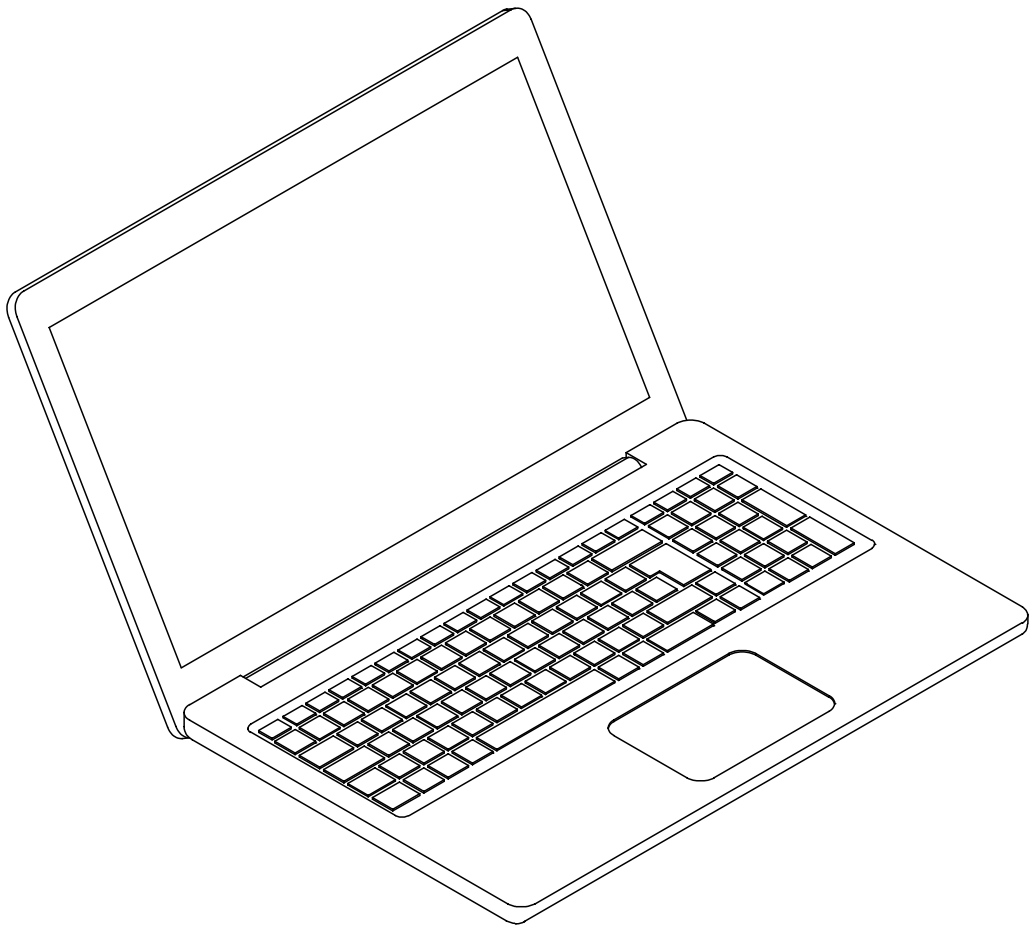




NIRWise PLUS Software

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 BÜCHI 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 |
|---------------------------|--|
| <i>Window</i> | Software Windows are marked-up like this. |
| <i>Tab</i> | Tabs are marked-up like this. |
| <i>Dialog</i> | Dialogs are marked-up like this. |
| <i>[Button]</i> | Buttons are marked-up like this. |
| <i>[Field names]</i> | Field names are marked-up like this. |
| <i>[Menu / Menu item]</i> | 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 32



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 32

| 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

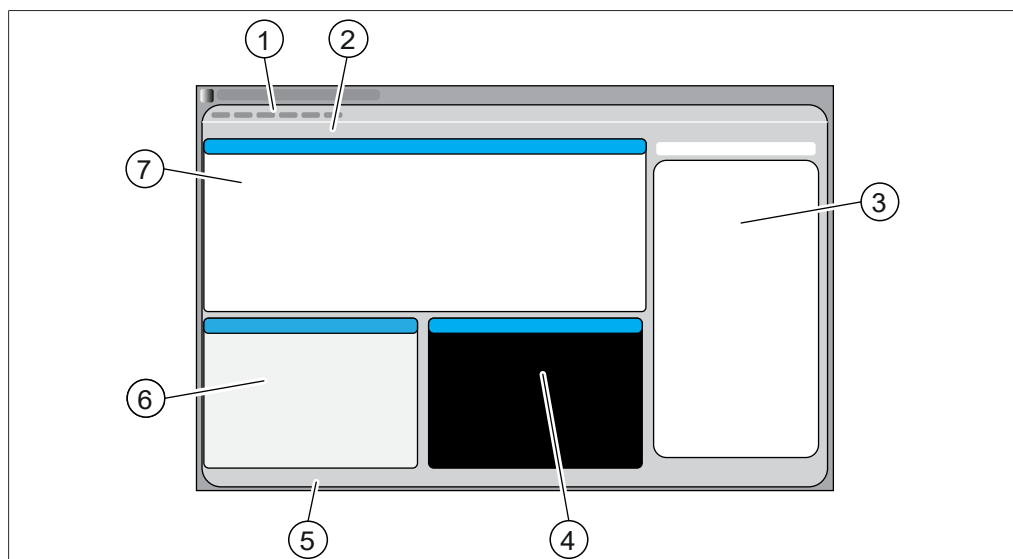


Fig. 1: User interface of the software

| No. | Description | Function |
|-----|---------------|---|
| 1 | Menu bar | Shows the program menu. See Chapter 6 "Menu bar", page 18 |
| 2 | Tool bar | Shows the available tools. See Chapter 7 "Tool bar", page 19 |
| 3 | Project panel | Editing project data and calibration settings. See Chapter 8 "Project panel", page 20 |
| 4 | Graph panel | Shows the graphic results of a calibration. See Chapter 9 "Table panel and graph panel", page 28 |
| 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 28 |
| 7 | Report panel | Shows the report generated after computing a calibration model. See Chapter 10 "Report panel", page 29 |

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.

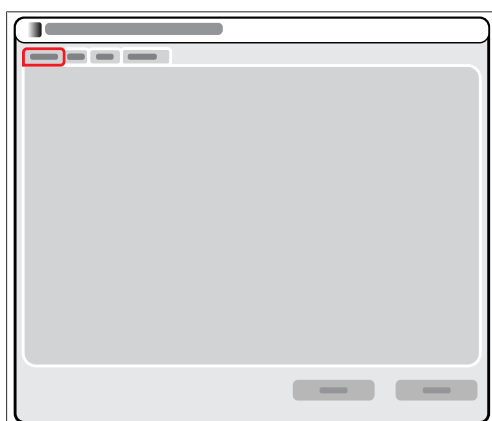
Navigation path

→ [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. |

| Action | Option | Explanation |
|---|---------------------------------|--|
| <i>[PC's to compute]</i> | Enter value | Maximum amount of PCs used for calculation. Used by PCR/PLS/XLS |
| <i>[PC Loading precision]</i> | Enter value | Precision to maximize the variance of the PC loadings |
| <i>[Plot X-Axis as Wavenumbers]</i> | Enable / disable | Option to show X-axis in wavenumbers instead of nanometer. |
| <i>[Sample ID repeat separator]</i> | Enter value | Defines the character used as an ID repeat. Default ID separator is [<u>] Sample named <i>[A_1]</i>, <i>[A_2]</i>, <i>[A_3]</i> represents the same sample.</u> |
| <i>[Delete outliers]</i> | Enable / disable | Outliers detected by the software are not used for the calculation. |
| <i>[Delete repeat]</i> | Enable / disable | Calculating until no more outliers are found. |
| <i>[Factors by minimum maximum residual]</i> | Enable / disable | Chooses the amount of factors based on the residuals, when the amount of factors is not entered manually. |
| <i>[Adjust Targets With ID]</i> | 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: <ul style="list-style-type: none"> • 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 |
| <i>[Adjust Targets for Hierarchical calibrations]</i> | Enable / disable | No function |
| <i>[Maximum Number of Samples per Table]</i> | Enter value | To reduce data in large structures. To use N fresh samples only. |
| <i>[Create root reference]</i> | - | No function |
| <i>[Exclude first N composition]</i> | - | 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.

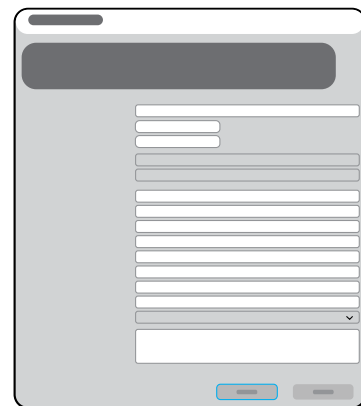
The following data is necessary for the license request:

- 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@buchicom.



3.3.2 Importing a license

Navigation path

→ *[Help]*

Precondition:

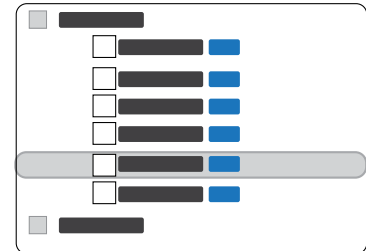
- The license file *.lic* is available on the instrument.
- ▶ Navigate to the action *[Import License]* via the navigation path.
 - ⇒ The display shows a dialog for choosing the folders on the instrument.
- ▶ Navigate to the saving folder of the license you wish to import.
- ▶ Select the file.
- ▶ Tap 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

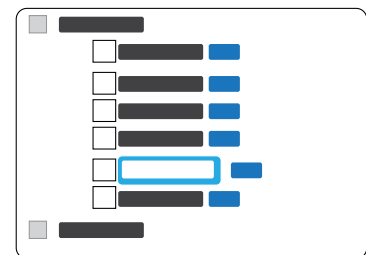
Red marked characters mean incomplete or wrong entry.



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.



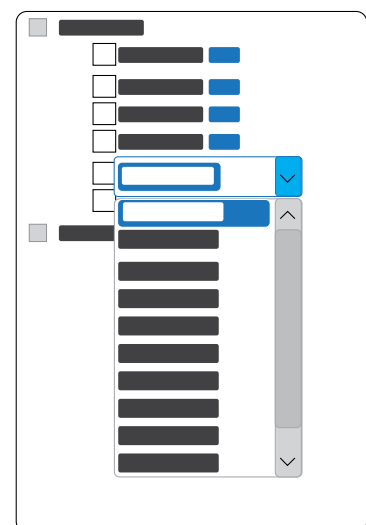
4.1.3 Entering a value from a drop-down menu



NOTE

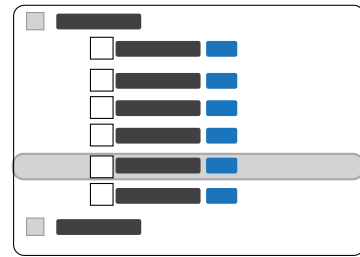
Only if the corresponding checkbox is activated, the entry will be processed.

- ▶ 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 cursor key **Up** or **Down**.
- ⇒ The entry moves according to your entry.



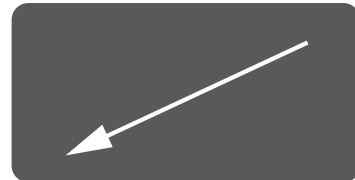
4.2 Operating graph panel and table panel

4.2.1 Select various entries

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

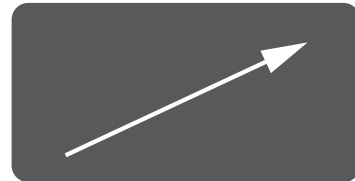
4.2.2 Zoom out

- ▶ 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 cursor 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 20

- ▶ 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 20
- ▶ Change the project selector settings according to your requirements. See Chapter 8.2 "Project selector settings", page 20
- ▶ Change the project pretreat settings according to your requirements. See Chapter 8.3 "Project pretreat settings", page 21
- ▶ Change the project model settings according to your requirements. See Chapter 8.4 "Project model setting", page 22
- ▶ 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 28
- ▶ 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 32
- ▶ 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 20
- ▶ 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 |
|------------------|---------------------------------|---|
| <i>[File]</i> | <i>[New]</i> | Create a new project. (BUCHI application support only) |
| | <i>[Open]</i> | Open a project. |
| | <i>[Open in History]</i> | Open a project from history folder. |
| | <i>[Merge]</i> | Merges .tsv files. (BUCHI application support only) |
| | <i>[Save]</i> | Save a project. |
| | <i>[Save as]</i> | Save a project as. |
| | <i>[Save project with data]</i> | Save a project incl. all available data. |
| | <i>[Exit]</i> | Exit a project. |
| | <i>[Import NAX]</i> | BUCHI application support only. |
| | <i>[Export NAX]</i> | BUCHI application support only. |
| <i>[Edit]</i> | <i>[Undo]</i> | Available according to the operation. |
| | <i>[Cut]</i> | Available according to the operation. |
| | <i>[Copy]</i> | Available according to the operation. |
| | <i>[Paste]</i> | Available according to the operation. |
| | <i>[Clear]</i> | Available according to the operation. |
| | <i>[Select All]</i> | Available according to the operation. |
| | <i>[Insert]</i> | Insert row or column. Available according to the operation. |
| | <i>[Remove]</i> | Delete row or column. Available according to the operation. |
| <i>[View]</i> | <i>[Tools bar]</i> | Enable / disable the tools bar. |
| | <i>[Status bar]</i> | Enable / disable the status bar. |
| | <i>[Options]</i> | See Chapter 3.2.1 "General settings", page 9 |
| <i>[Project]</i> | <i>[Export model]</i> | See Chapter 5.6 "Exporting a calibration", page 16 |
| <i>[Compute]</i> | | Carrying out a calculation. |
| <i>[Help]</i> | <i>[License Request]</i> | See Chapter 3.3.1 "Applying for a li- cense", page 11 |
| | <i>[Installed Licenses]</i> | Shows a dialog with details about the li- censes on this instrument. |
| | <i>[Import License]</i> | 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.

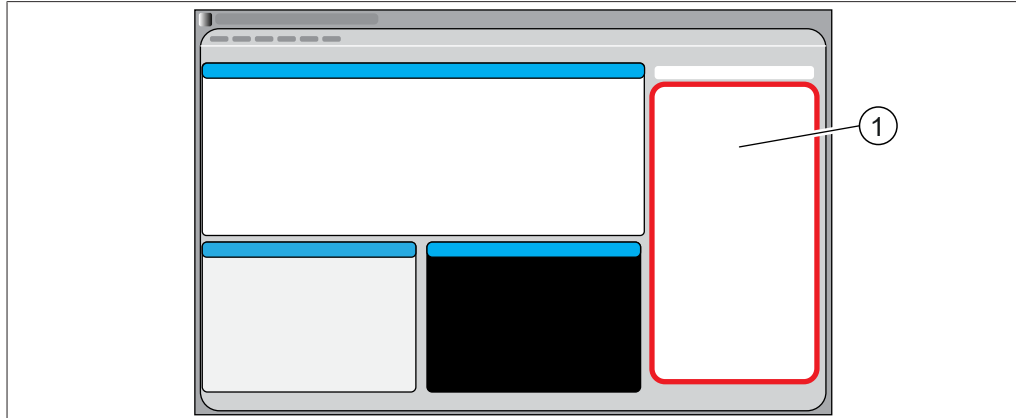


Fig. 2: Project panel

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 32
- A project is open. See Chapter 5.2 "Open an existing project", page 15
- ▶ Double click the action [*<DbiClick 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

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) | | Wave-length 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 |
|-----------|---|
| [MEAN] | Subtracts the mean of the spectra. |
| [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. |
| [OSC] | Computes a model of the data that is perpendicular to the modeling target and subtracts it from the observations. |
| [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 |
|-------------|---|
| PCR (Type) | Standard PCR-Method. |
| PLS (Type) | Standard PLS-Method. |
| PLS2 (Type) | Standard PLS2-Method. Uses SIMPLS method where several parameter predictions are made from a single set of regression coefficients. |

| Parameter | Explanation |
|-------------------|--|
| XLS (Type) | PLS with optimized first derivative. |
| RR (Type) | Ridge Regression (MLR). |
| PLS;XLS;RR (Type) | Compute model using all listed methods and automatically select the best option. |

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. |

| Parameter | Explanation |
|-----------------------|---|
| 99999 (CrossValidate) | <p>Leave out one, permutations equal to number of samples.</p> <p>Only one sample will be used for the validation at one time.</p> <p>All the other samples are used for the calibration.</p> |

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 wavelength calibrations | + | - |
| [Means] | Table of spectral means for each data-set | + | - |

| Result | Explanation | Output table | Output graph |
|--------------|--------------------------------------|--------------|--------------|
| [Targets] | Reference values | + | - |
| [OSC] | No function | + | - |
| [Variations] | Matrix of variance for each data-set | + | - |

8.6 Project model results



NOTE

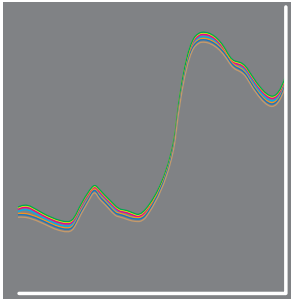
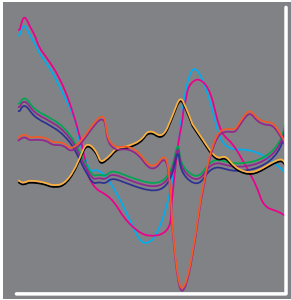
Only bold mark-up results contain data.

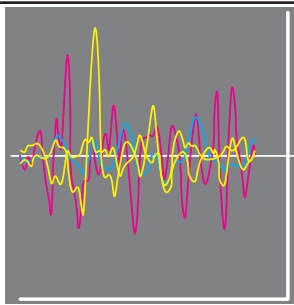
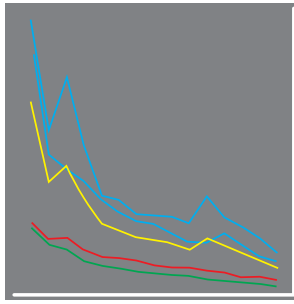
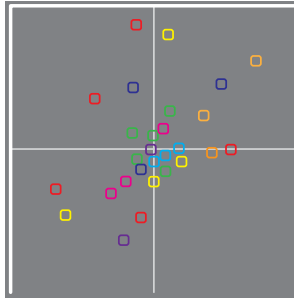
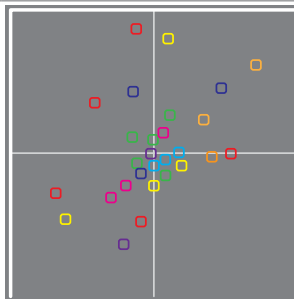
The results are shown in the graph panel and/or in the table panel. See Chapter 9 "Table panel and graph panel", page 28

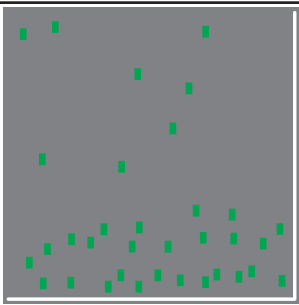
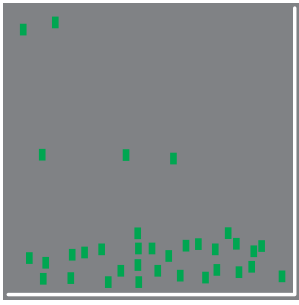
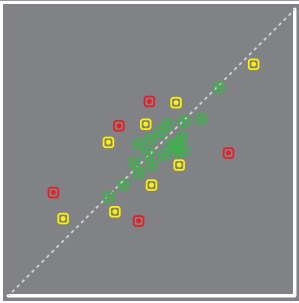
Navigation path

→ [Project panel] → [Model]

The following results are available:

| Result | Explanation | Output table | Output Graph |
|---|---|--------------|---|
| <i>Wavelengths</i> | Vector of the used wavelengths. | + | - |
| <i>Indexes</i> | List of sample indexes. | + | - |
| <i>IDs</i> | List of sample IDs. | + | - |
| <i>Center</i> | Average of all reference values. | - | - |
| <i>Target</i> | List of reference values. | - | - |
| <i>Zero</i> | Table of mean spectra. | + | - |
| <i>Observations</i> | Shows the spectra included in the calculation and validation of the calibration. (only spectra with reference values set as true and from selected data files are shown here) | + |  |
| <i>ObservationsZ</i> (=Observation Zero) | Shows spectra to find areas with high amount of spectral information. The mean spectrum is subtracted from each spectrum. | + |  |

| Result | Explanation | Output table | Output Graph |
|----------------------|--|--------------|---|
| <i>Weights</i> | 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) | + |  |
| <i>Loads</i> | Describe the correlation between original spectra and scores. | + | + |
| <i>Scale</i> | Standard deviation of the scores. | + | - |
| <i>Regressions</i> | Weights multiplied by the standard deviations of the spectra (by wavelengths/column). | + | + |
| <i>Press</i> | Visualizes the change of the SEC and SECV with the amount of factors. For optimizing the number of factors. | + |  |
| <i>Scores</i> | 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. | + |  |
| <i>Scores Scaled</i> | Table of standardized scores obtained by dividing the scores by the scales. | + |  |

| Result | Explanation | Output table | Output Graph |
|--------------------|--|--------------|---|
| <i>Mahalanobis</i> | The Mahalanobis is a measure of spectral similarity between the measured spectrum and the dataset used in the calibration. For identifying outliers. | + |  |
| <i>Residuums</i> | The (Euclidean) distance of the given spectra to the reconstructed spectra. | + |  |
| <i>Bias</i> | 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. | + | - |
| <i>Estimates</i> | Predictions based on calibration. | + |  |
| <i>Skew</i> | No function | - | - |
| <i>SkewBias</i> | No function | - | - |
| <i>Residuals</i> | Difference between reference and estimated values. | | |
| <i>CVEstimates</i> | Predictions based on the calibration during cross-validation executions. | | |
| <i>CVResiduals</i> | Difference between reference values and CVEstimates. | | |
| <i>TEstimates</i> | Estimates per sample. | | |
| <i>TResiduals</i> | Residuals per sample. | | |

9 Table panel and graph panel

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

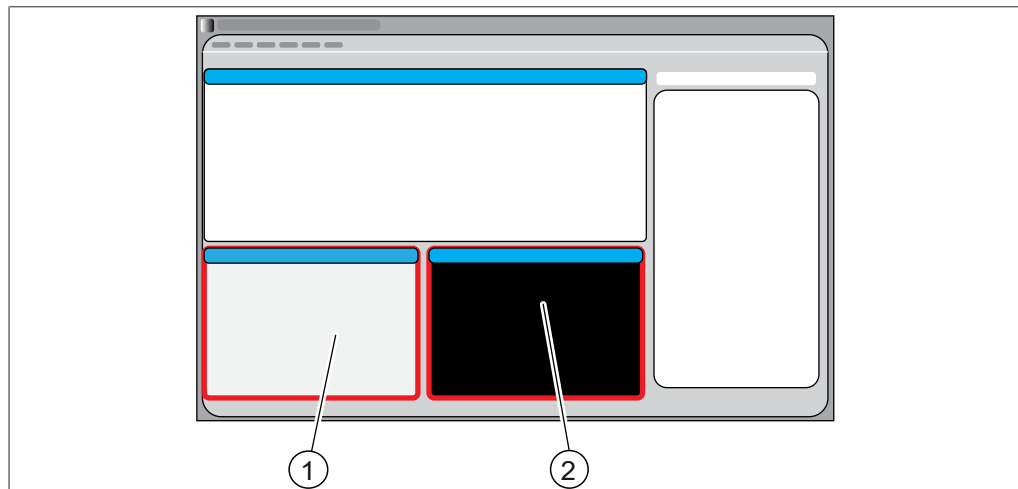


Fig. 3: Results

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 24 and Chapter 8.6 "Project model results", page 25

10 Report panel

The report panel shows report data about the calibration.

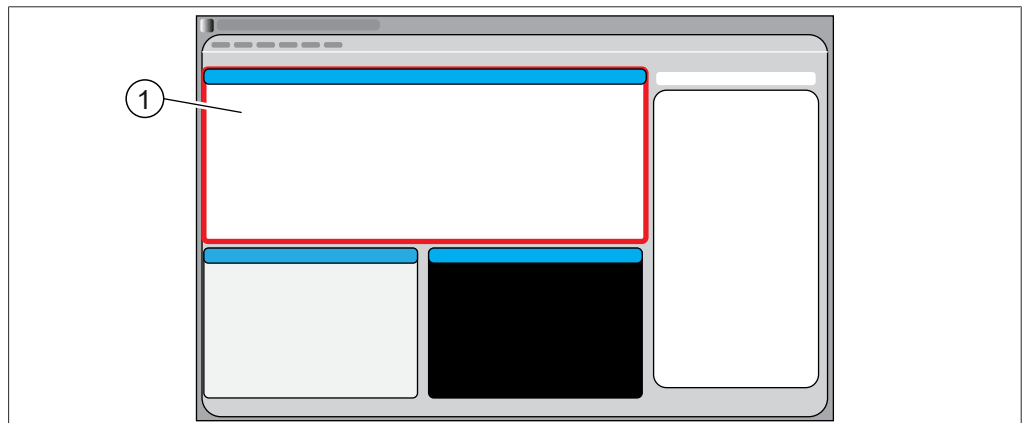


Fig. 4: Report panel

The data is exported together with the calibration export.

11 Troubleshooting

| Problem | Possible cause | Action |
|-------------------|--|--|
| Computation error | The project contains no data. | <ul style="list-style-type: none"> ▶ 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 [<i>file not found</i>], double click on data file and load it again from the correct directory. |
| | No data selected. | <ul style="list-style-type: none"> ▶ 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. | <ul style="list-style-type: none"> ▶ Less than three reference values in one of the data files. |
| Wrong results | The wavelength range is outside the range of available data. | <ul style="list-style-type: none"> ▶ 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 |

| Abbreviation | Explanation |
|--------------|---|
| 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 |
| 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\NIR-Wise\Calibrations |
| Data files for calibration | .tsv | C:\ProgramData\BUCHI\NIR-Wise\Calibrations\Data |
| Device specific data files for calibration | .tsv | C:\ProgramData\BUCHI\NIR-Wise\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 |

| Explanation | Type | Folder |
|---|-------------|---|
| 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 |
| 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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