

NANOOCOLOR® Data export software



Manual

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Dear Customer,

We congratulate you on buying one of our NANOCOLOR® photometers. To simplify working with the instrument and to make sure you can use everything the photometer has to offer, we have developed the NANOCOLOR® data export software.

Please read these software instructions carefully.

The NANOCOLOR® data export software essentially performs the following tasks:

- Reading out the test data from the photometer memory
- Online saving of test data
- Exporting test data
- Creating special photometric methods

This manual uses a few typographical conventions in the description of the NANOCOLOR® data export software program and how it is used in conjunction with your photometer. These conventions are described below.

- Keys or buttons that should be pressed on the computer keyboard or the photometer touch screen, for example the [ENTER] key, are printed in bold face upper-case letters and enclosed in square brackets.
- Program or data directories and file names are printed in italics, e.g. the default program directory, *c:\programme\macherey_nagel\datenexport*.
- Other software that are required for operating the NANOCOLOR® Data export software program or that can be used in conjunction with the software, for example, MS EXCEL, are printed in upper case letters.
- Buttons, screen keys, option buttons and text entry boxes in the NANOCOLOR® Data export software program, are printed in black.
- The majority of the software buttons are shown graphically. In this case, the relevant button is displayed as a picture
- Menu commands, such as *Scan/Open* in the NANOCOLOR® Data export software program are printed in *Verdana italic*.
- Important notices are identified using italic font and a light blue box.

1. Installation

1.1. System requirements

The NANOCOLOR® Data export software program requires at least a Pentium 4 / Athlon XP processor, 100 MB free space on the hard disk, 256 MB RAM (512 MB or more is recommended) running under Windows® XP or higher. The Microsoft .NET Framework V 2.0 program must be installed on the system. The VGA resolution should be at least 1024 * 768 pixels. The computer requires one free serial RS-232 port or one free USB port.

For creating MS EXCEL worksheets, MS EXCEL 2003/2007 or OpenOffice Version 3.2 or higher is also required. A DVD ROM drive is required for installing the program.

OFFICE 2003 / OFFICE 2007 / OpenOffice are not part of this software! No support can be guaranteed when the program is installed on other operating systems!

When using a USB port, the USB driver and the Virtual-Com driver supplied must be installed.

Administrator access rights are required for the installation.

1.2. Installing the software

Insert the installation DVD in the drive on your computer and open the file setup.exe. By default, the NANOCOLOR® Data export software is installed in the program directory on your computer (usually C:\Programs) in the sub-directory

MACHEREY-NAGEL\NANOCOLOR®_Data_Export. To ensure problem-free support, MACHEREY-NAGEL strongly recommends that the default installation directory is not changed.

With the installation and during the initial start of the software, the following sub-directories are created in the installation directory:

Data_Export\contract

Contains the software license agreement as an RTF file and the legal disclaimer as a TXT file in various languages

Data_Export\errorlog

Contains the files *error.log* and *error.crp* where information is saved regarding any possible software errors (see 8. LIMS configurator, page 14).

Data_Export\ini

Contains the initialization files *ini.xml* and *internet.ini*

Data_Export\language

Contains the file *mn_dataexport_language.xml*, that comprises all languages included in the software (see 11.1. Language Selection in the Software, page 17) and the LANGUAGE_TOOL program

Data_Export>manual

Contains the file *dataexportsoftware_en.pdf* (i.e. this manual in PDF format).

Data_Export\originals

After installation, this sub-directory is empty and is required for saving the original files (see 6. Original Files, page 13)

Data_Export\syslog

Contains the files *sys.log*, *sys.crp* and *environment.log* where technical information on your computer system is saved for possible future support purposes (see 8. LIMS configurator, page 14).

Data_Export\dataase

Contains the file *nanocolor_db.xml*, all results are saved there

Data_Export\exports

Standard folder for all exported data

Data_Export\graphics

Standard folder for all pictures

Data_Export\guids

Contains the file *guids.xml*, database for saving used GUIDs

Data_Export\logos

Standard folder for company logos used for the protocol layout

Data_Export\methods

Standard folder for calibrations

Data_Export\places

Contains the folder *sampleplaces_db.xml*, database for automatically allocating sample locations

1.3. Installing the USB driver

If you intend to connect the NANOCOLOR® Photometer to the computer via a USB port, two driver files must be installed on your PC. Normally, this is done automatically under Windows Vista / 7. For Windows XP, and in some cases Windows Vista and 7 as well, you need to install the drivers manually using the device manager menu, which you can access in the Windows control panel.

In the device manager menu, chose the respective connection and select the option **refresh drivers**. You can either search for the drivers online, or select the respective folder that comes on the software dvd. As two drivers need to be installed, you have to perform the driver installation twice!

1.4. Operating instructions

The NANOCOLOR® Data export-Software software has been developed to conform to all regulations of "Good Laboratory Practice" (GLP). This requires an unambiguous assignment of user rights in order to prevent, for example, the unintentional deletion of information. Consequently, some of the functions described in this manual can only be executed if the user has administrator access rights.

If functions in this software do not appear to operate correctly, please consult your system administrator.

1.5. GLP and FDA 21 CFR Part 11 Compliance

complies with GLP and 21 CFR Part 11 by virtue of the following measures:

- LOG-File

All changes to the software settings and deletions are logged together with details of the date, time and user ID.

- RIGHTS

Security-relevant changes and deletions can only be made by the system administrator.

- PRINTER OUTPUT

All printouts are marked with the date, user name, software version and device serial number.

- ORIGINAL DATA

All original data is stored in binary-coded non-editable files with checksum information.

- SYSTEM DATA

All system settings and the LOG file are encrypted and include a checksum.

- RECOGNITION OF MANIPULATION

The software automatically recognizes whether measured values or system data have been manipulated (checksums). There are two different security settings available: LOW (manipulation warning message, the user can open the relevant file if technically possible), HIGH (manipulated files cannot be opened).

- EXCHANGEABILITY OF DATA

NANOCOLOR® test data can be output in SDF or XML format, scan data can be saved as netCDF/ANDI files. The data complies with the ASTM E 1947 -98 (2004) and ASTM E 1948 -98 (2004) standards.

- SECURE DATA TRANSFER

Data transfer is performed via a bi-directional protocol with checks of the transmitted/received information.

In order to achieve full compliance with 21 CFR Part 11, the software must be installed on a certified computer with an NTFS file system. Access to the software must be conducted via Windows® authorization rights.

The security setting must be set to HIGH.

2. Supported photometer

The **NANOCOLOR®** data export software can be used together with the **NANOCOLOR®** 250 D, 300 D, 350 D, 400 D, 500 D, PF-12, Linus and our luminometer BioFix® *Lumi-10*.

All MACHERRY-NAGEL photometer can run with different serial interface settings,. To use the photometers with this software, you have to set the default interface mode. The following table shows the necessary settings for the respective photometers.

Photometer	Baud rate	Parity	Bits	Stop bits	Format	Protocol
NANOCOLOR® 250 D	9600	no	8	1	SDF	no
NANOCOLOR® 300 D	9600	no	8	1	SDF	no
NANOCOLOR® 350 D	19200	no	8	1	SDF	no
NANOCOLOR® 400 D	19200	no	8	1	SDF	no
NANOCOLOR® 500 D	19200	no	8	1	SDF	no
PF-12	19200	no	8	1	SDF	no
NANOCOLOR® LINUS	9600	no	8	1	SDF	no
BioFix® Lumi-10	38400	no	8	1	SDF	no

Tab. 1 : Interface settings of supported photometers

SDF = semicolon delimited fields

The format of some data, such as time, date and decimal is dependant on both the system configuration of your computer and the photometer settings.

3. Program start

Connect the photometer to your computer using a serial or USB cable.

Turn on the photometer (Method: . . . appears in the screen). Select the NANOCOLOR® data export software on your computer via the windows start menu (*Start\Programs\MACHEREY_NAGEL\Photometer_dataexport*).

The software start screen contains icons within the icon bar to select the most important functions and settings. All functions are also available via the menu bar.



Fig. 1: Start screen *NANOCOLOR*[®] data export software

4. System menu and software settings

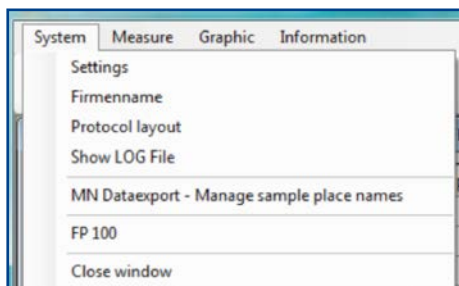


Fig. 2: System menu

4.1. Settings

The **Settings** function or the  button open the **Settings** window of the **NANOCOLOR®** data export software.

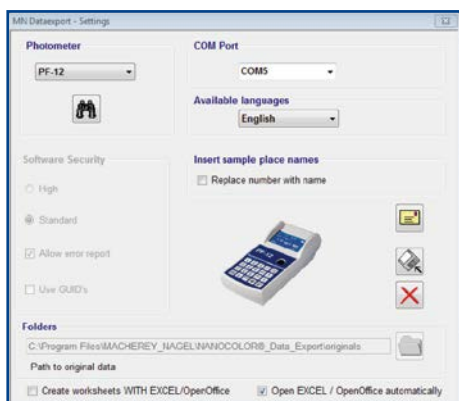


Fig. 3: Fenster Einstellungen




Some functions in the Settings window are greyed out if you do not have administrator access rights. In this manual, greyed out functions are identified by the ! symbol.

4.1.1. Instrument selection / interface search

To communicate with a computer, the photometer has to be in the method mode. In the photometer display **Method: . . .** appears.

For the **COM-Port** function area, select the interface your computer is using.

Then, choose your photometer in the **Photometer** function area.

All transmission parameters are set automatically. The program saves the data. Please set the connection you are using. The button search interface  is displayed when using a PF-12, 500 D and 400 D. If you don't know the port-number of your connection, you can find the interface with this function (for the 400 D, the function is dependant of the software version). As long as you don't connect a different photometer or change the interface, you only have to adjust the photometer settings once. Confirm your selection with the save settings button . If you press Close , the window is closed without making any changes.

4.1.2. Language selection and other settings

In the upper right of the settings window, you see the **Available languages** function area. There, you can choose the software language.

! In the **Software security** function area, the level of security for the software can be specified (see also Chapter 2, GLP and FDA 21 CFR Part 11 Conformity) (see 2. Supported photometer, page 6).


If the setting **High** has been selected, the software will not open damaged or manipulated files. This includes saved scans, photometer export files and the configuration file in the software.

Some information boxes that can record the data of a scan, are also changed to compulsory fields that must be completed.

! The **Normal** setting allows damaged or manipulated files to be opened (where it is technically still possible), after a warning prompt is accepted. The number of compulsory fields is also less when a scan is created.

The third option **Allow error report** With an existing internet connection, this button allows the user to automatically send an error report to MACHEREY-NAGEL without having to search for and summarize all the relevant information. The function transmits the files *error.log*, *sys.log* and *environment.log* (see 8. LIMS configurator, page 14) to the server www.mn-net.com via http.

If the administrator wishes to stop the automatic exchange of information via an internet connection, this option must be disabled.

When the  button is clicked, the software asks whether an error report is to be sent to MACHEREY-NAGEL. A click on **Ja** opens a window with text boxes for entering your name, telephone number and e-mail address, together with a text box for entering a short description of the fault. Now click on the **OK** button. The time taken for transmitting the information depends on the quality of the internet connection.

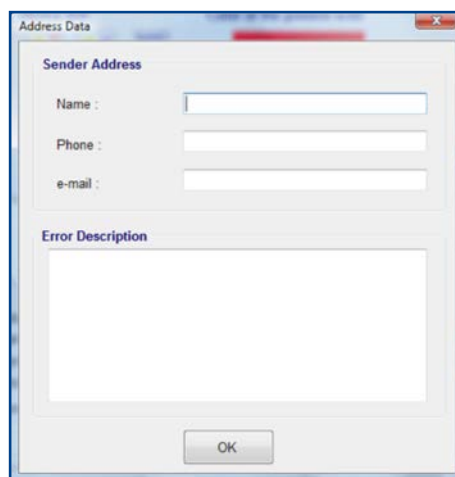





Fig. 4: Address window of the error report

This function uses port 25. This port on your local PC may be inhibited by a virus scanner or firewall. In this case, consult your system administrator. If there is no active Internet connection, this function is disabled.

The last security option is the **GUID's verwenden** button. If this option is enabled, a GUID is calculated for each document to be printed and is included in the printout (see 7. GUID administration, page 14).

The **Folders** area is located at the bottom of the window. Here, you can specify the directory on your PC or network to which the original files are to be saved following export from the photometer. By default, the **original** folder in the software installation directory is used. Click on the  button to open a browser window where another location can be selected if required, click on **OK**.

In the same way, the path for saving wavelength scans can be specified. By default, the scans folder in the installation directory of the software is used. When all settings have been completed, the data must be saved by clicking on the  button. The  button closes the settings window without saving.

4.2. Company name

In some cases, depending on the software installation on your PC, the NANOCOLOR® Data export software may not detect the name of your company from the Windows® settings. In this case, the name "MACHEREY-NAGEL" is output in the protocols as the name of the company by default. A different name for the company can be entered via the *System/Company name* function.

4.3. User-specific printouts

Frequently, the NANOCOLOR® data export software may ask you or require you to create a protocol printout after carrying out a measurement. By default, the MACHEREY-NAGEL logo will be printed in the header and the MACHEREY-NAGEL company address in the footer.

The view will always be shown in the background of the software's main window.



Fig. 5: Display of the protocol design

In the area at the top, you can see the graphic used for the logo. Below, you can see "Protocol language: German". This shows that the protocol is being created in German. In the area at the bottom of the picture, you can see the company address. There are three lines available, with the first line consisting of two parts which are printed in two different typefaces.

Below the menu function *System/Protocol layout*, you can set up your own header and footer. If you run a contract laboratory, for example, you can create client-specific protocols, as you can store an infinite number of addresses and logos.

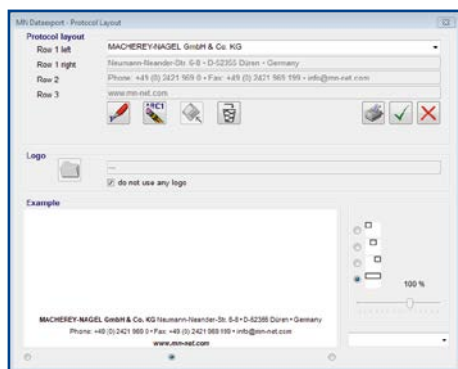



Fig. 6: The address settings window


The first text field **Row 1 left** is designed as a drop-down menu. If you have already saved addresses, then you will be able to select these stored addresses from this list. When the software is initially installed, it will only contain the address of MACHEREY-NAGEL. This entry can neither be deleted nor edited.

To create a new address, click on the button .

To edit an existing address, select this address from the drop-down menu **Row 1 left** and click on the button .

The content of this first row is displayed in bold on the left-hand side of the first line of text in the footer, and should generally contain the company name. The text of the second row appears in normal typeface on the right-hand side of the first line of text, and may contain the address. The third text box **Row 2** contains the second line of text in the footer. It is displayed in normal type-

face and is intended for telephone and fax numbers. The fourth text box **Row 3** is used for the third line of text in the footer, and appears in bold italics.

Once all the text boxes have been completed with the relevant data, click the button  to load up a graphic (GIF, JPG) to use as a logo. If the protocols are to be printed without a logo, then enable the option **No logo**.

To delete an address, select the address and click on the button .

Once all the text has been entered and a graphic has been chosen, all these elements may be positioned individually as shown below.





Fig. 7: Positioning the text elements

In the top right-hand corner, there are four option buttons represented by an icon in the shape of a small box. These determine the position of the logo. The first three are for either left, centre or right alignment. The fourth option resizes the logo across the entire breadth of the page. Below these four buttons is a slide adjuster. If the option "Resize across the entire page" is not enabled, then the size of the logo can be adjusted in %.

Below the protocol example, there are three more option buttons, one each in the left-hand corner, the middle and the right-hand corner. Use these to adjust the alignment of the lines of text in the footer. In the example shown, the text is aligned flush right. In the list box, you can also set the output language of the protocol. It is possible to print protocols in a different language than the one set in the software itself.

Ensure that logo graphics are stored in such a way that the software can always find them. If the graphics file is moved or deleted, then it can no longer be used for printing the protocol.

Once you have completed all the settings, save your individual design by clicking on the button . Your settings are now saved in the database. If this design is to be used for printing the protocol, then you also need to click on the button .

5. NANOCOLOR® photometer functions

5.1. Allocate sample locations

NANOCOLOR® photometers from MACHEREY-NAGEL assign numbers from 00 to 99 to sample locations (see photometer manual).

To these numbers, you can add clear text, which is transferred automatically when creating a table. That means, in your MS EXCEL sheet or database, for example sample location number "01" is replaced by "Inflow 1". To assign sample locations, please use the menu command *System/MN data export – administer sample locations*.

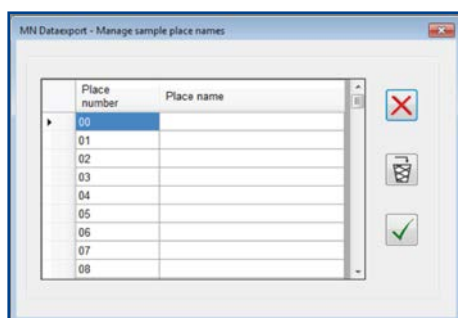


Fig. 8: Assigning sample locations

To do so, select the numbers you are using for your photometric measurements in the left column and enter the respective sample location name into the right column. Once you have assigned a name to all sample locations, press . If you have enable "Sort tables according to sample locations", the sample location names are also used to label the different tabs in your EXCEL sheet.

The settings of this function are ignored when using a NANOCOLOR® 500 D or PF-12. For these photometers, just use the inbuilt sample location function.

5.2. Export the photometer memory

To export the photometer memory, initially connect the instrument to the computer as described (see 4.1.1. Instrument selection / interface search, page 7).

Due to the different technical set-up, the data export function is slightly different between the photometers.

5.2.1. NANOCOLOR® 250 D, 300 D, 350 D, 400 D, 500 D, PF-12

Start the data export by pressing the menu command *Measure/Read photometer memory*. Alternatively, click on the button .

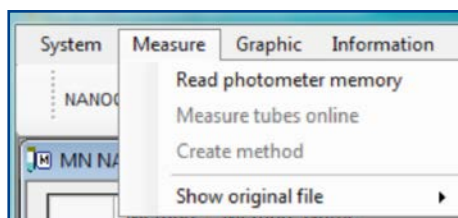


Fig. 9: Menu command *Measurement/read photometer memory*

The software opens the data window and fills the table with the data from the photometer.

Normally, data transmission takes about 1 to 5 minutes, depending on the amount of data. The photometers NANOCOLOR® 250 D and 300 D are a little slower, which means exporting a full memory may take up to 8 minutes.

For all these models, the data export is fully automatic. The end of transmission is recognized and the data base or table is created right away.

5.2.2. NANOCOLOR® LINUS

These instruments don't tell the computer when the data transmission has been completed. Therefore, you need to do the following: Press *Measurement/Photometer data export*. Alternatively, you can also press .

Then, set the photometer to the memory mode (Mem. button). The display will show two words saying **Memory** and **Print?**. Press **OK** on the photometer. The data export starts. Once the sending has been completed, the display goes blank for a brief moment. As soon as **Memory** and **Print** is displayed again press in the software. The data export to the computer has been completed.

The software automatically inserts the photometer data into the table. Normally, data export take between 1 to 5 minutes. In case of a completely full memory, export time may be up to 8 minutes.

5.2.3. BioFix® Lumi-10

Press *Measurement/Photometer data export*. Alternatively, you can also press .

Then, set the luminometer to the memory mode (Mem. button). Turn on the luminometer and select the menu function **Results/PC** from the LCD display. Then, select the option **Start transmission**. While the data is exported, the luminometer display shows **data transmission**. Once the notice has vanished, press .

The software automatically inserts the photometer data into the table. Normally, data export take between 1 to 5 minutes. In case of a completely full memory, export time may be up to 8 minutes, as the luminometer has a very large memory.

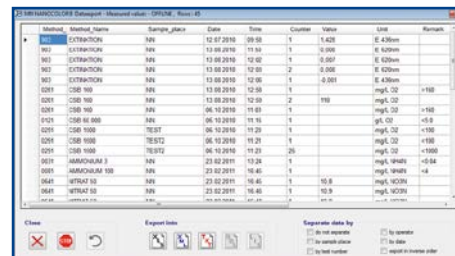


Fig. 10: Data window with data sets

5.2.4. Data export

The table shown is intended only as a summary. The data here cannot be edited. The table can be sorted by clicking on the column titles. The window allows you to save the measured values in one of four possible formats in order to process the data in other software products, or for archiving. In the lower area of the window, there are five buttons that can be used to initiate the corresponding export function




Fig. 11: Buttons for data export

With the options under the heading **Separate data by** the data can be split into individual tables. The measured values can be split into individual tables, according to: by sample place, by test number, by date and by operator.

These options are not relevant when the export is to a text file.

5.2.4.1. Export to MICROSOFT EXCEL

To use this function, Microsoft® EXCEL 2003 or higher must be installed on your computer. The button  exports the data to an MS EXCEL worksheet. The software opens a file selection window.

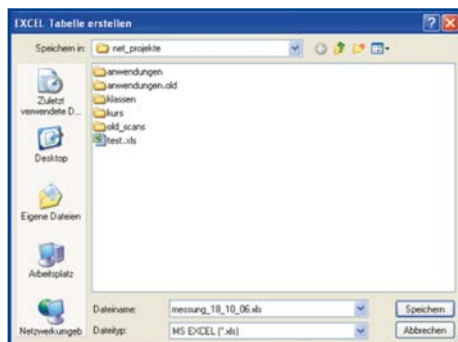


Fig. 12: File selection window "Create EXCEL Worksheet"

Select an appropriate file path and in the **File name:** box enter a valid name for your EXCEL file and then click the **Save** button.

The NANOCOLOR® Data export software opens MICROSOFT EXCEL and fills the worksheet with the measured values. The MS EXCEL worksheet is automatically saved with the selected file name.

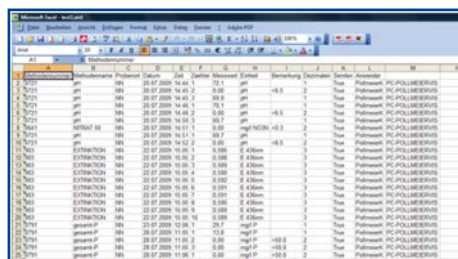


Fig. 13: Measured values in MS EXCEL


If one of the options from **Separate data by** has been selected, an individual table is created for each sample place, NANOCOLOR® test number, user and date. The tables are automatically labeled with the selected criteria.

If MS EXCEL is already opened or the selected file already contains data, the new data is added after a blank line.

If the values measured are outside the measurement range (< or > symbol), the values are shown in the Remark column.

User name, sample place and dilution are output if they have been entered in the photometer during the measurement. If no user name is entered, the Windows® logon name is output.


5.2.4.2. Export in the database format XML

The second export button  is used to create an XML database. The software opens a data selection window. Select an appropriate file path and in the **File name:** box, enter a valid name for your XML database and then click the button **Save**.

The XML database can be read by all database programs, regardless of the operating system being used. Any questions regarding import to an existing database system should be addressed to your database administrator.


If one of the options from **Separate data by** has been selected, an individual table for each selection is created in the XML file. When importing into a database system, the measured values are automatically assigned to the various tables.

5.2.4.3. Export in the TEXT-format

The third export button  is used to create a formatted text file with semicolons as separators. The software opens a data selection window. Select an appropriate file path and in the **File name:** box enter a valid name for your TEXT file and then click the button **Save**.

5.2.4.4. Export to OpenOffice-SCALC

To use this function, OPENOFFICE, Version 3.2 or higher must be installed on your computer.


The button  exports the data to an OPENOFFICE SCALC table. The software opens a file selection window. Select an appropriate file path and in the **File name:** box, enter a valid name for your SCALC file and then click the button **Save**.

The NANOCOLOR® PC Software for Spectrophotometers opens OPENOFFICE SCALC and fills the table with the measured values. The OpenOffice SCALC table is automatically saved with the selected file name.


If one of the options from **Separate data by** has been selected, an individual table is created for each sample place, NANOCOLOR® test number, user and date. The tables are automatically labeled with the selected criteria.

If OPENOFFICE SCALC is already opened or the selected file already contains data, the new data is added after a blank line.

5.2.4.5. Export to a laboratory information system

The last export button  sends the data records to a laboratory information system. This button is active only if the "send" function is activated in the laboratory information system configurator. (see 8. LIMS configurator, page 14).

5.3. Online measurements


Click on the menu command *Measure/Measure tubes on-line*. Alternatively, click on the second button in the icon bar .

The software opens the data window with an empty table and waits for the data.

Complete your measurements. The measured values are transferred to the PC when the cuvette is removed. Before removing the cuvette, you can enter your settings for the sample place, the dilution and the user ID on the photometer display.



Fig. 14: Online measurement, waiting for data input

In online mode, the  button is shown at the lower left of the data window. This button allows you to quit online mode without closing the data window.

The buttons for data export are shown at the lower edge of the data window (see 5.2. Export the photometer memory, page 9).

This function is not available in the BioFix® Lumi-10, PF-12 and PF-3

5.4. Calibrating Special Methods

With the NANOCOLOR® Data export software you can create your own special methods. All you require is a series of cuvettes each with a specified test concentration. After measuring the cuvettes, all relevant statistical parameters are automatically measured and displayed. If required, a measurement log can be printed.

This function is not available in the BioFix® Lumi-10 and PF-3

5.4.1. Measuring Special Method Data

To create a special method, click on the menu function *Measure/Create method*. Alternatively, click on the  button.

A Method window is opened.

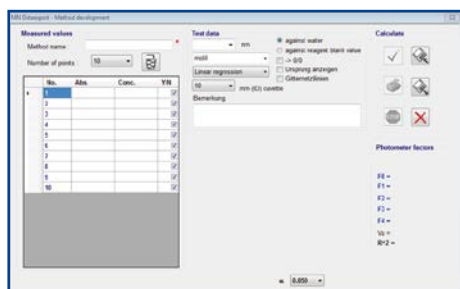


Fig. 15: Method development window

In the **Number of points** list, enter the number of measurement points. We recommend that at least 10 concentrations are measured.

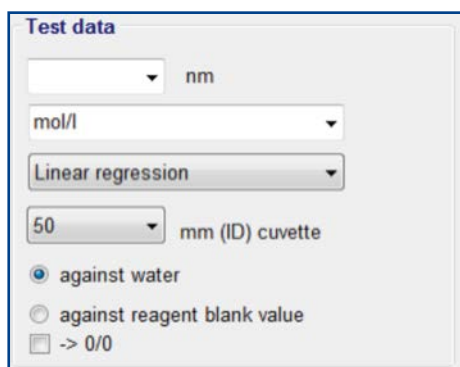


Fig. 16: Measured value settings

In the **Test data** box enter the required wavelength. If the required wavelength is not included in the drop-down list, the value can be directly entered in the text box (smallest permissible value 190 nm, largest value 1100 nm, no decimal places (the software cannot check if the wavelength exists in the photometer and that the correct wavelength has been selected for the measurement!)).

In the second box, select the concentration unit you are using. If the required unit is not included in the drop-down list, the value can be directly entered in the text box (see 11.2. Selection of Units, page 17).

In the third box, the type of regression to be calculated is selected.

The type of cuvette used in your method must be entered in the fourth box.

In the lower section of the field, you must specify whether the measurements in your method are to be made against water or against a reagent blank value.

If you measure absorbance values, the photometer requests a blank solution. Set the type of blank solution used via the **against water** and **against reagent blank value** option buttons. If the option **against reagent blank value** is selected, the program assumes that all regression curves must pass through zero. If you want to force the curve passing through zero while measuring against water, activate the function **-> 0/0**.

Now, click in the first field of the **Conc.** column and enter the concentration set for the first cuvette.


	No.	Abs.	Conc.	Y/N
	1		10	<input checked="" type="checkbox"/>
	2			<input checked="" type="checkbox"/>
	3			<input checked="" type="checkbox"/>
	4			<input checked="" type="checkbox"/>
	5			<input checked="" type="checkbox"/>
	6			<input checked="" type="checkbox"/>
	7			<input checked="" type="checkbox"/>
	8			<input checked="" type="checkbox"/>
	9			<input checked="" type="checkbox"/>
	10			<input checked="" type="checkbox"/>

Fig. 17: Entry for the concentration, cuvette 1

Next, click in the second field of the **Conc.** column or press the **ENTER** key on your PC keyboard and enter the concentration set for the second cuvette


	No.	Abs.	Conc.	Y/N
	1		10	<input checked="" type="checkbox"/>
	2		20	<input checked="" type="checkbox"/>
	3			<input checked="" type="checkbox"/>
	4			<input checked="" type="checkbox"/>
	5			<input checked="" type="checkbox"/>
	6			<input checked="" type="checkbox"/>
	7			<input checked="" type="checkbox"/>
	8			<input checked="" type="checkbox"/>
	9			<input checked="" type="checkbox"/>
	10			<input checked="" type="checkbox"/>

Fig. 18: Entry for the concentration, cuvette 2

Finally, click in the third field of the **Conc.** column or press the **ENTER** key on your PC keyboard. Entries are made automatically in the subsequent fields with equidistant values


	No.	Abs.	Conc.	Y/N
	1		10	<input checked="" type="checkbox"/>
	2		20	<input checked="" type="checkbox"/>
	3		30	<input checked="" type="checkbox"/>
	4		40	<input checked="" type="checkbox"/>
	5		50	<input checked="" type="checkbox"/>
	6		60	<input checked="" type="checkbox"/>
	7		70	<input checked="" type="checkbox"/>
	8		80	<input checked="" type="checkbox"/>
	9		90	<input checked="" type="checkbox"/>
	10		100	<input checked="" type="checkbox"/>

Fig. 19: Automatic column entries

If you are working with non-equidistant concentration steps, simply overwrite the value in the third field. Subsequent fields are then automatically deleted.

The complete table can be deleted with the  button.

Now, in the **Calculate** area of the window, click on the  button.

The software asks you now to measure the first sample tube

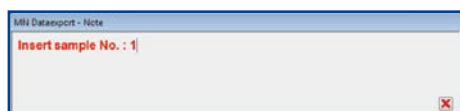


Fig. 20: Pop-up – insert sample tube 1

To do so, activate absorbance measurements (Method 903) in the photometer. Set the required wavelength and perform a zero measurement. Then, insert the tube with the first sample into the photometer for measurement.

Once the cuvette has been removed, the measurement value is sent and inserted into the table within the software.

	No.	Abs.	Conc.	Y/N
	1	0,056	10	<input checked="" type="checkbox"/>
	2		20	<input checked="" type="checkbox"/>
	3		30	<input checked="" type="checkbox"/>
	4		40	<input checked="" type="checkbox"/>
	5		50	<input checked="" type="checkbox"/>
	6		60	<input checked="" type="checkbox"/>
	7		70	<input checked="" type="checkbox"/>
	8		80	<input checked="" type="checkbox"/>
	9		90	<input checked="" type="checkbox"/>
	10		100	<input checked="" type="checkbox"/>

Fig. 21: Transfer the first result

Now insert all cuvettes, one after the other in the correct sequence, in the photometer. When the last cuvette is removed from the photometer, all static parameters are calculated and displayed graphically.

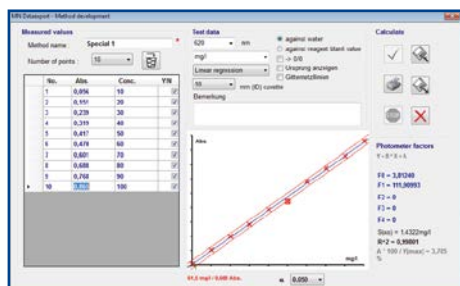




Fig. 22: Photometer factors and graphic display

Confidence intervals are indicated as red hyperbolas if linear or quadratic functions are calculated. Decision limit, detection limit and determination limit are displayed as green markers (see 11.3. Outlier elimination and multiple measurements, page 17).

5.5. Change Regression Type and Print the Log

A measurement log of your calibration can be printed via the  button. To cancel the measurement prematurely, click the  button. If it is seen from the curve that an incorrect regression has been selected, a different type of regression can be selected from the list. The parameters are immediately converted automatically.

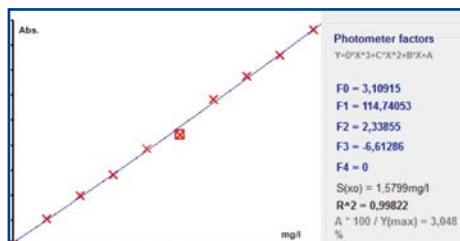



Fig. 23: Switch-over to cubic regression

The measurement points of the calibration can also be saved in a file, if for example, it is not possible to print at the present time. For this, click on the  button and in the selection box, enter

an appropriate file name. To re-load a saved measurement, click on the  button.

The factors F0 to F4 are the photometer factors, not the parameters of the displayed curve. The curve parameters A0 to A4 are printed with the measurement protocol.

5.6. Menu function Graphic/Copy to clipboard

Using the menu command *Graphic/Copy to clipboard*, the curve can be copied to the Windows® clipboard and used in other applications if required.

5.7. Menu function Graphic/Save to file

The function *Graphic/Save to file* allows you to store the calibration curve as a graphics file. A file selection window opens and you will need to enter the save location and the name. You can save the graphic in the following formats: JPG, GIF, BMP, TIF and WMF.

6. Original Files

The strict regulations of GLP and 21 CFR Part 11 state that all data measured using an instrument and saved on a computer via PC software must be stored in a form that prevents any accidental or intentional manipulation. The software must also be able to automatically detect any manipulation of measured values. To this end, the MACHEREY-NAGEL NANOCOLOR® Data export software writes all exported NANOCOLOR® test data to a protected, binary-coded file, the original file. This original file cannot be read or edited without causing damage, unless the appropriate software is used. An original file is created, even if the exported data is not saved in one of the suggested formats. As default, the directory used for saving is:

c:\Programme\MACHEREY-NAGEL\NANOCOLOR_data_export\originals

! It is possible to specify a different path for saving the original files via the Settings window, for example to save the original files to an external server. (see 4.1.2. Language selection and other settings, page 7).

Administrator access rights are required to allow the use of functions that work in conjunction with original files.

6.1. Reading Original Files

Regulation 21 CFR Part 11, specifies that original files may be read at any time by authorized persons or testers.

! If you wish to see what is contained in the original files, click on the menu command *Measure/Show original file*. A file selection window is opened.

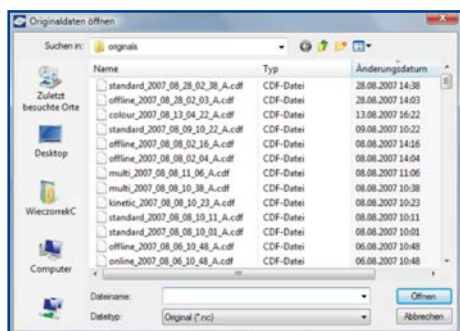


Fig. 24: Selection of original files

Switch to the directory where the original files are saved. By default, the original files are saved in the directory: *c:\Programme\MACHEREY-NAGEL\NANOCOLOR_data_export\originals*

Die Namen der Original-Dateien werden automatisch vergeben und bestehe aus typ_jahr_monat_tag_stunden_minuten_Buchstabe.cdf.

As will be seen, the file name is automatically formed and consists of type_year_month_day_hours_minutes_letter.cdf. The letter, usually an "A", represents a counter in case more than one process is completed within one minute. For the type, the terms online, offline, can be displayed, depending on the type of measurement completed.

Select a file and click on the button. A window displaying the contents of the original file opens.

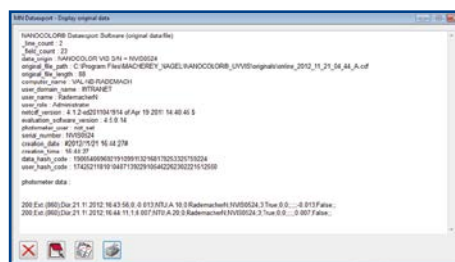


Fig. 25: Display of original files

A printout of the original file can be created by clicking on the button. The text window is copied to the clipboard with a click on the button. The button closes the window.

7. GUID administration

A Globally Unique Identifier (GUID) is a globally unique number of 128 bit (that is 16 bytes) and that comes into play in distributed computing systems. GUID's enable you to implement the Universally Unique Identifier Standards (UUID) whereby documents etc. may be uniquely identified across the world.

For additional security, you have the option to identify the printout of the document with such a GUID. This function is enabled via the settings menu with the function *Manage GUID's*. When this function is used, all GUIDs created by the software are saved in a database. The *Manage GUID's* menu function opens this database and displays the GUIDs that have been created. By comparing the entries, it is possible to ascertain that a GUID associated with a document, has actually been created by this software.

Counter	Sample	W/V	Date	Time	Operator	GUID
1	MLL_EXCEL	Blank	2010/12/11	13:37	RademacherH	c20a8f09-cd05-43d9-a011-42301f5a63ca
2	offen...	original file	2010/12/11	13:38	RademacherH	68c8a910-30ad-4a8f-8796-66337a7147
3	mutual...	original file	2010/12/11	13:37	RademacherH	0086d642-7e42-43d2-80d4-8001174b1564
4						a5058076-8b6c-4f6a-b8d1-7a7199154baf

Fig. 26: GUID database

The GUID that has been used is shown in the last line. This GUID is identical to the eleventh line in the database.



Fig. 27: GUID on a print out

8. LIMS configurator

In principle, there are two ways of sending measurement data from the photometer to the laboratory information system:

8.1. Direct connection

Connect the photometer to the LIMS using the serial interface. After each measurement, the data is transmitted every time the cuvette is removed. It is not possible, however, to alter the data format. Your LIMS must be able to accept the MACHEREY-NAGEL data format.

8.2. Indirect connection via PC

Connect your photometer to your PC using an RS-232 or USB interface. Then connect your LIMS to the same PC using another RS-232 interface. The NANOCOLOR® data export software is now able to send the photometer data on to the LIMS.

The advantage of this option is that you can control the data as well as the format in which they are transmitted.

Now click on the menu command *System/LIMS configurator*.

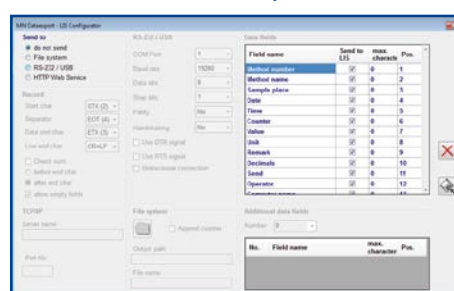


Fig. 28: LIMS Configurator

In the left upper part of the windows you see the frame *Send to*. Select here the way of data transmission. The first option do not send deactivates the LIMS function. The second option *File system* sends the data as text file. If you activate this option the frame *File system* is activated.

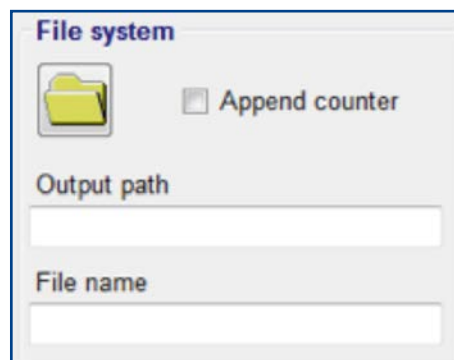



Fig. 29: Send records as file

With the button , you can open a file selection window. Set the file to which you want the data to be written. Enter the name of the text file to be created by the software in the cell *File name*. If you enable the function *Append counter*, then a counter is attached automatically to the file name, e.g. *sample.txt* becomes *sample_3.txt*.

The function *File system* requires that your LIMS is able to collect and process files automatically.

The third function in the frame *Send to*, *RS-232/USB*, sends the measurement data via a serial interface or a virtual USB adapter. If the function is enabled, the frame *RS-232/USB* is activated.

Fig. 30: Send data via a serial interface

The options of this frame are self-descriptive. Set all parameters that are required by your LIMS.

Finally, data may be sent by setting up the option **HTTP web service**. The data is sent via the PC network in TCP/IP format. If you enable this option, the frame TCP/IP is activated.

Fig. 31: Send data via TCP/IP

Enter the correct name of the server on which the LIMS-TCP/IP Listener runs into the box **Server name**. Alternatively, you can enter the IP address. Enter the number of the TCP/IP port on which the Listener is listening into the box **Port no.**. Using these settings, you are able to send the measurement data via the internet, provided you instruct your Firewall that the **NANOCOLOR®** data export software is permitted to send via the internet. This function requires that your LIMS is capable of reading data via a TCP/IP port.

Having determined how you are going to send the data, you now have to configure the data record yourself. The most important settings are made using the frame **Data record**.

Fig. 32: Configuring a data record

In general, a data record looks like this:

`<startcharacter>datafield_1<separator>datafield_2<endcharacter><checksum><lineend>`

Some of the elements in `< >` brackets may be absent. Usually, STX = ASCII 2 is used as a start character and ETX = ASCII 3 is used as end character. To mark the end of the record line either CR = ASCII 13 or CR+LF = ASCII 13 + ASCII 10 is used as line end character. As separator, the semicolon (;) is commonly used, but its use as separator then prohibits its use within the data fields.

Simplified, a data record may look like this:

`STXdatafield_1;datafield_2;datafield_3ETXCR`

Which characters you have to use depends on your LIMS system. Using the options in the frame **Data record**, it is possible to set the most common formats.

As there are several methods of check-sum calculation in use, the **NANOCOLOR®** data export software will probably have to be re-programmed, if you have to use a check-sum. Please contact us, if this is the case.

You will find an overview of the data fields provided by the photometer on the right-hand side of the window.

Data fields			
Field name	send to LIS	max. character	Pos.
Method number	<input checked="" type="checkbox"/>	0	1
Method name	<input checked="" type="checkbox"/>	0	2
Sample place	<input checked="" type="checkbox"/>	0	3
Date	<input checked="" type="checkbox"/>	0	4
Time	<input checked="" type="checkbox"/>	0	5
Counter	<input checked="" type="checkbox"/>	0	6
Value	<input checked="" type="checkbox"/>	0	7
Unit	<input checked="" type="checkbox"/>	0	8
Remark	<input checked="" type="checkbox"/>	0	9
Dilution	<input checked="" type="checkbox"/>	0	10
Operator	<input checked="" type="checkbox"/>	0	11
Serial number	<input checked="" type="checkbox"/>	0	12

Fig. 33: Data fields of the photometer

The first column displays the field name. If the checkmark in column two is activated, the data field is sent to the LIMS. If you do not need one of the data fields provided, just deactivate the option (depends on your LIMS setting). Usually, the number of characters for each data field is limited. In this case, write the allowed number of character for each field in column 3. A ZERO (0) means no character limitation. Data fields marked with a ZERO (0) may hold any number of characters. If the data field is marked with a number greater than ZERO (0), the software will shorten the field content to the allowed number of characters, if the

photometer is sending more characters than allowed. The last column determines the position of the data field within the LIMS data record.

In some cases, it is necessary to integrate additional data fields into the data record. For example, if you wish to add the job number to each measurement, an extra field has to be inserted. Then proceed as follows:

In the lower right-hand area of the window, you see the frame Extra data fields.

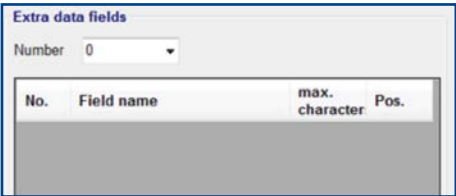


Fig. 34: Extra data fields frame

In the drop-down menu **Number**, enter the number of extra fields required. Create a unique name for the data field in the column **Field name**. As in the table with the fields of the photometer, you can now enter the maximum number of characters and the position within the data record

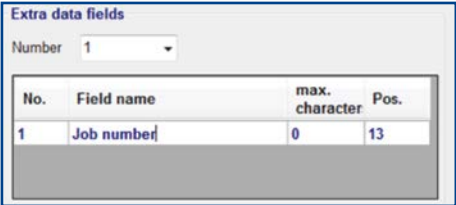



Fig. 35: Definition of an additional data field

Once you have defined an extra data field and saved the settings using the button , the software will open a text box after every cuvette measurement (and for each data export line), asking for the extra information to be entered. This can also be done by a barcode reader that has been correctly connected.

9. Show LOG Files

The Show LOG file menu function opens a window that allows the user to read all LOG files that have been created.

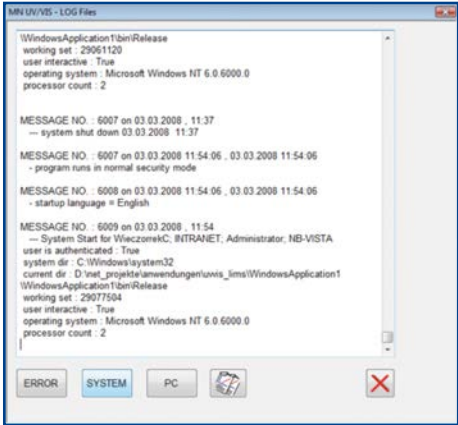






Fig. 36: Show LOG files

The ,  and  buttons open the corresponding LOG files for display in the text window. The button  copies the log file or selected text into the windows clipboard.

10. **NANOCOLOR®** FP-100 Sipper

The *FP-100* menu function opens a window that allows the user to set the parameters of our FP-100 sipper pump. In contrast to the **NANOCOLOR®** spectrophotometers however, using the Sipper with our filter photometers is not automated. Hence, the sipper cannot be connected to the photometer, which means measurements have to be conducted manually.

11. Appendices

11.1. Language Selection in the Software

Version 3.0 of the **NANOCOLOR®** data export software is issued in German, English, French, Polish and Spanish versions. MACHEREY-NAGEL is endeavoring to include other languages. If you wish to program a language yourself, follow the procedure given here:

1. First, make a backup copy of the file *mn_dataexport_language.xml* from the language folder in the installation directory of this software.
2. Start the program LANGUAGE_TOOL from the *language* folder in the installation directory of this software.
3. Click on *Language File / Open Language File*
4. In the file selection window, select the file *mn_dataexport_language.xml*
5. Click on *Modify Language File / New Language*
6. Enter the name of the language without special characters (i.e. "Francais" and not "Français")
7. Translate all texts and complete the new language column.
8. Click on *Language File / Save Language File*

The new language is now available in the **NANOCOLOR®** data export software.

11.2. Selection of Units

At various locations in this software, physical units can be selected from list boxes. The lists contain numerous units commonly used in photometry. However, if you require a particular unit that is not included in the list, there are two possibilities available: a) simply click in the text box of the list and enter the unit required from the keyboard or, b) open the Windows® Editor and enter the unit in the form

Unit 1 [ENTER] Unit 2 [ENTER] Unit 3

in the Editor and save the text under the file name *units.ini* in the *ini* subdirectory of your **NANOCOLOR®** data export software. The next time the software is started; the units are read from the *units.ini* file and added to the units list upon start-up.

11.3. Outlier elimination and multiple measurements

During a calibration outliers may appear by measurement errors or weighing/dilution errors of the calibration solutions. This chapter shows you how to handle outliers and gives you measures to improve the accuracy of your calibration.

11.3.1. Outlier

In mathematical statistics, several tests exist to determine, with a given probability, if a measured value is an outlier or not. One of these tests, the Grubbs outlier test, is integrated in the NANOCOLOR® data export software. The software detects automatically if a measured value should be declared as an outlier or if its deviation is within the confidence interval.

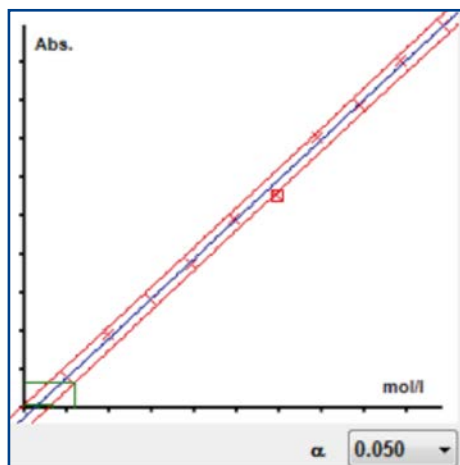


Fig. 37: Calibration curve with outlier

The software draws a red square around all detected outliers. In the figure above, the value no. 6 is obviously not correct. The result is a quite wide confidence interval.

No.	Abs.	Conc.	Y/N
1	0,057	10	<input checked="" type="checkbox"/>
2	0,135	20	<input checked="" type="checkbox"/>
3	0,202	30	<input checked="" type="checkbox"/>
4	0,265	40	<input checked="" type="checkbox"/>
5	0,347	50	<input checked="" type="checkbox"/>
6	0,392	60	<input checked="" type="checkbox"/>
7	0,499	70	<input checked="" type="checkbox"/>
8	0,557	80	<input checked="" type="checkbox"/>
9	0,641	90	<input checked="" type="checkbox"/>
10	0,705	100	<input checked="" type="checkbox"/>

Fig. 38: Calibration data with outlier at position 6

There are now two possibilities to handle the outlier: The first and simplest way is to deactivate the option button in the column Y/N.

No.	Abs.	Conc.	Y/N
1	0,057	10	<input checked="" type="checkbox"/>
2	0,135	20	<input checked="" type="checkbox"/>
3	0,202	30	<input checked="" type="checkbox"/>
4	0,265	40	<input checked="" type="checkbox"/>
5	0,347	50	<input checked="" type="checkbox"/>
6	0,392	60	<input type="checkbox"/>
7	0,499	70	<input checked="" type="checkbox"/>
8	0,557	80	<input checked="" type="checkbox"/>
9	0,641	90	<input checked="" type="checkbox"/>
10	0,705	100	<input checked="" type="checkbox"/>

Fig. 39: Disabling the outlier

The calibration curve is created new automatically.

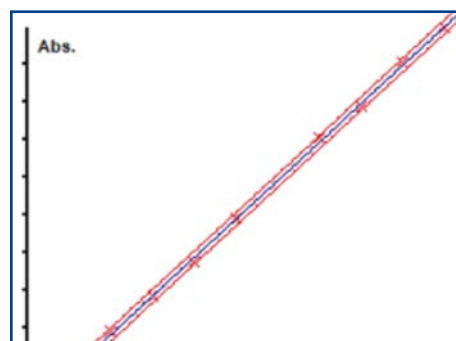


Fig. 40: Calibration curve without outlier

The confidence interval is now significantly narrower. In this way, you can either exclude or include any given measured value. The second possibility for outlier correction is to prepare the incorrect solution again and re-measure it. To do this double-click with the left mouse button on the data field with the incorrect value which in the example is field "0.454". The software will then prompt you to insert the new solution into the photometer.



Fig. 41: Re-measuring a sample

The new measured value is immediately incorporated into the spreadsheet. When the cuvette is removed, the graphic will also be updated.

4	0,319	40	<input checked="" type="checkbox"/>
5	0,418	50	<input checked="" type="checkbox"/>
6	0,475	60	<input checked="" type="checkbox"/>

Fig. 42: Displaying the new measured value

11.3.2. Multiple measurements

The example above shows a calibration series with 10 test solutions of different concentrations. There is a statistical trick how to improve the accuracy of your measurement and reduce your workload at the same time. The method is called multiple measurement. Instead of preparing 10 different solutions with concentrations ranging from 10 to 100, you prepare only 4 different solutions with concentrations let's say for example 20, 40, 60 and 80. However, the solutions with concentrations of 20 and 80 are used to carry out 3 to 4 single experiments, and the other ones with concentrations of 40 and 60 are used to carry out say 2 single experiments.

No.	Abs.	Conc.	Y/N
1		20	<input checked="" type="checkbox"/>
2		20	<input checked="" type="checkbox"/>
3		20	<input checked="" type="checkbox"/>
4		40	<input checked="" type="checkbox"/>
5		40	<input checked="" type="checkbox"/>
6		60	<input checked="" type="checkbox"/>
7		60	<input checked="" type="checkbox"/>
8		80	<input checked="" type="checkbox"/>
9		80	<input checked="" type="checkbox"/>
10		80	<input checked="" type="checkbox"/>

Fig. 43: Creating multiple measurements

If you are carrying out three experiments each with the solutions that have a concentration of 20 and 80, and two experiments each for the solutions that have a concentration of 40 and 60, then altogether this amounts to 10 photometric measurements. In the spreadsheet in figure 126, you can see that the solutions 1 to 3 all have the required concentration "20", then twice "40", twice "60" and again three times "80".

	No.	Abs.	Conc.	Y/N
	1	0,134	20	✓
	2	0,132	20	✓
	3	0,133	20	✓
	4	0,265	40	✓
	5	0,263	40	✓
	6	0,392	60	✓
	7	0,399	60	✓
	8	0,558	80	✓
	9	0,562	80	✓
	10	0,561	80	✓

Fig. 44: Measurement data of multiple measurements

As you have performed different experiments with those individual solutions, you will not get the exact same results. However, using the principle of multiple measurement increases the statistical accuracy.

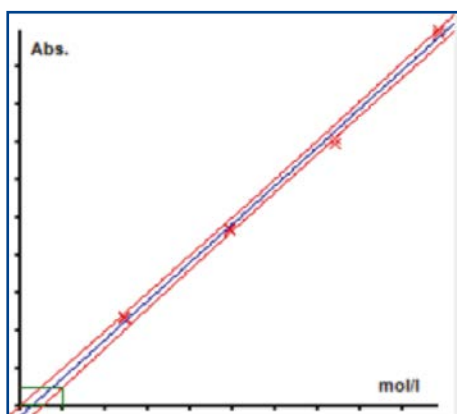


Fig. 45: Narrow confidence interval using multiple measurements

What does “different experiments mean? It does not mean measuring one cuvette three times! You have to prepare three tests with three different cuvettes, but for this you only need one test solution. This method covers all cuvette errors, measuring errors, and test errors, but reduces the influence of weighing/dilution errors and reduces your workload.

This method only works with linear calibrations! Always enter concentrations in increasing order as shown in the example!

11.3.3. Level of significance α

For the calculation of the Grubbs outlier test and the confidence intervals as well as the detection limit, decision limit and determination limit, it is necessary to provide the accuracy with which the results are to be calculated. This probability or level of significance α can be selected from the list box below the graphics area. For the Grubbs test, the levels $\alpha = 0.1$, $\alpha = 0.05$ and $\alpha = 0.01$ can be used. For the confidence intervals and the detection limit, decision limit and determination limit, the α values 0.005 and 0.001 are also possible. If you select these small values, the Grubbs test is calculated with $\alpha = 0.05$.

A value of $\alpha = 0.05$ means that the probability of the value that was identified as an outlier actually being an outlier is 95 %. Or to put it another way: There is a probability of 5 % that the value may not be an outlier after all.

11.4. Software Errors

Despite all checks and test runs, errors in software cannot be completely ruled out. Please help to improve our software products by reporting to us any errors or faults that may have occurred.

Send a short e-mail to: info@mn-net.com, Ref.: “Data export software errors” with a brief description of the fault (what happened or did not happen after clicking on a particular button or menu item) and include an attachment with the following three files:

1. *error.log* from the folder *errorlog*
2. *sys.log* from the folder *syslog*
3. *environment.log* from the folder *syslog*

Both folders can be found in the installation directory of your **NANOCOLOR®** data export software.

If possible, use the software function “Allow error report” to send an error report to MACHEREY-NAGEL (see 4.1.2. Language selection and other settings, page 7).

11.5. Data set structure

The following table describes the data structure of **NANOCOLOR®** photometers (250 D, 300 D, 350 D, 400 D, 500 D, PF-12 and LINUS):

Column description	Meaning	Example
Method number	NANOCOLOR® method number	061
Method name	NANOCOLOR® method name	Ammonium 200
Sample location	Number you can enter using the photometer	03
	The 500 D has the option to enter up to 12 characters for a sample location	Outflow 2
Date	From the photometer	21.10.2001
Time	From the photometer	14:23:15
Measurement counter	Number indicating the amount of measurements for a specific method	2
Result	Measured value	35
Remark	Is used if result is outside the measuring range	< 30
Unit	Unit used for the method	mg/L NH ₄ -N

Tab. 2: Data structure of **NANOCOLOR®** photometers

Data from the BioFix® *Lumi-10* are exported in the following way:

Column description	Meaning	Example
Date	Datum aus <i>Lumi-10</i>	10.12.2001
Time	Zeit aus <i>Lumi-10</i>	10:24:31
Protocol name	verwendetes Messprotokoll	RLU
Limit 1	Result evaluation	50000
Limit 2	Result evaluation	20000
Measurement time (RLU) place (BioTox)	Differs according to measurement protocol	10 min
Place (RLU) series (BioTox)	Differs according to measurement protocol	3
Number	Ongoing number	15
Result	Measured value	15000
Measured variable	Protocol unit	RLU
Remark	Is used if result is outside the measuring range	< 10

Tab. 3: Data structure of BioFix® *Lumi-10*

Apart from numeric measurement data, all data / columns are exported as text files.

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12.7. Contact

Should you have any questions concerning this Agreement, or if you desire to contact MACHEREY-NAGEL, please use the following address:

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