular to start the Operator Wizard.

Wizard

Select Application

	Application	Version	State	App Type	Description	License
▶	Meat	0	Created Idle	Quantification		
	SST Fiber Optic Solids	0	Created Idle	Identification	OQ Test	
	Rice	0	Created Idle	Quantification		
	Soft Wheat Flour	1	Created Idle	Quantification		

Select an application.

Wizard

Enter measurement description

Meat

Batch	Title	Values
	Meat 52	



Create a new batch or choose an existing one.

Wizard

Enter measurement description

Meat

AnalysisID

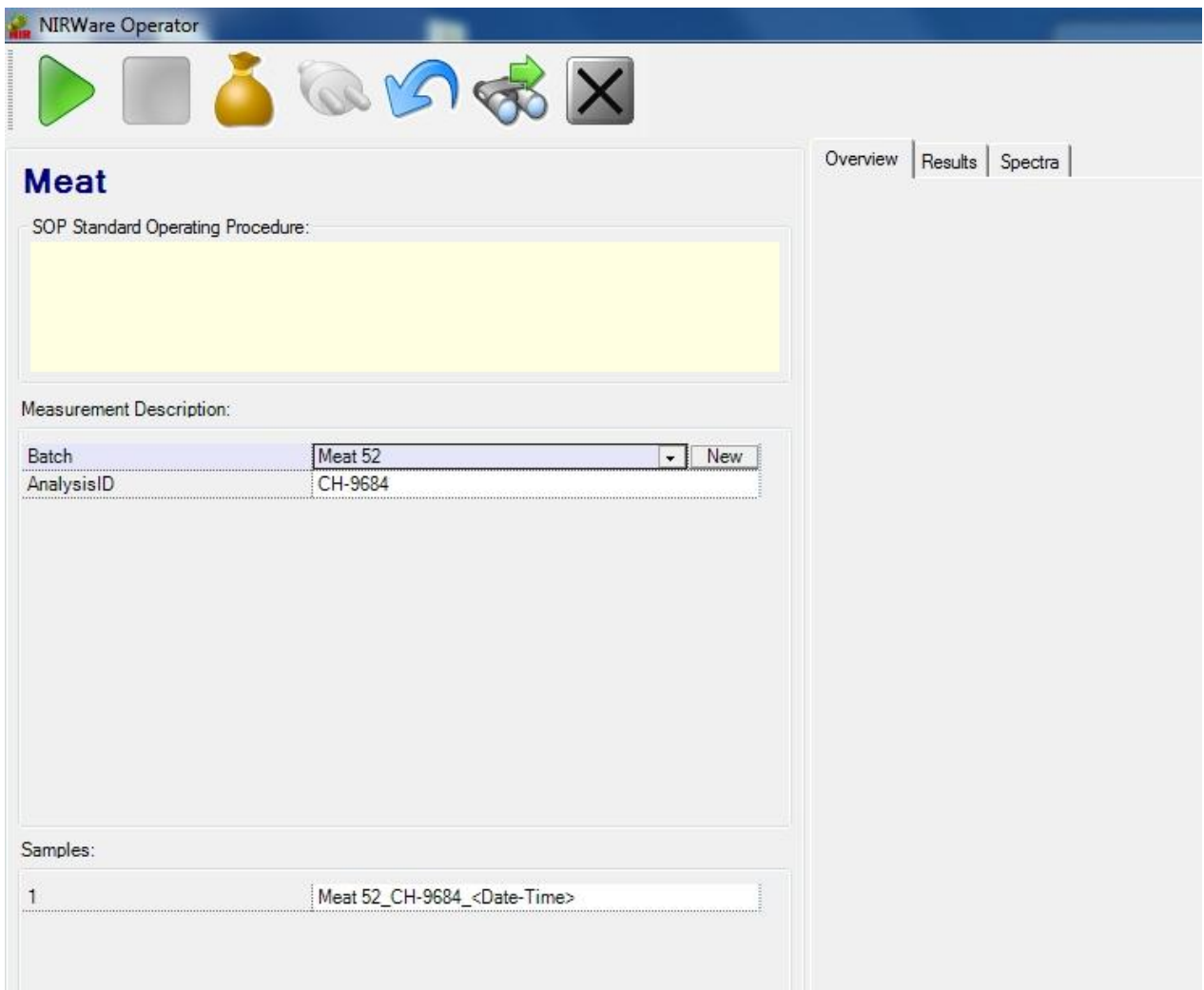
CH-9684



Enter all information that was selected in the Management Console (e.g. Analysis ID).



Confirm your settings in the final overview.



The application will be loaded and the measurement can be started.

NOTE

The Operator Wizard contains no menu bar. That means e.g. that it is not possible to measure an external reference manually.

7.4. Select Application

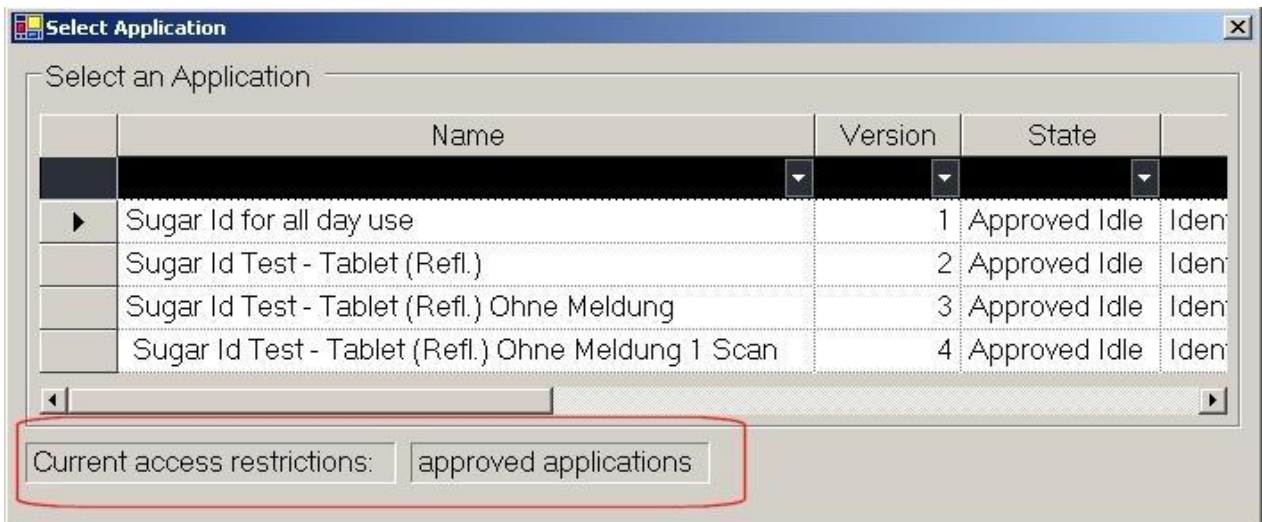


Clicking the Icon opens a dialog with all accessible applications.

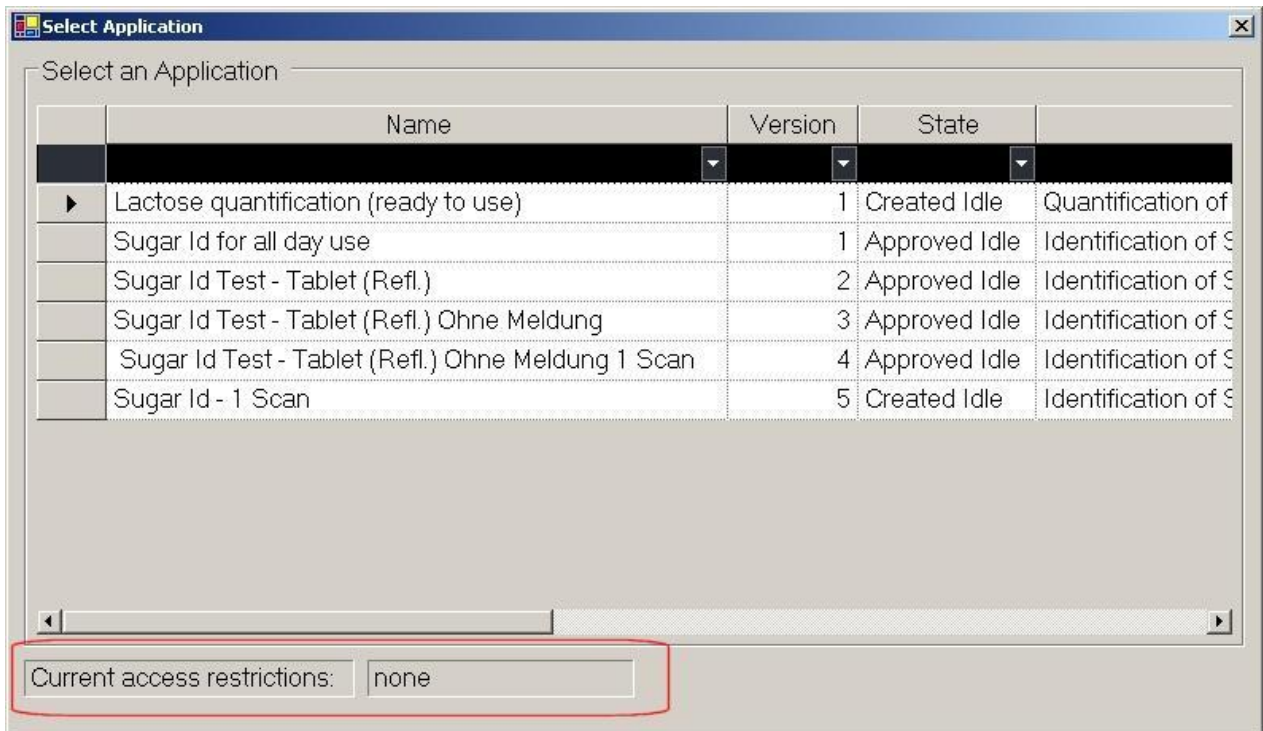
NOTE

Depending on the logged on user the list can differ. The default access restrictions for the user group "Operators" is set so that only applications which are in the lifecycle state "Approved" can be selected. "Administrators" have no access restrictions which allow them to use applications e.g. which are in the state "Created". Using such applications is not recommended.

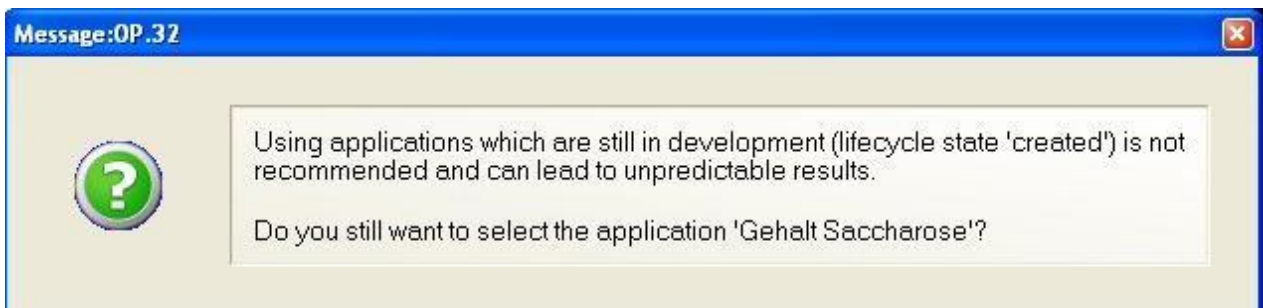
Example of Select Application Dialog for the User "Operator"



Example of Select Application Dialog for the User "Administrator"



Selecting an Application which is in the Lifecycle State Created the following message appears.



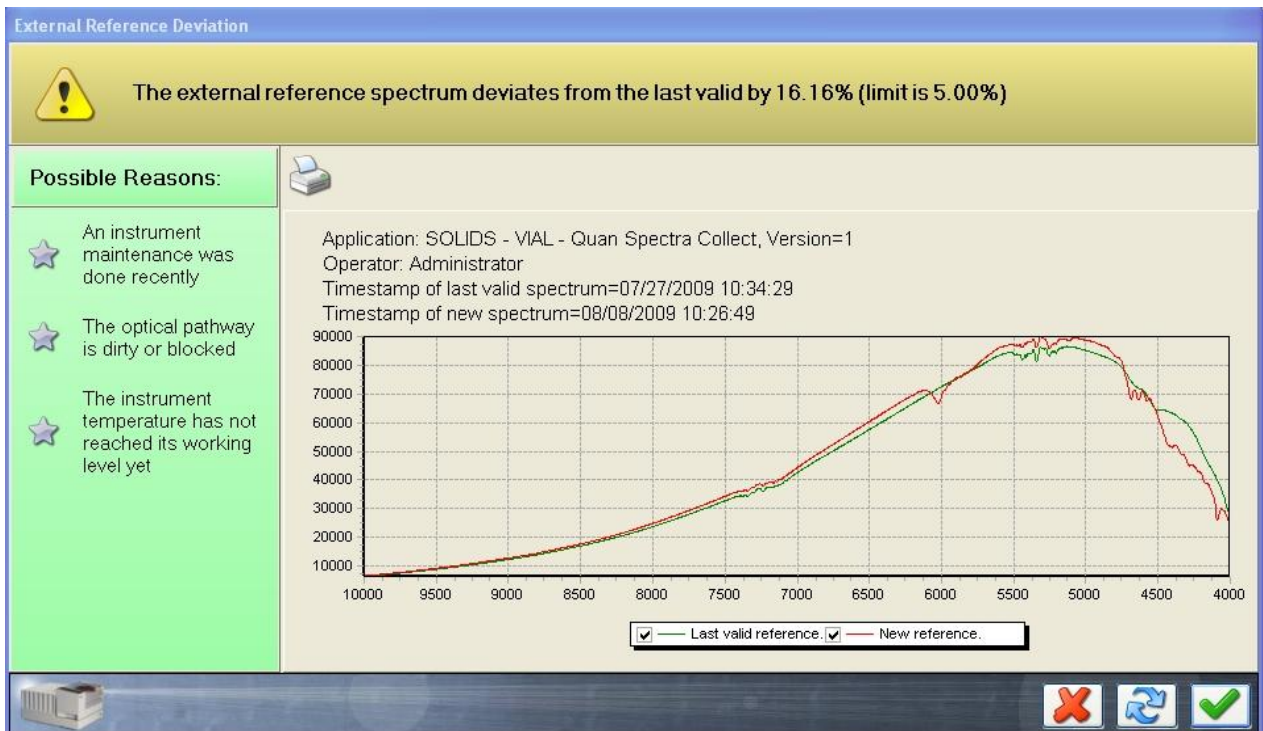
7.5. Deviating reference spectrum

7.5.1. Introduction

Spectral references are used to compensate for signal drift and other unwanted effects that could compromise the measured spectra. This is best done by using the 'External Reference', because it is measured at exactly the same position as the sample. NIRWare now offers an improved automatic test of the measured spectrum. This test compares the currently measured reference spectrum against the previous reference spectrum for the respective application.

7.5.2. Description

The test procedure generates a value for spectral deviation, expressed as relative number (%). If this value is below the acceptance limit, the new spectrum is automatically accepted as current reference. Otherwise, the user will see the following dialog:



The graphic enables to compare both spectra, so that experienced users can get an idea about the cause of the observed deviation (see Tips and Tricks section).

Furthermore, helpful information is given in the green column on the left-hand side of the dialog.

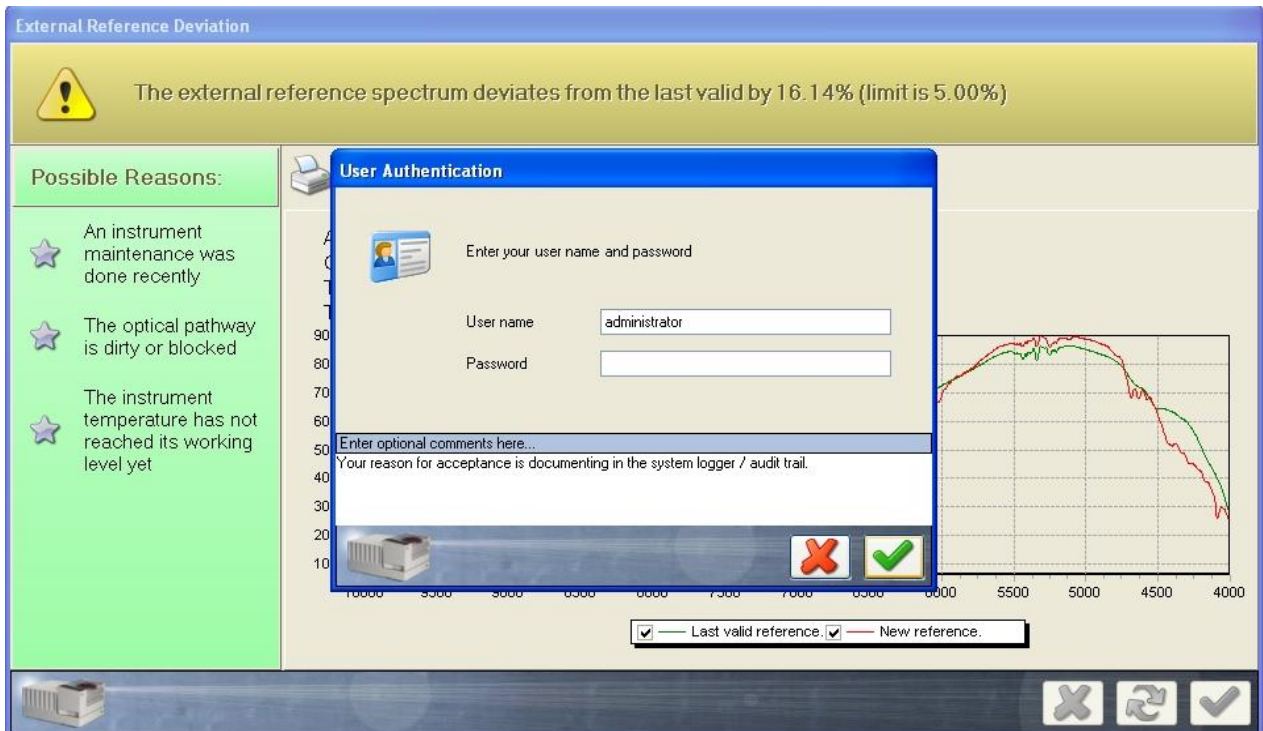
The user can now decide on how to proceed:

Pressing the red X button will discard the 'new reference' spectrum, and abort the measurement.

Pressing the blue arrows-button will discard the 'new reference' spectrum, and automatically repeat the external reference measurement. This enables to correct obvious operation errors.

Pressing the blue arrows-button will accept the 'New reference' spectrum as valid.

If you have decided to accept a deviating reference spectrum, you will see the following dialog, where you have to confirm your decision with your user log-in, and give a reason for the decision:



NOTE:

By default, only administrators are allowed to give the signature for acceptance. Everyone else will get an error message. -This security setting can be configured within the **Management Console under Security Designer – Security Policies: Acceptance of External References**.

7.5.3. Tips and Tricks

Frequent causes for deviations

Temperature drift

The performance of lamp, detector and electronics is influenced by the temperature. Despite many ingenious compensation techniques (like using a thermostated detector), a slight temperature dependence is inevitable. Therefore, you should operate the instrument in a thermostable environment (avoid direct sunlight or strong illuminating spots, cold winds from open windows or air condition,...) and let the instrument warm up to operating temperature several minutes after start up, before using it.

Temperature effects mainly cause intensity differences, while the spectrum curve shape basically remains the same.

Dirty reference or optics

Any extra material in the optical pathway can alter the spectrum. Therefore, keep your reference and optics clean. Extra bands suddenly showing up in the spectrum indicate extra substance in the optical pathway.

Error in hardware setup

If the external reference has simply been forgotten, or was mounted incorrectly, this will obviously result in faulty spectra. Therefore, always check your hardware if you encounter a deviation warning.

Interpretation of the spectra in the example above

The two spectra shown in the picture further above show pretty similar max. intensities (ca. 85.000 vs. 90.000 AU); furthermore, we can see an extra band at around 6.000 1/cm, and around 4.500 1/cm; in addition, the curves are well separated from each other in the range of 4.000 – 4.500 1/cm.


These extra bands hint an extra material in the optical pathway as most probable cause of the observed spectral deviation, rather than just a simple temperature drift.

7.6. Using the LIMS Interface

7.6.1. Using LIMS Export only

Select an application from the available list.

Enter all required information (keyboard or barcode reader) and start the measurement by clicking the

"Start" button  .

If the measurement is interrupted no export file will be generated.

If the measurement is finished successfully, but also in case the measurement is out of specification or the expected substance does not match, and after signing the measurement (depending on the lifecycle state), the result files will be written to the outbox. There is a separate file for each sample.

Using LIMS Import and Export

In the Operator toolbar the following icon is used for the LIMS import. This option is only visible with an active LIMS Interface license.



By clicking this icon the Operator selects an import file. The type of job selection can be defined in the [LIMS General Options](#) in the Management Console (oldest first, newest first, manual file selection).

Various checks will be performed to ensure the compatibility of the import file with the LIMS and application configuration:

The syntax of the file is checked as it is defined for XML and CSV types.

LIMS further checks, if:

- Mandatory fields are selected
- A valid license is active
- The batch name already exists or the batch is closed
- More samples than defined in the sample plan or in the measuring cell option are present
- Unicode compatibility is fulfilled

If the test passes, the Operator loads the job, starts the corresponding application and fills in the selected fields in the input mask. All fields activated for LIMS should be also activated in "**Operator Configuration - Sample Description Fields**".



To start the measurement, click the "Start" button .

During the measurement the import file is locked.

If the measurement is interrupted no export file will be generated.

If the measurement is finished successfully, but also in case the measurement is out of specification or the expected substance does not match, and after signing the measurement (depending on the lifecycle state), the result files will be written to the outbox. There is a separate file for each sample. The import file will be deleted automatically.

NOTE:

An export file is only generated if the import file could be read properly.

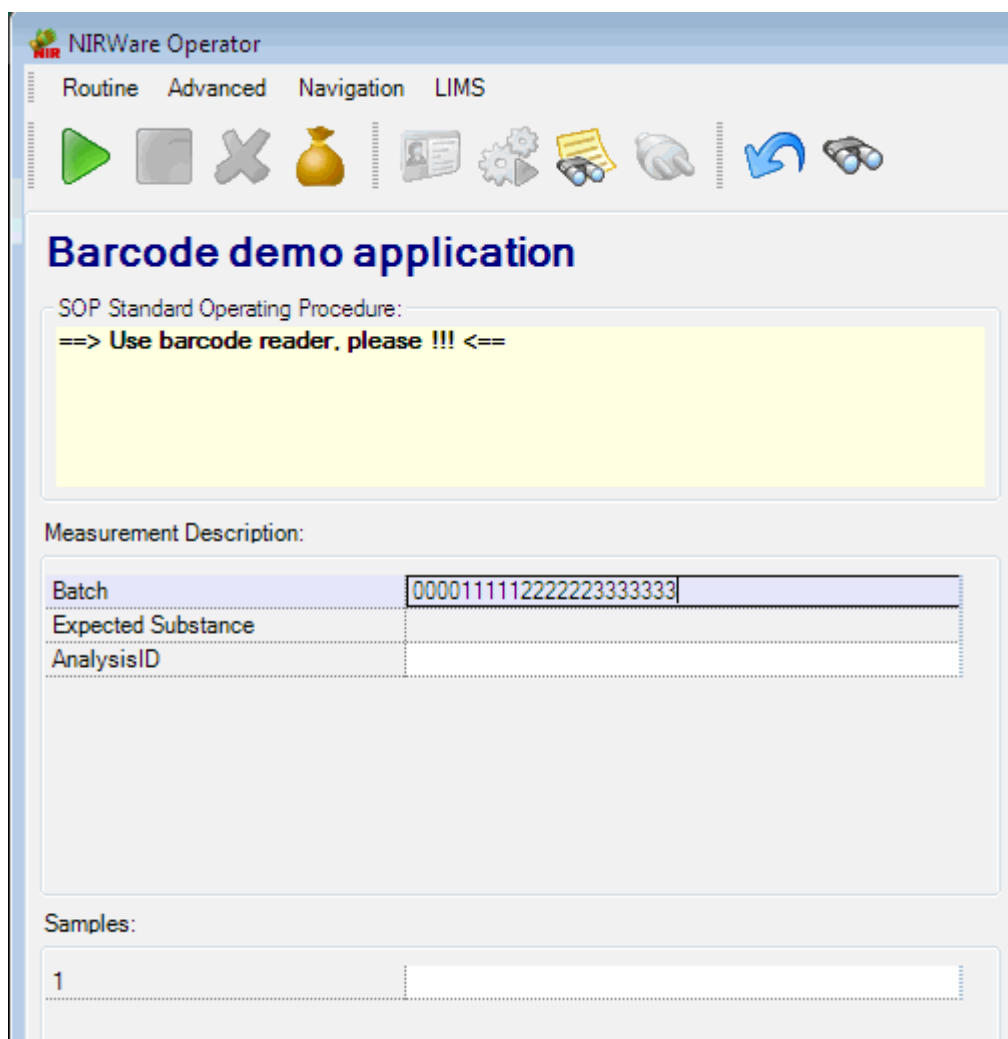
In the Application Designer it is recommended to select the options "Field Reset" and "Read Only", so that the input fields are cleared after the measurement.

If the configuration in the LIMS Interface is changed, the Operator and the Control System Service have to be restarted.

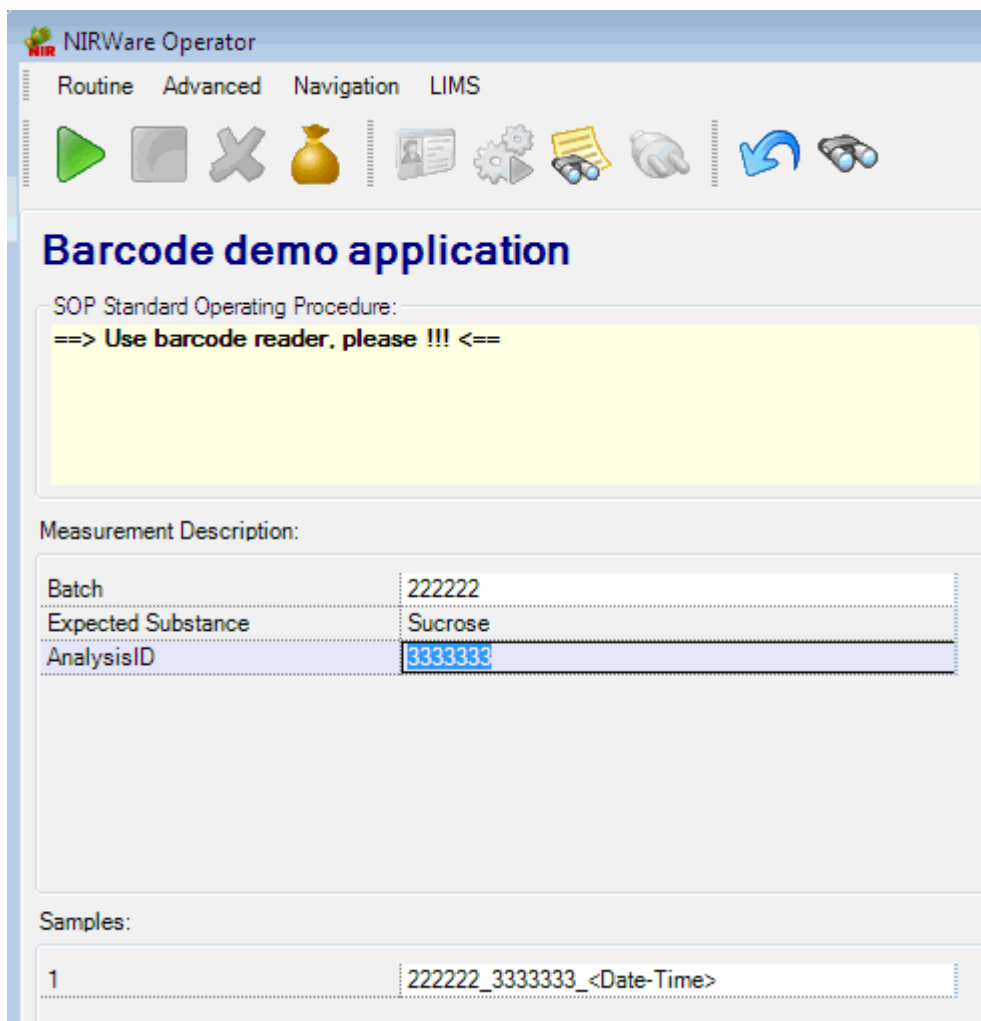
7.7. Using bar codes

After the configuration of application and property-IDs, we are ready to use the NIRWare Operator with the bar code reader:

After loading the application, we read the bar code into the 'Batch'-field:




This input will automatically be fractionated into the following fields:

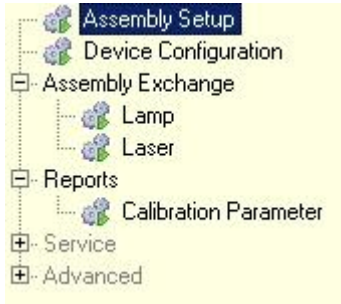


Please note that “11111” was automatically translated into “Sucrose” as “Expected Substance” by means of the respective PropertyID.

7.8. Service module

7.8.1. Introduction to the Service module

Menu:	NIRWare Operator / Advanced / Service
Icon:	



























The Service module is intended mostly for a service engineer to see and change instrument parameters.

The default setup only allows the User "Service" with the corresponding password access these advanced functions of the service module. Users other than "Service" have restricted access to the Service module in order to do the following maintenance work on the system:

- **Assembly Setup** to reset sensors when the covers were opened
- **Device Configuration** to change the IP address of the NIRFlex N-500
- **Assembly Exchange Lamp** to reset the lifetime counter of the lamps
- **Assembly Exchange Laser** to reset the lifetime counter of the laser
- **Reports Calibration Parameter** to view or print instrument parameter settings

Assembly Setup

	Assembly	Article	State	Access		
1	Main Board	46134	done	denied		
2	Optical Fiber Transmission	48494	done	denied		
3	Interferometer	42725	done	denied		
4	Fiber Optic Liquids	48441	done	denied		
5	Detector Board	45360	done	denied		
6	Standard Wheel	46119	done	denied		
7	Lamp	42774	done	granted		
8	Laser Module	42787	open	granted		
9	Application Board	45365	done	denied		
10	Cell Detector Unit	45323	done	denied		

Assembly	List of assemblies with their description
Article	Order No. of an assembly
State	State of an assembly
Access	Access indicates whether the current user has the right to access a specific assembly.
	Start an assembly
	Reset an assembly

The screen shot above is an example when the cover of the laser module was opened.

- To reset the sensor of the laser click the **Reset** icon.
- To reset the lifetime counter of the laser click the **Start** icon.

Device Configuration



The screenshot shows a software window titled "Device Configuration" with two tabs: "Device" and "Host". The "Device" tab is active. It contains two radio button options: "Obtain an IP address automatically" (which is unselected) and "Use the following IP address" (which is selected). Below these options are three rows of input fields, each with four boxes. The first row is labeled "Address", the second "Subnet Mask", and the third "Default Gateway".

The TCP/IP address of the instrument (NIRFlex N-500) can be changed from default (192.168.1.1) to any other address.

In order to change the IP address of the instrument see: [Change instruments TCP/IP address](#)

Assembly Exchange Lamp & Assembly Exchange Laser



The screenshot shows a software window titled "Assembly Exchange Lamp & Assembly Exchange Laser". It contains two rows of data. The first row is labeled "Primary Lamp hours of operation" and has a yellow input field containing the number "1619". To the right of the input field is a circular icon with a hand and a bird, representing a reset function. The second row is labeled "Secondary Lamp hours of operation" and has a yellow input field containing the number "3". To the right of this input field is a similar circular icon.

The lifetime counter of the laser and both lamps (primary- and secondary lamp) can be seen and reset.

See: [Resetting lifetime counter of lamp or laser](#)

Reports Calibration Parameter

The screenshot shows the NIRWare Operator software interface. The main window displays the 'Calibration Parameter' report. The report includes the following information:

- Cell Detector Unit**: Article: 45323, Version: 00.10, S/N: 0400000019
- Detector Board**: Article: 45360, Version: 00.10, S/N: 0437-0019
- Parameter Table**:

Parameter	Version	Value
Description		Default Value
DT DcMax	1	56000
<i>Common: max. Gain of DC</i>		56000
DT DcMaxFraction	1	0.9
<i>Common: Fraction of Dc Max for AutoGain examination</i>		0.9
DT DcOffset	1	-25241.88
<i>Common: DC Offset of the detector</i>		-25241.88
DT LifeTimeDetector	1	3370126
<i>LifeTime:[s] Passed operation time of detector</i>		0
DT PeltiCoolerBeta	1	2894.6
<i>PeltiCooler: Beta value for temperature calculation</i>		2794
DT PeltiCoolerBeta	1	0.000077073
<i>PeltiCooler: Beta value for temperature calculation</i>		


The interface also shows a navigation pane on the left with options like 'Assembly Setup', 'Device Configuration', 'USP Test', 'Assembly Exchange', 'Lamp', 'Laser', 'Reports', 'Calibration Parameter', 'Service', and 'Advanced'. The bottom status bar indicates 'Current Page No.: 1', 'Total Page No.: 4', and 'Zoom Factor: 100%'.

Hardware parameters of the instruments can be seen, printed or exported, e.g. to pdf.



Click on  to open the report view.

7.8.2. Changing the instruments TCP/IP address

Menu:	NIRWare Operator / Advanced / Service / Device Configuration
Icon:	

Every NIRFlex N-500 has the static IP-address 192.168.1.1 (Subnet 255.255.255.0) per default. It has been delivered with a crossed Ethernet patch cable to communicate directly to an ethernet network card on the PC where NIRWare is running.

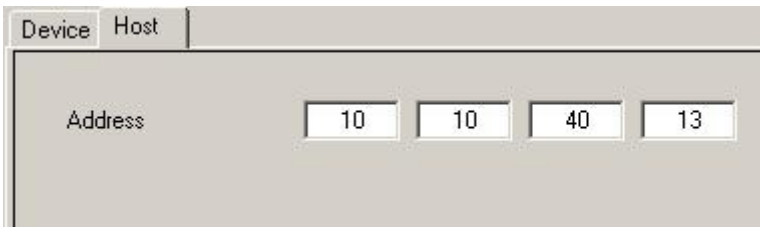
NOTE

In order to change the static IP-address of the NIRFlex N-500 (e.g. to the local requirements of the IT) the communication between PC and NIRFlex N-500 must be established. The user needs administrator rights on the OS.

1. Select **Device Configuration**

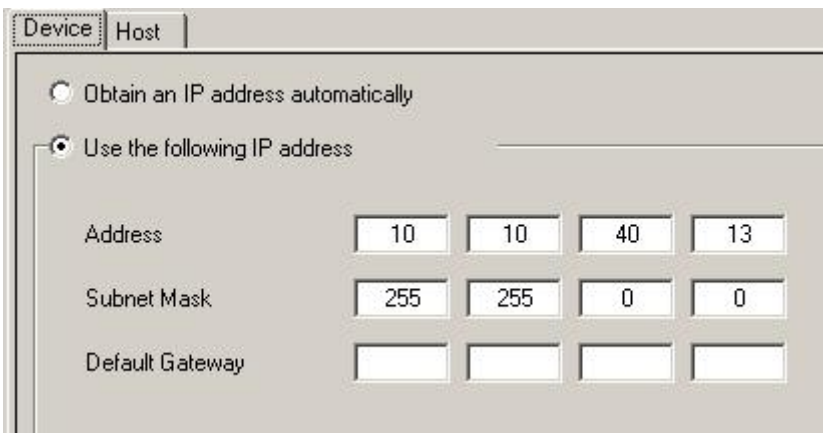


2. Select the **Host** tab



Edit the new IP-Address of the spectrometer and click the **OK** button.

3. Select the **Device** tab



Edit the new IP-address of the spectrometer including the Subnet mask again and click the **OK** button.

4. Confirm Security Message



Reconnect the control system afterwards in order to establish the connection.

NOTE

The configuration of the instrument IP and the connection information in the database have to match.

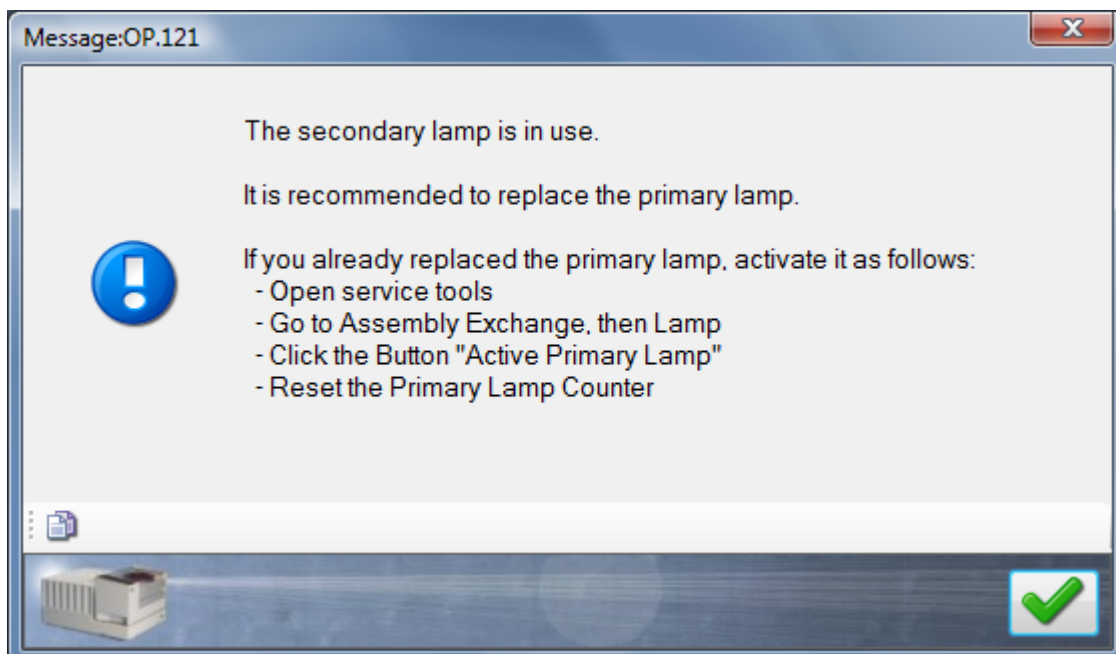
To connect to a different instrument, it will be necessary to edit the connection information in the database under Administrative Tools (NIRWare Management Console), [NIRWare Config](#) so that the Control System service connects to the new address.

Reset instruments TCP/IP address to its default

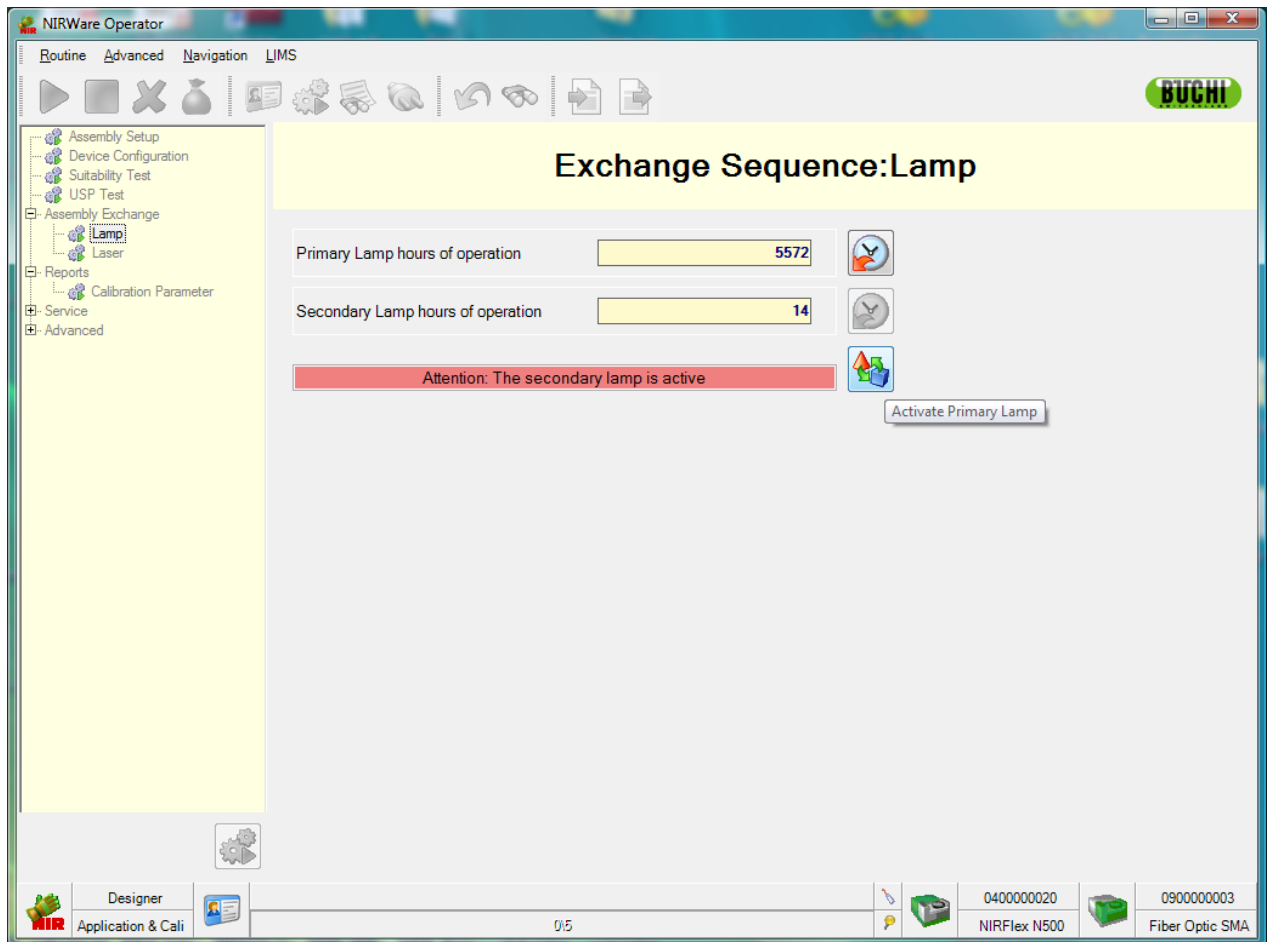
To reset the TCP/IP address of the NIRFlex N-500 to its default address (192.168.1.1) push both buttons **START** and **STOP** on the measurement cell continuously during power on for approximately 1 minute.

7.8.3. Activating the primary lamp after lamp change

When the system currently runs with the secondary lamp the following message will appear at the opening of the NIRWare Operator:




As soon as the primary lamp has been replaced, the described steps should be followed and the system should be switched back to the primary lamp. For this purpose, open the following dialog and click the button **Activate Primary Lamp**.



To reset the Primary lamp counter, see also [Resetting the lamp lifetime counter](#).



7.8.4. Resetting the lifetime counter of lamp or laser

Menu:	NIRWare Operator / Advanced / Service / Assembly Exchange Lamp (Laser)
Icon:	

After the installation of a new lamp or laser the corresponding lifetime counter should be reset.

To reset the lifetime counter of the primary lamp or the laser, open the Service module and select "**Assembly Exchange Lamp**" respectively **Assembly Exchange Laser**.

As instrument covers must be opened to replace the lamp or the laser, the sensors of the cover need to be reset in the Service module as well be means of **Assembly Setup**. See [Running an instrument setup](#)

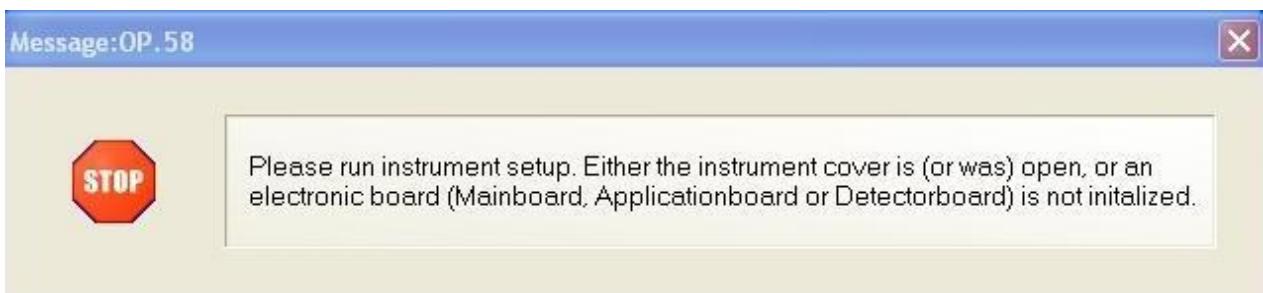
Primary Lamp hours of operation	<input type="text" value="1619"/>	
Secondary Lamp hours of operation	<input type="text" value="3"/>	



Click the icon Reset primary lamp counter to set it to 0 hours.
Confirm the following security message by clicking OK.


7.8.5. Running an instrument setup

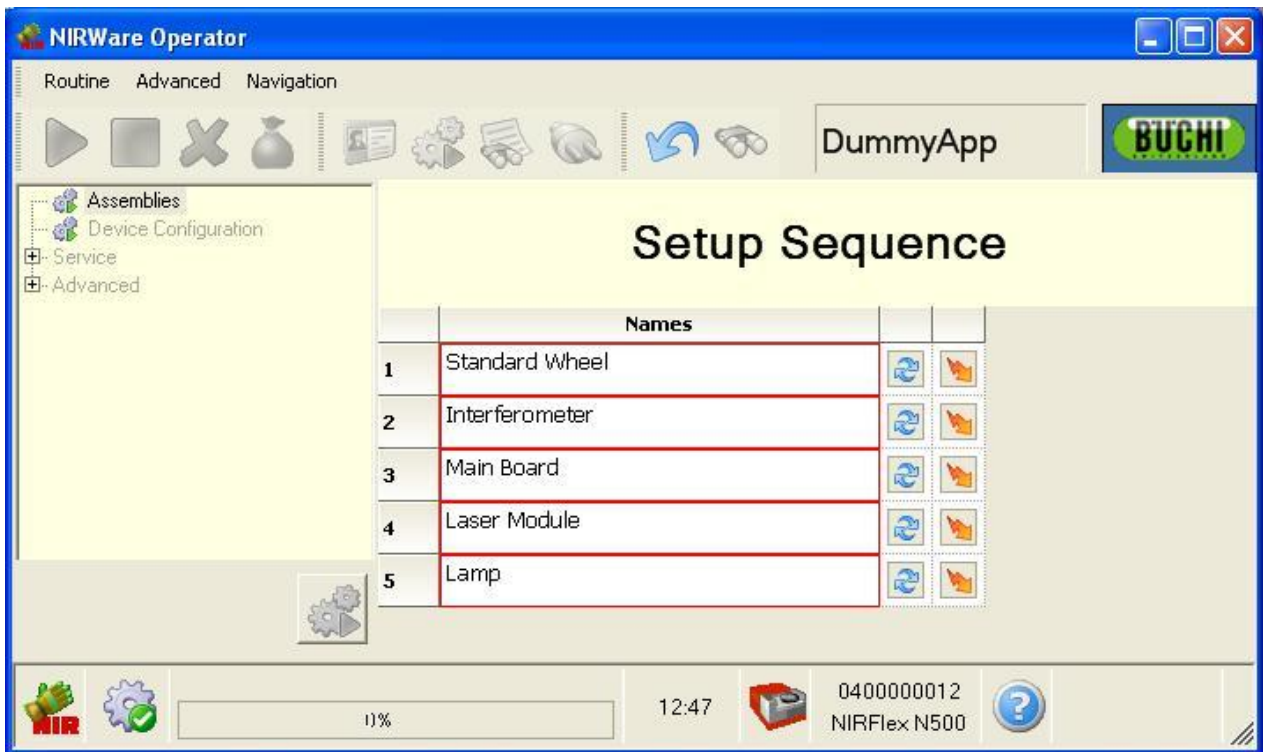
During the initialization process, the instrument recognizes when a cover was opened and the following message appears.




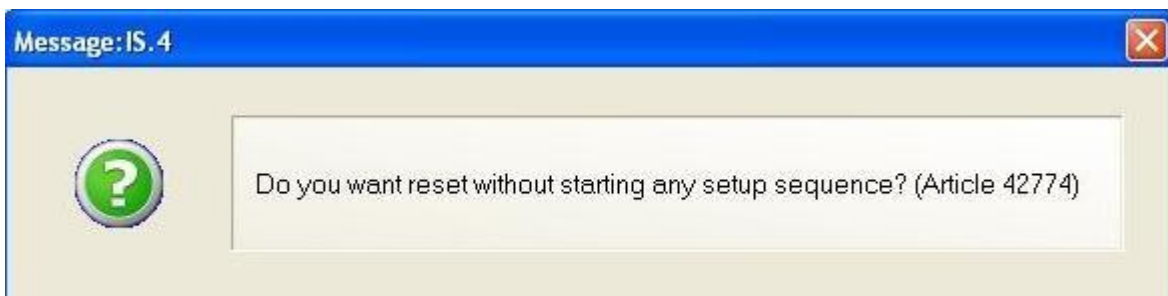
Click the green check mark button to confirm the message.



To run the **instrument setup** click the Service Icon  on the top of **NIRWare Operator** screen. Double click **Assemblies**, the following window appears.




Reset every position by clicking the Reset icon . The following message appears:



Confirming it by clicking the green check mark button.

After you have reset every parameter marked with the red frame around the name field, leave the

Assemblies menu by clicking the Back icon  twice.

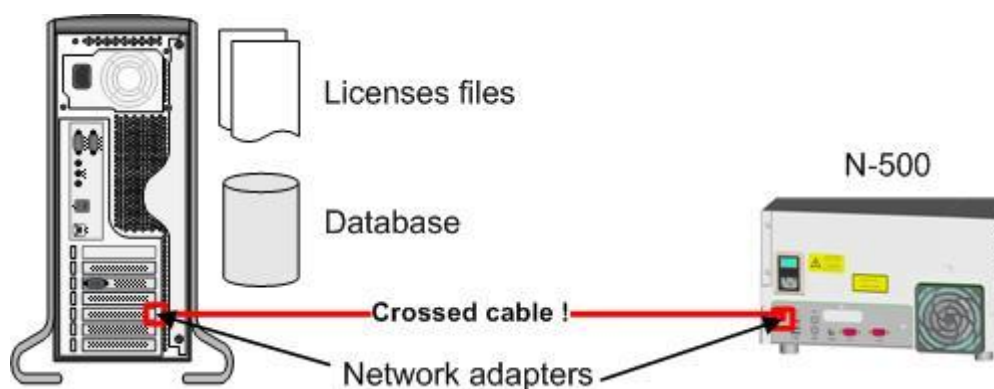
The Initialization process continues until the Instrument icon changes to green .

8. Server installation of a database

8.1. Typical installation scenarios

8.1.1. Standalone

In this scenario the PC is directly connected to the N-500, but to no other network device.



PC configuration:

Database	Free, but limited SQL Server SQL Express 2005 version, installed locally
Licenses	Installed and used locally
Network	Cable: crossed! Adapter: IP-address: 192.168.1.2 Subnet mask: 255.255.255.0
Data security	Burn database backups on several DVDs in regular intervals, e.g. daily or weekly.
NIRWare	Administrative Tools, NIRWare Config: 192.168.1.1

N-500 configuration:

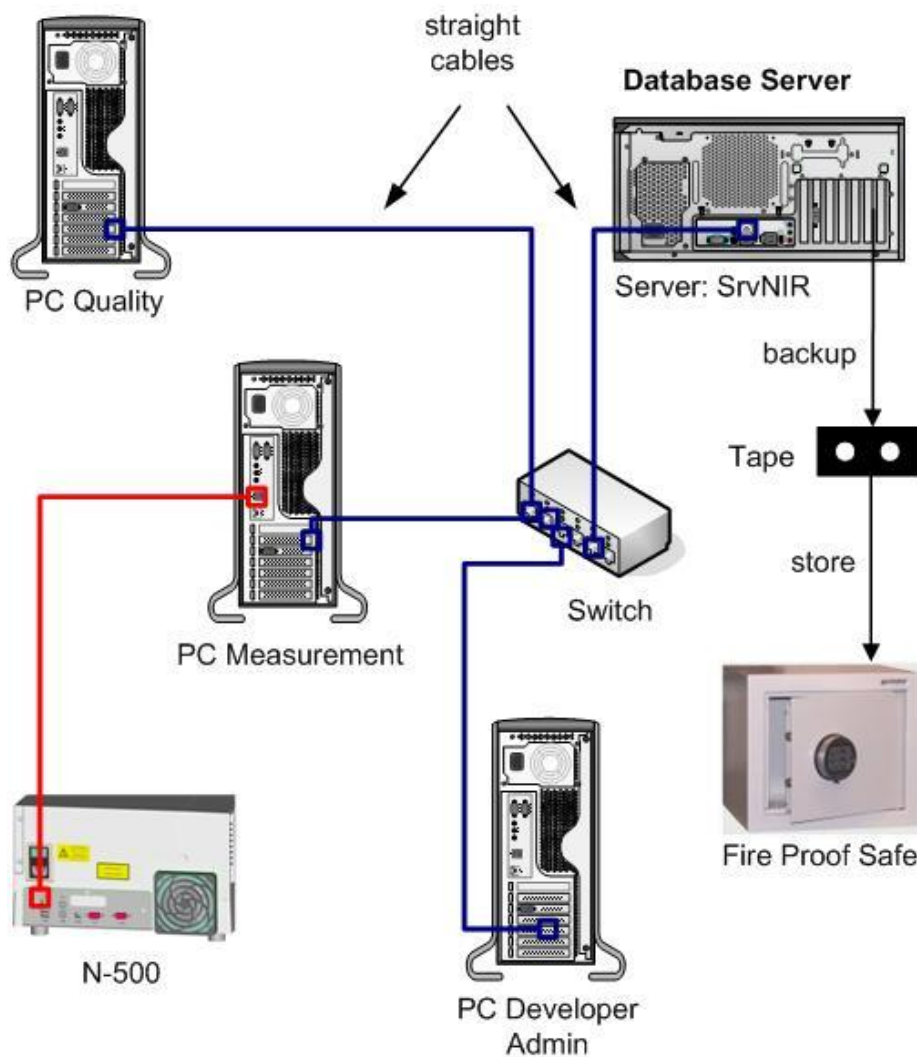
Network	Adapter: IP-address: 192.168.1.1 Subnet mask: 255.255.255.0
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8.1.2. Network installation

In this scenario three PCs are available for specific user roles (Measurement, QC, Administration). All data are stored on a dedicated database server computer with automated backup.

The following PCs are involved:

PC name	Role	Used software
PCMeas	Measurements	- NIRWare Operator
PCQuality	Quality Control	- NIRWare Management Console - NIRCal
PCDevAdmin	Calibration development Administration Users, Backup	- NIRCal - NIRWare Management Console



PCQuality configuration:

Database	Located on database server: SrvDB
Licenses	NIRCal / NIRWare
Network	Cable: straight

	Adapter: IP-address: Obtain automatically Subnet mask: Obtain automatically
Data security	solved on database server

PCMeas configuration:

Database	Located on database server: SrvDB
Licenses	NIRWare
Network	Cable: straight Adapter: IP-address: Obtain automatically Subnet mask: Obtain automatically Connection to N-500: Cable: crossed
Data security	solved on database server
NIRWare & N-500	N-500's IP-address: NIRWare Management Console > Administrative Tools > NIRWare Config > Connection Info: 192.168.1.1 (default)

PCDevAdmin configuration:

Database	Located on database server: SrvDB
Licenses	NIRCal / NIRWare
Network	Cable: straight Adapter: IP-address: Obtain automatically Subnet mask: Obtain automatically
Data security	solved on database server

Database server configuration:

Name	SrvDB
Database	Located on database server computer, accessed with an SQL - or Windows domain user as database owner
Licenses	No NIRFlex license required
Network	Provided and managed by customer's IT
Data security	Automated backup, e.g. every night, using a series of tapes (e.g. one for each workday), sotred away in a fireproof data safe.

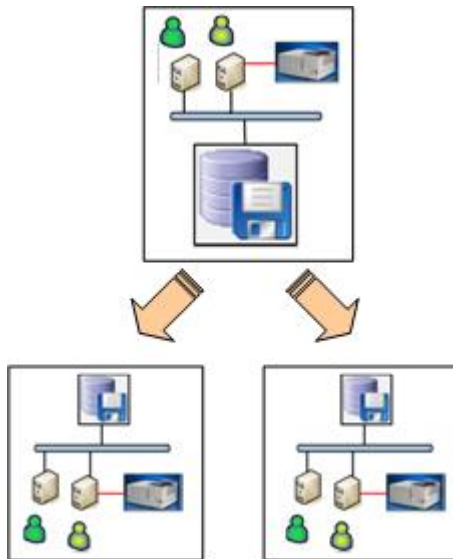
8.2. Worldwide connected N-500 network

This scenario describes a company with a headquarter and several production sites around the world. The plants work with local databases. The DB's in the plants are backed up periodically. Then the template database with actual applications at the headquarter is transferred to all plants.

NIRAnywhere takes over this function.

BUCHI has contract specialists, who do this in cooperation with the customer's IT.

Because the additional costs largely depend on the individual situation, it is essential to contact BUCHI Switzerland for a customer specific offer.



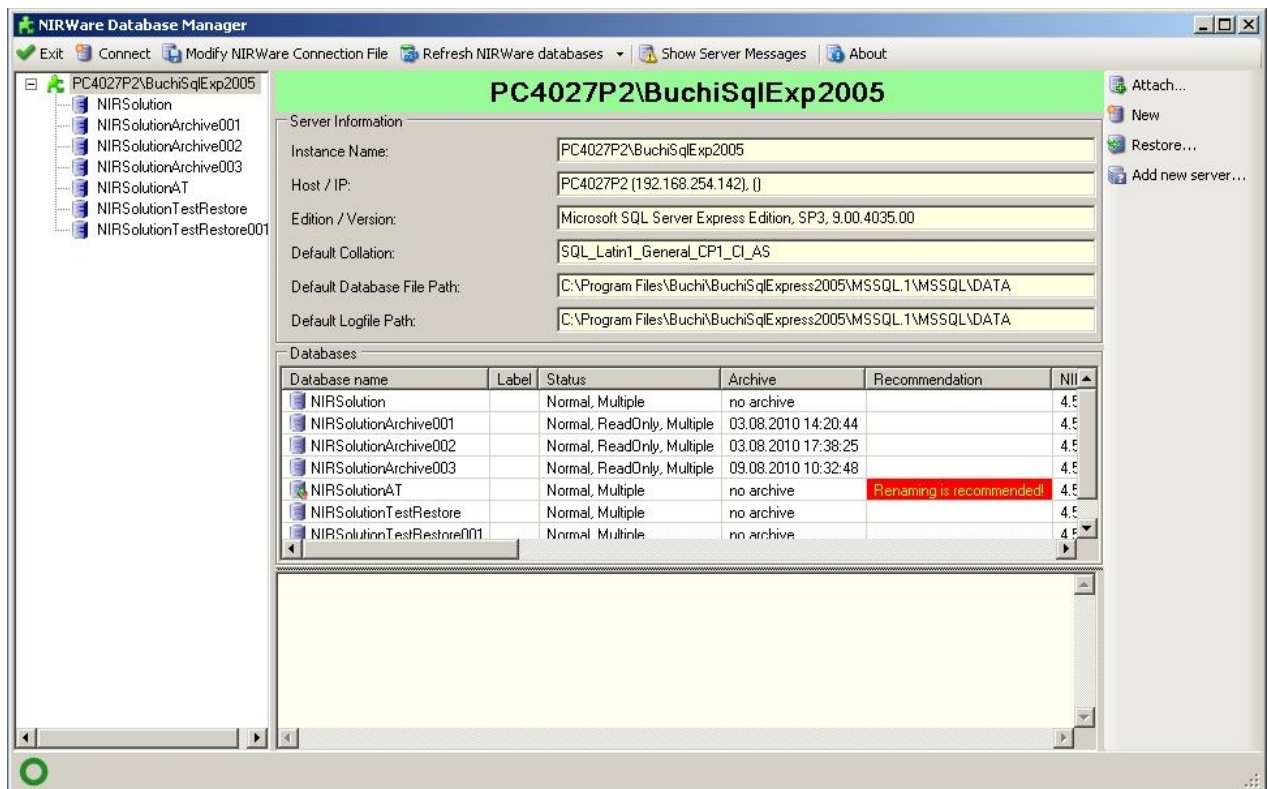
9. NIRWare Database Manager

9.1. NIRWare Database Manager

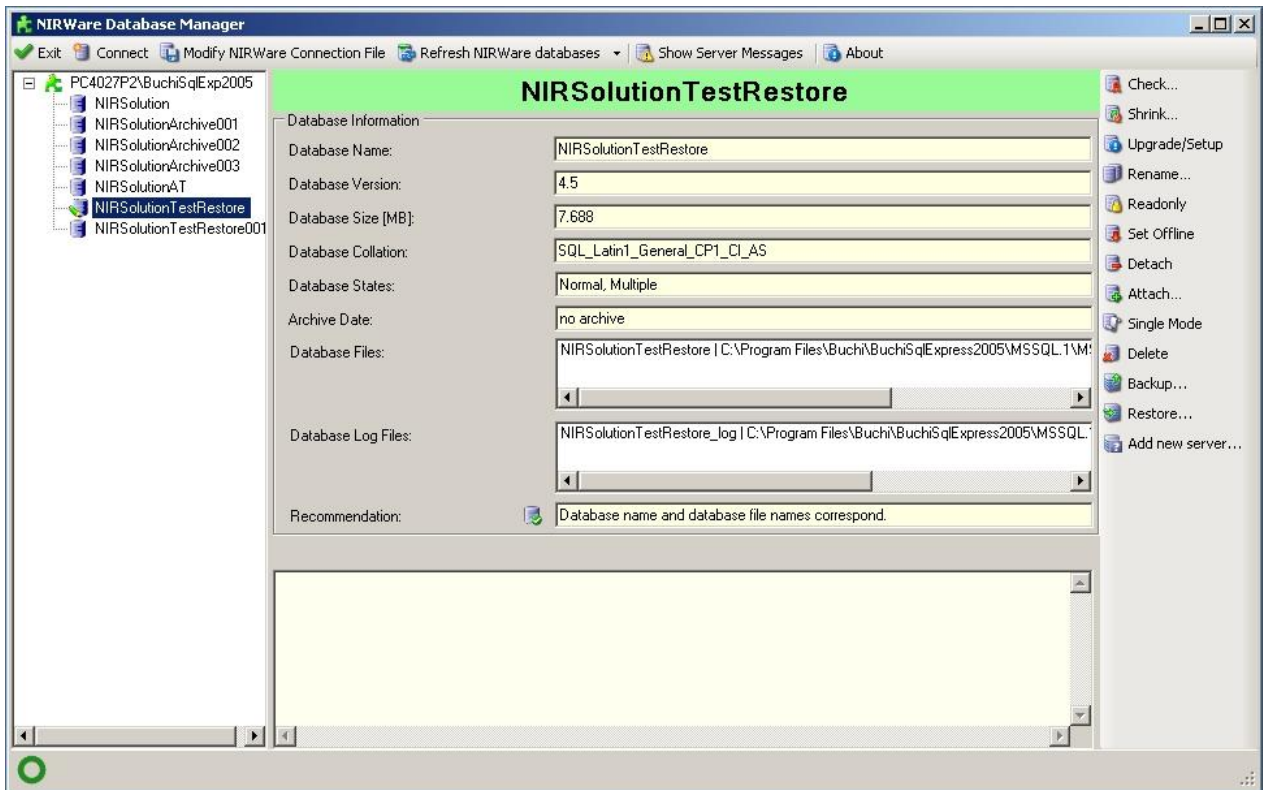
9.1.1. Introduction

Because the use is restricted to qualified personnel only, just a few functions are explained. Qualified personnel are certified MS SQL Server administrators or developers.

9.1.2. Main window of NIRWare Database Manager

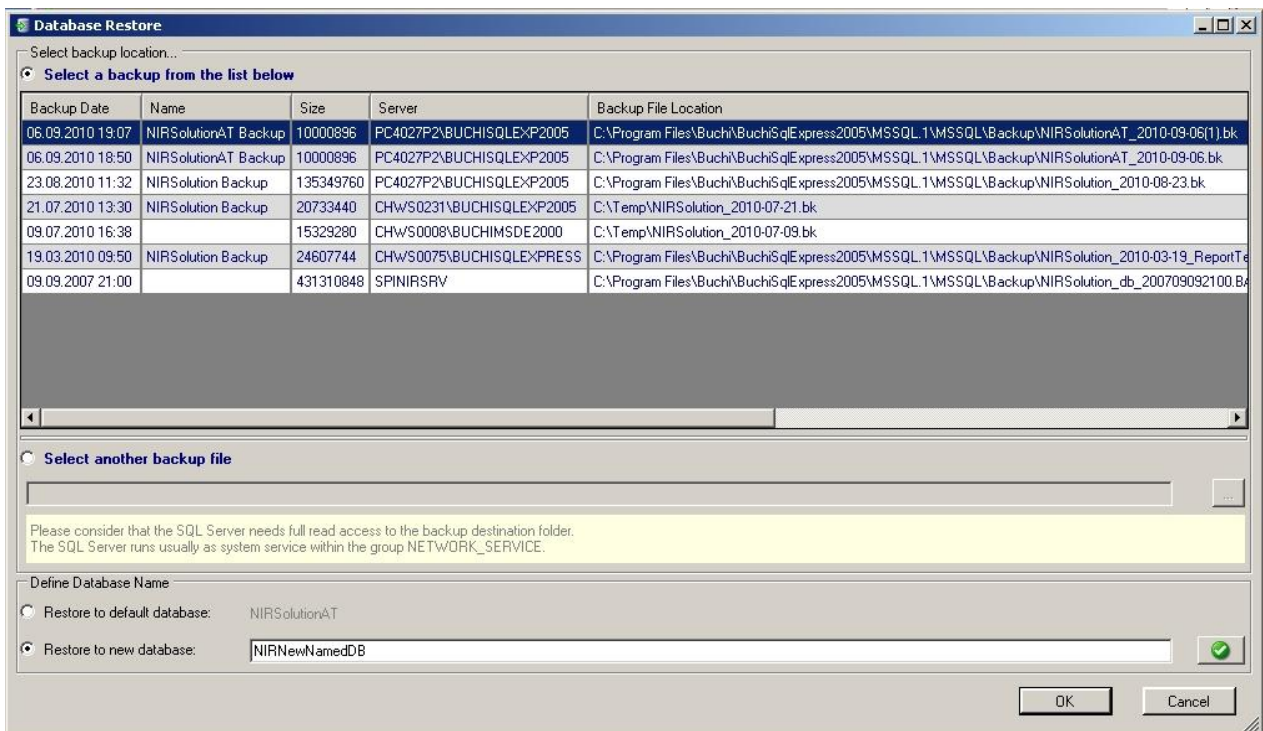


When a database is selected the main window looks as follows:



9.1.3. Restore database

To activate the restore function, click Restore... on the right of the main window with a database selected. The following window opens:



You have two possibilities for a restore:

Restore to default database: When this radio button is activated, the currently selected database will be overwritten with the content of the backup when clicking OK.

Restore to new database: When this radio button is activated, you have to enter a unique and valid name for the new SQL database. The content of the backup is then copied to this new database when clicking OK. This function is not available via NIRWare.

NOTE

After the restore of a databases from an earlier NIRWare version (less than 4.5), the database has to be upgraded to be able to use them with a current NIRWare version.

For this purpose, click 'Upgrade/Setup' on the right of the main window.

9.1.4. PC renamed

If the PC got renamed, the PC name has to be updated in the SQL server as well. For this purpose click on 'Add new server...' on the right of the main window.

NOTE

Activate the checkbox "Skip dropping. Only add new server name" only if you have good reasons.