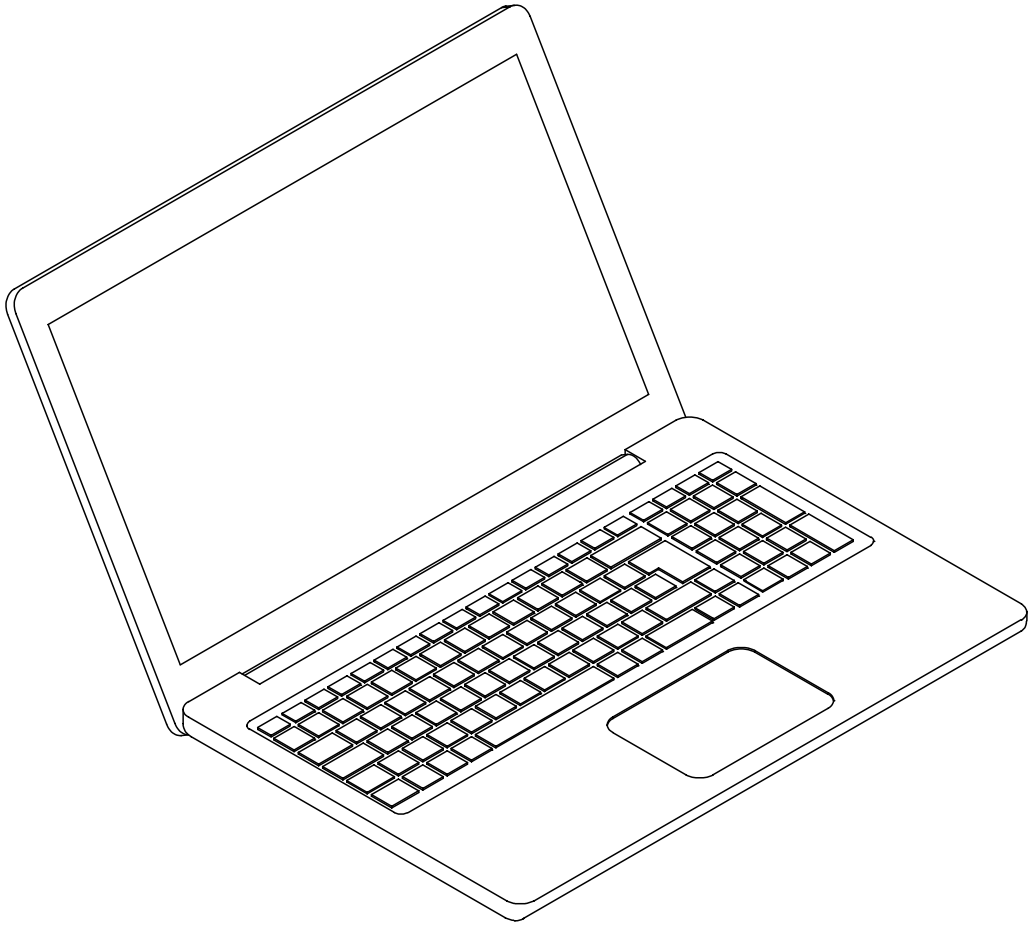
NIRWise PLUS Software
Operation Manual



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1 About this document

This operation manual is a part of the software. It describes the basic functions and provides information on the use of the software.
The software is used in conjunction with BUCHI instruments.
When operating the instrument, follow the respective operating instructions.
Keep this operation manual for later use and pass it on to any subsequent user or owner.
BÜCHI Labortechnik AG accepts no liability for damage, faults and malfunctions resulting from not following this operation manual.
If you have any questions after reading this operation manual:

▶ Contact BÜCHI Labortechnik AG Customer Service.

https://www.buchi.com/contact

1.1 Mark-ups and symbols

NOTE

This symbol draws attention to useful and important information.

☑ This character draws attention to a requirement that must be met before the instructions below are carried out.

▶ This character indicates an instruction that must be carried out by the user.

⇨ This character indicates the result of a correctly carried out instruction.

Mark-up	Explanation
Window	Software Windows are marked-up like this.
Tab	Tabs are marked-up like this.
Dialog	Dialogs are marked-up like this.
[Button]	Buttons are marked-up like this.
[Field names]	Field names are marked-up like this.
[Menu / Menu item]	Menus or menu items are marked-up like this.
Status	Status is marked-up like this.
Signal	Signals are marked-up like this.

1.2 Trademarks

Product names and registered or unregistered trademarks that are used in this document are used only for identification and remain the property of the owner in each case.

2 Product description

2.1 Description of function

The software is used for the maintenance and optimization of calibrations for ProxiMate™ instruments.
The software allows exploration, visualization and treatment of the calibration data.
The software maintains all data in project files.

2.2 Files and folders of a project

The project file contains references to other files e.g. calibration.
Exact location and explanations of the file types. See Chapter 12.3 "File explanations and folder locations", page 31

NOTE

Name the .prj, .cal, and .rtf files according to the following schematic:

- applicationname.property.filetype

A calibration consists of different files that are stored in different folders.

Navigation path

➔ *[Desktop]* ➔ *[Data]* ➔ *[Data]* ➔ *[Calibrations]*

NOTE

The location of the destination folder is fixed. See Chapter 12.3 "File explanations and folder locations", page 31

File structure		Explanation
[Calibrations] (folder)	*[Data]* (folder)	Additional .tsv files
	[History] (folder)	Old versions of the .cal/.prj/.rtf files. These files are labelled with date and time and are restorable.
	[Local] (folder)	Contains .tsv files that were generated by the AutoCal function.
	.cal (file)	Calibration file
	.prj (file)	Project file
	.rtf (file)	Calibration report file

2.3 User interface

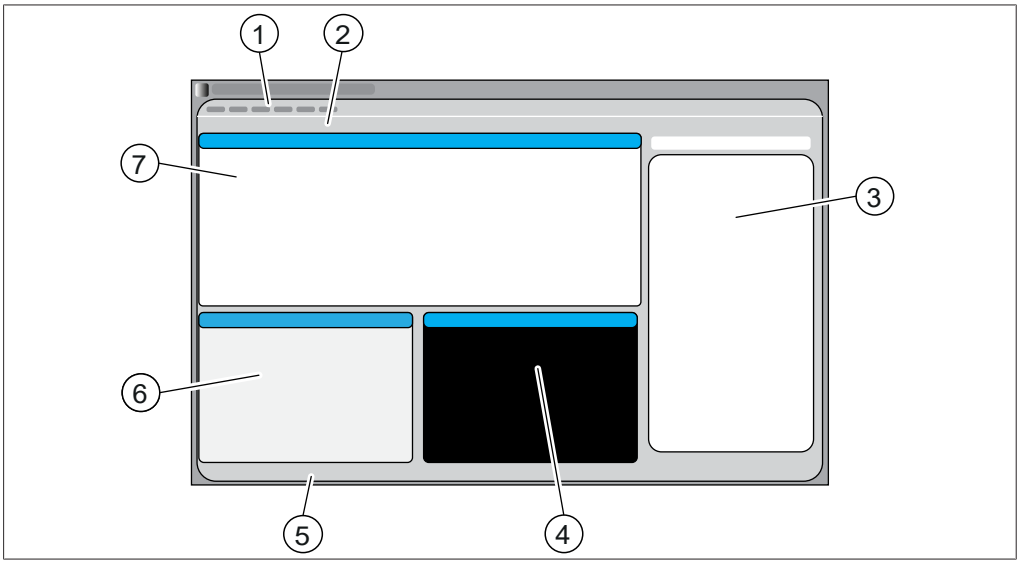


Fig. 1: User interface of the software

No.	Description	Function
1	Menu bar	Shows the program menu. See Chapter 6 "Menu bar", page 17
2	Tool bar	Shows the available tools. See Chapter 7 "Tool bar", page 18
3	Project panel	Editing project data and calibration settings. See Chapter 8 "Project panel", page 19
4	Graph panel	Shows the graphic results of a calibration. See Chapter 9 "Table panel and graph panel", page 27
5	Status bar	Shows the status of the software.
6	Table panel	Shows numeric results which depend on the selection in the project panel. See Chapter 9 "Table panel and graph panel", page 27
7	Report panel	Shows the report generated after computing a calibration model. See Chapter 10 "Report panel", page 28

2.4 Technical data

2.4.1 Computer system requirements

The software is designed to operate with the ProxiMate™ instrument.

3 Installation

3.1 Installing the software

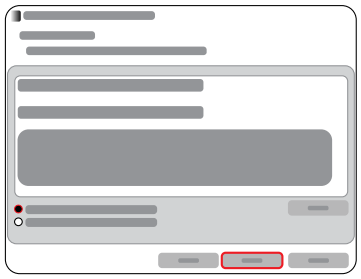
Precondition:
☑ The windows™ passwords are known.

▶ Double click the file Setup.exe.
⇨ The software installation client start.

▶ Single click *[Install NIRWise Plus™]*.
⇨ The software starts the installation process.

▶ Single click the button *[Next]*.

▶ Single click the Radio button next to **I accept the terms in the license agreement**.
▶ Single click the button *[Next]*.



▶ Single click the button *[Install]*.

▶ Wait until the software shows the dialog *[InstallationShield Wizard Completed]* .
▶ Single click the button *[Finish]*.
⇨ The software is installed.

3.2 Software settings

3.2.1 General settings

NOTE

Changing the default settings is at your own risk.

Navigation path

➔ *[View]*

- Navigate to the *[View]* menu.
- Single click the action *[Options]*.

⇨ The software shows the dialog box *Options*.

- Modify the options according to your needs.
- Single click *[OK]*.

⇨ The settings are saved.

⇨ The dialog box close.

The following settings are available:

General tab

Action	Option	Explanation
[Load the last project on startup]	-	No function
[Outlier sigma distance calibration]	Enter value	Defines the limit of outlier detection for the calibration set.
[Outlier Mahalanobis distance]	Enter value	Defines the limit of outlier detection in terms of the Mahalanobis distance.
[Outlier sigma distance validation]	Enter value	Defines the limit of outlier detection in validation set.
[MLR/SVD/RR Factors to compute]	Enter value	Determine maximum number of factors to compute.
[PC's to compute]	Enter value	Maximum amount of PCs used for calculation. Used by PCR/PLS/XLS
[PC Loading precission]	Enter value	Precision to maximize the variance of the PC loadings

Action	Option	Explanation
[Plot X-Axis as Wavenumbers]	Enable / disable	Option to show X-axis in wavenumbers instead of nanometer.
[Sample ID repeat separator]	Enter value	Defines the character used as an ID repeat. Default ID separator is *[_]* Sample named *[A_1]*, *[A_2]*, *[A_3]* represents the same sample.
[Delete outliers]	Enable / disable	Outliers detected by the software are not used for the calculation.
[Delete repeat]	Enable / disable	Calculating until no more outliers are found.
[Factors by minimum maximum residual]	Enable / disable	Chooses the amount of factors based on the residuals, when the amount of factors is not entered manually.
[Adjust Targets With ID]	Enable / disable Enter value	Makes a twofold calibration. 1. against original target values or laboratory reference values 2. original target values of selected measurements are replaced by their estimated value This function allows to: • balance weight of large and small data-sets • make optimization for e.g. temperature variation by having all samples but the temperature samples adjusted after first pass
[Adjust Targets for Hierarchical calibrations]	Enable / disable	No function
[Maximum Number of Samples per Table]	Enter value	To reduce data in large structures. To use N fresh samples only.
[Create root reference]	-	No function
[Exclude first N composition]	-	No function

Edit tab

Action	Option	Explanation
[Autocomplete]	Enable / disable	no function

Save tab

Action	Option	Explanation
[Create Backup files]	Enable / disable	Auto save function.
[Create restore information]	Enable / disable	Time between carrying out the Auto save function.

Expert tab

NOTE
BUCHI application support only.

3.3 License management

3.3.1 Applying for a license

NOTE
Only standard characters are allowed.

The following data is necessary for the license request:

- Article name
- Software license serial number (sticker on the cover page of the Quick Guide)
- Company name
- First name
- Last name
- Serial number (of the instrument)
- Country
- Email address

Navigation path
➔ *[Help]*

▶ Navigate to the *[Help]* menu.
▶ Single click the action *[License request]*.
⇨ The display shows a dialog with the mandatory information needed for application.
▶ Enter your data.
▶ Tap the button *[OK]*.
⇨ The dialog box closes.
▶ After entering all mandatory data tap the button *[OK]*.
⇨ The application file is created.
▶ Save the application file on your instrument.
▶ Send the file to registration@buchi.com.

3.3.2 Importing a license

Navigation path

➔ *[Help]*

Precondition:
☑ The license file .lic is available on the instrument.

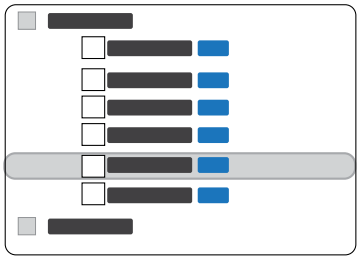
▶ Navigate to the action *[Import License]* via the navigation path.
⇨ The display shows a dialog for choosing the folders on the instrument.
▶ Navigate to the saving folder of the license you wish to import.
▶ Select the file.
▶ Tap the button *[OK]*.
⇨ The software imports the license.
▶ Start the software again.

4 Operating the software

4.1 Operating the project panel

4.1.1 Deleting an entry

▶ Single click on the parameter
▶ Press the key ***Delete***.
⇨ The entry is deleted.

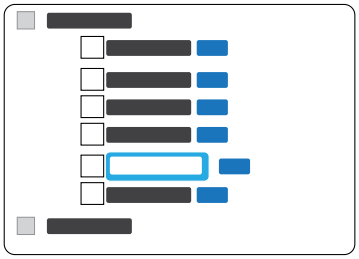


4.1.2 Entering a value

Red marked characters mean incomplete or wrong entry.

NOTE
Only if the corresponding checkbox is activated, the entry will be processed.

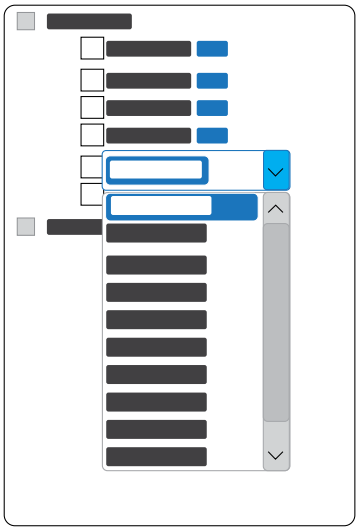
▶ Single click on the parameter.
▶ Press the key ***F2***.
⇨ The display shows an entry box.
▶ Enter a value.
▶ Press the key ***Enter***.
⇨ The value is saved.



4.1.3 Entering a value from a drop-down menu

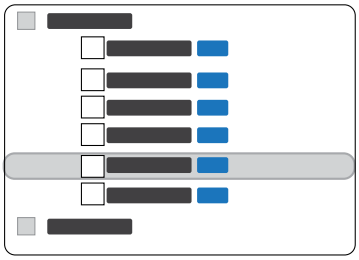
NOTE
Only if the corresponding checkbox is activated, the entry will be processed.

▶ Single click on the parameter.
▶ Press the key ***F2***.
⇨ The display shows a drop-down menu.
▶ Single click the entry you wish to use.
⇨ The drop-down menu close.
⇨ The value is saved.



4.1.4 Sorting entries

▶ Select the entry you wish to move.
▶ Press the key ***Shift***.
▶ Press the curser key ***Up*** or ***Down***.
⇨ The entry moves according to your entry.



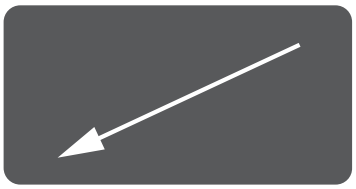
4.2 Operating graph panel and table panel

4.2.1 Select various entries

▶ Press the ***Shift*** button and select with the left mouse key the table entries.

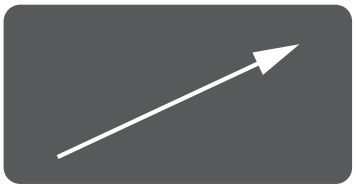
4.2.2 Zoom out

▶ Press the right mouse key and move the cursor diagonal from right up to left down.



4.2.3 Zoom

▶ Press the right mouse key and move the courser diagonal from left down to right up.



4.2.4 Rotate three-dimensional graphs

▶ Press the left ***Ctrl*** key, the left mouse key and move the mouse.

4.2.5 Carrying out a calculation

Navigation path

➔ *[Compute]*

Precondition:
☑ All settings have been selected. See Chapter 8 "Project panel", page 19

▶ Single click the *[Compute]* menu.
⇨ The status bar shows the progress of the calculation.
▶ Wait until the software shows the result.

5 Basic operations

5.1 Optimizing a calibration

Precondition:

☑ A calibration from the ProxiMate™ with reference values is available.

☑ If necessary, additional data files are available in the data folder.

- ▶ Open a project. See Chapter 5.2 "Open an existing project", page 15
- ▶ If necessary, add a data file to the project. See Chapter 8.1 "Project file settings", page 19
- ▶ Change the project selector settings according to your requirements. See Chapter 8.2 "Project selector settings", page 19
- ▶ Change the project pretreat settings according to your requirements. See Chapter 8.3 "Project pretreat settings", page 20
- ▶ Change the project model settings according to your requirements. See Chapter 8.4 "Project model setting", page 21
- ▶ Carry out a calculation. Chapter 5.5 "Carrying out a calculation", page 16
- ▶ Check the results. See Chapter 9 "Table panel and graph panel", page 27
- ▶ Adjust the settings according to your needs.
- ▶ Export the calibration. See Chapter 5.6 "Exporting a calibration", page 16
- ▶ Save the project.

5.2 Open an existing project

Navigation path

➔ *[File]*

- ▶ Navigate to the *[File]* menu.
- ▶ Single click the action *[Open]*.
- ▶ Select the project you wish to open.
- ▶ Single click the button *[Open]*.

⇨ The software opens the file.

⇨ The project is loaded into the software.

5.3 Creating a new project (BUCHI application support only)

Navigation path

➔ *[File]*

- ▶ Navigate to the *[File]* menu.
- ▶ Single click the action *[New]*.

⇨ The software shows the dialog box *Save project*.

- ▶ Select the save location according the rules. See Chapter 12.3 "File explanations and folder locations", page 31
- ▶ Enter the name of the project.
- ▶ Single click the button *[Save]*.

⇨ The new project is created.

5.4 Saving a project

Navigation path

➔ *[File]*

- ▶ Navigate to the *[File]* menu.
- ▶ Single click the action *[Save]*.

⇨ The project is saved.

5.5 Carrying out a calculation

Navigation path

➔ *[Compute]*

Precondition:
☑ All settings have been selected. See Chapter 8 "Project panel", page 19

- ▶ Single click the *[Compute]* menu.

⇨ The status bar shows the progress of the calculation.

- ▶ Wait until the software shows the result.

5.6 Exporting a calibration

Navigation path

➔ *[Project]*

- ▶ Navigate to the *[Project]* menu.
- ▶ Single click the action *[Export]*.
- ▶ Single click the button *[Save]*.

⇨ The calibration is exported.

⇨ The existing files are moved into the History subfolder.

5.7 Exporting a graph

Precondition:
☑ A graphic program is available (e.g. Paint).
☑ A calibration was carried out. See Chapter 5.5 "Carrying out a calculation", page 16

- ▶ Single click right in the graph panel.
- ▶ Select *[Copy as Picture]*.

⇨ The graph is saved in the catch.

- ▶ Past the graph in the graphic program.

5.8 Exporting a .tsv/excel file

Navigation path

➔ *[File]*

Precondition:
☑ A calculation was carried out. See Chapter 5.5 "Carrying out a calculation", page 16

- ▶ Click the table in the table panel.
- ▶ Navigate to the *[File]* menu according to the navigation path.

⇨ The *Save Matric...* dialog opens.

- ▶ Save the .tsv file in the requested folder.

6 Menu bar

The following menus are available:

Menu	Submenu / Action	Explanation
[File]	*[New]*	Create a new project. (BUCHI application support only)
	[Open]	Open a project.
	[Open in History]	Open a project from history folder.
	[Merge]	Merges .tsv files. (BUCHI application support only)
	[Save]	Save a project.
	[Save as]	Save a project as.
	[Save project with data]	Save a project incl. all available data.
	[Exit]	Exit a project.
	[Import NAX]	BUCHI application support only.
	[Export NAX]	BUCHI application support only.
[Edit]	*[Undo]*	Available according to the operation.
	[Cut]	Available according to the operation.
	[Copy]	Available according to the operation.
	[Paste]	Available according to the operation.
	[Clear]	Available according to the operation.
	[Select All]	Available according to the operation.
	[Insert]	Insert row or column. Available according to the operation.
	[Remove]	Delete row or column. Available according to the operation.
	[Name]	Rename a column. Available according to the operation.
[View]	*[Tools bar]*	Enable / disable the tools bar.
	[Status bar]	Enable / disable the status bar.
	[Options]	See Chapter 3.2.1 "General settings", page 9
[Project]	*[Export model]*	See Chapter 5.6 "Exporting a calibration", page 16
[Compute]		Carrying out a calculation.
[Help]	*[License Request]*	See Chapter 3.3.1 "Applying for a license", page 11
	[Installed Licenses]	Shows a dialog with details about the licenses on this instrument.
	[Import License]	See Chapter 3.3 "License management", page 11

7 Tool bar

Icon	Explanation
	Create a new project. (BUCHI application support only)
	Open a project.
	Open a project from history folder.
	Save a project.
	No function
	Cut Available according to the operation.
	Copy Available according to the operation.
	Paste Available according to the operation.
	Undo Available according to the operation.

8 Project panel

The project panel shows the project in a tree structure.

NOTE

Only if the corresponding checkbox is activated, the entry will be processed.

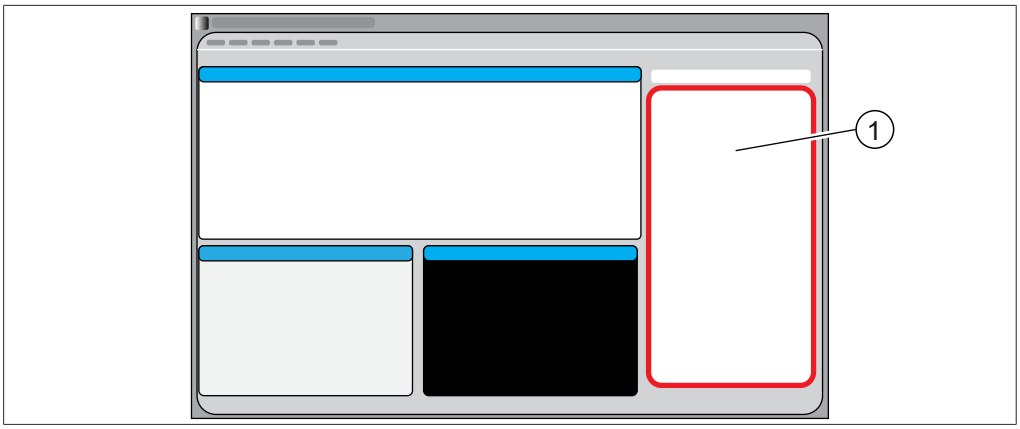


Fig. 2: Project panel

1 Project panel

8.1 Project file settings

8.1.1 Adding a data file to a project

Precondition:

☑ A .tsv file is in the data folder is available. See Chapter 12.3 "File explanations and folder locations", page 31

☑ A project is open. See Chapter 5.2 "Open an existing project", page 15

▶ Double click the action *[<DblClick to load data file>]*.

⇨ The software shows the dialog *Select Data File*.

▶ Select the data file you wish to add.

▶ Single click the button *[Open]*.

⇨ The software adds the file to the project.

8.2 Project selector settings

Navigation path

➔ *[Project panel]* ➔ *[Selector]*

The Selector allows to add further criteria to define which samples are included in the calculation of the calibration.

8.2.1 Changing the query of the project

Defines the mask used to search the data in the data files.

NOTE

The option true and false is defined by the ProxiMate™ firmware.

The following queries are possible:

Action	Option	Explanation
[Check]	*[true]*	The sample is activated.
	[false]	The sample is deactivated.
[Recipe]		BUCHI application support only.
[Composition]		BUCHI application support only.

8.2.2 Changing the target parameter

Select the property for a calibration.

The commands for target parameter follow the following syntax:

Syntax:	<parameter>	<min>	<max>	<format>
Explanation:	Name of the parameter	Parameter range		Unit and decimal e.g. 0.00 %

8.3 Project pretreat settings

Navigation path
➔ *[Project panel]* ➔ *[Pretreat]*

8.3.1 Changing the basic pretreatment

NOTE

It is essential that the wavelength range (end wavelength – start wavelength) is a multiple of the resolution (step size).

The instrument has a diode array detector.
Every diode detects the intensity for a certain wavelength.
The diodes are distributed over the whole wavelength range.
The .tsv file contains absorbance data collected at each pixel by the detectors.
To display spectra from these single values, a spline function is applied according to the below settings.
The commands for basic treatment follow the following syntax:

Syntax:	<Spline>	[#]X1	[#]X2	[#]X3	<number> <number>	<number>
Explanation:		Index of the first pixel	Index of the last pixel(s)	A string with the set(s) of polynomial coefficients	Wavelength range (depending on the instrument configuration)	Wavelength step size

8.3.2 Changing the advanced pretreatment

Mathematical pre-treatment is used to minimize artifacts and enhance the spectral data.

NOTE

The order of the pretreatments affects the result of the calculation of the calibration.

The following pretreatments are available:

Parameter	Explanation
[SMOOTH]	Smoothing over 5 data-points along each spectrum.
[DG]	1. Number: derivative
	2. Number: number of data points
	3. Number: number of data points for smoothing
[SNVT]	Subtracts the average and divides by the standard-deviation of the vector.
[AVG]	Calculates the average of repeated measurements. Repeated measurements hold same sample ID.
	Calculates the average of two consecutive x and y values. The sample ID does not matter.
[NOIMAGE]	No function

8.4 Project model setting

Navigation path

➔ *[Project panel]*➔ *[Model]*

8.4.1 Changing the regression method

NOTE

If a plus sign is added to the method the software will automatically select significant wavelengths (68% Relevance) for each factor. E.g. PLS+ or RR+. A double plus e.g. PLS++ will select 95% relevance.

The following regressions are available:

Parameter	Explanation
PLS (Type)	Standard PLS-Method.
XLS (Type)	PLS with optimized first derivative.

8.4.2 Changing the validation

NOTE

Choose either validation or cross validation.

Validation determines the number of samples used to validate the calculation.
The following codes are possible:

Code	Explanation
x	Selects every x spectra for the validation.
x:y	Selects y samples in each group of x samples for the validation.
x:-y	Selects the last y samples in a group of x for the validation.
-x	Selects the last x spectra for the validation.
ID x	Selects every x spectra by ID for the validation.

8.4.3 Changing the cross validation

NOTE

Choose either validation or cross validation.

Each sample will be used for the calculation and the validation of the calibration. Therefore, the samples are divided into groups.

Parameter	Explanation
5 (CrossValidate)	Divides all calibration samples into five groups. One of the five groups will be used to validate the calibration (20%), while the other 4 groups are used to calculate the calibration. The classification of the groups changes with each calculation. In a cycle of five calculations, each group is once the validation group.
10 (CrossValidate)	Divides the samples into 10 groups. 10% of the samples will be used for the validation at one time. The classification of the groups changes with each calculation.
99999 (CrossValidate)	Leave out one, permutations equal to number of samples. Only one sample will be used for the validation at one time. All the other samples are used for the calibration.

8.4.4 Changing the factors

Select the number of factors for the calculation.

NOTE

If the checkbox is not selected, the software selects the number of factors.

8.4.5 Changing the auto delete

Determine what samples to remove from the calibration and validation data, according to the settings for Mahalanobis and residual.

Number	<Number>	<Number>	<Number>
Explanation	Standardized calibration residual	Mahalanobis distance	Standardized validation residual

8.4.6 Delete

Defines a sample which will not be used for the calculation (after the first calculation when it is clear which sample does not fit the model).

▶ Enter the sample ID manually in the field.

or

▶ Copy paste the samples from the calibration plot.

8.5 Project pretreat results

NOTE

Only bold mark-up results contain data.

Navigation path
➔ *[Project panel]* ➔ *[Pretreat]*

The following results are available

Result	Explanation	Output table	Output graph
[Wavelengths]	Table of used wavelengths	+	-
[SNRs]	Vector of instrument serial-numbers	+	-
[WLCs]	Vector of instrument wave-length calibrations	+	-
[Means]	Table of spectral means for each data-set	+	-
[Targets]	Reference values	+	-
[OSC]	No function	+	-
[Variations]	Matrix of variance for each data-set	+	-

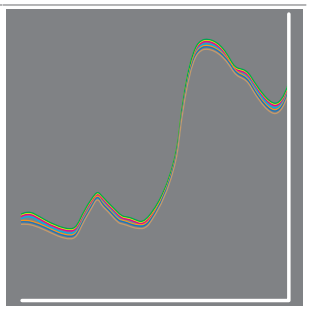
8.6 Project model results

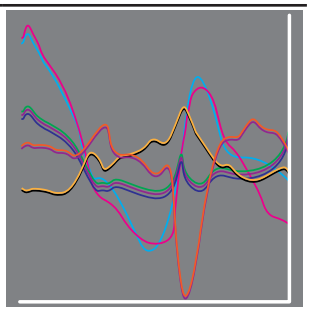
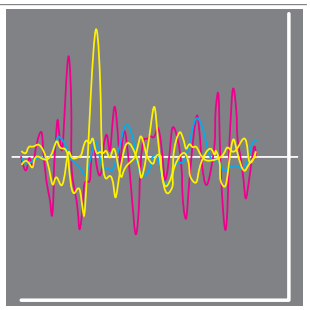
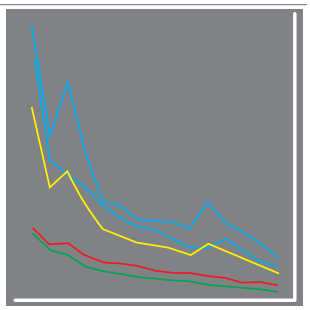
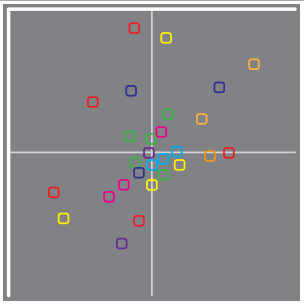
NOTE
Only bold mark-up results contain data.

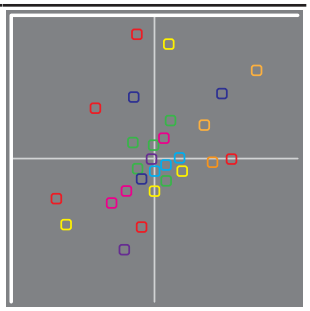
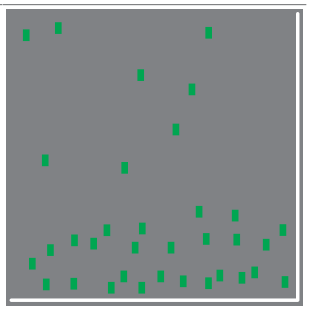
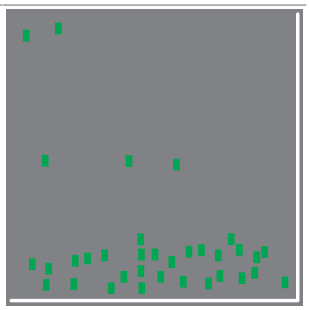
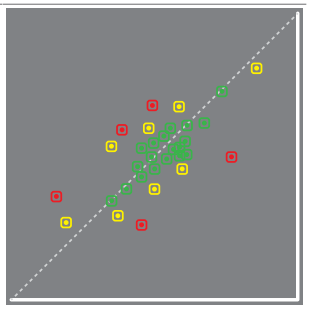
The results are shown in the graph panel and/or in the table panel. See Chapter 9 "Table panel and graph panel", page 27

Navigation path
➔ *[Project panel]* ➔ *[Model]*

The following results are available:

Result	Explanation	Output table	Output Graph
Wavelengths	Vector of the used wave-lengths.	+	-
Indexes	List of sample indexes.	+	-
IDs	List of sample IDs.	+	-
Center	Average of all reference val-ues.	-	-
Target	List of reference values.		
Zero	Table of mean spectra.	+	-
Observations	Shows the spectra included in the calculation and valida-tion of the calibration. (only spectra with reference values set as true and from selected data files are shown here)	+	

Result	Explanation	Output table	Output Graph
ObservationsZ (=Observation Zero)	Shows spectra to find areas with high amount of spectral information. The mean spectrum is subtracted from each spectrum.	+	
Weights	Matrix of projected values. Represents extracted features of the spectra. (e.g. for PLS, the correlation between spectra and reference values; for PCR, maximized the variance of the spectra)	+	
Loads	Describe the correlation between original spectra and scores.	+	+
Scale	Standard deviation of the scores.	+	-
Regressions	Weights multiplied by the standard deviations of the spectra (by wavelengths/column).	+	+
Press	Visualizes the change of the SEC and SECV with the amount of factors. For optimizing the number of factors.	+	
Scores	Matrix of projected spectra, as defined by the weights. Contains information on the estimations of the reference values based on the used number of factors. For identifying groups of samples. If there is more than one group, change the calibration.	+	

Result	Explanation	Output table	Output Graph
Scores Scaled	Table of standardized scores obtained by dividing the scores by the scales.	+	
Mahalanobis	The Mahalanobis is a measure of spectral similarity between the measured spectrum and the dataset used in the calibration. For identifying outliers.	+	
Residuums	The (Euclidean) distance of the given spectra to the reconstructed spectra.	+	
Bias	A bias is a constant value. This value is added to the result of a prediction to correct a constant deviation between predicted values and reference values.	+	-
Estimates	Predictions based on calibration.	+	
Skew	No function	-	-
SkewBias	No function	-	-
Residuals	Difference between reference and estimated values.		
CVEstimates	Predictions based on the calibration during cross-validation executions.		

Result	Explanation	Output table	Output Graph
CVResiduals	Difference between reference values and CVEstimates.		
TEstimates	Estimates per sample.		
TResiduals	Residuals per sample.		

9 Table panel and graph panel

The table panel and the graph panel are showing the results of the calculation.

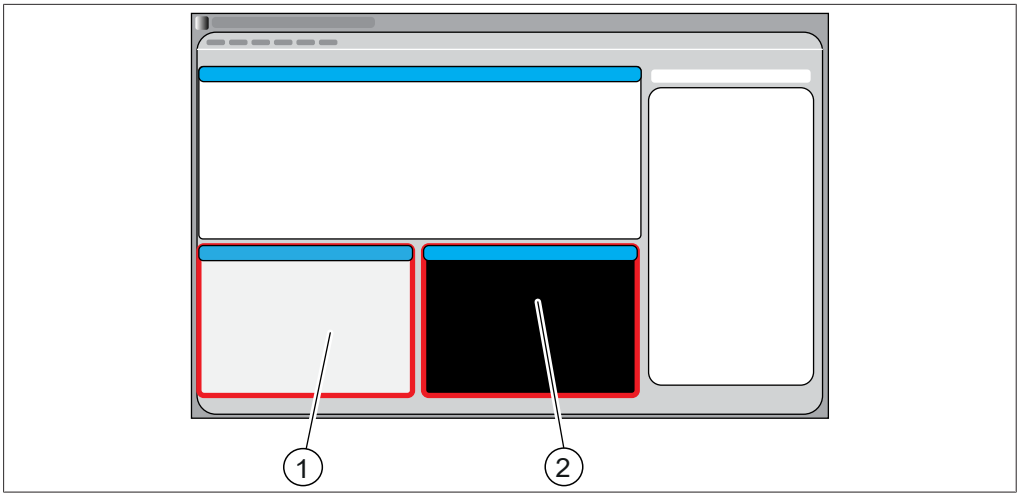


Fig. 3: Results

1 Table panel 2 Graph panel

NOTE

A selected table entry in the table panel is highlighted in the graphic in the graph panel. See Chapter 8.5 "Project pretreat results", page 22 and Chapter 8.6 "Project model results", page 23

10 Report panel

The report panel shows report data about the calibration.

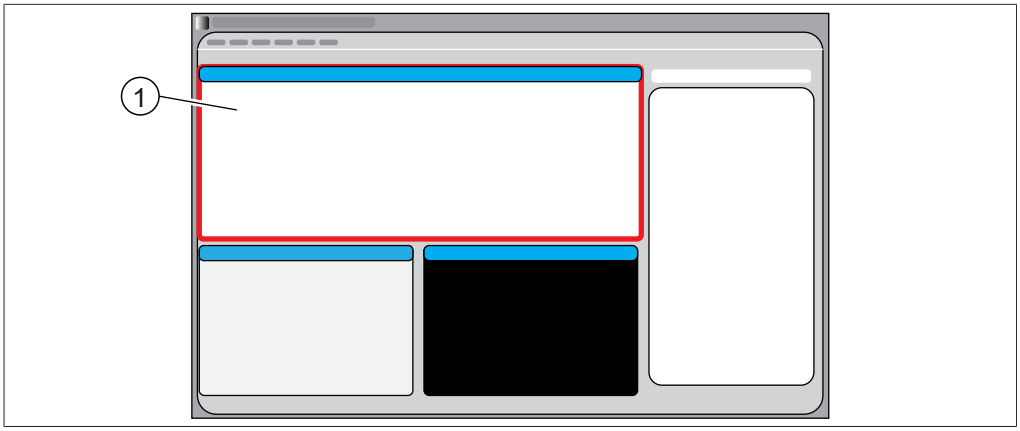


Fig. 4: Report panel

The data is exported together with the calibration export.

11 Troubleshooting

Problem	Possible cause	Action
Computation error	The project contains no data.	▶ Check if there is a data file attached to the project (project window, file). ▶ Check if the directory of the data file is still correct by clicking on it. ▶ If message says *[file not found]*, double click on data file and load it again from the correct directory.
	No data selected.	▶ Check if data file contains reference values by clicking on the file in the project window. ▶ If so, check if 'Check' is set to 'True' for samples exhibiting reference values.
	Too few data.	▶ Less than three reference values in one of the data files.
Wrong results	The wavelength range is outside the range of available data.	▶ Press abort and check if the wavelength range in the chosen spline (project window, pretreat) fits the measurements.

12 Appendix

12.1 Explanation of terms

Term	Explanation
Chemometrics	The interpretation of spectral data to determine chemical composition with the use of mathematical and statistical methods.
Regression	Solving an equation for its unknowns.
Regression methods	The mathematical or procedural way by which the equation is determined.
Multiple Linear Regression	Is a method of solving equations where you have many variables that in a linear combination represent the target. Various methods are used depending on numerical and stability properties of your data, SVD (Singular value decomposition) or RR (Ridge Regression).
Principal Component Regression	This method is a combination of data-reduction and Multiple Linear Regression, where the data is approximated by a fewer number of variables that are later used to solve the equation.
Partial Least Squares	This method is similar to the Principal Component Regression though the eigenvectors are calculated to maximize the covariance to the target / target residuum.
Mahalanobis	Orthonormal distance of a sample relative to its multivariate structure.
Standard -deviation, -errors	Standard deviations are used to determine the quality of a model. Given a normal distribution the value represents the spread of 68% of the population examined.
Standardized residuals	Divide the individual residual with its population standard deviation. <1 = 68%=GOOD, <2=95%=OK, <3=99%=QUESTIONABLE, >3=WRONG!
Pre-treatment	Pre-treatments are mathematical reformatting functions of the original measured signal. These pre-treatments are needed to e.g. cancel particle size effects, remove baselines etc.

12.2 List of abbreviations

Abbreviation	Explanation
MLR	Multiple Linear Regression
PC	Principal Component
PCR	Principal Component Regression
PLS(R)	Partial Least Squares
XVAR	Data Set Observation Variation
XCVAR	Calibration-set observation variation
XVVAR	Validation-set observation variation
SEC	RMS of calibration residuals
CMAX	Maximum calibration residual
SECV	RMS of cross-validation residuals
CVMAX	Maximum cross-validation residual

Abbreviation	Explanation
SEP	RMS of validation residuals
VMAX	Maximum validation residual
QVAL	Standardized ratio of residual when in and outside of calibration-set. (negative if outside yields lesser residual than in)
N	Number of instances
X	Observations
Y	Target
XLS	An extension of Partial Least Squares; to only use derivative information in the data. Replaces Partial Least Squares with derivative pretreatment.
Press	Predicted Residual Error Sum Square The difference between the predicted values and the original reference values.
RMS	Root mean square

12.3 File explanations and folder locations

NOTE

Hidden folders

By default settings the following folder locations are hidden.

- ▶ Start the software *[Windows Explorer]* on the instrument.
- ▶ Navigate to folder options via the following navigation path: View ➔ Folder Options ➔ View
- ▶ Activate the function *[Show hidden files, folders and drives]*.

Explanation	Type	Folder
Calibration files	.cal	C:\ProgramData\BUCHI\NIRWise\Calibrations
Data files for calibration	.tsv	C:\ProgramData\BUCHI\NIRWise\Calibrations\Data
Device specific data files for calibration	.tsv	C:\ProgramData\BUCHI\NIRWise\Calibrations\Local
Manually exported files with different content	diverse	C:\ProgramData\BUCHI\NIRWise\Export\Data
LIMS system files	.xml .csv	C:\ProgramData\BUCHI\NIRWise\Export\LIMS
License request file	.xml	C:\ProgramData\BUCHI\NIRWise\Export\LicenseRequests
External References	.brf	C:\ProgramData\BUCHI\NIRWise\References
Measurement Reports	.xls / .pdf	C:\ProgramData\BUCHI\NIRWise\Reports
System Test Reports	.pdf	C:\ProgramData\BUCHI\NIRWise\Reports\SystemTests
Measurement report templates	.xls	C:\ProgramData\BUCHI\NIRWise\Templates

Explanation	Type	Folder
Licenses	.xml	C:\ProgramData\BUCHI\LicenseManager\License
History files for NIRWise Plus	diverse	C:\ProgramData\BUCHI\NIRWise\Calibrations\Local\History
Report from latest calibration	.rtf	C:\ProgramData\BUCHI\NIRWise\Calibrations
NIRWise Plus project file, containing all .tsv files and the settings for the calibration	.prj	C:\ProgramData\BUCHI\NIRWise\Calibrations

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