analytikjena
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Operating manual

ASpect UV
Software for
UV/Vis Spectrometer

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To ensure correct and safe use, follow these instructions. Keep these instructions for later reference.

General information http://www.analytik-jena.com

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1 About this document

What is ASpect UV

The ASpect UV program is used to control and analyze measurement data from devices that are part of Analytik Jena's SPECORD PLUS series.

Program versions

The description in this manual is based on the following program versions:

- ASpect UV from version 2.0
- SPECORD PLUS firmware from version 4.4.2

The program version is displayed if you select **Info** | **About ASpect UV** from the menu in the main window.

Target group

This manual is aimed at qualified specialist personnel with knowledge of UV/Vis analysis. Basic knowledge of working with a computer and programs, such as choosing an option by clicking with the mouse or saving and opening files, is assumed.

For safe operation of the SPECORD PLUS with ASpect UV, knowledge of the operating instructions "SPECORD PLUS UV/Vis - Spectral Photometer" and "SPECORD PLUS UV/Vis Spectral Photometer Accessories" is required.

Typographical conventions

Instructions for action are numbered or grouped into blocks of instructions, shown as bullet points.

The elements of the ASpect UV program are indicated as follows:

- All elements, such as menu items, window names, buttons etc. are indicated in **bold**, e.g. **Options**.
- Menu items in a sequence of commands are joined together by a vertical line, e.g. **File** | **Save**.
- Some windows contain tabs. When labeling a specific tab, the window name and tab are joined together by a vertical line in the same way as menu items, e.g. **Options** | **General**.

The following pictograms and signal words are used:

NOTE

This is a note to be followed to avoid operating errors and obtain correct results.

Tip

The notes identified in this manner provide you with useful information concerning the program control.

2 Install ASpect UV

NOTE

The installation of ASpect UV requires administrator rights for the computer.

For the correct installation of the USB driver and to update the firmware the following sequence must be adhered to:

1. First install the ASpect UV program on the computer.
2. Only then connect the SPECORD PLUS to the computer and switch on the SPECORD PLUS.

When the SPECORD PLUS is connected for the first time, a device recognition procedure is performed and the drivers are allocated after the device is switched on.

Install ASpect UV

- Switch on computer.
- Insert the ASpect UV installation CD into the CD-ROM drive.
  On most computers, the installation will start automatically after a brief delay. If this does not happen, start the file setup.exe in the top directory of the CD.
- Click on **Install** and follow the instructions of the installation program:
- Select the language of installation.
- Select the target folder for the installation.
  ✓ The installation completes automatically.
- Connect the SPECORD PLUS to the computer vis the USB connections.
- Switch on the SPECORD PLUS.
  ✓ The required USB drivers will be installed automatically.

Install optional modules

The optionally available modules are also supplied on CDs.

- Insert the installation CD into the drive.
  If the installation does not start automatically, start the file setup.exe on the CD.
- Install the programs in the same folder as ASpect UV.
  ✓ The optional modules are integrated into the program when ASpect UV starts.

3 Starting and exiting ASpect UV

With the default settings of Aspect UV installed the main window is displayed after starting the program and the connection to the SPECORD PLUS and connected accessories is established. However, you may also configure the program in such a way that an application module opens straight away or the quick start menu is shown with a collection of selected methods.

3.1 Starting ASpect UV

By default the connection between the computer and SPECORD PLUS is established during the start of ASpect UV. The connection sequence must be observed:

- Install the accessories for the measurement in the sample chamber and switch on the SPECORD PLUS via the mains switch on the right side of the housing.
- Start ASpect UV by clicking on the desktop icon, or select **ASpect UV** | **ASpect UV** in the windows Start menu.
- Only if using module FDA 21 CFR Part 11 Compliance:
  Enter your **Login** (user name) and **Password** in the login window.
  - ✓ ASpect UV starts and connects to the SPECORD PLUS. The monochromator of the SPECORD PLUS moves and the message **Initialization** is displayed on the monitor. The SPECORD PLUS is now ready to measure.

If the connection to SPECORD PLUS could not be established, ASpect UV is started in simulation mode. Review the settings in the window **Options** | **Start** | **Start ASpect UV**. The **Initialize instrument** checkbox must be activated there. If necessary, connect by selecting the menu item **Instrument** | **Initialization**.

3.2 Configuring the start of ASpect UV with module or Quickstart

By default ASpect UV starts with the main window as start screen. However, the program start can also be configured for a favorite module or the quick start menu to be displayed.

- Select the menu item **Settings** | **Options**.
- Select the desired module or the **Quickstart** from the **Open element** list in the **Options** | **Start** | **Start ASpect UV** window. If the option **None** is selected, ASpect UV starts with the main window.
- When selecting **Quickstart**, configure the Quick Start menu.
  - ✓ During the next start of ASpect UV the selected element is displayed as start screen.

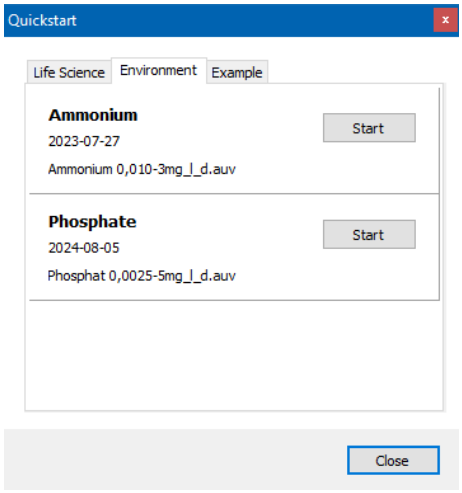
See also

Configuring quick start [▶ 138]

3.3 Using Quickstart

You can collect and start frequently used methods in the Quick Start. You can define the content of Quick Start in the **Options** | **Quickstart** window.

- Select the menu item **Modules** | **Quickstart**.
  - ✓ The **Quickstart** window appears. The methods are grouped into tabs.
- Select a method and click on **Start**.
  - ✓ The measurement module opens with the default method. You can use the sample sequence saved there immediately for the measurement, or edit the sample sequence beforehand.



See also

Configuring quick start [138]

3.4 Exiting ASpect UV

With the software-assisted shut-down routine, the monochromator of the spectrometer is locked into the original position. In this position the transport lock of the monochromator can be attached (see "SPECORD PLUS UV/Vis Spectral Photometer" operation instructions).

- Close all document windows.
- Select the menu item **File** | **Close**.
- The systems displays the message "Shut down routine is running.".
- After exiting the ASpect UV program, switch off the SPECORD PLUS via the mains switch.
  - ✓ The SPECORD PLUS is shut down.

When the measurements with the SPECORD PLUS have been completed, and you are only analyzing data in ASpect UV, first switch to simulation mode. The USB connection to the device is thus closed and you can switch off SPECORD PLUS at the power switch. The ASpect UV program can be ended later.

4 Basic structure and functions of ASpect UV

This section includes information about the program structure and cross-module program functions of ASpect UV.

4.1 ASpect UV program structure

4.1.1 Modules in ASpect UV

The ASpect UV program is of modular design. Each application area of the UV/Vis spectroscopy has a module assigned to it, in which the measuring parameters to be configured are adapted to the application and the connected accessories. This permits a quick orientation when selecting the required analysis parameters and simplifies data analysis.

The following applications/modules are available:

Photometry

Measurements at selected wavelengths are carried out in the **Photometry** module. Quantitative analyses at selected wavelengths for routine analysis, as well as all analyses integrating the measured values at selected wavelength into a formula, e.g. biochemical analyses, can be implemented.

Spectrum

The **Spectrum** module permits the measuring of spectra or spectral ranges. Based on this mathematic data processing of the spectra or a peak search can be performed. Sophisticated quantitative determinations based on the spectral analysis are also possible (automatic peak search, peak areas, analysis of spectral derivations, etc.).

Kinetics

The **Kinetics** module permits the recording of time-dependent reactions, i.e. registration of the change of transmittance or absorbance at a wavelength. The graph and measured values for the selected points in time are analyzed.

Quick measurement

The **Quick measurement** module can be used to determine the absorbance at a wavelength. Further processing, saving or printing of the values is not possible.

Thermometry

The **Thermometry** module is used to evaluate temperature-dependent absorbance or transmittance changes. The temperature curves can, for example, be used to determine the DNA melting point. The temperature curves are recorded by means of Peltier-tempered accessories.

Colormetric

The **Colormetric** module determines the color coordinates of reflecting surfaces or optically transparent samples. Moreover, different color numbers can be determined.

Optional modules

Optionally the following modules are available:

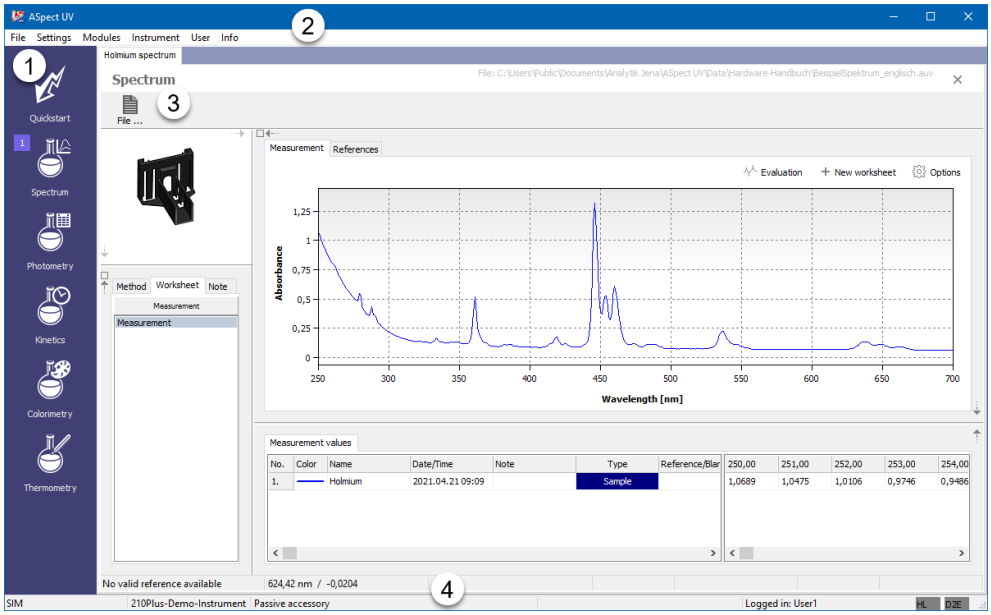
- ASpect UV Validation AJ
- ASpect UV Validation Standard Ph. Eur.
- ASpect UV Validation USP
- ASpect UV Maintenance economic
- AJ File Protection
- SOAP Web Server
- FDA 21 CFR Part 11 Compliance with user administration and data signing

4.1.2 The main window of ASpect UV

The main window opens after starting ASpect UV. It provides the following functions:

- Open the modules with the related measuring and analysis functions
- Configuration of module-independent basic functions for measurement and analysis (options)
- Functions for testing the SPECORD PLUS
- Access to user administration if the module FDA 21 CFR Part 11 Compliance has been installed

Components in the main window



No.	Description
1	The **task bar** contains the module icons and icons of basic program functions.
2	In the **menu bar** the general functions of ASpect UV have been arranged in menus.
3	The documents are arranged in the **workspace**.
4	The **status bar** contains information about the device and the logged-in user.

Menu bar

The menu bar of the main window includes the following functions:

Menu	Subitem	Description
File	**Open method**	Open a saved method for a subsequent measurement
	Open results	Open saved file with results in its module environment
	Close	Exiting ASpect UV
Settings	**Hide menu**	Hide menu bar
	Hide launchbar / Display launch bar	Show/hide task bar
	Options	Make basic configurations for ASpect UV
Modules	**Quick measurement**	Start absorbance measurements at a selected wavelength
	Spectrum	Open a new document in the **Spectrum** module / Switch to the module
	Photometry	Open a new document in the **Photometry** module / Switch to the module

Menu	Subitem	Description
	Kinetics	Open a new document in the **Kinetics** module / Switch to the module
	Colormetric	Open a new document in the **Colormetric** module / Switch to the module
	Thermometry	Open a new document in the **Thermometry** module / Switch to the module
	Quickstart	Open the quick start menu
Instrument	**Info**	After initialization, display information about the device, ASpect UV, firmware, and connected accessories
	Initialization	Establish the connection between SPECORD PLUS and ASpect UV
	Simulation	Put ASpect UV in simulation mode
	Test	Test the functionality of the SPECORD PLUS Validate SPECORD PLUS (optional modules)
	Correction	Start software-supported device corrections
	Zeroth order	Set the monochromator mesh to the zero order for adjusting accessories and testing the beam paths
	Accessory	Switch accessories off and on, start pump time optimization of the sipper system, query temperatures of Peltier accessories
User	**Log off**	Log off the user and lock ASpect UV
	Lock ASpect UV	Lock ASpect UV
	Change password	Change password of logged-on user
	User management	Opening the user management
Info	**Help**	Open help for ASpect UV
	About ASpect UV	Information about the program version

Task bar

The task bar on the left side of the main window includes icons providing quick access to the most frequently used program functions. The task bar can be configured in the **Options** window. The following functions can be arranged:

Icon	Description
	Open **Photometry** module / Add new document
	Open **Spectrum** module / Add new document
	Open **Kinetics** module / Add new document
	Open **Thermometry** module / Add new document
	Open **Colormetric** module / Add new document
	Load saved method for next measurements
	Open saved measurement results and analyses

Icon	Description
	Initialize SPECORD PLUS
	Display quick start menu with method selection
	Open **Options** window
	Exiting ASpect UV
	Logging out a user

The current absorbance value at the current wavelength position of the monochromator can be displayed at the bottom of the task bar.

Status bar

The following information is displayed in the status bar:

- SIM: The software is in simulation mode.
- INIT: The device was initialized at the indicated time.
- Device type and serial number
- Connected accessories
- Module: Measurement is being performed in the indicated module.
- Logged in user
- HL/D2E: Lamp status

The lamp status is indicated via colored fields:

Status color	Description
Gray	The lamps are not switched on or the software is in simulation mode.
Green	The lamps are in operation.
Red	The lamps are defective.

Show and hide the menu and task bar

If required, the menu and start bar can be shown and hidden to enlarge the workspace of the main window.

- To hide the menu, select the menu item **Settings** | **Hide menu**.
- To show the menu again, click on the drop-down menu icon in the top left corner of the main window.

- The task bar can be hidden and shown using the menu items **Settings** | **Hide launch-bar** and **Display launch bar**.

Use help

Help on the operation of ASpect UV is available via the menu item **Info** | **Help**. In the ASpect UV windows, you can click on the **Help** button at the bottom left of the window or press the **F1** function key to obtain information relating to the window settings.

See also

Configuring the launch bar [▶ 138]

4.2 The document window

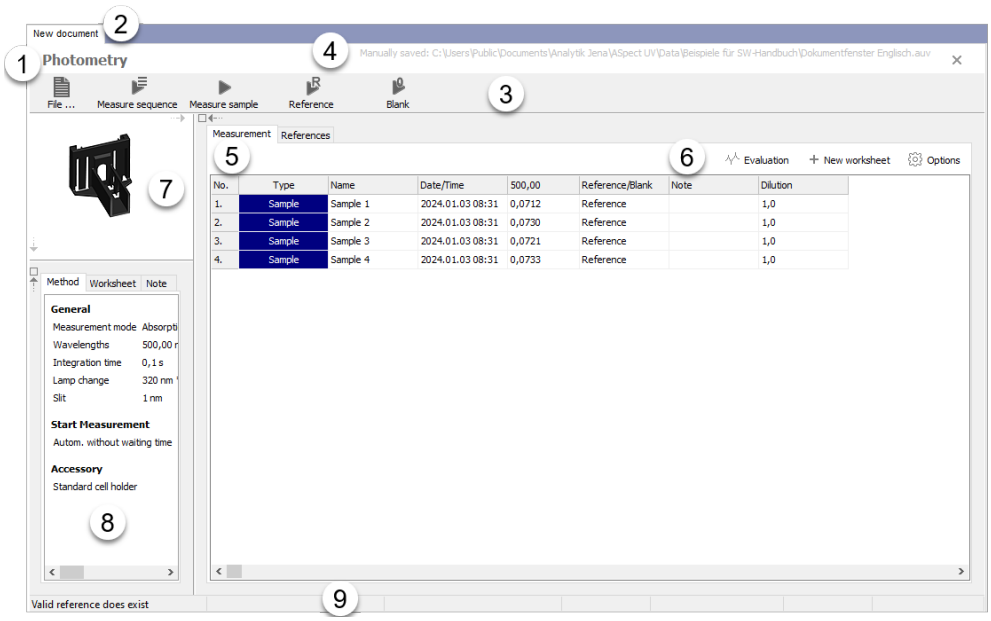
ASpect UV uses a single structure for all files, referred to below as documents, which includes all method configurations, sample information, measurement data, and analyses.

The document window in which a document is opened is of similar design in all modules. It includes functions for measurements, data administration and analysis. This section explains the general control elements and functions of the document windows. Functions that are only available in individual modules are described in the chapters relating to the corresponding modules.

Change between open documents

If several documents of the same module have been opened, these are arranged behind each other in the form of tabs in the workspace of the main window. Only the documents of one module are displayed simultaneously. If documents have been opened in different modules, it is necessary to change to the corresponding module by clicking on the module icon in the task bar or selecting the menu item in the **Modules** menu in order to display them.

4.2.1 Overview of the document window



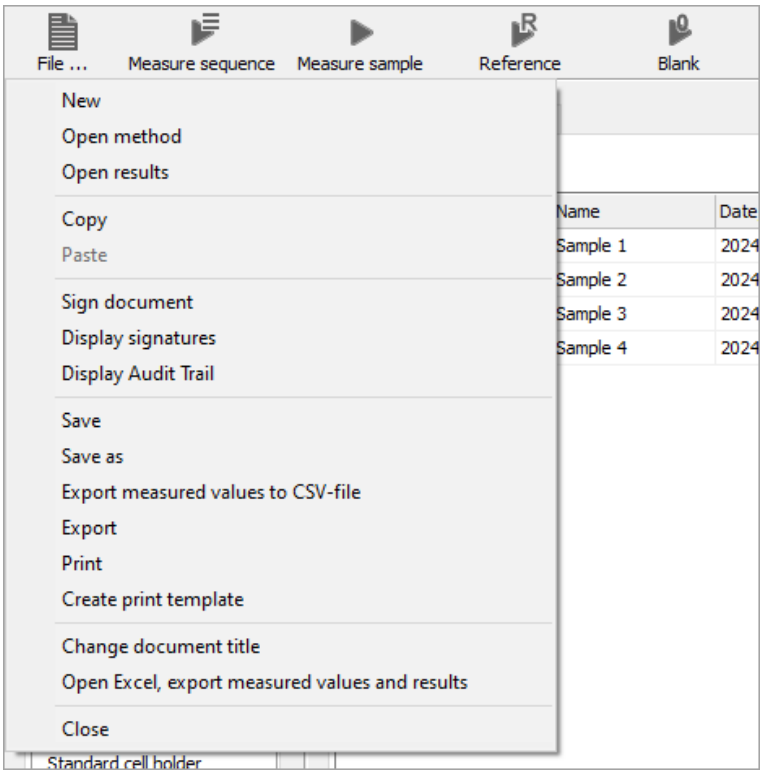
No.	Description
1	The module name indicates which module is open.
2	The document title is used to differentiate the opened documents. It is defined during the method configuration and may be later edited. If several documents in a module are opened, it is possible to change to the corresponding document by clicking on the document title.
3	The menu bar and toolbar provide functions for measurements and file administration in the document.
4	The complete file name of the document is displayed after saving.
5	The worksheet includes measured values, analyses, data processing and audit trail. Several work sheets with different analyses can be created in a document.
6	The function menu of the worksheet includes the menus for analysis and the view of the worksheet.
7	Display of the accessories used in the method. A method is always tailored to an accessory and can only be used with this accessory.
8	The tabs display the method parameters of the method stored in the document, the note on the measurement and the data processing carried out in the worksheet.
9	Information on the reference and the measurement (current measured values and measurement time) is displayed in the status bar of the document window. A progress bar is displayed during the measurement.

See also

Worksheets in the document [▶ 17]

4.2.2 Toolbar and File menu in the document window

Each document has its own toolbar and **File** menu.



Toolbar

The toolbar of the document window contains functions for file management and measurement. The display of the bar is automatically adjusted dependent on the current analysis status and the accessories used.

Icon	Description
	File menu with function for data administration in the module window
	Open the method window and configure the method
	Start the individual sample measurement independent of the sequence configured
	Measure the sequence specified in the method The sequence may temporarily change if the function is called up repeatedly.
	Start reference measurement independent of the settings in the sequence
	Start blank measurement independently of the settings in the sequence
	Stop sequence The ongoing sample measurement is completed and the sample sequence still pending is shown. The sample sequence may be re-edited.
	Only for kinetic measurements: Pause Interrupt the current measurement and continue at a later time
	Stop Stop the current measurement without continuing later
	Available for cartridge sipper system and APG sampler: Switch pump on or off and convey sample or stop conveying

Icon	Description
	Available for APG sampler: Lower or raise sample cannula
	Available for APG sampler with stirring function: Switch stirrer on or off
	Available for Peltier-tempered accessories: Configure starting temperature in accessories

File menu

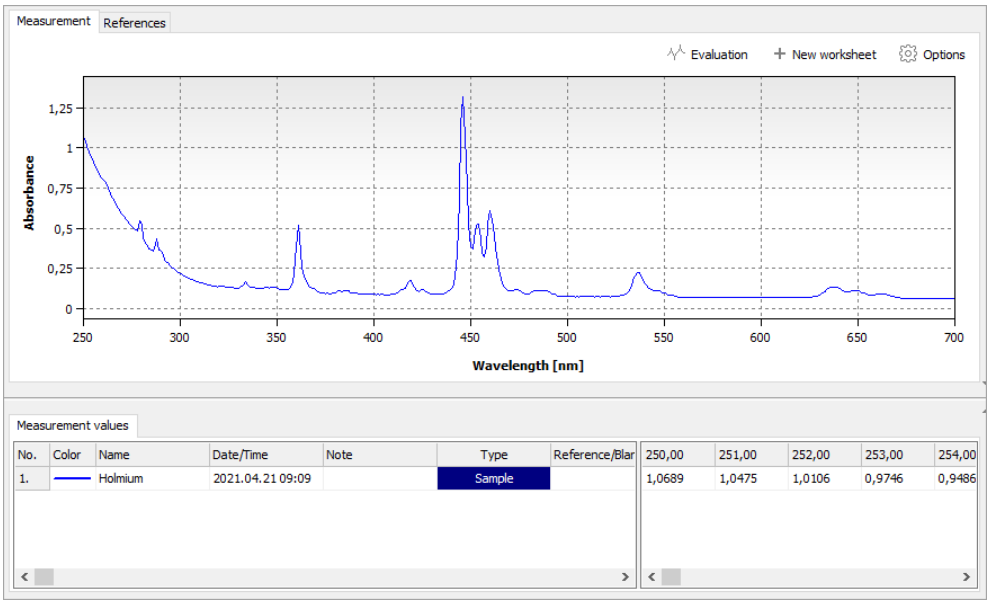
The functions in the **File** menu of the document window are always applied to the current document. Some functions may overwrite already existing data. In this case, there will be a security prompt before overwriting the data. The following functions are available in the **File** menu of the document window:

File	Description
New	Empty the current document and prepare for a new analysis
Open method	Open a method from a saved document The method can be modified for subsequent measurements.
Open results	Open measured values, method and analyses Additional data can be added to the document through measurements with an unchanged method.
Copy / **Paste**	Available in the **Spectrum** and **Colormetric** modules: Copy measured results and insert into a different document
Sign document	Add an electronic signature to the document
Display signatures / **Hide signatures**	Display signatures of a document / Close display
Display Audit Trail / **Hide Audit Trail**	Show or hide audit trail
Save	Save measured values, method and analyses in a file
Save as	Save measured values, method and analyses in a new file
Export measured values to CSV-file	Export measured values of the document to CSV format
Export	Export measured values and analyses via the report functions
Print	Print measured values, method and analyses with selected report template
Create print template	Create your own print templates
Edit document title	Change the document title on the document tab
Open Excel, export measured values and results	Export measured values and results to an Excel file and open this file in Excel Note: This function requires that Excel is installed.
Close	Close the document

4.2.3 Worksheets in the document

Measured values and references are displayed on the worksheets in the document.

The **Measurement** worksheet contains the measured values of the samples and standards, which you can analyze using the functions of the respective analysis module. These functions are also available in the module's method. The measured references can be found on the **References** worksheet. The **Measurement** and **References** worksheets cannot be deleted, which means the original measurement data is always retained.



Function bar in worksheet

The worksheet has its own function bar on the top right side:

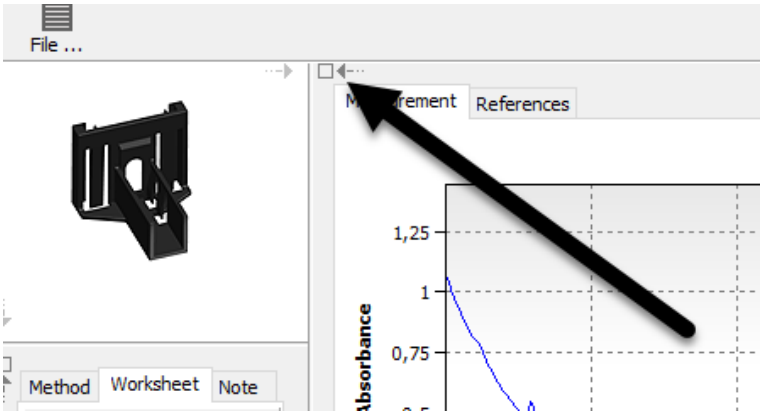
Function	Description
Evaluation	Menu with module-specific analyses
New worksheet	Only available on the **Measurement** and **References** worksheets: Copy measured values to a new worksheet
Options	Scale graph view, create text boxes, rename worksheet
	Delete worksheet

Divide the worksheet

The worksheet is divided into a lower and an upper area for the output of spectra, measurement data, and analyses. The output depends on the analyses in the module. You can move the area boundaries with the mouse.

- Move the mouse pointer on to a boundary line and once the double arrow appears, move the boundary line with the left mouse button held down.
- Move the boundaries into predefined areas by clicking on the separating line arrows at the ends of the separating lines.

Example of separating line arrows to adjust the window areas



Note: You will also find the separating line arrows in the method window on the **Sample sequence** screen between the graphical input and the sample table.

Add new worksheet

You can copy the measurement data into a new worksheet in order to carry out various analyses side by side in one document.

- In the **Measurement** worksheet, click on + **New worksheet**.
- You can copy the **References** worksheet in the same way.
  - ✓ In the document, an additional worksheet with the title **New worksheet** and a copy of the data from the **Measurement** worksheet appears.

Tip

Only the measurement data activated on the **Measurement** worksheet will be copied. Deactivate the measurement data which does not need to be processed further by right-clicking on the sample and selecting the **Hide** function in the context menu.

Rename a worksheet

For a better overview, you can give the new worksheets a new title. You cannot rename the **Measurement** and **References** worksheets.

- On the worksheet, select the menu item **Options** | **Rename worksheet**.
- Edit the name in the input field.
  - ✓ The current worksheet is renamed.

4.2.4 Show spectra and measurement curves on the worksheet

Spectra or measurement curves are displayed in the following modules:
- Spectrum
- Kinetics
- Thermometry
- Color measurement

Spectra or other measured curves are represented in the same way in all modules. The following functions can be applied to the representation of the curves:
- Scaling curves
- Adding text to curves (text box)
- Marking curves/samples
- Changing the color of curves
- Hiding a curve (deactivating a sample)

Scale curves

In the graphical representation of the curves, you can change the display ratio and enlarge the display. You define the curve section interactively with the mouse or in a dialog box.

Draw a frame around the area with the mouse

- With the mouse button held down draw a rectangle across the area to be enlarged.
  - ✓ When releasing the mouse button the display is updated for the selected area.
- Double-clicking on the curve restores the original display.

Run via dialog window

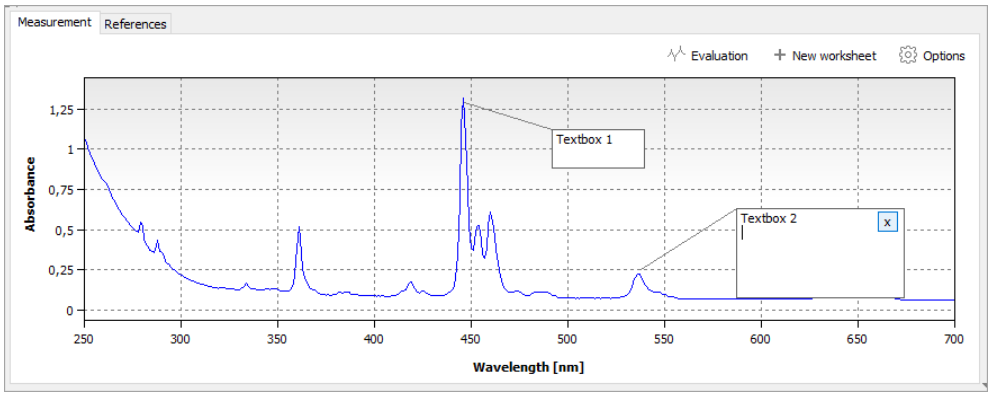
- On the worksheet, select the menu item **Options** | **Scaling**.
- Select the **User defined** option from the **Scaling** list.
- Enter the new limits in the **X-Axis** and **Y-Axis** input fields.
  If the **Fixed** option has been activated, the diagram can no longer be changed with the mouse.

✓ The curve display is updated.

Note: Selecting the option **Automatic** in the **Scaling** list will restore the original view.

Create text box

A text box is a text field that can be positioned freely on the diagram and be modified in size. A reference line from the text box can refer to a specific location in the diagram. This allows you to add notes on details of the measurement curve to the diagram. Text boxes are saved and printed with the data.



- On the worksheet, select the menu item **Options | Create textbox**.
  The cursor changes to a crosshair with the label "T".
- Click on the position in the curve where the reference line should start and move the cursor with the mouse button held down to the position where the text box should be placed.
- Click in the text box and edit the text.

  ✓ The text box is now anchored to the graph and is saved and printed with the data.

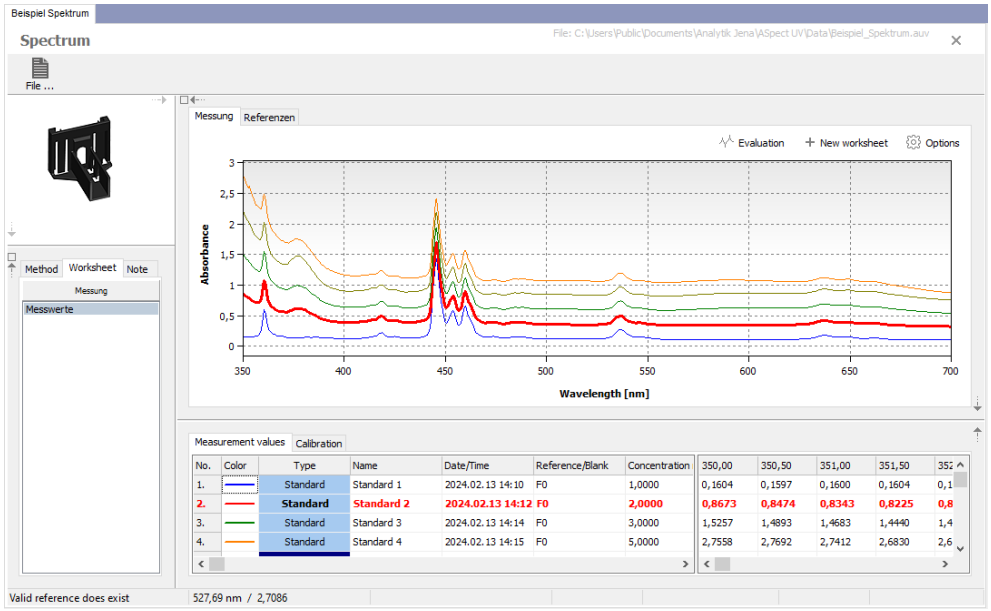
Additional text box functions

- The size of the text box can be adjusted later. To this end, move the cursor on to one of the frame lines and move the frame line with the mouse button held down to the desired position.
- To move a text box, move the mouse pointer to the top of the text box until it changes to a directional cross and then, holding the mouse button down, drag the text box to the new position.
- To delete the text box move the cursor on to the upper right corner in the text box.

  When the ✕ icon appears, click on it.

Highlight samples

For a better overview in a group of graphs, graphs can be highlighted using a bold line.



- Right click on a sample in the **Measurement values** sample table.
- Select **Highlight multiple samples** in the context menu. In the selection window, only enable the checkboxes whose samples are to be highlighted in the graphic and the sample table. To undo the highlighting, clear the corresponding checkboxes.
- Alternatively, individual samples can also be highlighted or their highlighting removed directly. To do this, select the option **Highlight in chart** or **Remove highlight in chart**.
  - ✓ The selected sample curves are highlighted in bold in the graph and marked in bold in the sample table.

Changing the color of curves

The curves are automatically assigned a color. You can change the colors of individual sample curves for a better overview.

- In the **Measurement values** sample table, click on the **Color** table cell of the sample.
- In the **Color** dialog, select a new color by clicking with the mouse.
  - ✓ The display of the curve is updated with the new color.

Hide curve / (de)activate samples

Samples can be disabled and hidden from the display. At the same time the sample is excluded from analyses if disabled but not completely deleted from the record.

- Right click on a sample in the **Measurement values** sample table.
- In the context menu, select **Show/Hide multiple samples** . In the selection window, only enable the checkboxes whose samples are to be shown and analyzed.
- Alternatively, an individual sample can also be enabled or disabled. To do this, select the option **Hide** or **Show**.
  - ✓ The sample spectra that are not activated are hidden from the graph and highlighted in light gray font in the sample table.

4.3 Managing, printing and exporting documents

Documents in ASpect UV have a uniform data structure and include the following information:

- Measured values of samples, standards, references and blanks
- Method parameters
- Analyses of the measured values/calibration graphs

- Parameters for data processing
- Audit trail
- Signatures

The files are identified with the file extension "*.auv" in the Microsoft Windows file system.

4.3.1 Opening and saving documents

Documents can be opened both in the main window and in the modules. The easiest way to load measuring results or extract methods is by clicking on the corresponding icon in the task bar of the main window. If the icons are not yet displayed in the task bar, you can activate their display in the **Options** | **General** | **Launch bar** window.

Open results

Using the **Open results** function loads the entire document to the workspace of ASpect UV. You can view previous measuring results and analyses, add additional measured values or edit or amend the analysis. When loading the results, the accessory settings and the connected SPECORD PLUS with accessories are checked (switched on and initialized or simulated). Additional measurements may only be added to the document if the accessories currently connected in SPECORD PLUS are consistent with the accessory settings in the method. Further analysis of the measurement data is always possible.

Note: You can also open measuring results with the extension "*.dat", which have been created with WinASPECT or WinASPECT PLUS.

- In the task bar, click on the **Open results** icon or select the menu item **File** | **Open results** in the main window.

- In the **Load** default window, select the file types "*.auv" for ASpect UV files or "*.dat" for WinASPECT or WinASPECT PLUS files.
- Select the file and open it by clicking on **Load**.
  - ✓ The results are displayed in the respective module.

Alternatively, in the document window of a module you can select the menu item **File** | **Open results**. The following restrictions for loading into the document window of a module should be noted:

- Only results created with this module can be opened. Otherwise an error message is displayed.
- The data are opened in the current document. Previous content of the document is overwritten after a query. If the current document has already been saved, the saved file will not be changed.
- WinASPECT and WinASPECT PLUS files can only be opened in the main window.

Opening a method

Using the function **Open method**, the method is extracted from an existing document. The method contains the measurement parameters, parameters for analyses and the parameters of the measuring sequence. The method may be edited or use it to immediately start a measurement.

When opening the method, it is checked whether the initialized device (accessories and SPECORD PLUS type) are consistent with the settings in the method. If this is not the case, the method will not be loaded. Install the corresponding accessories or load a suitable method. If you are working in simulation mode, select the SPECORD PLUS type and the accessories from the settings in the **Options** window.

- In the task bar, click on the **Open method** icon or select the menu item **File** | **Open method** in the main window.

- Alternatively, in the document window you can select the menu item **File** | **Open method**. When loading the method, the same restrictions apply as those for loading results (see above).
- Select the file in the default window **Load** and open it by clicking on **Load**.
  - ✓ The method is loaded. You can start a measurement with the method or use it as a template and edit it.

Save document

Documents are saved in the document window using the standard functions **Save** and **Save as**. When saving the files, methods, original data and changes are saved in the document.

- If you want to save changes to an existing file, select the menu item **File** | **Save**.
- If you want to save changes in a file to another file, select the menu item **File** | **Save as**. In the standard window **Save as**, enter a file name and a file path and save the file by clicking on **Save**.
  - ✓ The document is saved.

4.3.2 Creating a new document

A new document is the starting point for creating a method with subsequent measurement. When starting a module, a new document appears without data. Alternatively, the current document in the module can also be overwritten by a new document.

- By clicking on a module icon in the task bar or selecting the module menu item, a new document is created in the module, e.g. **Module** | **Spectrum** or .
  - ✓ A new document with the title "New document" appears.
- Repeatedly clicking on the icon opens further new documents in the module. The number of documents opened in a module is displayed next to the icon in the task bar.
- If several modules are open at the same time, you must first click on the icon to bring the module back to the foreground before you can create further documents.
- Alternatively, you can select **File** | **New** in the current document. Data already existing in the current document window will be deleted after a query and the document updated.

4.3.3 Edit document title

The document title is displayed in the document tab. If several documents are open in a module, you can use the title to identify the document. When creating a document, it displays the title "New document". The title is first defined in the method settings on the **General** screen. You can change the document title after the first measurement has been started via a menu item in the document.

- In the document, select the menu item **File** | **Edit document title**.
- Edit the name in the **New title** field.
  - ✓ The document title is updated.

4.3.4 Tracking changes in the audit trail

All operations in a document are always recorded in an audit trail. The audit trail is therefore the logbook for the created method, the measurements carried out, and the data processing.

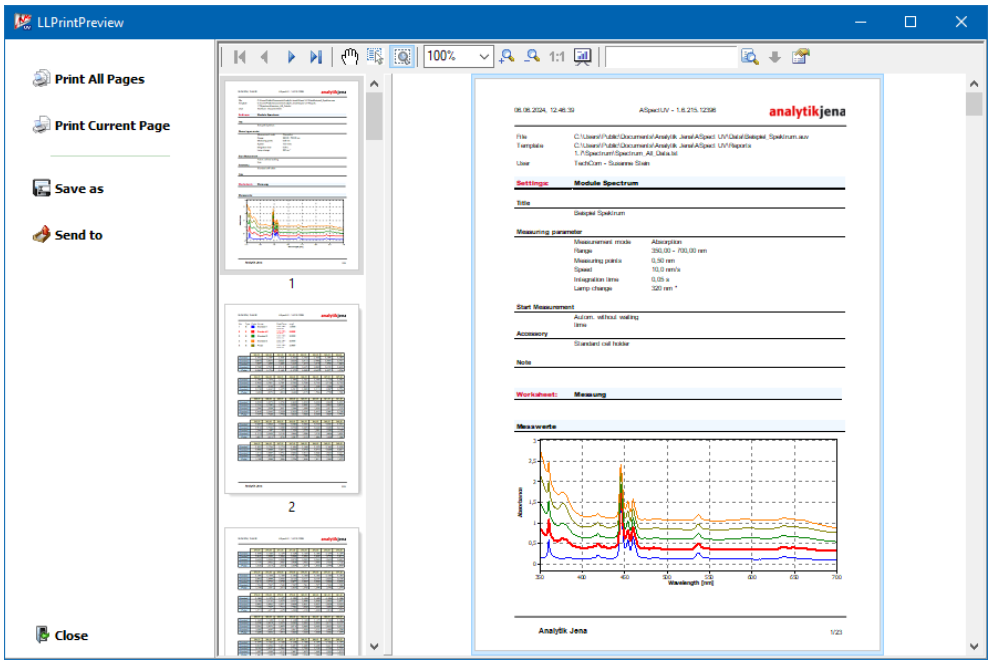
Display the audit trail

- To display the audit trail of the current document in the module, select the menu item **File | Display Audit Trail**.
  - ✓ The audit trail is shown in a spreadsheet in the lower half of the worksheet.
- To hide the audit trail, select the menu item **File | Hide Audit Trail**.

4.3.5 Print documents

You can print the contents of the documents or send them as an e-mail. The print function in the respective modules is controlled via the **LLPrint Preview** window, which contains the print preview, print functions, data export, and send by e-mail. To print, you must select the print content using a report template.

LLPrint Preview window with print preview and selection for printing



The following options are available for printing:

Option	Description
Print all pages	Print the entire report
Print displayed page	Only print the currently selected page
Save as	Export report in various formats
Send to	Send the report by e-mail using the e-mail program installed on the computer. The same formats as for export are available.

Print document / Send email

- In the document window, select the menu item **File | Print**.
- In the window **Load** in the folder *\\Users\Public\Documents\Analytik Jena\ASpect UV\Reports*, select the report template required for the current module.
- In the **LLPrint Preview** window, select one of the listed options.
- Only when printing the report: Configure printer if necessary.
  - ✓ The report is printed or the email is sent.

See also

Report templates for print and export [▶ 26]

4.3.6 Exporting the data

The ASpect UV files with the extension *.auv are encrypted and thus protected against tampering. However, to allow the use of the data in other programs, the data can be exported. For the output of data ASpect UV has a large number of output formats available. Along with being output to the printer, the data can be exported into PDF, HTML, CSV, Excel or Text format or can be saved as an image file. If there is an Excel program installed on your computer, you can use the menu command **Open Excel, export measured values and results** to export to a new Excel folder.

Export data using the report functions

The following export formats are available under the report functions:

- HTML
- PDF
- Rich Text Format (RTF)
- Text format (*.txt)

Tip

Export the measurement data to a TXT or CSV file if you want to open the data in a spreadsheet program.

The content of the exported file is controlled by the report templates. Different templates are available for each module.

- In the document window, select the menu item **File** | **Export**.
- In the **Load** window, select the template in the folder \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports.
- In the **Print Options** window, choose the desired export format from the **Direct to** list and click on **Start**.
- In the **Save as** window, enter the name for the export file.
  - ✓ The measurement data is exported in the selected format.

Tip

Exporting via Reports is also possible via the Print function. To do this, use the **Save as** function in the **LLPrint Preview** window.

Export measured values to CSV format

The measured values may be exported to a CSV file.

- In the document window, select the menu item **File** | **Export measured values to CSV-file**.
- In the standard **Save as** window, enter or select a file name and click **Save**.
  - ✓ The data is exported to a CSV file with the selected name.

Export measured values to Excel

If you have installed an Excel program on your computer, the measured values can be directly exported to the program without being saved.

- In the document window, select the menu item **File** | **Open Excel, export measured values and results**.
  - ✓ Excel opens and the data is exported to a new Excel folder.

See also

Report templates for print and export [▶ 26]

4.3.7 Report templates for print and export

Report templates with different content are used for printing and exporting measurement data and analysis results. The selection of a report template can thus determine the scope and content of the output. There are special report templates available for every module which are adapted to the measurement data and the possible analyses.

A set of report templates is installed as standard. If required these templates can be adapted individually with the report designer "Report/Print module List & Label" by programmers or experienced users. A description of the Report designer is included on the installation CD of ASpect UV.

After program installation, the templates are stored in the following folders:

- In the installation path C:\Program Files (x86)\ ASpect UV\Reports
- In the library path \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports 2.0

Spectrum module

\\Spectrum

Template	Content of the printout or export
Spectrum_All_Data.lst	All available data: method, spectra, calibration, results table, analyses
Spectrum_All_Data_wo_MeasureData.lst	(all data without measured data) Results table (incl. Variables and statistics, if activated) and the calibration curve (if available)
Spectrum_Audit Trail.lst	Audit trail of the document
Spectrum_Calibration.lst	Calibration curve and calibration parameters
Spectrum_Chart.lst	Spectra (with thick lines), results and calibration curve
Spectrum_Measure_Values.lst	Measured values of the document
Spectrum_Measure_Values_Transposed.lst	Transposed output of the document's measured values
Spectrum_Method.lst	Method of the document
Spectrum_Results.lst	Analyses of the measured values

Photometry module

\\Photometry

Template	Content of the printout or export
Photometry_All_Data.lst	All available data: Method, calibration, results table, analyses
Photometry_Audittrail.lst	Audit trail of the document
Photometry_Calibration.lst	Calibration curve and calibration parameters
Photometry_Evaluation.lst	Analyses of the measured values
Photometrie_Measure_Values.lst	Measured values of the document
Photometry_Measure_Values_Transposed.lst	Transposed output of the document's measured values
Photometry_Method.lst	Method of the document
Photometry_Results.lst	Results table (incl. Variables and statistics, if activated) and the calibration curve (if available)

Kinetics module

\\Kinetics

Template	Content of the printout or export
Kinetics_All_Data.lst	All available data: method, spectra, calibration, results table, analyses
Kinetics_Audit Trail.lst	Audit trail of the document
Kinetics_Calibration.lst	Calibration curve and calibration parameters
Kinetics_Charts.lst	Results table, kinetic curves (with thick lines) and calibration (if available)
Kinetics_Evaluation.lst	Analyses of the measured values
Kinetics_Measure_Values.lst	Measured values of the document
Kinetics_Measure_Values_Transposed.lst	Transposed output of the document's measured values
Kinetics_Method.lst	Method of the document
Kinetics_Results.lst	Results table (incl. Variables and statistics, if activated) and the calibration curve (if available)

Thermometry module

\\Thermometry

Template (de/en)	Content of the printout or export
Thermometry_All_Data.lst	All available data: method, temperature curves, results table, analyses

Colormetric module

\\Colometric

Template (de/en)	Content of the printout or export
Colormetric_All_Data.lst	All available data: method, spectra, results table, color coordinates/color numbers

Validation module AJ

\\Validation\AJ

Template (de/en)	Content of the printout or export
Compact_AJ.lst	Short log with overview of validation results
Detailed_AJ.lst	Detailed validation protocol with target values, measurement data or spectra, validation results and audit trail

Validation module Standard Ph. Eur.

\\Validation\Standard Ph Eur

Template (de/en)	Content of the printout or export
Compact_EUP.lst	Short log with overview of validation results
Detailed_EUP.lst	Detailed validation protocol with target values, measurement data or spectra, validation results and audit trail

Validation module Economic maintenance

\\Validation\Eco maintenance

Template (de/en)	Content of the printout or export
Compact_ECO.lst	Short log with overview of validation results
Detailed_ECO.lst	Detailed validation protocol with target values, measurement data or spectra, validation results and audit trail

Validation module USP

\\Validation\USP

Template (de/en)	Content of the printout or export
USP_All_Data.lst	Detailed validation protocol with target values, measurement data or spectra, validation results and audit trail

User management

\\User Management

Template	Content of the printout or export
UM_Audittrail.lst	Audit trail about the changes in the user profiles
UM_LoginList.lst	List of successful and failed user logins in ASpect UV
UM_UserList.lst	List of user profiles created and their status
UM_UserRights.lst	List of rights for a selected user profile

Service documentation

The report templates in the \\Service folder are used for service purposes.

4.3.8 Automatically archive measurement data

Data can be automatically archived. The following options are available for this:

- Automatic save
- Automatic print with selected report template
- Automatic export with selected report template
- Automatic export to a CSV file

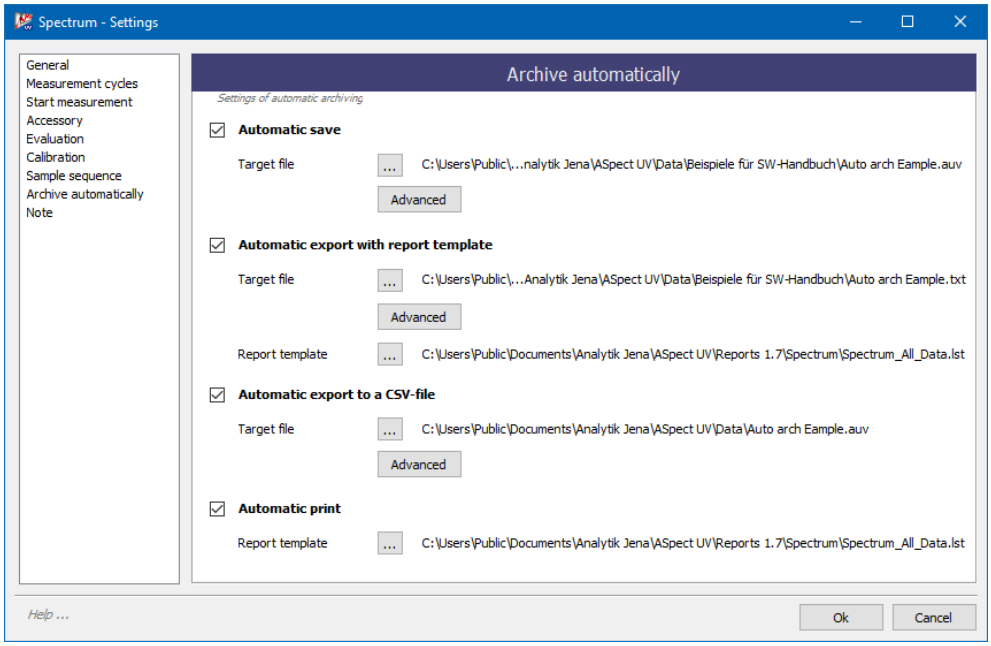
For automatic archiving, the target files and the report template must be specified **in the method**. The time and activation of this function is defined program-wide in the **Options** window.

Defining the target files and the report template in the method

- Switch to the **Archive automatically** screen in the method parameters.
- Activate the archiving function.
- For the automatic save or the automatic export, select the target file. Click on ... next to Target file and enter the path and the file name in the **Save as** window.
- Optionally, open a window with options for the target file name with **Advanced** and define the following:
  - **Addition in the file name**: Add a character string in front of the selected name (prefix) or after the name (suffix).
    This function can be used together with the **Allow user change before saving** option to add a serial ID in front of or behind the defined sample name, for example.
  - **Time stamp**: Add the measurement start time to the name.
    The start time is output in the format yyyy-mm-dd_hh_mm-ss,sss, e.g. "auto-save-photometry 2020-10-22_13-59 50,022.auv". The timestamp can also be added in front of or behind the file name.
    This option is activated by default.
  - **Allow user change before saving**: When activated, a window appears with an entry field to change the file name at the time of archiving. The file path cannot be changed.
- Select the report template for the automatic print or the automatic export. Click on ... next to Report template and select the report template in the **Load** window.

Note: Automatic archiving must be activated program-wide in the **Options** | **Advanced** | **Automatically archiving** window. If archiving is not activated, a notification will be displayed when a method with automatic archiving is closed or loaded. The **Options** window can be opened via the link in the notification and archiving activated. If archiving is kept deactivated, measurements can be started with the method, but the data must be saved, printed or exported manually.

Example of method settings in the Spectrum module



See also

Activating automatic archiving [▶ 145]

4.4 Sample sequences

A sample sequence contains a list with the sequence of the samples to be processed, with information about sample type, name and other data important for the analysis. After starting the measurement, the sequence is automatically processed and the results are displayed in the results window. Sample sequences can be viewed after the measurement and additional samples can be added to them

4.4.1 Sample types and special samples in ASpect UV

Various sample types are used in the sample sequences in ASpect UV. The sample types have specific functions in the analysis. The sample types are defined in the sample table in the **Sample type** column. In the sample sequence chart, the sample types are identified by a small symbol (circle with letters) and can be changed by clicking with the mouse.

Sample	Icon	Sample with unknown analyte concentration
Reference	R	Each absorbance, transmittance, or reflectance measurement requires a previous measurement of the baseline as a device-specific reference value. The reference measurement can be carried out with an empty sample chamber or reference sample (sample matrix without analytes). In most cases, the reference sample is also measured in the reference measurement. The subsequent measurements of the sample and standard are corrected with the reference measurement.
Sample	P (En: S)	Sample with analytes
Blank	0	Sample without analytes (sample matrix only)

Sample	Icon	Sample with unknown analyte concentration
		This value is required if you want to display the measured value of the sample matrix. Otherwise, you can also measure the sample matrix in the reference. To record the blank, you must set the sequence (reference – blank – sample) in the sample sequence. The reference measurement (baseline) is carried out with an empty sample chamber or a sample without a sample matrix, e.g. a cell with water. All subsequent sample measurements are corrected with the blank.
Standard	Std	Sample with known concentration of the analyte for analyses with calibration

For some accessories, there are special samples on which no measured values are recorded. They are also specified as a sample type.

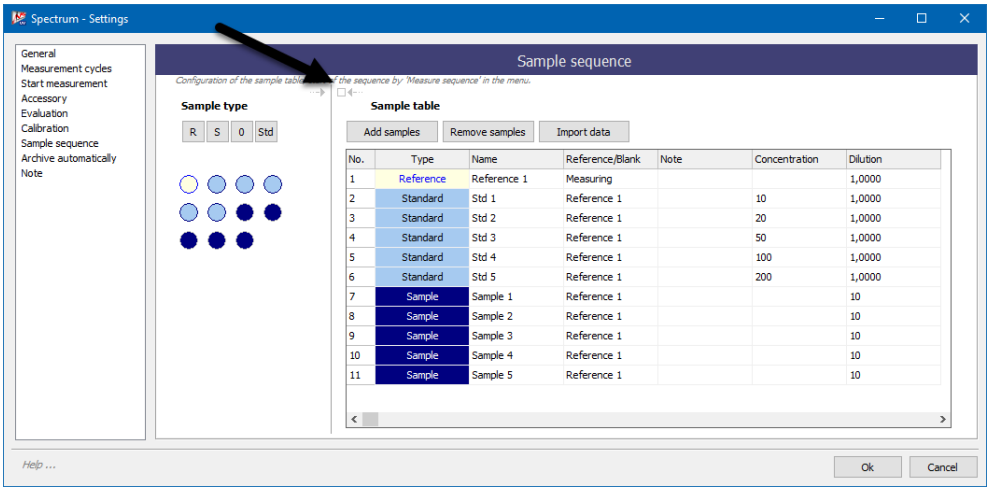
Sample type	Icon	Description
No measurement	?	For cell changer and APG The relevant accessory slot is not filled.
Wash	W	For cartridge sipper system and APG The sample in this accessory slot is used to rinse the sample paths (cannula, tubes).

4.4.2 Structure of the Sample sequence screen

The **Sample sequence** screen of the method parameters is identical in all ASpect UV modules. The screen is divided into two areas: the chart area on the left and the sample table on the right. In the chart area, you get a quick overview of the sample sequence and can assign the sample type by clicking with the mouse. In the table, you can edit all sample properties such as sample type, sample name, standard concentrations, and others.

If the chart area is not displayed, click on the dividing line arrows (arrow in figure below) to open the chart area. Then move the dividing line to the correct position by holding down the mouse button.

Example for Sample sequence methods screen in the Photometry module



Buttons in the Sample sequence window

Use the buttons to add further samples to the table or delete samples that are not required.

Button	Description
Add samples	Add one or several samples of a sample type to the sequence from a selected list place in the list
Remove samples	Remove one or several samples of a sample type from the sequence
Import data	Import sample data from a CSV or TXT file

Sample table

You can configure the columns of the sample table yourself.

- Right-click on the column header and activate all required columns in the context menu.
- To move a column to a different position, click on the column title and drag the column to the desired position while holding down the mouse button.

  ✓ The table is configured.

The table columns contain the sample properties.

Column	Description
No.	Row in the sample sequence
Pos.	Position in the accessory
Batch	Loading of the accessory
Type	Sample type or special sample
Name	Sample name
Reference/Blank	Reference or blank with which the measured sample value is corrected
Note	Optional note on the sample
Initweight	Sample weight during sample digestion This value is used for analyses with calibration when calculating the concentration for samples and blank values. It can also be used for all sample types (including standard) in the formula editor.
Concentration	Concentration of the standard
Dilution	Dilution of the sample This value is used for analyses with calibration when calculating the concentration for samples and blank values. It can also be used for all sample types (including standard) in the formula editor.
Variable A ... H	Sample-dependent variables that can be calculated in a formula Example: If you calculate a concentration analysis with factor, you can include the dilution as a sample-dependent variable in the formula.

4.4.3 Creating and editing sample sequences

Sample sequences are dependent on the accessories. With manual sample changing, the samples follow each other without gaps. For cell changers and automatic autosamplers, the loading (batch) is taken into account.

As of ASpect UV 2.0, references and blanks are saved in the document so that they can be loaded in other methods and reused for the calculation. To do this, you must enter a unique name in the sample table for each reference and each blank.

When confirming the method parameters with **Ok**, the system checks, among other things, whether the sample table is sufficiently filled out or whether data required for the analysis is missing. Among other things, the standard concentrations and the names of the references/blanks must be entered.

NOTE

At the start of the sample frequency, there should be a reference. All subsequent measurements are corrected with the reference. It is valid until a new reference is measured or the method (document) is changed.

If no reference has been defined in the sequence, a reference measurement must be carried out manually before the sequence is started.

Sample sequences with manual sample change

When using cell holders and accessories for solid samples, the sample must be manually replaced after every measurement. The samples are consecutively added to the sample table, without any gaps.

- Switch to the **Sample sequence** screen in the method parameters.
- Click **Add samples**.
- In the **Add samples** window, enter the following data for the first samples of a type:

Option	Description
Paste	Select the insertion range of the samples **At the begining** Insert samples from row 1 of the sample table **At the end** Add samples to the end of the sample table **From line number** Add samples in consecutive order starting from the selected row number If there are already entries in the selected sample location, they are moved down in the sample table. No sample entries are overwritten.
Sample type	Selection of sample type
Number	Number of samples of the same type to be inserted

- Click **Ok** to confirm the entered data.
- Click on **Add samples** again and make the other entries until all samples/sample types have been created.
- If references and blanks have been created, enter a sample name for these samples.
- Enter the known analyte concentrations for standards.
  - ✓ The sample table is created. You can make further entries for the sample properties (see below).

Sample sequences with automatic sample change

When using cell changers or autosamplers, the samples are approached and measured automatically according to the loading of the accessories (batch). After the first batch has been measured, you can fill the accessory again and carry out the next measurements automatically. You therefore define the sample sequence by batch in the sample table. Within a batch, the sample positions do not have to be filled without gaps.

If not already shown, when using a cell changer or autosampler, show the **Batch** column for a better overview of the sample placement in the accessories.

- Switch to the **Sample sequence** screen in the method parameters.
- Click **Add samples**.
- In the **Add samples** window, enter the following data for the first samples of a type:

Option	Description
Paste	Select the insertion range of the samples

Option	Description
	At the begining Insert samples from row 1, first batch of the sample table **At the end** Add samples to the end of the sample table **From line number** Add samples in consecutive order starting from the selected row number **From position in batch** Add samples from the selected position in the batch **From first free position in batch** Automatic search for the next free position to add the samples
Sample type	Selection of sample type
Number	Total number of samples of the same type to be inserted
Total per batch	Total number of samples within one loading of accessories, regardless of the sample type

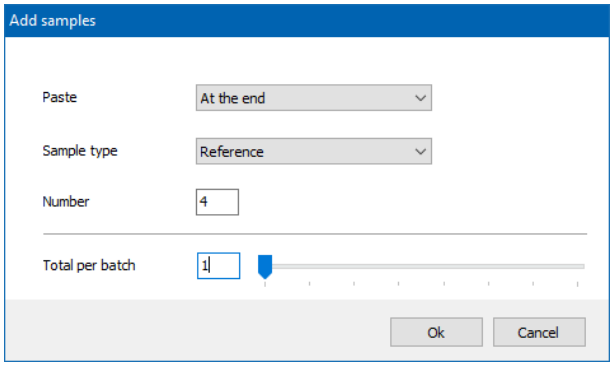
- Click **Ok** to confirm the entered data.
- Click on **Add samples** again and make the entries until all samples/sample types have been created.
- If references and blanks have been created, enter a sample name for these samples.
- Enter the known analyte concentrations for standards.

  ✓ The sample table is created. You can make further entries for the sample properties (see below).

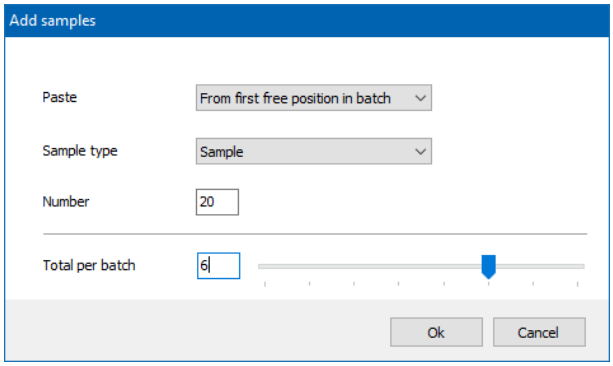
Example of a sample sequence with 8-cell changer

Within the sample sequence, you can distribute the samples of different types over different batches in the cell changer or autosampler. In the example, the settings for a measurement of 4 batches with 5 samples respectively and the associated reference are applied for the 8-cell changer.

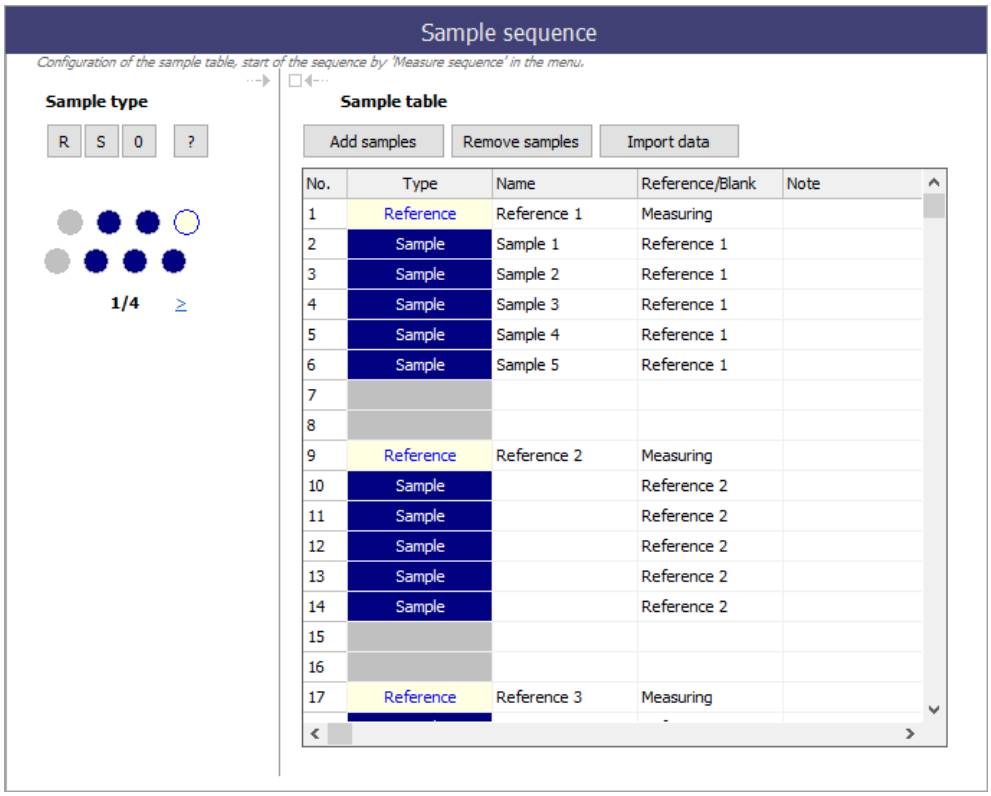
- Click on **Add samples** and first allocate the 4 reference samples to the first sample position of each individual batch of the cell changer:



- Click **Ok** to confirm the entered data.
- Click again on **Add samples** and allocate the samples to the various batches (5 samples * 4 batches = 20; 1 reference + 5 samples = 6 samples in total per batch):



- Click **Ok** to confirm the entered data.
  - ✓ There are 4 batches created, in each of which there is first a reference, followed by 5 samples. For each batch (load), 2 sample slots in the cell changer remain empty.



Enter sample name

Entering the sample names for the sample types **Sample** and **Standard** is optional. They can also be entered after the measurement. For sample types **Reference** and **Blank**, unique sample names must be assigned.

- In the sample cell, click on the **Name** column and enter the name.
  If you select the name with the mouse, the standard editing functions (cut, copy, paste and delete) are available to you after right-clicking in the context menu.

Consecutive samples can be assigned the same name or, for numbers with numbering, also an ascending index.

- Click once in the first cell of the sequence, enter the name and confirm with the Enter key.
- Highlight the cell with the name and the following cells with the mouse button held down.
- Right click on the highlighted choice and select **Fill with same value** or **Fill with ascending values**.

✓ All samples have been assigned the same name or the name with ascending numbering.

Enter additional sample data

- When activating the calibration, the concentration of the standard samples must be entered in the **Concentration** column of the sample table.
- If applicable, enter the factors for sample weight and dilution for samples and standard samples.
- In other table columns, individual variables A ... H, Note and other sample data may be entered for each sample.
- The parameters **Initweight** and **Dilution** are only taken into account in the calculation for analyses with calibration. For all other analyses, this data is only additional information about the sample. If you want the sample weight and dilution to be calculated in a concentration analysis with factor, use the variables A ... H in the formula.

Edit sample types

You can change the sample types in the sample table. For references and blanks, the measurement in the sequence is preset when first inserted into the sample table. You can define the use of saved data instead.

- Right-click in the sample type field in the sample table and select the new sample type in the context menu.
- For references and blanks, select one of the two options **Measuring** or **Load from file**. If required, select a suitable saved reference with the same method parameters.

Alternatively, you can edit the sample types using the sample icons in the chart.

- Enlarge the chart area by moving the dividing line arrows until the sample symbols appear with their numbering. The numbering indicates the row in the sample table for manual sample changes or the position in the accessories for automatic changes.
- Enable the button of the sample type (**Sample type**) and click on the sample icon. To select several adjacent samples together, hold down the mouse button and draw a frame around the sample icons.

✓ The sample types are changed accordingly.

Remove samples from the sequence

You can remove unnecessary samples from the sample table.

- Click **Remove samples**.
- Select the samples to be removed using the following settings:

Option	Description
Clear	**At the begining** Delete number of samples at start of sample table
	At the end Delete number of samples at end of sample table
	Number from line number Delete number of samples from selected row number
	Line number from - to Delete samples between the row numbers specified
Type	**All** Delete samples, regardless of type
	Sample type Delete samples of the selected sample type
Number	Number of samples to be removed

Editing the sample sequence during the measurement

An ongoing measurement may be interrupted in order to edit samples of the sequence not yet edited or to add further samples to the sequence.

- In the document window, interrupt the measurement by clicking on .
  The **Sequenz settings** window is displayed.
- Add further samples from the sequence or edit any samples not yet edited (see above) and confirm with **Ok**.
- Acknowledge the prompt with **Yes** to start the measurement.
  ✓ The measurement is resumed.

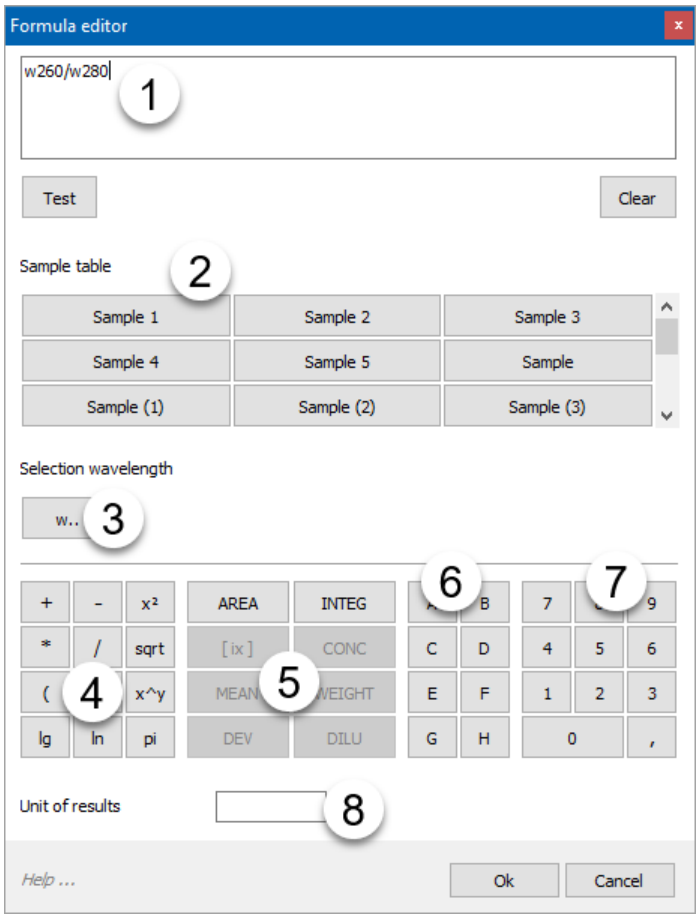
4.5 Using formulae

In ASpect UV, measurement results of one or more samples of a sequence can be analyzed in a formula (function).

In the method, you can create the formulas on the **Evaluation** or **Calibration** screens. These formulas are then applied to the samples measured with this method.

After the sample measurement, the results of the formula calculations are displayed in the analysis area of the document window on the **Formula** tab. You can supplement the analyses by entering additional formulas or editing existing formulas.

Structure of the formula editor



No.	Description
1	In the **input area**, you can either compile the formula (function) using the buttons or enter it directly using the keyboard. The buttons below the input area are used to check and correct the formulas: **Test** Test the correctness of the formula syntax

No.	Description
	Delete Delete last term in the formula
2	**Sample table** according to the set sample sequence If you want to link the values of selected samples (argument with sample reference) in the formula, first create a sample table on the **Sample sequence** screen and give the samples unique names. You will find the created samples in this area of the formula editor.
3	Function arguments
4	Operands
5	Functions
6	Sample-dependent variables There are 8 (A – H) sample-dependent variables available. The value of the variables is entered individually already in the sample table of the sequence or for subsequent calculations after the measurement in the results table.
7	Figures
8	Unit of the result

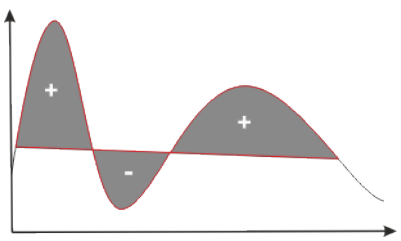
Function arguments

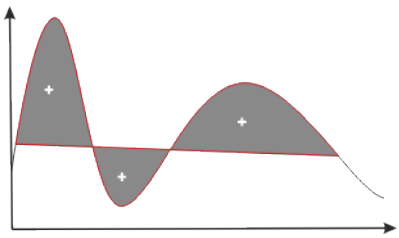
You can use measured values at defined wavelengths, times or temperatures as arguments in the functions. The availability depends on the selected module and the settings in the measurement parameter window.

Button	Description	Syntax example
w...	Measured value at a defined wavelength	w280
t...	For module **Kinetics** Measured value at a defined point in time in the format thh:mm:ss	t00:00:10
T...	For module **Thermometry** Measured value at a defined temperature	T38

Functions

The formula editor contains functions that can be used in the formulas. The functions are located at the bottom of the formula editor.

Button	Description	Syntax example
INTEG	For spectra, time curves, or temperature curves Integral between the measurement curve and a baseline The baseline is defined by two limit points whose abscissa values are entered. The ordinate values of the limit points correspond to the measured values associated with the abscissa values. If a baseline intersects several peaks, areas above and below the measurement curve and baseline are included. The integral is the difference between the areas above and below the baseline.  	INTEG[320~500]
AREA	For spectra, time curves, or temperature curves	AREA[320~500]

Button	Description	Syntax example
	Amount of the area between the measurement curve and a baseline As with the integral, the baseline is defined by two limit points. The area is the sum of the areas above and below the baseline. 	
SLOPE	For module **Kinetics** Slope of the kinetic curve in a defined time range	SLOPE[00:00:10 ~ 00:01:00]
TIME	For module **Kinetics** Time at a defined absorbance value If the time lies between 2 measured values, the time of the absorbance value is determined using linear interpolation.	TIME(2)
Y[i]	For module **Kinetics** Measured value at a selected measuring point	Y[1]
CONC	For methods with calibration Concentration value of a sample or a standard	CONC
WEIGHT	Factor for the weight of a sample from the sample table	WEIGHT
DILU	Dilution factor of a sample from the sample table	DILU
[ix]	Multiple measurements and time-cyclic measurements Value of a selected individual measurement The individual measurements within a multiple measurement or a cyclic measurement are numbered consecutively starting with 1. Add the desired value directly to the index of the individual measurement.	[5]w560
MEAN	Multiple measurements and time-cyclic measurements Mean of the individual measurements	MEANw560
DEV	Standard deviation of the individual measurements	DEVw560
	Sample reference Use the value of a selected sample from the sample table in the formula.	{Sample 1}w560

Function arguments for energy measurements

With dual-beam devices, the energy spectra of both beam paths are recorded. With the SPECORD 50, an internal reference is determined with a second diode in the monochromator. For energy measurements, you must specify the channel M (measurement channel) or R (reference channel) before the function argument, for example measured value at the 560 nm wavelength in the measurement channel: Mw560.

Formulas with and without reference to a selected sample

You can create formulas with and without reference to a specific sample. In a formula without a sample reference, the function is applied to all samples, e.g. calculate the quotient from the absorbance values at wavelengths 260 and 280: w260/w280.

With a sample reference, the function argument of a selected sample is generated from the sample sequence and used in the formula, e.g. subtract the measured value at the wavelength 560 nm of the first sample "Sample 1" from the measured value at 560 nm for all other samples: w560-{Sample 1}w560. For a sample reference, the sample name is placed in curly brackets in front of the function argument.

You can also apply the sample reference to the functions in the formula editor, e.g. {Sample 1}INTEG[320~500] or {Sample 1}conc.

Entering the formula

The easiest way is to compile the formula by clicking on the buttons in the formula editor. Alternatively, you can enter the formulas directly in the field using the syntax described above. If you want to create a sample reference, first click on the sample button and then add the desired value (argument).

Example 1 (with sample reference)

Subtract the absorbance value of sample 1 at wavelength 560 from the absorbances of the other samples at wavelength 560 nm.

- Click on **w...**, enter the value "560" and confirm with the ENTER key.
- Click on the **–** button.
- Click on the **Sample 1** button.
- Click on **w...**, enter the value "560" and confirm with the ENTER key.
  - ✓ The formula "w560-{Sample 1}w560" is displayed in the editor. The results of the calculation are displayed in the document on the **Formula** tab.

Example 2 (without sample reference)

As a measure of DNA purity, calculate the quotient of the absorbance values at the wavelengths 260 nm and 280 nm.

- Click on **w...**, enter the value "260" and confirm with the ENTER key.
- Click on the **/** button.
- Click on **w...**, enter the value "280" and confirm with the ENTER key.
  - ✓ The formula "w260/w280" appears in the editor. The results of the calculation are displayed in the document on the **Formula** tab.

4.6 Using accessories

Connected accessories are detected automatically when switching on the SPECORD PLUS and are taken into account in the method parameters. This chapter provides an overview of the accessory-specific method parameters and program functions organized by accessory type and module.

Observe the information on assembly, adjustment and function of the accessories in the "SPECORD PLUS accessories UV/Vis Spectrphotometer" operating manual.

In the method the accessory parameters are always arranged on the **Accessory** screen.

4.6.1 Passive accessories

Passive accessories are accessories that are not electronically controlled or automatically detected via an identification plug:

- Standard cell holder
- Holder for 100mm cells
- Holder for round cells
- Holder for microcells
- Adjustable cell holder for microcells
- Thermostated cell holder 10 mm and 50 mm
- Holder for cylindrical cells up to 50 mm and 100 mm

- Fiber optic coupling set
- Holder for solid samples

Method parameters

The following method parameters are available in all modules on the **Accessory** screen:

Option	Description
Select passive accessory	Selection of the accessories listed above The accessories are displayed in the document. The selection does not affect the method parameters further.
Change meas. channels	Swap beam paths in the sample space. The beam path for the sample measurement (M) becomes the reference beam path (R) and vice versa.

4.6.2 Cartridge sipper system

Method parameters

The following method parameters are available in all modules:

Option	Description
Pump time [s]:	This time is required to optimally transport the sample into the flow cell.
Wash time [s]:	During this time, the cell is rinsed with the rinsing solution. **Note:** The order of samples and rinsing solution is defined in the method sequence.
Slow run	The pump speed has been reduced by up to one half. This can reduce degassing or segregation of the samples. Smaller sample volumes may be dosed more accurately.
Change meas. channels	Swap beam paths in the sample space. The beam path for the sample measurement (M) becomes the reference beam path (R) and vice versa.

Functions in the document window

When using the cartridge sipper system, the following icons are additionally displayed in the toolbar of the document window:

Icon	Description
 Run sipper / **Stop sipper**	Switch pump on and off This function can be used to fill, purge, or empty the system additionally or after the end of the measurement.

Functions in the main window

The optimum pump time can be determined using the program using the menu command **Instrument** | **Accessory** | **Optimization pumping time** .

See also

Optimizing the pump time of the cartridge sipper system [▶ 135]

4.6.3 Autosampler

The following samplers are available for the SPECORD PLUS:

- APG 49
- APG 64
- APG 116
- APG S

Method parameters

The following method parameters are available in all modules:

Option	Description
Pump time [s]:	This time is required to optimally transport the sample into the flow cell.
Wash time [s]:	During this time, the cell is rinsed with the rinsing solution. **Note:** The order of samples and rinsing solution is defined in the method sequence.
Manual start	Start the measurement at a sample only after pressing another button. This option must be enabled if multiple measurements are run per sample.

Option	Description
Change meas. channels	Swap beam paths in the sample space. The beam path for the sample measurement (M) becomes the reference beam path (R) and vice versa.
Stirrer enable	Enable the stirring function for samplers with stirrer
Stirring speed	Set stirring speed The maximum stirring speed corresponds to 100 %.
Stirring time [s]	During this time, the sample is stirred before it is aspirated and transported into the cell.
Test strirring	Switch stirrer on and off to determine the optimum stirring speed
Slow run	The pump speed has been reduced by up to one half. This can reduce degassing or segregation of the samples. Smaller sample volumes may be dosed more accurately.

Functions in the document window

When using an autosampler, the following icons are also displayed in the toolbar of the module:

Icon	Description
Run sipper / Stop sipper	Switch pump on and off This function can be used to fill, purge, or empty the system additionally or after the end of the measurement.
Needle down **Needle up**	Lower or raise the sampler needle in the sample container
Run stirrer **Stop stirrer**	Switch the magnetic stirrer on and off

Functions in the main window

In the menu item **Instrument** | **Accessory** of the main window, additional functions are released for adjusting the autosampler.

See also

Adjusting the APG autosampler, moving to individual positions, and optimizing the pump time [▶ 136]

4.6.4 Cell changer

The following cell changers available in the SPECORD PLUS:

- Cell carousel
- 6-cell changer (also Peltier tempered)
- 8-cell changer (also Peltier tempered)
- Simultaneous use of two 6-cell or 8-cell changers in the measurement and reference channel of the SPECORD PLUS.
- Combination of a Peltier-tempered cell changer with the Peltier-tempered cell holder

Method parameters

The following method parameters are available in all modules:

Option	Description
Cyclic for	Only when cyclical measurement is activated Sample processing sequence **Sample** All repeat measurements are first performed at one sample. Then the next sample in the cell changer is indexed and the measurements are performed there. All samples are consecutively processed in this manner. **Batch** First, the first measurement is performed in each sample in the cell changer, then the cell changer returns to position 1 and starts the next measurement in each sample. This is repeated until the last measurement. **Note**: If a sequence contains more than one batch, the batches are processed one after the other.
Manual start	Every measurement of a sample in the cell changer must be started by pressing a button.
Synchronous	Only when using two cell changers If enabled the two cell changers move synchronously. A separate reference can be used for each sample. If deactivated, the cell changers are moved consecutively through the beam paths (offset mode). In this way, both cell changers are used for the sample measurement. At first, the samples in the reference channel are measured followed by the samples in the measuring channel. In offset mode, the measuring and reference channels are swapped during the measurement. In order to determine the respective beam ratios for this process, **the first position of the cell changer in the measuring channel and the last position of the cell changer in the reference channel must remain empty.** With two 8-cell changers you therefore have 14 measuring positions available and with two 6-cell changers there are 10 measuring positions.

Reference measurements for kinetic curve and temperature curve

If the measurement of the reference within a sequence has been agreed for batch processing, this is only carried out once at the start of the sequence. All sample measurements are corrected with this reference. You can record or correct time or temperature-dependent changes in the sample matrix by agreeing a blank measurement in the sequence.

Functions in the main menu

In the menu item **Instrument** | **Accessory** of the main window, the following functions are available for cell changers:

- Index specific individual sample positions
- Switch cell changer on and off
  When switching off, the cell changer travels to the park position in facilitate a simple removal and installation and for packing into the storage box.
- Adjust cell changers
- Detect accessories

See also

- Adjusting the cell changer and moving to individual positions [▶ 134]
- Peltier-tempered accessories [▶ 43]

4.6.5 Peltier-tempered accessories

The following Peltier-tempered accessories are available for the SPECORD PLUS:

- Peltier-tempered cell holder
- 6-cell changer, Peltier-tempered
- Two 6-cell changers, Peltier-tempered
- 8-cell changer, Peltier-tempered
- Two 8-cell changers, Peltier-tempered
- 8-cell or 6-cell changers, Peltier-tempered (in measuring channel) and cell holder, Peltier-tempered (in reference channel)

Method parameters

With the Peltier-tempered accessories the following temperature operation modes are possible:

- **None**
- **Fixed temperature**
- **Variable**

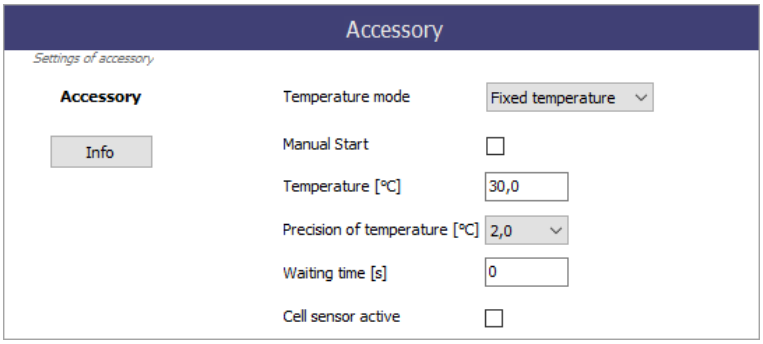
None temperature mode

The temperature mode **None** is available in the modules **Photometry**, **Spectrum**, **Kinetics** and **Colormetric**. In this mode, the temperature of the Peltier temperature controlled accessory is not controlled via the ASpect UV program, but can be directly specified at the temperature control unit (see also the operating instructions on "SPECORD PLUS UV/Vis Spectrophotometer Accessories").

Click on the **Info** button to display information about the adjustable temperature range and the current temperatures in the accessories.

Fixed temperature temperature mode

The temperature mode **Fixed temperature** is available in the modules **Photometry**, **Spectrum**, **Kinetics** and **Colormetric**. In this temperature mode, the Peltier temperature controlled accessory is kept at a constant temperature. The optical measurement (measurement of transmittance or absorbance) is taken 5 s after reaching the temperature in the range of the agreed temperature accuracy plus any selected waiting time.



Option	Description
Temperature mode	**Fixed temperature** Set a constant temperature
Temperature [°C]	Enter the target temperature
Precision of temperature [°C]	Select the accuracy of the temperature control
Waiting time [s]	Enter the waiting time from reaching the target temperature to starting the optical measurement
Cell sensor active	At the start of the measurement when the target temperature is reached, the registered cell temperature is recorded. The measured value (absorbance/%T) is assigned to the cell temperature. The temperature measurement is therefore more accurate than the sample block temperature. If the option is not enabled, the block temperature (standard temperature) is recorded and indicated as an abscissa value in the **Thermometry** module.
Info	Display information about the adjustable temperature range and the current temperatures in accessories

Variable temperature mode

The temperature mode **Variable** allows you to record temperature-dependent measurement curves. Each optical measurement is taken 5 s after reaching the temperature within the agreed temperature accuracy range plus a potential waiting period.

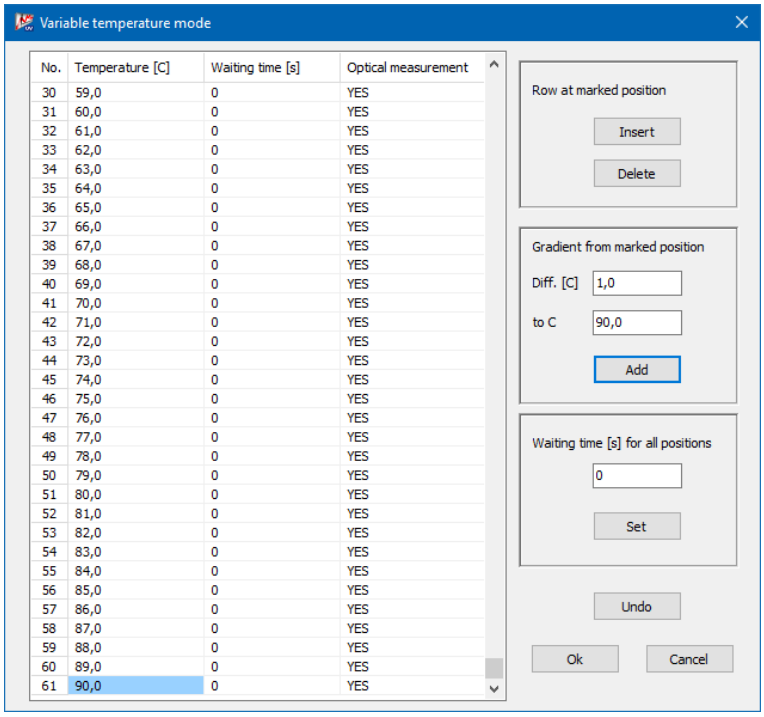
The temperature mode **Variable** is available in the modules **Thermometry**, **Spectrum** and **Colormetric**. In the **Thermometry** module, the measurement is carried out at a wavelength. In the **Spectrum**, a spectrum is recorded at each specified temperature level. A section may be applied to the resulting spectra array at a wavelength and the intersection curve evaluated in the **Thermometry** module.

The temperature mode **Variable** cannot be combined with a kinetic measurement (**Measuring time [sec]**). When using Peltier temperature controlled cell changers, the samples are processed in batches. The first temperature is set in the cell changer and the measured value is recorded in all samples. The next temperature is then set and the measured value is determined again in all samples. The measurements are continued until all samples have been processed.

Option	Description
Temperature mode	**Variable** Recording a temperature curve at a fixed wavelength (module **Thermometry**) or a spectra array (module **Spectrum** or **Colormetric**)
Precision of temperature [°C]	Select the accuracy of the temperature control
Cell sensor active	At the start of the measurement when the target temperature is reached, the registered cell temperature is recorded. The measured value (absorbance/%T) is assigned to the cell temperature. The temperature measurement is therefore more accurate than the sample block temperature. If the option is not enabled, the block temperature (standard temperature) is recorded and indicated as an abscissa value in the **Thermometry** module.
Temp. after sequence	Activate holding temperature after optical measurement This temperature is approached and held after the last optical measurement.
Temperature values	Click on **Setup...** to open the **Variable temperature mode** window for entering the temperature values.
Info	Display information about the adjustable temperature range and the current temperatures in accessories

Settings in the Variable temperature mode window

After clicking on **Setup...** in the method sequence, the **Variable temperature mode** window appears. The parameters of the temperature stages can be edited individually in the table rows or defined automatically using the checkboxes and input fields.



Option/button	Description
Paste	Enter a new temperature step after the highlighted table row
Delete	Delete the highlighted table row
Gradient from marked position	Automatically generate a temperature gradient from a highlighted table row. Starting with the start temperature of the highlighted table row further temperature stages are inserted into the table in steps until the final temperature has been reached. **Diff. [C]** Temperature difference of a temperature stage **to C** Final temperature of the gradient **Add** Append temperature gradient at the highlighted position
Waiting time [s] for all positions	Waiting time from reaching the setpoint temperature to the start of the optical measurement Click on **Set** to transfer the entered temperature to all temperature levels in the table. **Note**: Regardless of the set waiting time, the optical measurement is carried out no less than 5 s after reaching the temperature within the agreed temperature accuracy range in the block. The waiting time is added to this 5 s period.
Undo	Reverse the last action
Optical measurement	**Yes** Perform an optical measurement at temperature step **No** No optical measurement takes place at the temperature step.

Functions in the document window

The following icon is also displayed in the toolbar of the document window.

Icon	Description
Set temperature	Set the accessory temperature to the defined value (**Fixed temperature** temperature mode) or the starting temperature of the temperature curve (**Variable** temperature mode).

4.6.6 Integrating sphere

The integrating sphere is used for the measurement of scattering solid, liquid or powder samples in transmittance, absorbance or reflectance.

Method parameters

The following measurement mode options are available in the method parameters:

- **Transmittance**
- **Absorption** (not in module **Colormetric**)
- **Reflectance**

4.6.7 Scanning attachment for solid samples

The scanning attachment for solid samples is used for the locally resolving determination of transmittance or the absorbance of small transparent solid samples.

Method parameters

The following method parameters are available in all modules:

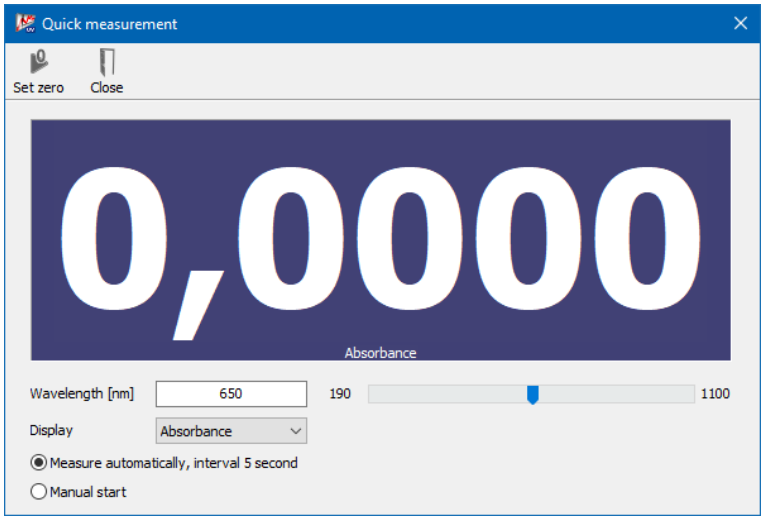
Option/button	Description
Start	Start coordinate of a measurement
Finish	End coordinate of a measurement
Stepwidth	Measuring point spacing on the sample
Set	Move the scanning attachment to the start or end coordinate of the measurement
Zeroth order	Set the monochromator mesh to the zero order. The undispersed (white) light of the Vis lamp passes through the sample chamber and due to its good visibility facilitates the adjustment of the sample in the scanning attachment.

5 Quick measurement module and online measurement

Quick measurement module

The **Quick measurement** module is used to determine a single measured value. The data is only displayed on the screen and cannot be saved or printed. The measured value can be determined either in a single measurement or automatically and continuously. In this measurement, electrically controlled accessories are not supported. The cell changer can only be used as a cell holder. The cartridge sipper system or the autosampler cannot be used.

Structure of the Quick measurement window



Option/Icon	Description
Measure	Start measurement
Set zero	Determine reference value The reference value is used as a base value, i.e. is set to zero.
Close	Close the **Quick measurement** window
Value display	Displays the measured value
Wavelength [nm]	Enter the wavelength in the input field or set it using the slider
Display	Select display: **Absorbance** or **Transmittance [%T]**
Measure automatically, interval 5 sec	Determine measured value continuously every 5 seconds
Manual start	Determine the measured value after clicking on .

Manual start

In this mode you select a wavelength and start the measurement via mouse click.

- Select the menu item **Modules** | **Quick measurement**.
- Edit the wavelength in the input field or set it using the slider.
- As value display, select the option **Transmittance [%T]** or **Absorbance**.
- Enable the **Manual start** option.
- Insert reference sample into the cell holder where applicable and click on .
  - ✓ The reference measurement is performed. The display shows "0.000" for absorbance measurements and "100.0" for transmittance.
- insert samples into the cell holder and click on .
  - ✓ The results display is updated. Read the measured value.

- For subsequent sample measurements insert the next sample into the cell holder and click on .

Continuous measurement

In this mode a measured value is determined continuously at time intervals of 5 s.

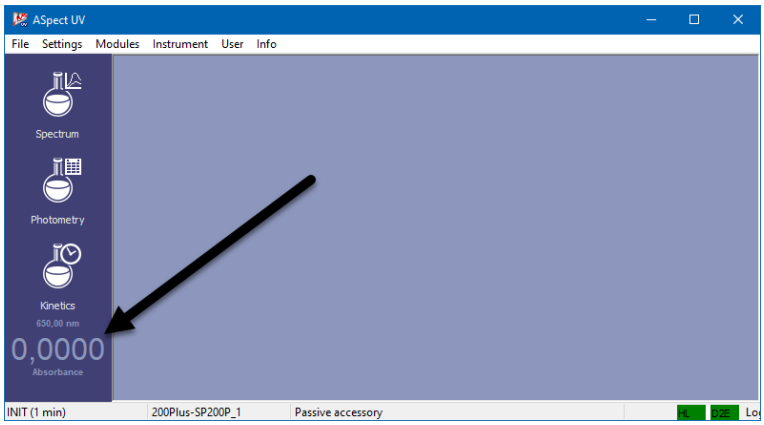
- Select the menu item **Modules** | **Quick measurement**.
- Edit the wavelength in the input field or set it using the slider.
- As value display, select the option **Transmittance [%T]** or **Absorbance**.
- Enable the **Measure automatically, interval 5 sec** option.
- Insert reference sample into the cell holder where applicable and click on .
  - ✓ The reference measurement is performed. The reference value appears in the display.
- Insert samples into the cell holder. Wait until the new measured value is displayed and read the measured value.
- For the subsequent measurement, insert samples and wait each time until the measured value is updated.

Online measurement

During online measurement, the measured values at the currently set wavelength are continuously determined every second and displayed in the task bar of the main window. The online measured values are only shown after the first measurement. The online measurement can be enabled in the **Options** | **General** | **Launch bar** window.

Like the module **Quick measurement**, the online measurement can be used for a quick sample value determination. The measurement is not saved and cannot be printed. To use the online measurement, the wavelength must be set in the quick measurement and the reference value determined (set to zero). The measurand shown complies with the value last measured in the active document.

- Enable the **Quick measurement** window.
- Set the wavelength and click on .
- Close the **Quick measurement** window.
- Insert samples into the cell holder and read the current measured values in the task bar.
  - ✓ The measured values are continuously updated.



See also

Configuring the launch bar [▶ 138]

6 Photometry module

The **Photometry** module enables the measurement of transmittance or absorbance at selected wavelengths. You can evaluate the measurements quantitatively in a calibration or formula. Together with the preparation of measurement methods and easily editable sample sequences, the **Photometry** module satisfies the requirements of routine analysis with high sample throughput.

Open Photometry module

- Open the **Photometry** module by clicking on the icon in the task bar.

- Alternatively, select the menu item **Modules** | **Photometry**.
  - ✓ A new document is opened in the workspace.
- Each additional click on the icon opens another new document on the workspace.

All functions of the document windows of the **Photometry** module are assigned to the measurements at individual wavelengths and the corresponding analysis. You can now create a method and start a measurement with analyses based on it.

See also

Basic structure and functions of ASpect UV [▶ 11]

6.1 Method settings in the Photometry module

This section includes all configurations that can be made for a method in the **Photometry** module.

Tip

Methods for enzymatics, water analysis, and biochemical analyses are already pre-installed in the ASpect UV program.

Creating a method

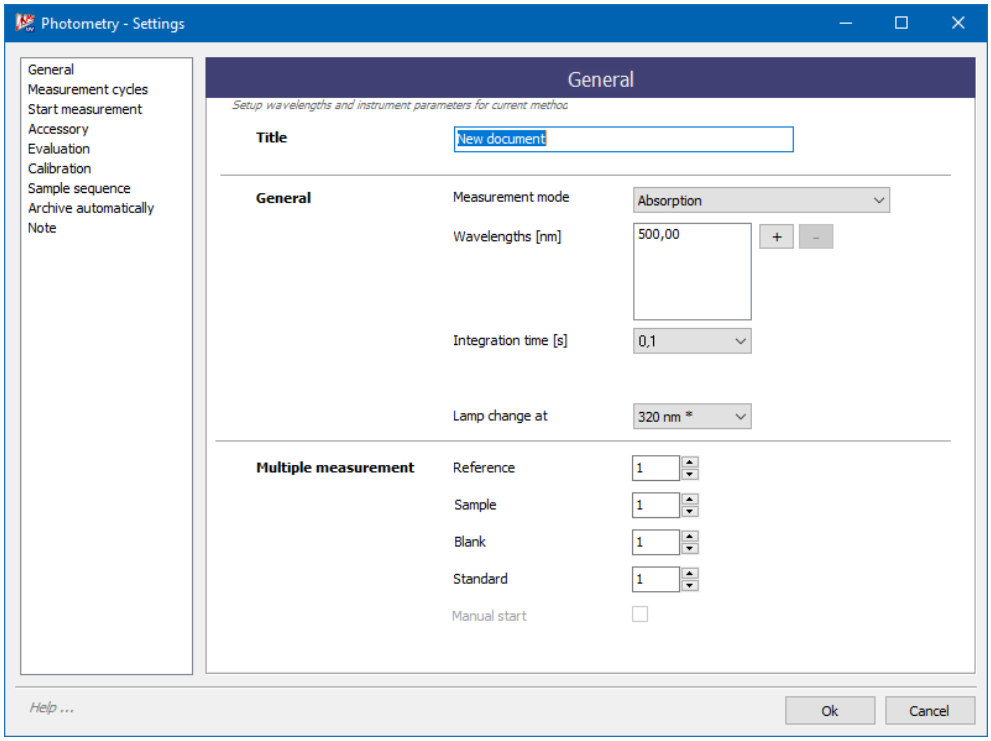
- Click on **Method setup** in the document window to open the method window.
- Make the settings on the screens of the method window.
- Finish entering the parameters by clicking on **Ok**.
  - ✓ The method parameters are output on the left side of the document window on the **Method** tab. The icons for starting the measurement appear in the toolbar of the document window.

See also

Pre-installed methods [▶ 178]

6.1.1 Photometry - Settings | General

On the **General** screen, the basic measurement configurations are made.



Title

Enter the title of the document here, which is displayed in the document tab. You can edit the title later.

General

In this area, select the parameters for the optical measurement.

Option	Description
Measurement mode	The following measurement modes can be selected: ■ **Transmittance** ■ **Absorption** ■ **Reflectance** (only for reflectance measuring attachments and integrating sphere)
Wavelengths [nm]	Select the wavelengths for the analysis: Click on + , enter the desired wavelength in the input field and click on + again to transfer it to the list. To remove a wavelength from the list, highlight the wavelength in the list and click on - .
Integration time [s]	Select the time for recording a measuring point
Slit [nm]	For SPECORD 210/250 PLUS Select spectral width (optical resolution): 0.2; 0.5; 1; 2; 4 nm **Note**: The 0.2 nm slit was not yet installed in older SPECORD 210/250 PLUS. It is not available for selection for these devices.
Lamp change	Select the wavelength of the change from UV lamp to Vis lamp The preset lamp change at 320 nm guarantees an optimal distribution of energy across the entire wavelength range of the spectrometer. If you are only working in UV or Vis range, you may also measure with the selected lamp using the options **UV only** or **Vis only**.

Multiple measurement

You can carry out a measurement several times in succession and use the mean for further calculations and analyses. For measurements with very little energy, e.g. samples with high absorbance, this procedure can improve the signal-to-noise ratio and increase the measurement accuracy.

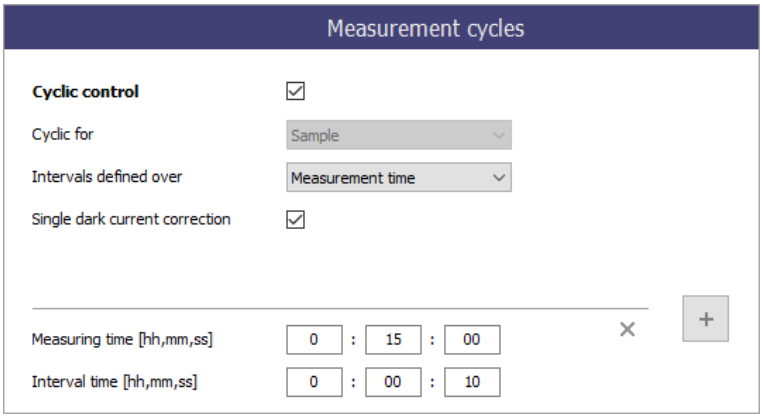
Option	Description
Multiple measurement	If necessary, enter the number of measurement repetitions for the sample types **Reference**, **Blank**, **Sample** and **Standard**. If the **Manual start** option is enabled, a request to start is made for each individual measurement within a repetition.

See also

Edit document title [▶ 23]

6.1.2 Photometry - Settings | Measurement cycles

On the **Measurement cycles** screen, you can arrange time-staggered measurement repetitions (kinetic measurements) in a sample. One measurement value is recorded for each sample in each cycle. If you have defined the measurement at several wavelengths on **General**, the measuring points are recorded for each wavelength. You can export the measurement data as a CSV file (measured value/time).



Parameters for the kinetic measurements

Option	Description
Cyclic control	When activated, enables the inputs for cyclical measurements
Cyclic for	Only when using cell changers or autosamplers **Sample** The entire reaction-kinetic measurement is performed in one sample and then the measurement started in the next sample. All samples in the sequence are processed consecutively in this manner. The measurement is suitable for fast reaction kinetics. If the reaction is to be started immediately before the measurement, option **Manual start** must be enabled on the **Start/Stop measurement** screen. **Batch** In this mode the sample measurements are staggered. Within an interval, all samples of the sequence are measured, starting with the first sample. The next interval then re-starts with measuring the first sample. In this manner the measurement is continued until the last interval. One batch of the cell changer/APG is measured at a time. Once all measurements for this batch (either by sample or batch) have been processed, the samples are replaced in the accessories and the measurement of the next batch is started.

Option	Description
Intervals defined by	**Measurement points** The number of measuring points/repeated measurements and the interval time must be defined for the measurement. The resulting total measuring time is calculated automatically. **Measurement time** The interval time and a total measurement time must be defined for the measurement. The resulting number of measuring points is calculated automatically.
Single dark current correction	By default, this option is enabled. The dark current is determined before the first measurement and the measured values are corrected accordingly. If the option is disabled, a dark current correction is performed before each measurement.
+	Insert time period For time-controlled cyclical measurements, several time periods can be defined, each with different interval times.

Further information on the settings for kinetic measurement can be found in the **Kinetics** module.

See also

Kinetics - settings | Measurement cycles [▶ 87]

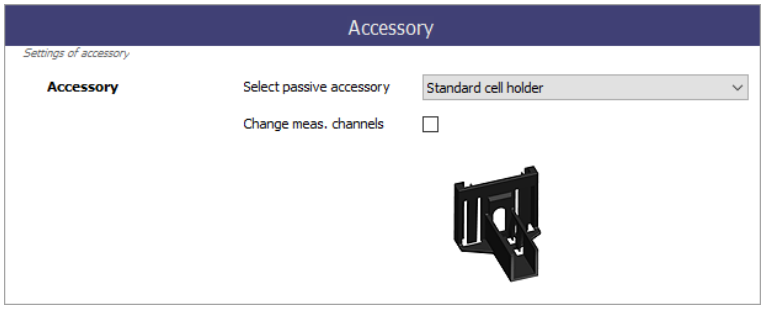
6.1.3 Photometry - Settings | Start measurement

You define the measurement start of a sample on the **Start measurement** screen. The following start options are available:

Option	Description
Autom. without waiting time	The measurement starts immediately after you click on or .
Autom. with waiting time	After clicking on or , the measurement only starts after the wait time has elapsed.
Manually without waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the measurement starts immediately.
Manually with waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the wait time elapses first and then the measurement starts.
Waiting time	Time delay for start options with wait time

6.1.4 Photometry - Settings | Accessory

The parameters in the **Accessory** screen depend on the installed accessories.



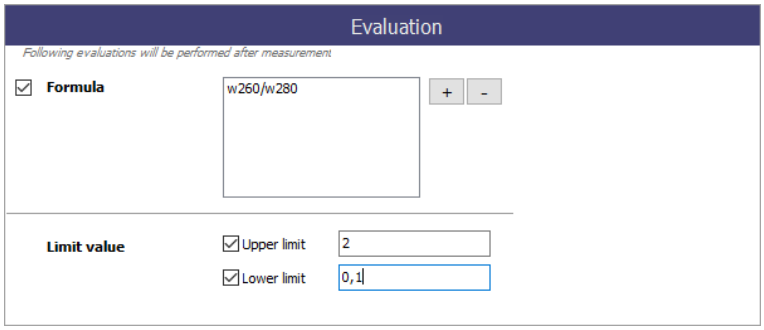
See also

Using accessories [▶ 39]

6.1.5 Photometry - Settings | Evaluation

On the **Evaluation** tab, the following settings are configured:

- Input of formulae
- Input of a limit value for the measuring results



Formula

You can link the measured values in a formula and, for example, perform a concentration analysis based on the multiplication of the measured values by a factor.

Limit value

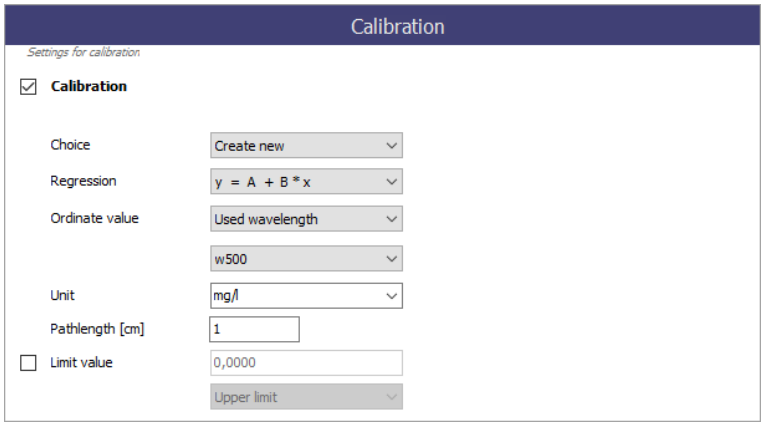
You can activate and enter an upper and a lower limit. The measured values that are above or below the limit value are marked with "!" in the results table.

See also

Using formulae [▶ 36]

6.1.6 Photometry - Settings | Calibration

You can define analysis parameters for a quantitative analysis with calibration on the **Calibration** screen.



To determine the concentration using a calibration with standards, activate the **Calibration** option and configure the following settings:

Option	Description
Selection	**Create new** Record calibration within the following measurement series You must define the standard samples and their concentration in the sample sequence. **Load from file** Load calibration parameters from an existing method

Option	Description
Regression	Regression type of the calibration function $y = B * x$ $y = A + B * x$ $y = A + B * x + C * x^2$
Ordinate value	Ordinate value for the calibration function **Value at wavelength** Select a measured value at one of the wavelengths for the calibration in the list field. The wavelengths are determined on the **General** screen. **Formula** Use the result of a formula calculation for the subsequent calibration. Clicking on ... displays the formula editor. **Note**: The formula used on the **Calibration** screen is independent of any formula entered on the **Evaluation** screen.
Unit	Unit of the analysis result
Thickness	Pathlength of the cell This value is for information only and is saved with the method parameters.
Limit value	Define an upper or lower limit value for the analysis result Results above or below this limit value are identified with "!" in the results table.

See also

Using formulae [▶ 36]

6.1.7 Photometry - Settings | Sample sequence

On the **Sample sequence** screen, you can specify the sequence of samples for a subsequent measurement, which you can start using the icon in the document window. You can also create a sample sequence directly before a measurement.

Requirements for the sample sequence

- Activating the calibration requires entering a sequence with standard samples.
- When using cell changers and autosamplers, the samples are assigned to the sample positions in the accessories.
- If the sample sequence is empty, the **Sequenz settings** window will first appear when starting the measurement of the sample sequence. This window may only be exited once there has been at least one sample defined.

See also

Sample sequences [▶ 29]

6.1.8 Photometry - Settings | Archive automatically

You can automatically save, export, and print the measurement data and its analysis. This allows you to standardize your data archiving processes and ensure that data is not lost. Select the target files and report templates in the **Archive automatically** screen. Additionally, automatic archiving must be activated program-wide in the **Options** window and the times for the individual archiving functions must be selected.

See also

Automatically archive measurement data [▶ 28]

6.1.9 Photometry - Settings | Note

A note on the method may be optionally entered on the **Note** screen.

6.2 Performing measurements in the Photometry module

The prerequisite for starting a measurement is that a new method has been created or loaded in the document window. The measurement can be started with a sample sequence stored in the method or as individual measurement.

The following icons are displayed for the measurements:

Icon	Description
Measure sample	Start individual sample measurement independent of the sample sequence configured
Measure sequence	Start sample sequence If you have not saved any sample sequences to the measurement parameters, the **Sequenz settings** window will appear after you click on this icon. This window may only be exited once there has been at least one sample defined.
Reference	Measure reference A separate reference measurement is required if the sample sequence does not start with a reference measurement or no reference is available that matches the current method parameters.
Stop	Stop current measurement and do not continue
Suspend sequence	Interrupt the measurement and continue at a later time The current sample measurement is completed. The pending sample sequence is then displayed and can be edited.
	Available for cartridge sipper system and APG sampler: Switch pump on or off and convey sample or stop conveying
	Available for APG sampler: Lower or raise sample cannula
	Available for APG sampler with stirring function: Switch stirrer on or off
	Adjust the temperature in a Peltier temperature controlled accessory

Measure reference

If the sample sequence does not have a reference at the first location, the reference must be recorded separately.

- Place the reference into the sample space.
- Click on **Reference** and confirm the prompt about the reference measurement.
  - ✓ The reference measurement is run. All subsequent measurements are corrected with this reference until the measuring parameters are modified by a new method configuration or the next reference measurement takes place.

Start first sequence

With the start of the sample sequence the samples are processed in the order specified in the sample table.

- Place the first sample of the sequence in the sample space or fill cell changer/autosampler with samples.
- Click on **Measure sequence**.

- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  - ✓ The sample sequence is processed. The measured values and analyses are displayed in the document window.

Interrupting or stopping the sequence

An ongoing measurement may be interrupted and then continued or stopped completely.

- Click on **Stop** to stop the measurement.
  - ✓ The measurement of the sequence is stopped and cannot be continued. Measurement data recorded up to this point remain intact and may be processed further.
- Click on **Suspend sequence** to interrupt a measurement and continue it later.
  - ✓ The current sample measurement is ended and then the processing is interrupted. The measurement pause may be used to view and edit the ongoing sample sequence.

Start next sequence

After processing the first sample sequence, the sequence may be started again or re-edited on other occasions. This is also possible if the document has already been saved and re-opened to display the results.

- Click .
  The **Edit sequence** window appears with the sequence stored in the method.
- If necessary, compile a new sequence.
- Confirm the setting in the **Edit sequence** window by clicking on **Ok**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  - ✓ The current sequence is processed and the data appended to the existing measurement table and analyses.

Performing single measurements

Regardless of the sequence configured, single samples of sample type **Sample** may be measured and appended to the measurement table and analyses.

- Place the sample into the sample space.
- Click on **Measure sample**.
- Follow further on-screen prompts for starting the measurement.
  - ✓ The measurement is run and the data is appended to the existing measurement table and analyses.

Tip

If measurements of other sample types are to be appended, click on **Measure sequence** and enter a sequence with the corresponding samples.

Re-measuring samples

Outliers of a measurement may be re-measured and thus values from a measuring series that differ greatly replaced by new values. The re-measurement of samples is always recorded in the audit trail. For the re-measurement of a probe, you will need to switch to the **Measurement** worksheet.

- Place the sample in the sample space.
- Right click on the row of the sample to be re-measured. For multiple measurements, you can select a single value by clicking with the right mouse button.
- In the context menu, select **Remeasure sample**.
- Follow further on-screen prompts for starting the measurement.

✓ The measurement is run and the measured value replaced in the sample table. The existing analyses are updated.

NOTE

If additional worksheets besides the **Measurement** worksheet are already available in the document, these are not updated during a re-measurement.
When using cell changers or APG the sample to be re-measured must be placed in the same position in the accessories. The position in the accessories can be displayed in the sample table on the worksheet.
Time-cyclical measurements cannot be re-measured.

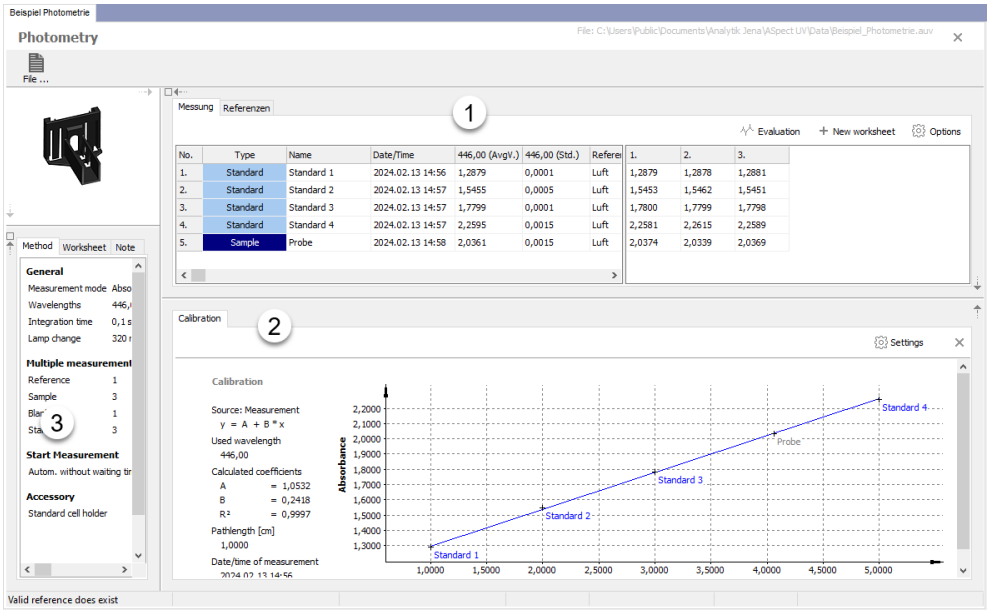
See also

Creating and editing sample sequences [▶ 31]

6.3 Displaying, evaluating, and processing results in the Photometry module

This section explains the particularities of the results display and analysis in the **Photometry** module.

Photometry document window with measured values and quantitative analysis



No.	Description
1	Worksheets with measurement data, reference data and further analyses
2	Tabs with analyses for the active worksheet
3	Tabs with information on method settings and mathematical analyses on the worksheets

Measurement worksheet

The sample table with the measurement data is located in the upper part of the **Measurement** worksheet. The lower part of the worksheet contains the data analyses that have already been defined in the method, each on separate worksheets. You can add to and edit these analyses.

Sample table

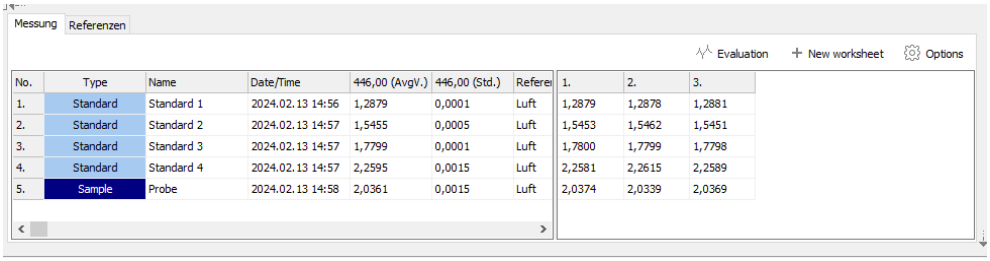
The display of the sample table can be configured freely. After right clicking on the table header the following parameters can be selected in the context menu:

- Number in the sequence
- Position in accessories when using cell changer or autosampler
- Batch when using cell changer or autosampler
- Sample name
- Sample type
- Date and time of the measurement
- Measured value or average value for multiple measurements
- Standard deviation for multiple measurements
- Reference or blank with which the sample was corrected
- Temperature for methods with Peltier-tempered accessories
- Notes
- Sample concentration for concentration determination with calibration
- Dilution and sample weight
  These entries are only taken into account for concentration determinations with calibration.
- Sample-specific variables A – H for calculations in formulae

Via Drag&Drop the order of the table columns can be changed.

Sample table for multiple measurements

For multiple measurements, the mean value is displayed in the sample table and used for further analyses. The individual measurements are listed adjacent in a separate table.



No.	Type	Name	Date/Time	446,00 (AvgV.)	446,00 (Std.)	Referer	1.	2.	3.
1.	Standard	Standard 1	2024.02.13 14:56	1,2879	0,0001	Luft	1,2879	1,2878	1,2881
2.	Standard	Standard 2	2024.02.13 14:57	1,5455	0,0005	Luft	1,5453	1,5462	1,5451
3.	Standard	Standard 3	2024.02.13 14:57	1,7799	0,0001	Luft	1,7800	1,7799	1,7798
4.	Standard	Standard 4	2024.02.13 14:57	2,2595	0,0015	Luft	2,2581	2,2615	2,2589
5.	Sample	Probe	2024.02.13 14:58	2,0361	0,0015	Luft	2,0374	2,0339	2,0369

Reference worksheet

The reference values are listed on the **Reference** worksheet.

New worksheet

You can create additional worksheets in the document window and carry out further analyses on them. In this way, you can create different analyses side by side in one document (file). The **New worksheet** worksheet is created after clicking on + **New worksheet** in the **Measurement** worksheet. The unedited, original measurement data is first copied to the new worksheet and can then be edited.

6.3.1 Edit sample table in the Photometry module

Edit sample table

You can subsequently edit the following values in the sample table:

- Sample name
- Notes
- Dilution and sample weight
  These entries are only taken into account for concentration determinations with calibration.
- Sample-specific variables A – H for calculations in formulae

▶ Click on the table cell and edit the value.

✓ The changes are documented in the audit trail. Existing analyses are re-calculated and updated.

Reassign reference

By default, samples are always corrected with previous references or blanks. If you have several references/blanks in the sample table, you can also assign one of the other references/blanks to samples and correct the samples again in this way.

▶ In the sample row, right-click in the **Reference/Blank** column and select the new reference from the context menu.

✓ The reference is applied to the sample. The name of the reference is shown in the **Reference/Blank** cell.

Highlight samples

You can select samples in the sample table and highlight them in bold.

- Right click on a sample in the sample table.
- In the context menu, select **Highlight multiple samples**.
- In the selection window, enable the sample checkboxes.
  - ✓ The selected samples are shown in bold font in the sample table and highlighted with a thick outline in the calibration graph display.

Note: Alternatively, individual samples can also be highlighted or their highlighting removed directly. To do this, select **Highlight in chart** or **Remove highlight in chart** in the context menu.

Hide samples

You can hide samples in the sample table. The hidden sample is not included in the analysis, but is not deleted from the data record. You can show a hidden sample again.

- Right click on a sample in the sample table.
- In the context menu, select **Show/Hide multiple samples** .
- In the selection window, only enable the checkboxes whose samples are to be shown and analyzed.
  - ✓ The analysis results are recalculated. The hidden samples are highlighted in light gray in the sample table.

Note: Alternatively, you can also show or hide an individual sample. To do this, select **Hide** or **Show** in the context menu.

6.3.2 Analyzing photometry data

The data analyses offered in this method can also be performed later. The functions have been compiled in the menu **Evaluation** that is available on every worksheet. The analyses always relate to the measured values of the respective worksheet. If the measured values are processed with mathematical functions, the analysis on this worksheet is adjusted accordingly.

The analyses are output in their own spreadsheet in the bottom part of the worksheet.

The following functions are available in the **Photometry** module in the method for the analysis and can be used or edited subsequently:

- **Formula**
- **Calibration**
- **Limit value**

Edit analysis

The analysis parameters can be edited for existing analyses.

- Click on **Settings** in the spreadsheet of the analysis and change the analysis parameters in the dialog window.
  - ✓ The analysis is updated.

Delete analysis

Analyses that are not required may be deleted.

- At the top right of the spreadsheet of the analyses click on .
  - ✓ The analysis is removed from the worksheet.

Formula

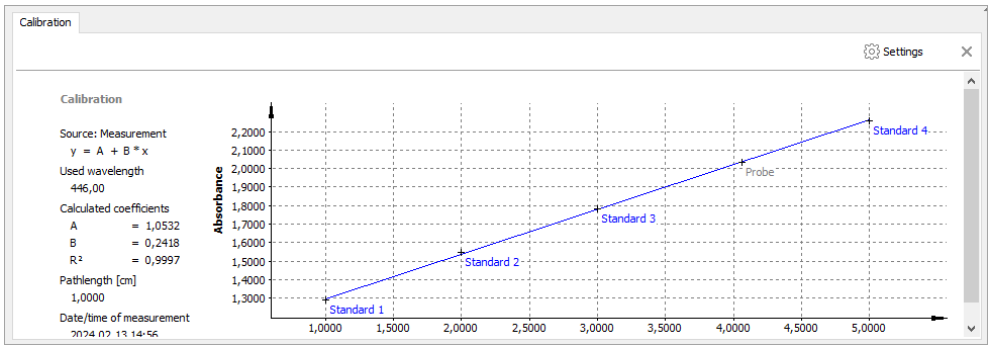
Use the **Formula** function to link the measured values of one or more samples in a formula.

- On the worksheet, select the menu item **Evaluation | Formula**.
- Click on + and create the formula using the formula editor.
- If necessary, add further formulae in the same way.
  - ✓ The results are displayed on the **Formula** tab.

Calibration

The **Calibration** function is available if a document does not contain its own calibration with standards. You can use this function to subsequently load the calibration data from other files and carry out a quantitative analysis of the measured values. Only the calibration parameters are loaded and not the standards.

- On the worksheet, select the menu item **Evaluation | Calibration**.
- Enable the **Calibration** option.
- Click on **Load** and select the document with the calibration graph.
  - ✓ The **Calibration** spreadsheet with the current calibration graph and the calculated calibration parameters is displayed. The results of the concentration analysis with calibration are entered directly into the sample table. Concentrations outside of the calibrated range are placed in brackets.



The **Calibration** spreadsheet contains the following information:

- Source of the calibration graph (measured in this document or loaded from a file)
- Regression model
- Analyses wavelengths or calibration formula used
- Regression coefficients A, B and C if calculated in the regression model
- Coefficient of determination R^2
- Pathlength of the cell (for information only, not used in the calculation)
- Date and time of the measurement

Limit value

The **Limit value** function permits the identification of measured values above or below a defined value.

- On the worksheet, select the menu item **Evaluation | Limit value**.
- Enter the value in the **Limit value** input field.

- In the list, select the option **Upper limit** or **Lower limit**.
  - ✓ On the **Limit value** spreadsheet, the samples that are below/above the specified value are shown. In addition, the values in the sample table are highlighted in bold and marked with a "!".

See also

Using formulae [▶ 36]

6.3.3 Processing photometric data mathematically

You can apply mathematical functions, e.g. the addition of a constant, to the measurement data. The measurement data and existing analyses on a worksheet are then recalculated and updated. You can apply the mathematical operations consecutively in the same worksheet.

NOTE

If the measurement data in the **Measurement** worksheet is changed, e.g. due to re-measurement or by disabling a sample, the data in the other worksheets is not updated.

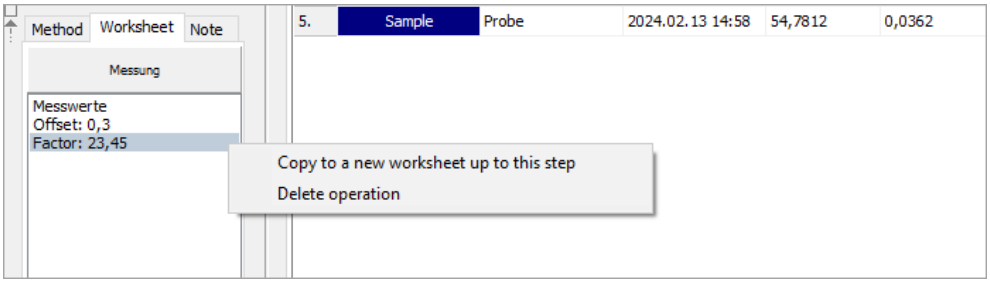
The following functions are available in the **Evaluation** menu:

- Addition of an offset
- Multiplication with a factor
- Convert values to transmittance [%T] or absorbance

Reverse data editing

The operations report can be found on the left-hand side of the document on the **Worksheet** tab. Here, the operations are listed one after the other. By clicking on the corresponding operation, the editing step is displayed. You can undo operations on this tab.

- Right click on the last operation to be reversed.
- Select one of the two options in the context menu:
  - **Copy to a new worksheet up to this step**
    A new worksheet is opened and the data is copied with the change history up to the selected operation. All operations remain intact in the previous worksheet.
  - **Delete operation**
    All steps including the selected operation are deleted in the current work sheet.
  - ✓ The operations are copied to a new worksheet or undone according to the selected option.



Offset

This function is used to add a constant to the measured values. The value of the constant may be both positive or negative. This allows for interferences to be simulated or compensated.

- On a new worksheet, select the menu item **Evaluation | Offset**.
- Enter the value in the **Offset** field.

✓ The measured values and analyses are re-calculated and the displays updated.

Factor

This function is used to multiply the measured values by a constant. The multiplication of an absorbance value by a constant theoretically corresponds to a change in the path-length or concentration of the sample.

- On a new worksheet, select the menu item **Evaluation** | **Factor**.
- Enter the value in the **Factor** field.

✓ The measured values and analyses are re-calculated and the displays updated.

Convert to transmittance[%T] / Convert to absorbance

These functions make it possible to convert the measured values from absorbance to transmittance [%T] and vice versa.

- On a new worksheet, select the menu item **Evaluation** | **Convert to transmittance[%T]** or **Convert to absorbance**.

✓ The measured values are converted and the displays are updated.

6.4 Example measurement in the Photometry module

In the example, the concentration in three samples is determined using the formula c = A(446 nm) * 24.3. The standard cell holder is used for the measurement. The gray filters of the Hellma standard filter set can be used as samples.

The following steps must be carried out:

1. Create the document in the module.
2. Open method and enter parameter.
3. Start measurement.

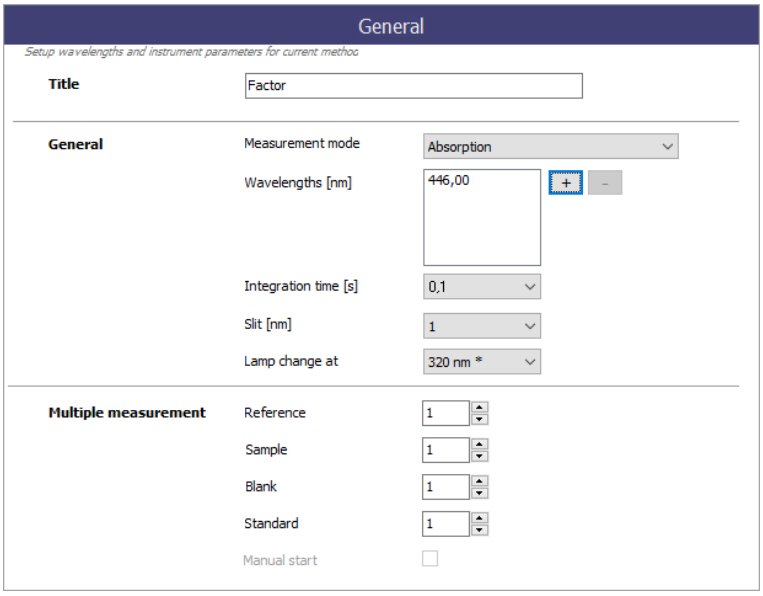
Preparing a document

- Select the menu item **Modules** | **Photometry** or click on the icon in the task bar.

Defining method parameters

- Click on **Method setup** in the document window.
- Enter the parameters according to the screenshot on the screens of the **Photometry - Settings** method window (see below).
- Confirm the parameters in the method window by clicking on **Ok** and return to the document window.

General screen



Enter 446 nm as wavelength:

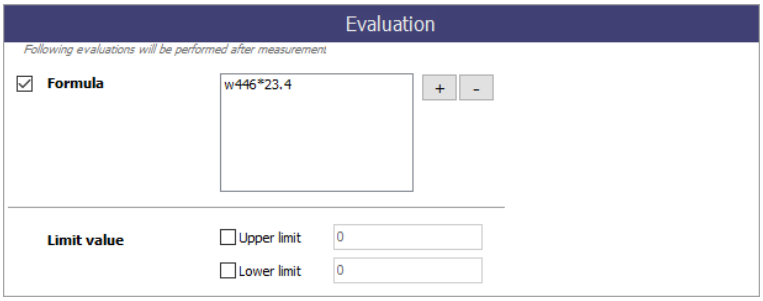
- Double click on the preset value "500".
- Enter the value "446" and click on + to transfer it to the list.

Note: The slit setting only applies for the SPECORD 210/250 Plus.

Measurement cycles, Start measurement, Accessory screens

Make no entries.

Evaluation screen



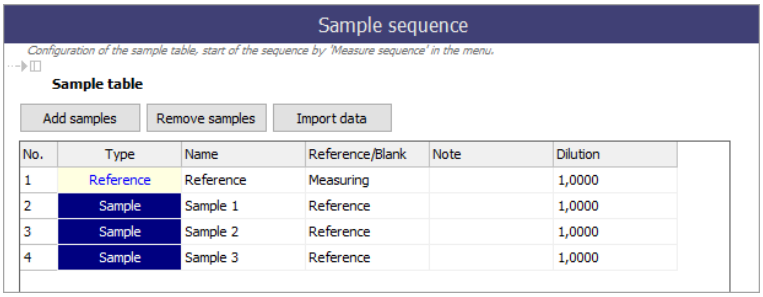
Enter the formula "w446 * 24.3":

- Click +. The formula editor appears.
- Click on **w446**.
- Click on "*", click at the end of the formula in the editor field and then enter the value "24.3".
- Enter "mg/l" in the Unit of results field. Click **Ok** to confirm the entries.

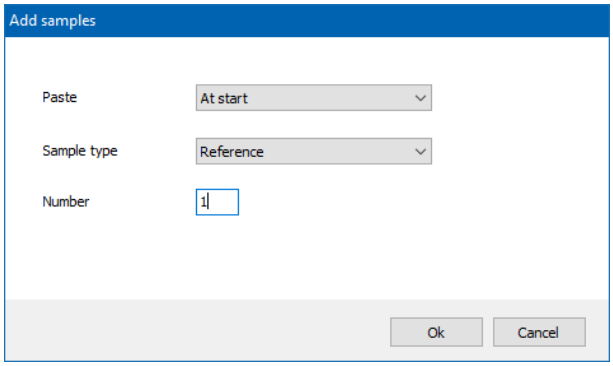
Calibration screen

Make no entries.

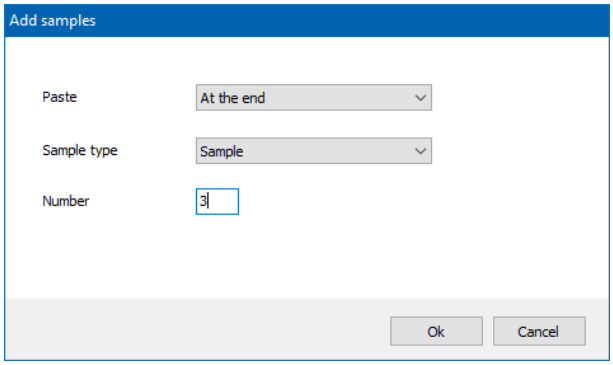
Sample sequence screen



- Click on **Add samples** and set a reference at the start of the sample table:



- Click on **Add samples** again and add 3 samples to the end of the sample table:



- In the first line of the sample table, enter "Reference" in the **Name** field and confirm with the Enter key.
- In the second line, enter "Sample 1" as the name and confirm with the Enter key.
- Hold down the mouse button and select the three consecutive sample name fields, including the "Sample 1" field.
- Right click on the highlighted choice and select the command **Fill with ascending values** from the context menu.

Archive automatically screen

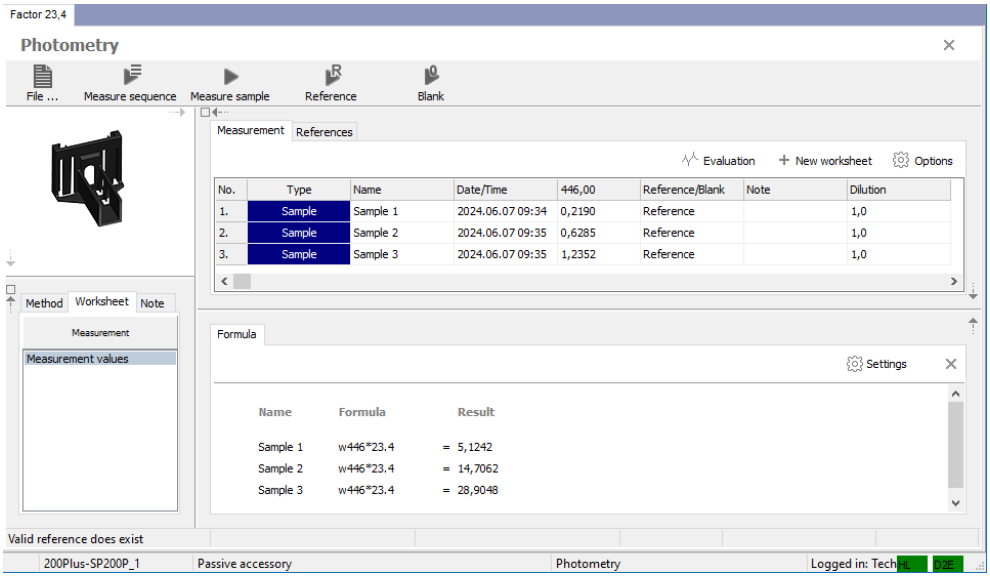
Make no entries.

Note screen

Enter the text "Example of a concentration analysis with factor".

Performing the measurement

- Click on in the document window.
  The start information for measuring the reference is displayed.
- Insert the reference sample and click on **Yes** to start the measurement.
- The reference measurement is performed. A prompt to measure sample 1 is displayed.
- Insert sample 1 and click on **Yes** to start the measurement.
- Measure sample 2 and sample 3 in the same manner.
  - ✓ The measurement results are displayed in the sample table of the **Measurement** worksheet. The results of the formula calculation are displayed on the **Formula** tab at the bottom of the worksheet.


Factor 23,4
Photometry
File ...
Measure sequence
Measure sample
Reference
Blank
Measurement
References
Evaluation
New worksheet
Options
No. Type Name Date/Time 446,00 Reference/Blank Note Dilution
1. Sample Sample 1 2024.06.07 09:34 0,2190 Reference 1,0
2. Sample Sample 2 2024.06.07 09:35 0,6285 Reference 1,0
3. Sample Sample 3 2024.06.07 09:35 1,2352 Reference 1,0
Method
Worksheet
Note
Measurement
Measurement values
Formula
Settings
Name Formula Result
Sample 1 w446*23.4 = 5,1242
Sample 2 w446*23.4 = 14,7062
Sample 3 w446*23.4 = 28,9048
Valid reference does exist
200Plus-SP200P_1
Passive accessory
Photometry
Logged in: Tech

7 Spectrum module

In the **Spectrum** module, spectra are recorded and analyzed. The module contains the following functions:

- Quantitative analysis with calibration function
- Analysis of measured values at defined wavelengths of the spectrum
- Comprehensive mathematical data processing of the spectra
- Automatic peak search
- Sections through a spectra array as a result of a kinetics measurement or a measurement with Peltier temperature controlled accessories

Open **Spectrum** module

- Open the **Spectrum** module by clicking on the icon in the task bar of the main window.

- Alternatively, select the menu item **Modules** | **Spectrum**.
  - ✓ A new document is opened in the workspace.
- Each additional click on the icon opens another new document on the workspace.

All functions of the document windows of the **Spectrum** module are assigned to the measurements of spectra and their analyses. You can now create a method and start a measurement with analyses based on it.

7.1 Method configuration in the Spectrum module

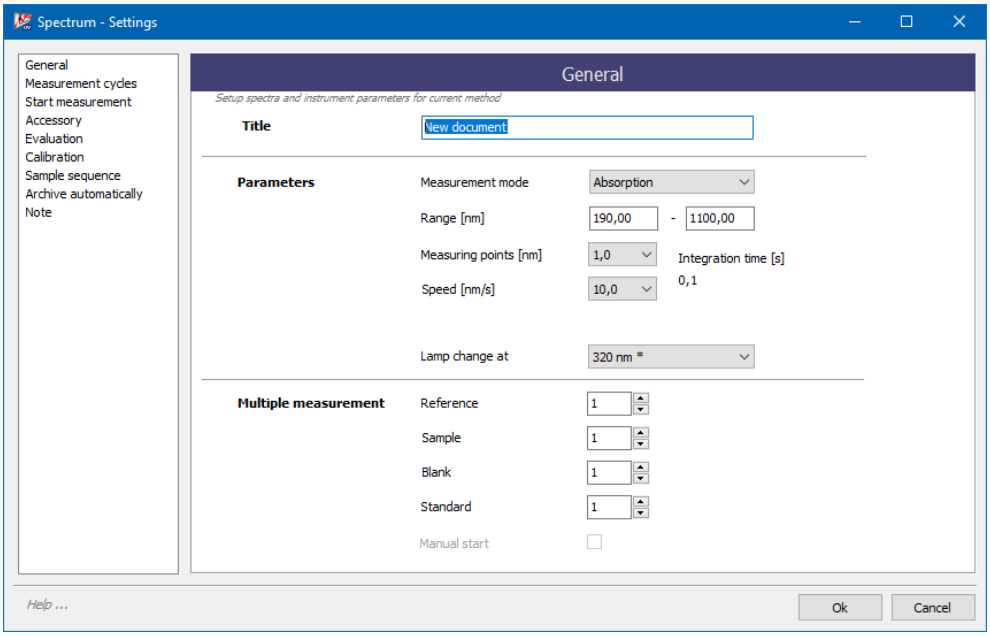
This section includes all configurations that can be made for a method in the **Spectrum** module.

Creating a method

- Click on **Method setup** in the document window to open the method window.
- Make the settings on the screens of the method window.
- Finish entering the parameters by clicking on **Ok**.
  - ✓ The method parameters are output on the left side of the document window on the **Method** tab. The icons for starting the measurement appear in the toolbar of the document window.

7.1.1 Spectrum - Settings | General

The basic measurement settings are configured in the **Spectrum - Settings** | **General** window.



Title

Enter the title of the document here, which is displayed in the document tab. You can edit the title later.

Parameters

In this area, select the parameters for the optical measurement.

Option	Description
Measurement mode	The following measurement modes can be selected: ■ **Transmittance** ■ **Absorption** ■ **Reflectance** (only for reflectance measuring attachments and integrating sphere)
Range [nm]	Enter the wavelength range for the measurement in the input fields
Measuring points [nm]	Select distance between measuring points.
Speed [nm/s]	Select measuring speed
Integration time	Time for recording a measuring point This value is calculated automatically.
Slit [nm]	For SPECORD 210/250 PLUS Select spectral width (optical resolution): 0.2; 0.5; 1; 2; 4 nm **Note**: The 0.2 nm slit was not yet installed in older SPECORD 210/250 PLUS. It is not available for selection for these devices.
Lamp change	Select the wavelength of the change from UV lamp to Vis lamp The preset lamp change at 320 nm guarantees an optimal distribution of energy across the entire wavelength range of the spectrometer. If you are only working in UV or Vis range, you may also measure with the selected lamp using the options **UV only** or **Vis only**.

Multiple measurement

You can carry out a measurement several times in succession and use the mean for further calculations and analyses. For measurements with very little energy, e.g. samples with high absorbance, this procedure can improve the signal-to-noise ratio and increase the measurement accuracy.

Option	Description
Multiple measurement	If necessary, enter the number of measurement repetitions for the sample types **Reference**, **Blank**, **Sample** and **Standard**.

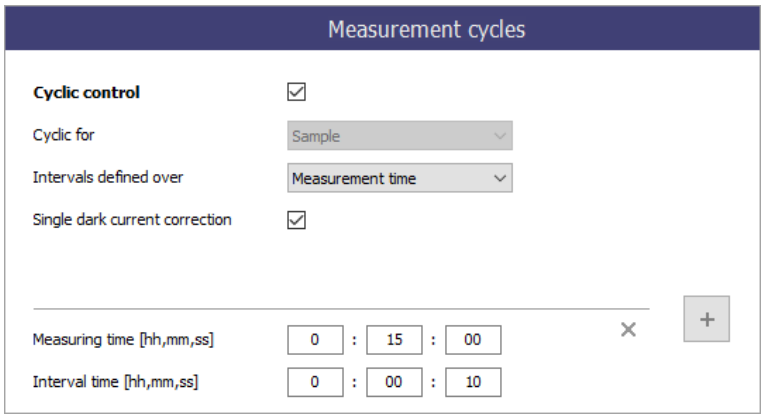
Option	Description
	If the **Manual start** option is enabled, a request to start is made for each individual measurement within a repetition.

See also

Edit document title [▶ 23]

7.1.2 Spectrum - Settings | Measurement cycles

On the **Measurement cycles** screen, you can define time-staggered measurement repetitions (kinetic measurements) in a sample. As a result of the measurement, a spectra array is created for each sample, through which sections are made at defined wavelengths. The resulting kinetic spectra (change in absorbance/transmittance over time) can be further analyzed in the **Kinetics** module.



Option	Description
Cyclic control	When activated, enables the inputs for cyclical measurements
Cyclic for	Only when using cell changers or autosamplers **Sample** The entire reaction-kinetic measurement is performed in one sample and then the measurement started in the next sample. All samples in the sequence are processed consecutively in this manner. The measurement is suitable for fast reaction kinetics. If the reaction is to be started immediately before the measurement, option **Manual start** must be enabled on the **Start/Stop measurement** screen. **Batch** In this mode the sample measurements are staggered. Within an interval, all samples of the sequence are measured, starting with the first sample. The next interval then re-starts with measuring the first sample. In this manner the measurement is continued until the last interval. One batch of the cell changer/APG is measured at a time. Once all measurements for this batch (either by sample or batch) have been processed, the samples are replaced in the accessories and the measurement of the next batch is started.
Intervals defined by	**Measurement points** The number of measuring points/repeated measurements and the interval time must be defined for the measurement. The resulting total measuring time is calculated automatically.

Option	Description
	Measurement time The interval time and a total measurement time must be defined for the measurement. The resulting number of measuring points is calculated automatically.
Single dark current correction	By default, this option is enabled. The dark current is determined before the first measurement and the measured values are corrected accordingly. If the option is disabled, a dark current correction is performed before each measurement.
+	Insert time period For time-controlled cyclical measurements, several time periods can be defined, each with different interval times.

Further information on the settings for kinetic measurement can be found in the **Kinetics** module.

See also

Kinetics - settings | Measurement cycles [▶ 87]

7.1.3 Spectrum - Settings | Start measurement

You define the measurement start of a sample on the **Start measurement** screen. The following start options are available:

Option	Description
Autom. without waiting time	The measurement starts immediately after you click on or .
Autom. with waiting time	After clicking on or , the measurement only starts after the wait time has elapsed.
Manually without waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the measurement starts immediately.
Manually with waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the wait time elapses first and then the measurement starts.
Waiting time	Time delay for start options with wait time

7.1.4 Spectrum - Settings | Accessory

The parameters in the **Spectrum - Settings** | **Accessory** window depend on the installed accessory.

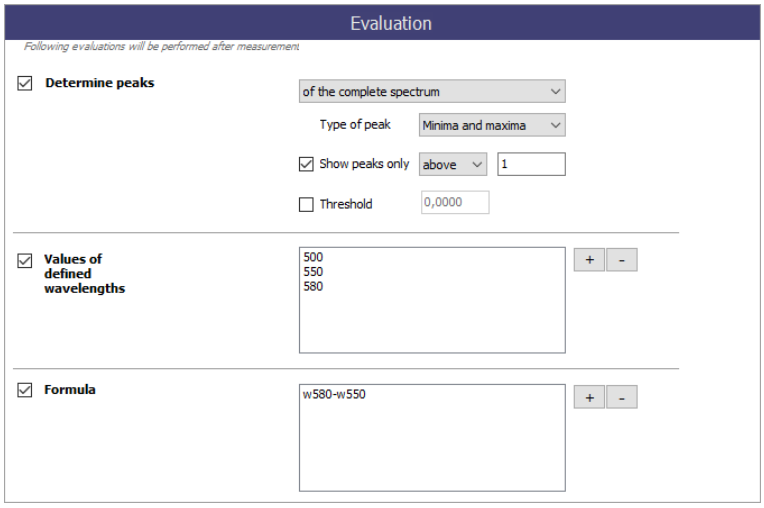
See also

Using accessories [▶ 39]

7.1.5 Spectrum - Settings | Evaluation

You can perform the following analyses in the **Spectrum - Settings** | **Evaluation** window:

- Peak determination
- Display of the measured values at selected wavelengths
- Input of formulae



Determine peaks

By enabling the checkbox **Determine peaks** extreme values are automatically searched for based on specified criteria. The peaks are highlighted in the graphical display of the measurement curve and displayed on a separate tab in the analysis area.

Option	Description
Selection list	**of the complete spectrum** Search for all peaks in the measuring range **only in defined ranges of the spectrum** Search for peaks in defined spectral ranges
Type of peak	Select the type of peak: **Minima**, **Maxima** or **Minima and maxima**
Show peaks only	Absolute limit for the display of peaks Peaks are only displayed if they are above or below the entered ordinate value.
Threshold	Difference between peak height and the adjacent local maximum/minimum Peaks are only displayed if they exceed (maximum) or fall below (minimum) the entered threshold value.

Values of defined wavelengths

You can select measured values at defined wavelengths of the spectrum. These measured values are displayed in the sample table in the analyses of the document window.

- Activate the **Values of defined wavelengths** checkbox.
- Click on + , enter the wavelength within the spectral range in the input field, and click on + again to transfer it to the list.

Formula

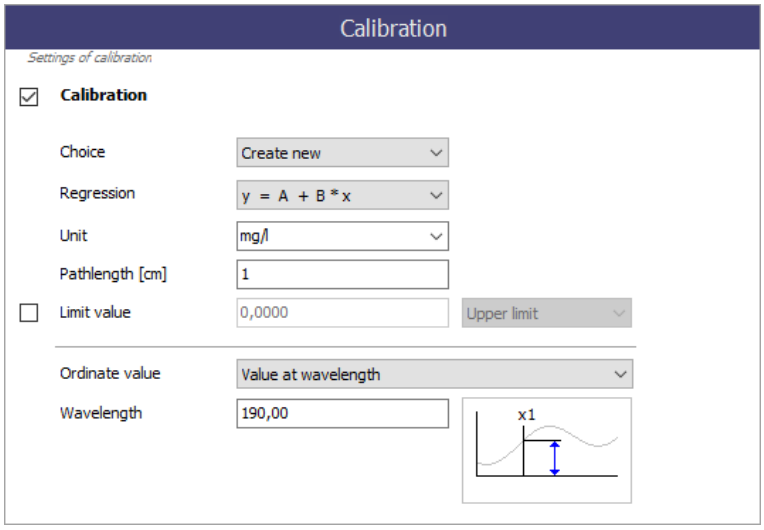
You can link the measured values of one or more samples in a formula. This enables complex analyses of the spectra.

See also

Using formulae [▶ 36]

7.1.6 Spectrum - Settings | Calibration

You can define analysis parameters for a quantitative analysis with calibration on the **Calibration** screen.



To determine the concentration using a calibration with standards, activate the **Calibration** option and configure the following settings:

Option	Description
Selection	**Create new** Record calibration within the following measurement series You must define the standard samples and their concentration in the sample sequence. **Load from file** Load calibration parameters from an existing method
Regression	Regression type of the calibration function $y = B * x$ $y = A + B * x$ $y = A + B * x + C * x^2$
Unit	Unit of the analysis result
Thickness	Pathlength of the cell This value is for information only and is saved with the method parameters.
Limit value	Define an upper or lower limit value for the analysis result Results above or below this limit value are identified with "!" in the results table.

The **Spectrum** module can use different values from the spectrum for the calibration:

Option	Description
Value at wavelength	Measured value at a selected wavelength
Formula	Result of a formula calculation Clicking on ... displays the formula editor. As functional argument, the peaks in defined partial ranges or the values at defined wavelengths selected on the **Evaluation** screen are available.
Band amplitude	Automatically determined peak maximum between **Wavelength 1** and **Wavelength 2**
Area	Peak area between **Wavelength 1** and **Wavelength 2** When enabling the **Correction** option, a baseline correction of the peaks is performed.
Corrected band	Baseline-corrected peak height

Option	Description
	Corrected band x Enter the wavelength of the peak **Wavelength 1** and **Wavelength 2** Enter the wavelengths between which the baseline correction takes place
Derivative	1st to 4th derivative of the spectrum between two wavelengths **Wavelength 1** and **Wavelength 2** Wavelength range for analyzing the derivative **order** Order of the derivative **Supporting points** Number of support points for the derivative with the integrated smoothing filter **Range** Value for the calibration (**from 0 to maximum**, **from 0 to minimum** or **from min. to max.**)

7.1.7 Spectrum - Settings | Sample sequence

On the **Sample sequence** screen, you can specify the sequence of samples for a subsequent measurement, which you can start using the icon in the document window. You can also create a sample sequence directly before a measurement.

Requirements for the sample sequence

- Activating the calibration requires entering a sequence with standard samples.
- When using cell changers and autosamplers, the samples are assigned to the sample positions in the accessories.
- If the sample sequence is empty, the **Sequenz settings** window will first appear when starting the measurement of the sample sequence. This window may only be exited once there has been at least one sample defined.

See also

Sample sequences [▶ 29]

7.1.8 Spectrum - Settings | Archive automatically

You can automatically save, export, and print the measurement data and its analysis. This allows you to standardize your data archiving processes and ensure that data is not lost. Select the target files and report templates in the **Archive automatically** screen. Additionally, automatic archiving must be activated program-wide in the **Options** window and the times for the individual archiving functions must be selected.

See also

Automatically archive measurement data [▶ 28]

7.1.9 Spectrum - Settings | Note

A note on the method may be optionally entered on the **Note** screen.

7.2 Performing measurements in the Spectrum module

The prerequisite for starting a measurement is that a new method has been created or loaded in the document window. The measurement can be started with a sample sequence stored in the method or as individual measurement.

The following icons are displayed for the measurements:

Icon	Description
Measure sequence	Start sample sequence If you have not saved any sample sequences to the measurement parameters, the **Sequenz settings** window will appear after you click on this icon. This window may only be exited once there has been at least one sample defined.
Measure sample	Start individual sample measurement independent of the sample sequence configured
Reference	Measure reference A separate reference measurement is required if the sample sequence does not start with a reference measurement or no reference is available that matches the current method parameters.
Stop	Stop current measurement and do not continue
Suspend sequence	Interrupt the measurement and continue at a later time The current sample measurement is completed. The pending sample sequence is then displayed and can be edited.
	Available for cartridge sipper system and APG sampler: Switch pump on or off and convey sample or stop conveying
	Available for APG sampler: Lower or raise sample cannula
	Available for APG sampler with stirring function: Switch stirrer on or off

Measure reference

If the sample sequence does not have a reference at the first location, the reference must be recorded separately.

- Place the reference into the sample space.
- Click on **Reference** and confirm the prompt about the reference measurement.
  - ✓ The reference measurement is run. All subsequent measurements are corrected with this reference until the measuring parameters are modified by a new method configuration or the next reference measurement takes place.

Start first sequence

With the start of the sample sequence the samples are processed in the order specified in the sample table.

- Place the first sample of the sequence in the sample space or fill cell changer/autosampler with samples.
- Click on **Measure sequence**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.

✓ The sample sequence is processed. The measured values and analyses are displayed in the document window.

Interrupting or stopping the sequence

An ongoing measurement may be interrupted and then continued or stopped completely.

- Click on **Stop** to stop the measurement.
  ✓ The measurement of the sequence is stopped and cannot be continued. Measurement data recorded up to this point remain intact and may be processed further.
- Click on **Suspend sequence** to interrupt a measurement and continue it later.
  ✓ The current sample measurement is ended and then the processing is interrupted. The measurement pause may be used to view and edit the ongoing sample sequence.

Start next sequence

After processing the first sample sequence, the sequence may be started again or re-edited on other occasions. This is also possible if the document has already been saved and re-opened to display the results.

- Click .
  The **Edit sequence** window appears with the sequence stored in the method.
- If necessary, compile a new sequence.
- Confirm the setting in the **Edit sequence** window by clicking on **Ok**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  ✓ The current sequence is processed and the data appended to the existing measurement table and analyses.

Performing single measurements

Regardless of the sequence configured, single samples of sample type **Sample** may be measured and appended to the measurement table and analyses.

- Place the sample into the sample space.
- Click on **Measure sample**.
- Follow further on-screen prompts for starting the measurement.
  ✓ The measurement is run and the data is appended to the existing measurement table and analyses.

Tip

If measurements of other sample types are to be appended, click on **Measure sequence** and enter a sequence with the corresponding samples.

Re-measuring samples

Outliers of a measurement may be re-measured and thus values from a measuring series that differ greatly replaced by new values. The re-measurement of samples is always recorded in the audit trail. For the re-measurement of a probe, you will need to switch to the **Measurement** worksheet.

- Place the sample in the sample space.
- Right click on the row of the sample to be re-measured. For multiple measurements, you can select a single value by clicking with the right mouse button.
- In the context menu, select **Remeasure sample**.
- Follow further on-screen prompts for starting the measurement.
  ✓ The measurement is run and the measured value replaced in the sample table. The existing analyses are updated.

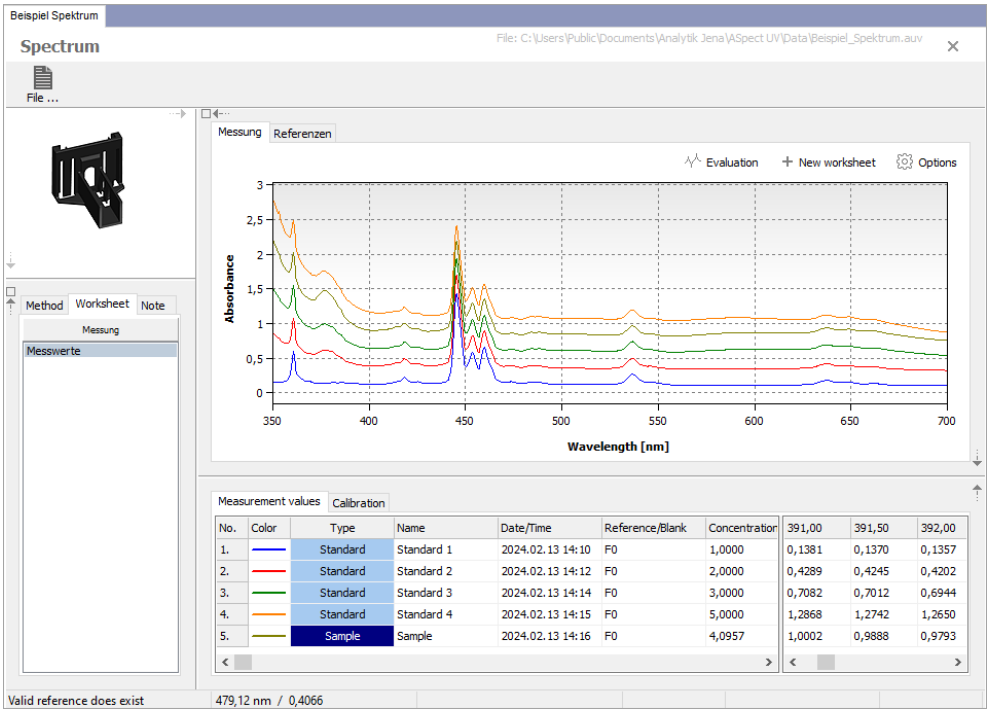
NOTE

If additional worksheets besides the **Measurement** worksheet are already available in the document, these are not updated during a re-measurement.
When using cell changers or APG the sample to be re-measured must be placed in the same position in the accessories. The position in the accessories can be displayed in the sample table on the worksheet.
Time-cyclical measurements cannot be re-measured.

7.3 Displaying, evaluating, and processing results in the Spectrum module

This section explains the particularities of the results display and analysis in the Spectrum module.

Document window in the Spectrum module with several spectra



No.	Description
1	Worksheets with the display of sample and reference spectra and further analyses
2	**Measurement values** tab with the individual measured values of the samples
3	Tab with data analyses
4	Tab with information on method settings and mathematical data handling on the worksheets

Measurement worksheet

The **Measurement** worksheet contains the measurement data. The spectra are displayed in the upper half of the worksheet.

The **Measurement values** tab in the lower half of the worksheet contains the sample table in the order of the measurements and the table with the digital measured values. The other tabs contain data analyses that have already been defined in the method. You can add to and edit these analyses.

Sample table

The display of the sample table can be configured freely. After right clicking on the table header the following parameters can be selected in the context menu:

- Number in the sequence
- Position in accessories when using cell changer or autosampler
- Color of the measurement curve in the chart
- Batch when using cell changer or autosampler
- Sample name
- Sample type
- Date and time of the measurement
- Temperature for methods with Peltier-tempered accessories
- Notes
- Sample concentration for concentration determination with calibration
- Dilution and sample weight
  These entries are only taken into account for concentration determinations with calibration.
- Sample-specific variables A – H for calculations in formulae

Via Drag&Drop the order of the table columns can be changed. The individual measurements for each sample are listed adjacent in a separate table.

Reference worksheet

The reference values are listed on the **Reference** worksheet.

New worksheet

You can create additional worksheets in the document window and carry out further analyses on them. In this way, you can create different analyses side by side in one document (file). The **New worksheet** worksheet is created after clicking on + **New worksheet** in the **Measurement** worksheet. The unedited, original measurement data is first copied to the new worksheet and can then be edited.

See also

Show spectra and measurement curves on the worksheet [▶ 19]

7.3.1 Display options for the results in the Spectrum module

The following functions are available for display in the **Spectrum** module:

- Scale curves
- Add text to curves (text box)
- Select curves/samples
- Change the color of curves
- Hide a curve (deactivate a sample)

See also

Show spectra and measurement curves on the worksheet [▶ 19]

7.3.2 Analyzing spectral data

The data analyses offered in this method can also be performed later. The functions have been compiled in the menu **Evaluation** that is available on every worksheet. The analyses always relate to the measured values of the respective worksheet. If the measured values are processed with mathematical functions, the analysis on this worksheet is adjusted accordingly.

The analyses are output in their own spreadsheet in the bottom part of the worksheet.

The following analyses are available in the **Spectrum** module:

- Automatic peak search
- Display measured values at defined wavelengths in tabular form
- Use measured values in a function/formula
- Load calibration data for a concentration analysis

Edit analysis

The analysis parameters can be edited for existing analyses.

- Click on **Settings** in the spreadsheet of the analysis and change the analysis parameters in the dialog window.
  - ✓ The analysis is updated.

Delete analysis

Analyses that are not required may be deleted.

- At the top right of the spreadsheet of the analyses click on .
  - ✓ The analysis is removed from the worksheet.

Peaks

An automatic peak search can be started with the **Peaks** function.

- On the worksheet, select the menu item **Evaluation** | **Peaks**.
- Select the following options in the **Settings peak list** window.

Option	Description
Selection list	**of the complete spectrum** Search for all peaks in the measuring range **only in defined ranges of the spectrum** Search for peaks in defined spectral ranges
Type of peak	Select the type of peak: **Minima**, **Maxima** or **Minima and maxima**
Show peaks only	Absolute limit for the display of peaks Peaks are only displayed if they are above or below the entered ordinate value.
Threshold	Difference between peak height and the adjacent local maximum/ minimum Peaks are only displayed if they exceed (maximum) or fall below (minimum) the entered threshold value.

- Click **Ok** to confirm.
  - ✓ The peak list is displayed.

Values of defined wavelengths

The **Values of def. wavelengths** function compiles measured values of selected wavelengths in a table.

- On the worksheet, select the menu item **Evaluation** | **Values of def. wavelengths**.
- Click on +, enter the desired wavelength in the input field and click on + again to transfer it to the list.
  - ✓ The value table is displayed.

Formula

Use the **Formula** function to link the measured values of one or more samples in a formula.

- On the worksheet, select the menu item **Evaluation** | **Formula**.
- Click on + and create the formula using the formula editor.
- If necessary, add further formulae in the same way.
  - ✓ The results are displayed on the **Formula** tab.

Calibration

The **Calibration** function is available if a document does not contain its own calibration with standards. You can use this function to subsequently load the calibration data from other files and carry out a quantitative analysis of the measured values. Only the calibration parameters are loaded and not the standards.

- On the worksheet, select the menu item **Evaluation** | **Calibration**.
- Enable the **Calibration** option.

- Click on **Load** and select the document with the calibration graph.
  - ✓ The **Calibration** spreadsheet with the current calibration graph and the calculated calibration parameters is displayed. The results of the concentration analysis with calibration are entered directly into the sample table. Concentrations outside of the calibrated range are placed in brackets.

The **Calibration** spreadsheet contains the following information:
- Source of the calibration graph (measured in this document or loaded from a file)
- Regression model
- Analyses wavelengths or calibration formula used
- Regression coefficients A, B and C if calculated in the regression model
- Coefficient of determination R^2
- Pathlength of the cell (for information only, not used in the calculation)

See also

Using formulae [▶ 36]

7.3.3 Processing spectral data mathematically

You can apply mathematical functions, e.g. the addition of a constant, to the measurement data. The measurement data and existing analyses on a worksheet are then recalculated and updated. You can apply the mathematical operations consecutively in the same worksheet.

NOTE

If the measurement data in the **Measurement** worksheet is changed, e.g. due to re-measurement or by disabling a sample, the data in the other worksheets is not updated.

The following functions are available in the **Spectrum** module for mathematical processing:
- Cut out
- Time cut
- Temperature cut
- Offset
- Factor
- Smooth
- Derivative
- Normalization
- Interpolation
- Baseline correction
- Auto baseline correction
- Convert to transmittance[%T] / Convert to absorbance
- Average spectrum
- Spectra formula

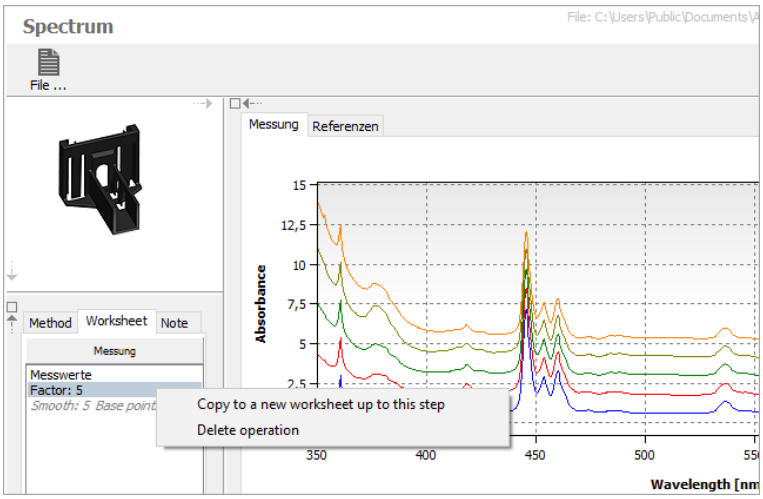
Reverse data editing

The operations report can be found on the left-hand side of the document on the **Worksheet** tab. Here, the operations are listed one after the other. By clicking on the corresponding operation, the editing step is displayed. You can undo operations on this tab.

- Right click on the last operation to be reversed.
- Select one of the two options in the context menu:
  - **Copy to a new worksheet up to this step**
    A new worksheet is opened and the data is copied with the change history up to the selected operation. All operations remain intact in the previous worksheet.

– **Delete operation**
  All steps including the selected operation are deleted in the current work sheet.

✓ The operations are copied to a new worksheet or undone according to the selected option.



Cut out

Use this function to select a curve section for display and further processing/analysis. The values outside the selected range are no longer taken into account.

- On the worksheet, select the menu item **Evaluation** | **Cut out**.
  ✓ The cursor changes to a vertical line with the label "Range".
- Click on the left or right limit of the x-coordinate range to be cut out and with the mouse button held down move the cursor to the opposite limit. Then release the mouse button.
- Alternatively enter the range limits in the **Cut out** window in the **Start** and **End at X :** fields.
- Confirm the entry in the **Cut out** window by clicking on **Ok**.
  ✓ The curve display is updated. Now only the selected area of the measurement graph is visible.

Time cut

If you define a time-controlled interval measurement in the method settings, a three-dimensional spectral array is created with the coordinates wavelength, absorbance or transmittance [%T] and time. With this function, a section is taken through the set of curves at a defined wavelength. The result is a curve with the time-related change of the measured value at the selected wavelength. This kinetic curve is displayed in a new document window of the **Kinetics** module and can be analyzed and further processed there.

- On the worksheet, select the menu item **Evaluation** | **Time cut**.
- In the input field enter the point on the x-axis (here wavelength) and click on the corresponding wavelength in the spectrum.
  ✓ The resulting kinetic curve is displayed in a new document of the **Kinetics** module.

Temperature cut

If you define a spectral measurement with Peltier temperature controlled accessory in the **Variable** temperature mode in the method settings, a three-dimensional spectral array is created with the coordinates wavelength, absorbance or transmittance [%T] and temperature. This function is used to make a section through the spectral array at a selected wavelength. The result is a temperature curve in which the absorbance or transmittance is plotted against the temperature. The temperature curve is displayed in a new document window of the **Thermometry** module and can be analyzed and further processed there.

- On the worksheet, select the menu item **Evaluation** | **Temperature cut**.
- In the input field enter the point on the x-axis (here wavelength) and click on the corresponding wavelength in the spectrum.
  - ✓ The temperature curve is displayed in a new document of the **Thermometry** module.

Offset

This function is used to add a constant to the measured values. The value of the constant may be both positive or negative. This allows for interferences to be simulated or compensated.

- On a new worksheet, select the menu item **Evaluation** | **Offset**.
- Enter the value in the **Offset** field.
  - ✓ The measured values and analyses are re-calculated and the displays updated.

Factor

This function is used to multiply the measured values by a constant. The multiplication of an absorbance value by a constant theoretically corresponds to a change in the pathlength or concentration of the sample.

- On a new worksheet, select the menu item **Evaluation** | **Factor**.
- Enter the value in the **Factor** field.
  - ✓ The measured values and analyses are re-calculated and the displays updated.

Smooth

This function is used to smooth the curve using the Savitzky-Golay method.

- On the worksheet, select the menu item **Evaluation** | **Smooth**.
- In the dropdown list **Base points**, select the number of points to be considered for smoothing in accordance with Savitzky-Golay.
  - ✓ The curve is recalculated and the display is updated.

Derivative

This function is used to calculate the derivative of the 1st to 4th order for the measurement curve with integrated constant smoothing over 5 points and a variable number of interpolation points for the Savitzky-Golay derivative filter (n points). The derived curve can suppress background signals that are superimposed on the measurement and emphasize the specific absorbances more clearly.

A curve can be derived several times. However, the algorithm is specifically adapted to the derivative type, therefore the fourth derivative does not result in the same y-coordinate values as four times the first derivative. Therefore, the same method should always be used for the quantitative analysis.

Especially the derivative of a higher order always results in the "coarsening" of the measurement graph. Therefore, dependent on the width of the measurement graph structure, always select the highest possible number of support points. Smoothing beforehand to suppress the statistical noise is sometimes also recommended. Note that the value range is reduced in accordance with the selected number of support points (n) by the number of values (n-1)/2+2 at both ends of the spectrum. To reduce this effect, you can carry out an interpolation beforehand.

- On the worksheet, select the menu item **Evaluation** | **Derivative**.
- In the **Derivative** list, select the order of the derivative.
- In the list **Base points** select the number of support points to be used for the derivative with integrated smoothing filter.
  - ✓ The derivative is calculated and the display updated. In the audit trail the order of the derivative and the number of support points are documented.

Normalization

This function can be used to spread or compress spectra so that a specified ordinate value is reached at a specific wavelength or peak. To do this, all measured values are multiplied by a normalization factor that was determined for the ordinate value at the wavelength or peak.

Execution - Normalization at a wavelength

- On the worksheet, select the menu item **Evaluation** | **Normalization** | **One point**. The cursor changes to a continuous vertical line with the label "W".
- In the graphic, click on the required wavelength.
- If necessary, edit the wavelength in the **Selected X:** field and enter the desired ordinate value in the **Value of normalization** field.
  - ✓ The normalization factor is determined and each measured value of the spectrum is multiplied by this factor. The measured values and the spectrum display on the worksheet are updated.

Execution - Normalization at a peak

- On the worksheet, select the menu item **Evaluation** | **Normalization** | **Maximum in band**.
  The cursor changes to a vertical line with the label "Range".
- Click on the left or right limit of the peak and with the mouse button held down move the cursor to the opposite limit.
- Edit the wavelengths of the peak limits in fields **Start at X:** and **End point at X:** and enter the desired ordinate value in the **Value of normalization** field.
  - ✓ The peak and the corresponding normalization factor are determined and each measured value of the spectrum is multiplied by this factor. The measured values and the spectrum display on the worksheet are updated.

Interpolation

This function calculates further measured values between the existing measured values of the spectrum. The function can be used to gain intermediate values for a more precise peak determination. The interpolation is optionally linear or with a cubic spline.

- On the worksheet, select the menu item **Evaluation** | **Interpolation**.
- In the **Calculation** list, select the calculation type.
- In the **Measuring points** field, enter the new measuring point distance. The new measuring point distance must be smaller than the original one.
  - ✓ The spectrum is re-calculated and the display updated.

Average spectrum

This function calculates the mean value spectrum from a set of curves.

- On the worksheet, select the menu item **Evaluation** | **Average spectrum**.
  - ✓ The mean value spectrum is calculated and the display updated.

Baseline correction

This function can be used to correct a rising or falling linear background of a band. The linear function of the baseline is determined by two points in the graph.

- On the worksheet, select the menu item **Evaluation** | **Baseline correction**.
  The cursor changes to a vertical line with the label "Range".
- Click with the mouse on the first point in the spectrum, drag the cursor with the mouse button held down to the second point and release.
- In the input window edit the two points (start point and end point) for the linear function, and confirm by clicking **Ok**.

Automatic baseline correction

With the automatic baseline correction a rising or falling baseline of a band is automatically corrected. The linear function of the baseline is placed through the minima on both sides of the peak.

- On the worksheet, select the menu item **Evaluation | Automatic baseline correction**.
  - ✓ The spectrum is re-calculated and the display updated.

Convert to transmittance[%T] / Absorbance

This function converts a spectrum from absorbance to transmittance and vice versa.

- On the worksheet, select the menu item **Evaluation | Convert to transmittance[%T]** (**Absorbance**).
  - ✓ The spectrum is converted and the display updated.

Spectra formula

You can use this function to link the spectra of different samples in a document arithmetically, e.g. to generate an overall spectrum for comparison purposes by adding the spectra of two (or more) known substances.

A condition for linking the spectra to each other is that the spectra are overlayed together in a window. Spectra from different files can be combined in a new window with Copy/Paste.

- On the worksheet, select the menu item Evaluation | Spectra formula.
- Enter the function in the formula editor. The spectra can be selected as arguments in the dropdown list Spectrum selection and inserted into the formula by clicking on . The spectra are numbered in accordance with their order in the Measured values worksheet.
  - ✓ The result is calculated and the display updated.

See also

- Merging spectra from different documents [▶ 83]
- Using formulae [▶ 36]

7.3.4 Merging spectra from different documents

You can use the **Copy** and **Paste** functions to merge and edit spectra from different documents in a new document. The spectra may have different wavelength ranges and measuring point distances.

- In the **Spectrum** module, open all files where the required spectra are located (e.g. Spektrum1.auv and Spektrum2.auv).
- Open a new document by clicking on .
- In the first document (Spektrum1.auv), select all spectra that are to be copied and select the menu item **File ... | Copy**.
- Switch to the new document and insert the spectrum with the menu item **File ... | Paste**.
- Copy the required spectra from the second document (Spektrum2.auv) into the new document in the same way.
  - ✓ The spectra in the new document can now be edited.

7.4 Example measurement in the Spectrum module

A spectrum measurement in the range of 300 ... 900 nm is used as an example. The holmium oxide filter from Hellma's standard filter set can be used as a sample, if available. The measurement is performed with the standard cell holder:

The following steps must be carried out:

1. Create the document in the module.
2. Open method and enter parameter.
3. Start measurement.

Preparing a document

▶ Select the menu item **Modules** | **Spectrum** or click on the icon in the task bar.

Defining method parameters

▶ Click on **Method setup** in the document window.

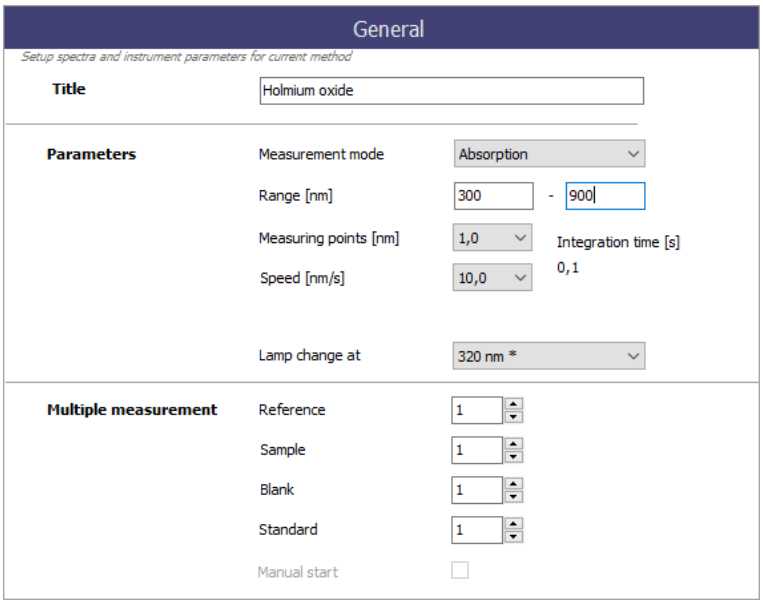
▶ Enter the parameters on the screens of the **Spectrum - Settings** method window (see below).

▶ Confirm the parameters by clicking on **Ok** and return to the document window.

Parameter entries

Enter the parameters as shown in the screenshot.

General screen



Measurement cycles screen

Make no entries.

Start measurement screen

Make no entries.

Accessory screen

Make no entries.

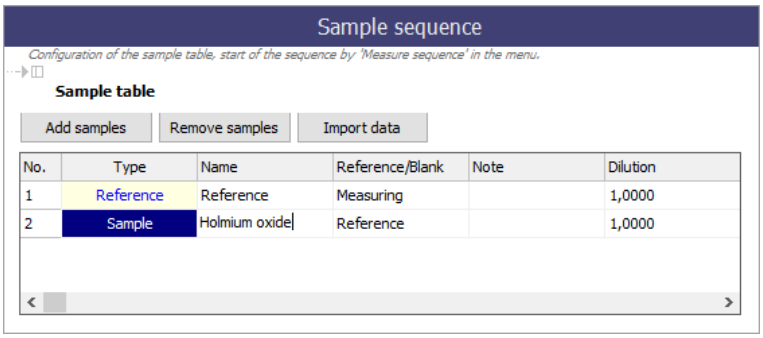
Evaluation screen

Make no entries.

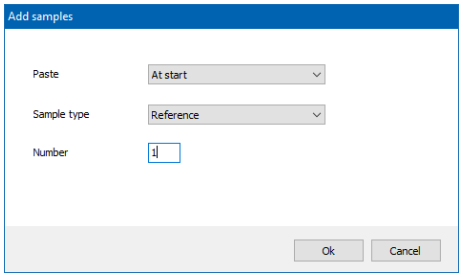
Calibration screen

Make no entries.

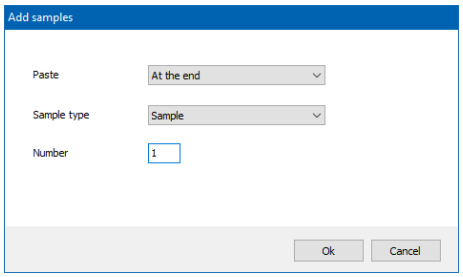
Screen Sample sequence



▶ Click on **Add samples** and set a reference at the start of the sample table:



- Click on **Add samples** again and add a sample to the end of the sample table:



- In the first row of the sample table, enter "Reference" in the **Name** field and confirm with the ENTER key.
- Enter "Holmium oxide" as the name in the second row of the sample table and confirm with the ENTER key.

Archive automatically screen

Make no entries.

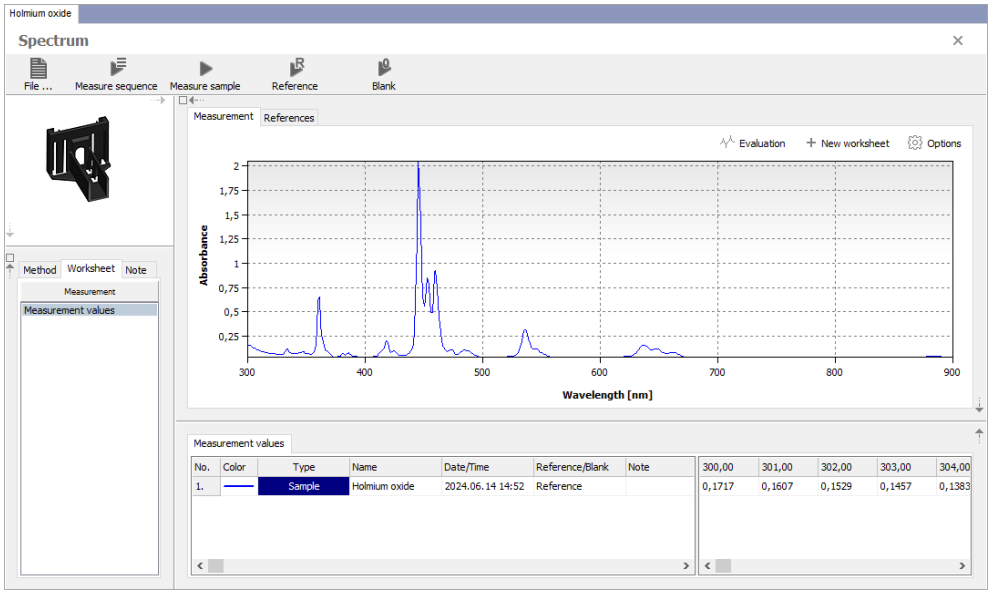
Note screen

Enter "Spectral scan example".

Performing the measurement

- Click on in the document window.
  The start information for measuring the reference is displayed.
- Insert the reference sample and click on **Yes** to start the measurement.
- The reference measurement is performed. A prompt to measure sample 1 is displayed.
- Insert sample 1 and click on **Yes** to start the measurement.

The spectrum and the measured values are output on the **Measurement** worksheet.



8 Kinetics module

In the **Kinetics** module, time-related changes of the measured values at a wavelength are recorded and analyzed.

Open **Kinetics** module

- Open the **Kinetics** module by clicking on the icon in the task bar.

- Alternatively, select the menu item **Modules** | **Kinetics**.
  - ✓ A new document is opened in the workspace.
- Each additional click on the icon opens another new document on the workspace.

All functions of the document windows of the **Kinetics** module are assigned to the kinetic measurements at an individual wavelength and the corresponding analysis. You can now create a method and start a measurement with analyses based on it.

8.1 Method configuration in the Kinetics module

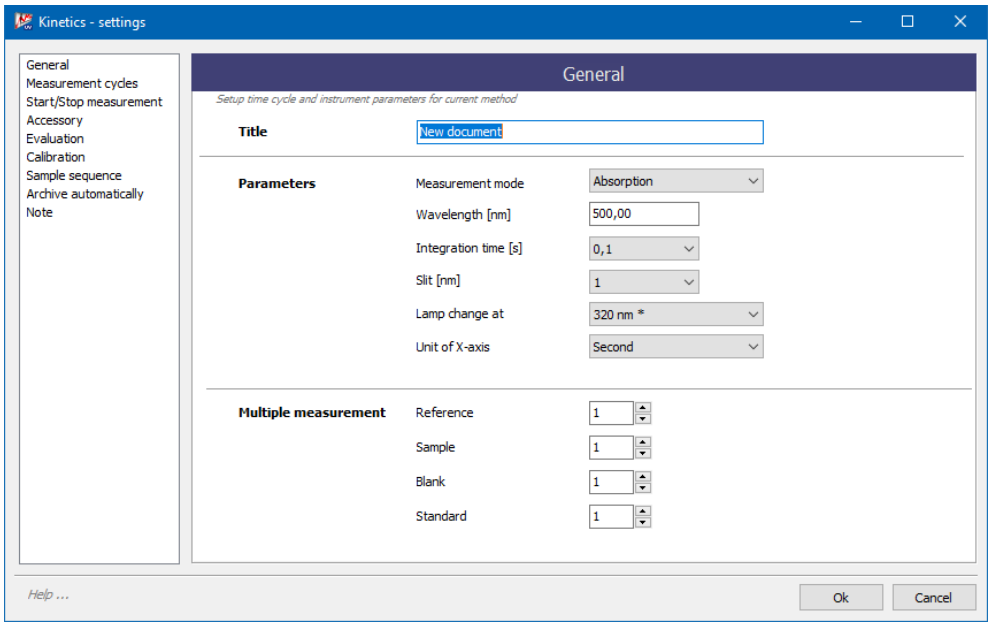
This section includes all configurations that can be made for a method in the **Kinetics** module.

Creating a method

- Click on **Method setup** in the document window to open the method window.
- Make the settings on the screens of the method window.
- Finish entering the parameters by clicking on **Ok**.
  - ✓ The method parameters are output on the left side of the document window on the **Method** tab. The icons for starting the measurement appear in the toolbar of the document window.

8.1.1 Kinetics - settings | General

On the **General** screen, the basic measurement configurations are made.



Title

Enter the title of the document here, which is displayed in the document tab. You can edit the title later.

Parameters

In this area, select the parameters for the optical measurement.

Option	Description
Measurement mode	The following measurement modes can be selected: ■ **Transmittance** ■ **Absorption**
Wavelength [nm]	Enter wavelength for the analysis
Integration time [s]	Select the time for recording a measuring point
Slit [nm]	For SPECORD 210/250 PLUS Select spectral width (optical resolution): 0.2; 0.5; 1; 2; 4 nm **Note**: The 0.2 nm slit was not yet installed in older SPECORD 210/250 PLUS. It is not available for selection for these devices.
Lamp change	Select the wavelength of the change from UV lamp to Vis lamp The preset lamp change at 320 nm guarantees an optimal distribution of energy across the entire wavelength range of the spectrometer. If you are only working in UV or Vis range, you may also measure with the selected lamp using the options **UV only** or **Vis only**.

Time Scan

Option	Description
Unit of X-axis	Select time unit for the X-axis of the kinetics curve

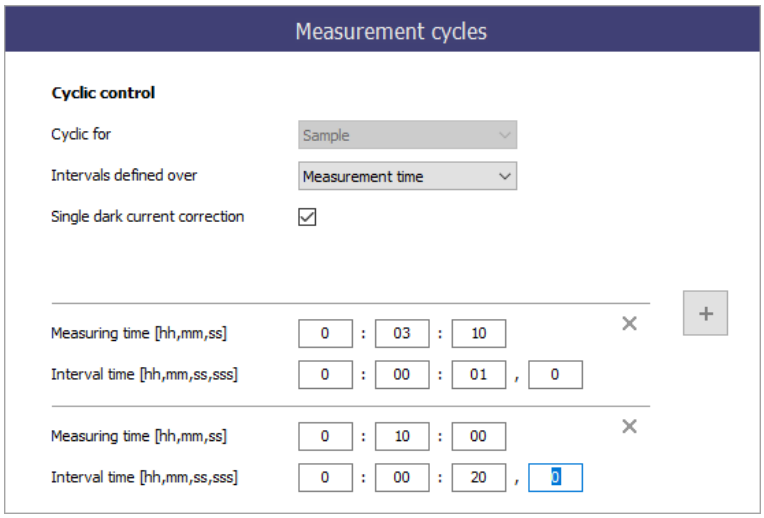
Multiple measurement

You can also define a measurement repetition for each measurement time of the time-cycled measurement. The mean value of the measurement repetition is always used in further analyses.

Option	Description
Multiple measurement	If necessary, enter the number of measurement repetitions for the sample types **Reference**, **Blank**, **Sample** and **Standard**.

8.1.2 Kinetics - settings | Measurement cycles

You define the parameters for the kinetic measurement on the **Measurement cycles** screen.



Parameters for the kinetics measurement

Option	Description
Cyclic for	Only when using cell changers or autosamplers **Sample** The entire reaction-kinetic measurement is performed in one sample and then the measurement started in the next sample. All samples in the sequence are processed consecutively in this manner. The measurement is suitable for fast reaction kinetics. If the reaction is to be started immediately before the measurement, option **Manual start** must be enabled on the **Start/Stop measurement** screen. **Batch** In this mode the sample measurements are staggered. Within an interval, all samples of the sequence are measured, starting with the first sample. The next interval then re-starts with measuring the first sample. In this manner the measurement is continued until the last interval. One batch of the cell changer/APG is measured at a time. Once all measurements for this batch (either by sample or batch) have been processed, the samples are replaced in the accessories and the measurement of the next batch is started.
Intervals defined by	**Measurement points** The number of measuring points/repeated measurements and the interval time must be defined for the measurement. The resulting total measuring time is calculated automatically. **Measurement time** The interval time and a total measurement time must be defined for the measurement. The resulting number of measuring points is calculated automatically.
Single dark current correction	By default, this option is enabled. The dark current is determined before the first measurement and the measured values are corrected accordingly. If the option is disabled, a dark current correction is performed before each measurement.
+	Insert time period For time-controlled cyclical measurements, several time periods can be defined, each with different interval times.

Settings for cyclical measurements over the total measurement time

In this setting, you enter the total measurement time and the interval times for the kinetic measurement.

- Select the **Measurement time** option from the **Intervals defined by** list.
- Select the **Intervals** option from the **Time intervals for** list.
- Click +.
  - ✓ The first time period is inserted.
- Enter the total measuring time in the **Total time** parameter.
- Enter the time between two consecutive measurements in the **Interval time** parameter.
  - ✓ The first time period is defined.
- If necessary, click on + again and add further time periods.

Settings for cyclical measurements via the number of measuring points

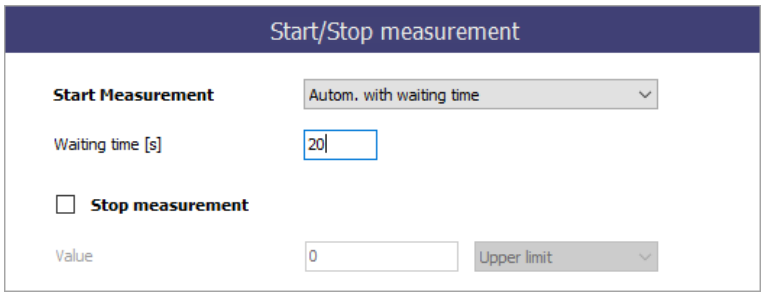
Here you define the kinetic measurement by entering the number of measuring points and the interval time.

- Select the **Measurement points** option from the **Intervals defined by** list.
- Select the **Intervals** option from the Time intervals for list.
- Click +.
  - ✓ The first time period is inserted.

- Enter the number of measurement repetitions in the **Measurement points** parameter. During the measurement, one more measuring point is created than the number entered because a measuring point is already created at the start of the measurement.
- Enter the time between two consecutive measurements in the **Interval time** parameter.
  - ✓ The first time period is defined.
- If necessary, click on + again and add further time periods.

8.1.3 Kinetics - settings | Start/Stop measurement

You define the measurement start of a sample on the **Start/Stop measurement** screen.



Option	Description
Autom. without waiting time	The measurement starts immediately after you click on or .
Autom. with waiting time	After clicking on or , the measurement only starts after the wait time has elapsed.
Manually without waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the measurement starts immediately.
Manually with waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the wait time elapses first and then the measurement starts.
Waiting time	Time delay for start options with wait time

Optionally, you can select a termination criterion for the kinetics measurements.

Option	Description
Stop measurement	**Value** The measurement stops when this limit value is reached. The unit depends on the measurement mode selected on the **General** screen. **Upper limit/Lower limit** Depending on the expected curve, one of the limit options must be selected.

8.1.4 Kinetics - settings | Accessory

The parameters in the **Accessory** screen depend on the installed accessories.

See also

Using accessories [▶ 39]

8.1.5 Kinetics - settings | Evaluation

The following measured value analyses can be defined on the **Evaluation** screen:

- Determine measured values at defined points in time
- Calculation of formulae

Values of defined times

Measured values at selected points in time are displayed in the sample table and can be used for the analysis in a formula or in the calibration.

- Activate the **Values of defined times** option to select the measured values.
- Click on + and enter the desired time in the input fields. Click + to transfer to the list.
- To delete the value select it in the list and click on -.

Formula

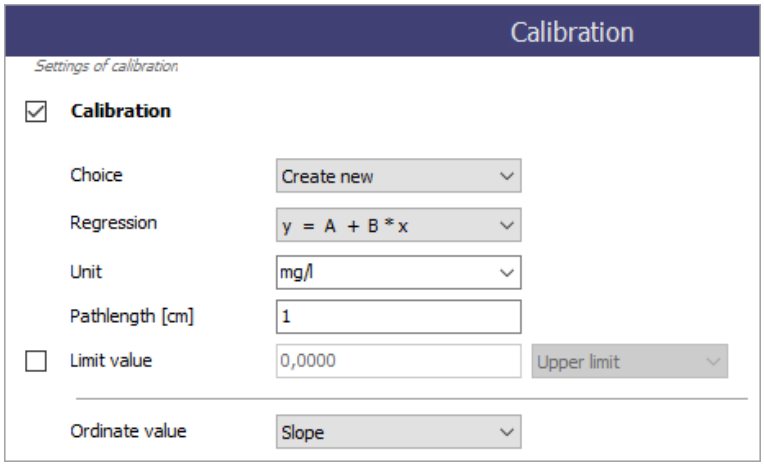
You can link the measured values of one or more samples in a formula.

See also

Using formulae [▶ 36]

8.1.6 Kinetics - settings | Calibration

On the **Calibration** screen, you can define an analysis with calibration.



For calibration with standards, enable the **Calibration** option and configure the following settings:

Option	Description
Selection	**Create new** Record calibration within the following measurement series You must define the standard samples and their concentration in the sample sequence. **Load from file** Load calibration parameters from an existing method
Regression	Regression type of the calibration function $y = B * x$ $y = A + B * x$ $y = A + B * x + C * x^2$
Unit	Unit of the analysis result
Thickness	Pathlength of the cell This value is for information only and is saved with the method parameters.

Option	Description
Limit value	Define an upper or lower limit value for the analysis result Results above or below this limit value are identified with "!" in the results table.

The **Kinetics** module can use different values from the time-related measuring curve for the calibration:

Option	Description
Slope	Slope of the entire kinetic curve from the start to the end of the measurement The range can be narrowed down after the measurement.
Maximum between t1 and t2	Maximum of kinetic chart between times **Time begin** and **Time end**
Formula	Result of a formula calculation Clicking on ... displays the formula editor.
Lineweaver Burk	Reciprocal reaction speed 1/v

See also

Using formulae [▶ 36]

8.1.7 Kinetics - settings | Sample sequence

On the **Sample sequence** screen, you can specify the sequence of samples for a subsequent measurement, which you can start using the icon in the document window. You can also create a sample sequence directly before a measurement.

Requirements for the sample sequence

- Activating the calibration requires entering a sequence with standard samples.
- When using cell changers and autosamplers, the samples are assigned to the sample positions in the accessories.
- If the sample sequence is empty, the **Sequenz settings** window will first appear when starting the measurement of the sample sequence. This window may only be exited once there has been at least one sample defined.

See also

Sample sequences [▶ 29]

8.1.8 Kinetics - settings | Archive automatically

You can automatically save, export, and print the measurement data and its analysis. This allows you to standardize your data archiving processes and ensure that data is not lost. Select the target files and report templates in the **Archive automatically** screen. Additionally, automatic archiving must be activated program-wide in the **Options** window and the times for the individual archiving functions must be selected.

See also

Automatically archive measurement data [▶ 28]

8.1.9 Kinetics - settings | Note

A note on the method may be optionally entered on the **Note** screen.

8.2 Performing measurements in the Kinetics module

The prerequisite for starting a measurement is that a new method has been created or loaded in the document window. The measurement can be started with a sample sequence stored in the method or as individual measurement.

The following icons are displayed for the measurements:

Icon	Description
Measure sequence	Start sample sequence If you have not saved any sample sequences to the measurement parameters, the **Sequenz settings** window will appear after you click on this icon. This window may only be exited once there has been at least one sample defined.
Measure sample	Start individual sample measurement independent of the sample sequence configured
Reference	Measure reference A separate reference measurement is required if the sample sequence does not start with a reference measurement or no reference is available that matches the current method parameters.
Suspend sequence	Interrupt the measurement and continue at a later time The current sample measurement is completed. The pending sample sequence is then displayed and can be edited.
Break	The measurement stops immediately and can be continued with **Continue**. You can use the pause to add a reagent to a sample.
Stop	Stop current measurement and do not continue
	Available for cartridge sipper system and APG sampler: Switch pump on or off and convey sample or stop conveying
	Available for APG sampler: Lower or raise sample cannula
	Available for APG sampler with stirring function: Switch stirrer on or off

Measure reference

If the sample sequence does not have a reference at the first location, the reference must be recorded separately.

- Place the reference into the sample space.
- Click on **Reference** and confirm the prompt about the reference measurement.
  - ✓ The reference measurement is run. All subsequent measurements are corrected with this reference until the measuring parameters are modified by a new method configuration or the next reference measurement takes place.

Start first sequence

With the start of the sample sequence the samples are processed in the order specified in the sample table.

- Place the first sample of the sequence in the sample space or fill cell changer/autosampler with samples.
- Click on **Measure sequence**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  - ✓ The sample sequence is processed. The measured values and analyses are displayed in the document window.

Interrupting or stopping the sequence

An ongoing measurement may be interrupted and then continued or stopped completely.

- Click on **Stop** to stop the measurement.
  - ✓ The measurement of the sequence is stopped and cannot be continued. Measurement data recorded up to this point remain intact and may be processed further.
- Click on **Suspend sequence** to interrupt a measurement and continue it later.
  - ✓ The current measurement step is stopped and then the processing interrupted. The measurement pause may be used to view and edit the ongoing sample sequence.
- With **Break** you can interrupt a running sample measurement immediately, e.g. to add reagents to a sample. Click on **Restart** to continue the sample measurement.

Start next sequence

After processing the first sample sequence, the sequence may be started again or re-edited on other occasions. This is also possible if the document has already been saved and re-opened to display the results.

- Click .
  The **Edit sequence** window appears with the sequence stored in the method.
- If necessary, compile a new sequence.
- Confirm the setting in the **Edit sequence** window by clicking on **Ok**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  - ✓ The current sequence is processed and the data appended to the existing measurement table and analyses.

Performing single measurements

Regardless of the sequence configured, single samples of sample type **Sample** may be measured and appended to the measurement table and analyses.

- Place the sample into the sample space.
- Click on **Measure sample**.
- Follow further on-screen prompts for starting the measurement.
  - ✓ The measurement is run and the data is appended to the existing measurement table and analyses.

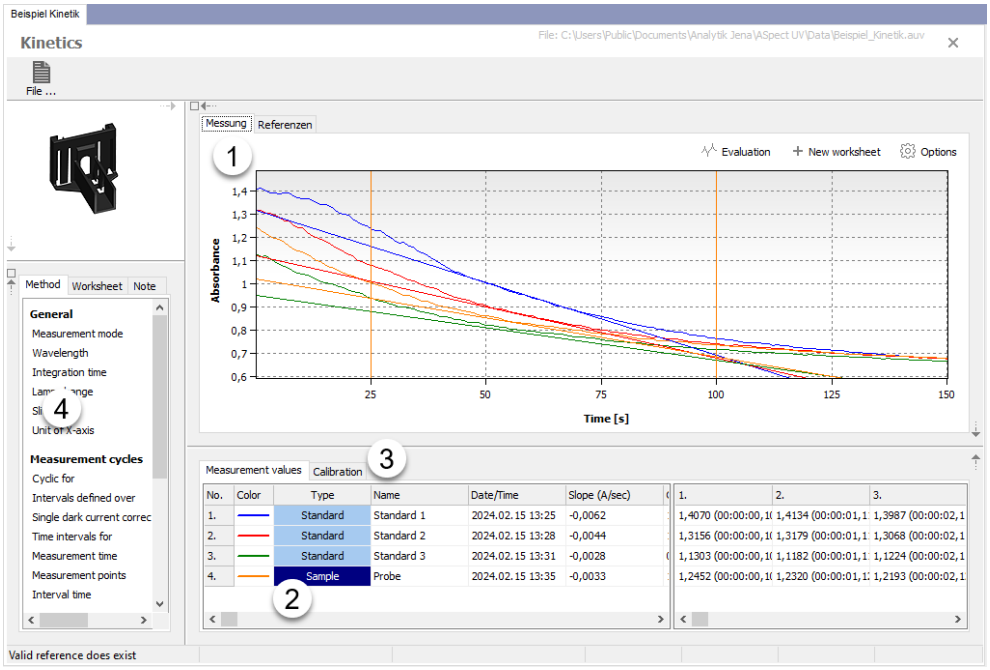
Tip

If measurements of other sample types are to be appended, click on **Measure sequence** and enter a sequence with the corresponding samples.

8.3 Displaying, evaluating, and processing results in the Kinetics module

This section explains the particularities of the results display and analysis in the **Kinetics** module.

Document window in the Kinetics module with several kinetics curves



No.	Description
1	Worksheets with the display of sample and reference spectra and further analyses
2	**Measurement values** tab with the individual measured values of the samples
3	Tabs with data analyses
4	Tab with information on method settings and mathematical data handling on the worksheets

Measurement worksheet

The **Measurement** worksheet contains the measurement data. The spectra are displayed in the upper half of the worksheet.

The **Measurement values** tab in the lower half of the worksheet contains the sample table in the order of the measurements and the table with the digital measured values. The other tabs contain data analyses that have already been defined in the method. You can add to and edit these analyses.

Time display for kinetic curve

The display of the x-coordinate in the kinetic curve can be changed between hours, minutes and seconds.

▶ Select the **Options** | **Unit of X-axis** menu item and enable the unit in the submenu.

✓ The display of the kinetic curve and the slope are updated.

New worksheet

You can create additional worksheets in the document window and carry out further analyses on them. In this way, you can create different analyses side by side in one document (file). The **New worksheet** worksheet is created after clicking on + **New worksheet** in the **Measurement** worksheet. The unedited, original measurement data is first copied to the new worksheet and can then be edited.

Sample table

The display of the sample table can be configured freely. After right clicking on the table header the following parameters can be selected in the context menu:

- Number in the sequence
- Position in accessories when using cell changer or autosampler
- Color of the measurement curve in the chart
- Batch when using cell changer or autosampler
- Sample name
- Sample type
- Date and time of the measurement

- Slope
- Absolute value (y-axis section of the linear regression function)
- Range limits of the slope
- R^2 adjust
- Temperature for methods with Peltier-tempered accessories
- Notes
- Sample concentration for concentration determination with calibration
- Dilution and sample weight
  These entries are only taken into account for concentration determinations with calibration.
- Sample-specific variables A – H for calculations in formulae

Via Drag&Drop the order of the table columns can be changed.

The individual measurements for each sample are listed adjacent in a separate table.

See also

Show spectra and measurement curves on the worksheet [▶ 19]

8.3.1 Evaluate kinetic curves

The data analyses offered in this method can also be performed later. The functions have been compiled in the menu **Evaluation** that is available on every worksheet. The analyses always relate to the measured values of the respective worksheet. If the measured values are processed with mathematical functions, the analysis on this worksheet is adjusted accordingly.

The analyses are output in their own spreadsheet in the bottom part of the worksheet.

Edit analysis

The analysis parameters can be edited for existing analyses.

- Click on **Settings** in the spreadsheet of the analysis and change the analysis parameters in the dialog window.
  - ✓ The analysis is updated.

Delete analysis

Analyses that are not required may be deleted.

- At the top right of the spreadsheet of the analyses click on ✕.
  - ✓ The analysis is removed from the worksheet.

Range for slope calculation

The slope is initially calculated over the entire kinetic curve. After the end of the measurement, you can limit this range and only use a section of the reaction kinetics, ideally the linear part, for the calculation.

- If the slope is only calculated for individual samples, highlight these samples on the worksheet.
- On the worksheet, select the menu item **Evaluation | Range for slope calculation**.
- Enter times for the start and end of the linear range.
- In the list select the samples for which the slope will be calculated:
  Set to all measurements: The calculation is performed for all samples.
  Set only to marked measurements: The calculation is only performed for the previously highlighted samples.
  - ✓ The values **Slope** and **Offset** are updated in the measured value table. Any analyses are also re-calculated.

Values of def. times

The **Values of def. times** function compiles measured values at selected times in a table.

- On the worksheet, select the menu item **Evaluation | Values of def. times**.

- Click on + , choose the measuring time in the input fields and click on + again to transfer it to the list.
  - ✓ The value table is displayed.

Formula

Use the **Formula** function to link the measured values of one or more samples in a formula.

- On the worksheet, select the menu item **Evaluation** | **Formula**.
- Click on + and create the formula using the formula editor.
- If necessary, add further formulae in the same way.
  - ✓ The results are displayed on the **Formula** tab.

Calibration

The **Calibration** function is available if a document does not contain its own calibration with standards. You can use this function to subsequently load the calibration data from other files and carry out a quantitative analysis of the measured values. Only the calibration parameters are loaded and not the standards.

- On the worksheet, select the menu item **Evaluation** | **Calibration**.
- Enable the **Calibration** option.
- Click on **Load** and select the document with the calibration graph.
  - ✓ The **Calibration** spreadsheet with the current calibration graph and the calculated calibration parameters is displayed. The results of the concentration analysis with calibration are entered directly into the sample table. Concentrations outside of the calibrated range are placed in brackets.

The **Calibration** spreadsheet contains the following information:

- Source of the calibration graph (measured in this document or loaded from a file)
- Regression model
- Analyses wavelengths or calibration formula used
- Regression coefficients A, B and C if calculated in the regression model
- Coefficient of determination R^2
- Pathlength of the cell (for information only, not used in the calculation)

8.3.2 Processing kinetic data mathematically

You can apply the following mathematical operations to a kinetic curve:

- Trim
- Smoothing

The measurement data and existing analyses on a worksheet are then recalculated and updated. You can apply the mathematical operations consecutively in the same worksheet.

Reverse data editing

The operations report can be found on the left-hand side of the document on the **Worksheet** tab. Here, the operations are listed one after the other. By clicking on the corresponding operation, the editing step is displayed. You can undo operations on this tab.

- Right click on the last operation to be reversed.
- Select one of the two options in the context menu:
  - **Copy to a new worksheet up to this step**
    A new worksheet is opened and the data is copied with the change history up to the selected operation. All operations remain intact in the previous worksheet.
  - **Delete operation**
    All steps including the selected operation are deleted in the current work sheet.
  - ✓ The operations are copied to a new worksheet or undone according to the selected option.

Cut out

Use this function to select a curve section for display and further processing/analysis. The values outside the selected range are no longer taken into account.

- On the worksheet, select the menu item **Evaluation** | **Cut out**.
  - ✓ The cursor changes to a vertical line with the label "Range".
- Click on the left or right limit of the x-coordinate range to be cut out and with the mouse button held down move the cursor to the opposite limit. Then release the mouse button.
- Alternatively enter the range limits in the **Cut out** window in the **Start** and **End at X :** fields.
- Confirm the entry in the **Cut out** window by clicking on **Ok**.
  - ✓ The curve display is updated. Now only the selected area of the measurement graph is visible.

Smooth

This function is used to smooth the curve using the Savitzky-Golay method.

- On the worksheet, select the menu item **Evaluation** | **Smooth**.
- In the dropdown list **Base points**, select the number of points to be considered for smoothing in accordance with Savitzky-Golay.
  - ✓ The curve is recalculated and the display is updated.

8.4 Example measurement in the Kinetics module

A kinetics measurement at 500 nm over a period of 30 s is used as an example. The example measurement can be carried out with an empty sample chamber.

The following steps must be carried out:

1. Create the document in the module.
2. Open method and enter parameter.
3. Start measurement.

Preparing a document

- Select the menu item **Modules** | **Kinetics** or click on the icon in the task bar.

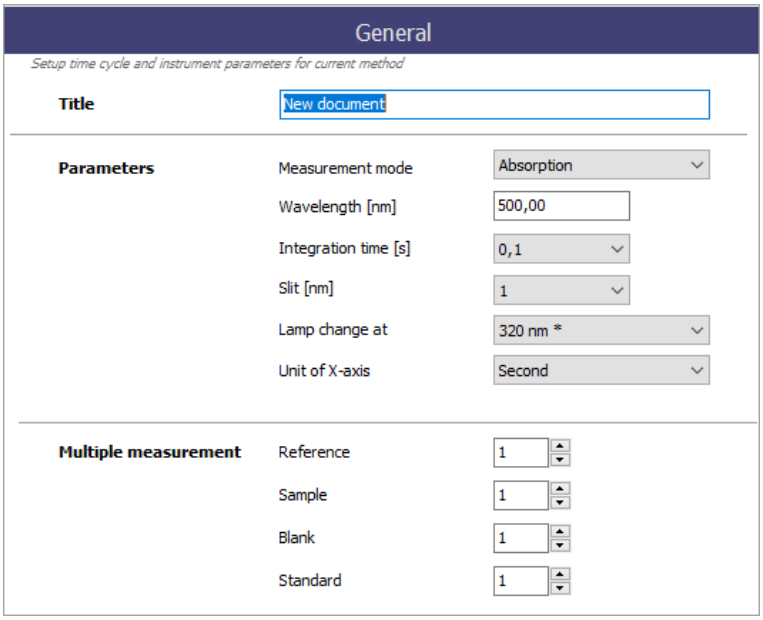
Defining method parameters

- Click on **Method setup** in the document window.
- Enter the parameters on the screens of the **Kinetics - settings** method window (see below).
- Confirm the parameters in the method window by clicking on **Ok** and return to the document window.

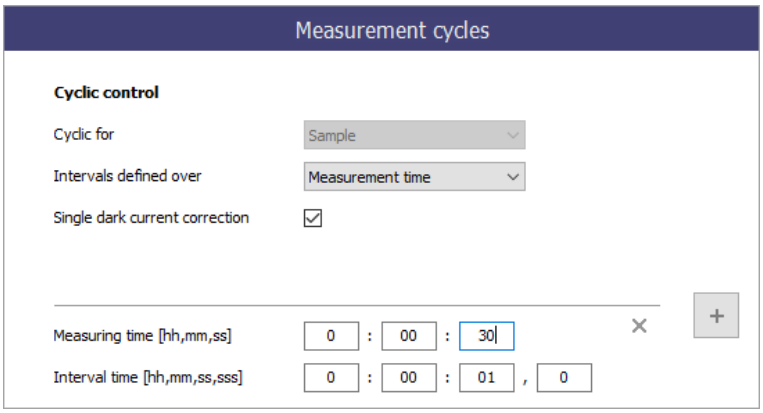
Parameter entries

Enter the parameters as shown in the screenshot.

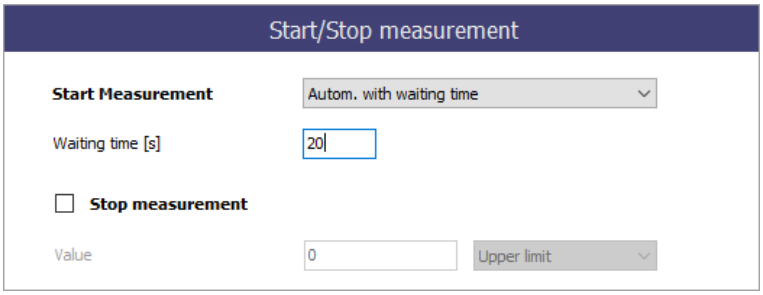
General screen



Measurement cycles screen



Start/Stop measurement screen



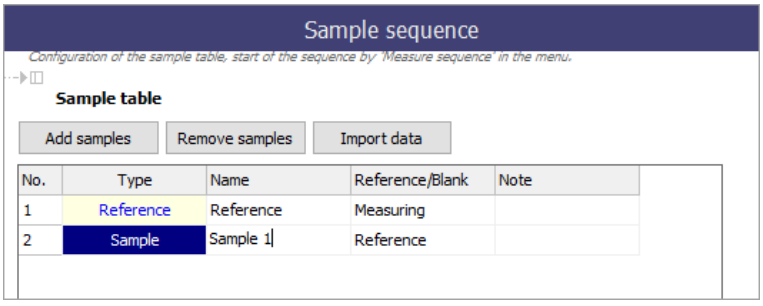
Evaluation screen

Make no entries.

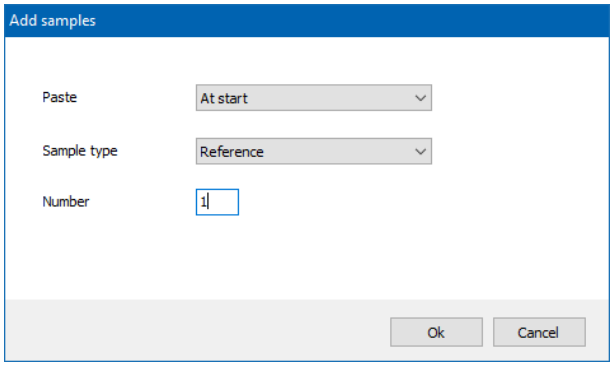
Calibration screen

Make no entries.

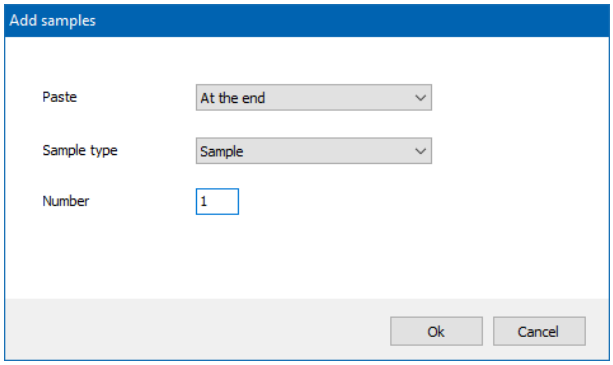
Sample sequence screen



▶ Click on **Add samples** and set a reference at the start of the sample table:



- Click on **Add samples** again and add a sample to the end of the sample table:



- Enter "Reference" as the name in the first line of the sample table and confirm with the Enter key.
- In the second line of the sample table, enter "Sample 1" as the name and confirm with the Enter key.

Archive automatically screen

Make no entries.

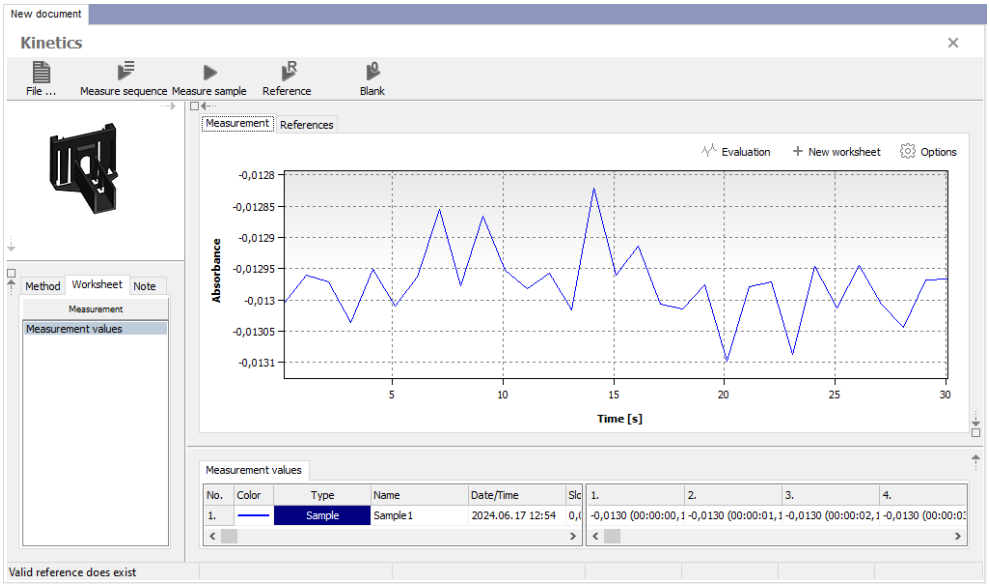
Note screen

Make no entries.

Performing the measurement

- Click on in the document window.
  The start information for measuring the reference is displayed.
- Insert the reference sample and click on **Yes** to start the measurement.
- The reference measurement is performed. A prompt to measure sample 1 is displayed.
- Insert sample 1 and click on **Yes** to start the measurement.

The kinetic curve and the measured values are output on the **Measurement** worksheet.


New document
Kinetics
File ...
Measure sequence
Measure sample
Reference
Blank
Measurement
References
Evaluation
New worksheet
Options
-0,0128
-0,01285
-0,0129
-0,01295
-0,013
-0,01305
-0,0131
Absorbance
5
10
15
20
25
30
Time [s]
Method
Worksheet
Note
Measurement
Measurement values
Measurement values
No.
Color
Type
Name
Date/Time
1.
Sample
Sample1
2024.06.17 12:54
1.
2.
3.
4.
Valid reference does exist

9 Thermometry module

In the **Thermometry** module, temperature-resolved measured curves can be recorded and analyzed with a Peltier-tempered accessory. The following analyses are available:

- DNA melting point determination
- Peak determination
- Output of measured values at selected temperatures
- Linking of the measured values in a formula

Open Thermometry module

- Open the **Thermometry** module by clicking on the icon in the task bar of the main window.

- Alternatively, select the menu item **Modules** | **Thermometry**.
  - ✓ A new document is opened in the workspace.
- Each additional click on the icon opens another new document on the workspace.

All functions of the document windows of the **Thermometry** module are assigned to the measurements of temperature curves and their analyses. You can now create a method and start a measurement with analyses based on it.

9.1 Method configuration in the Thermometry module

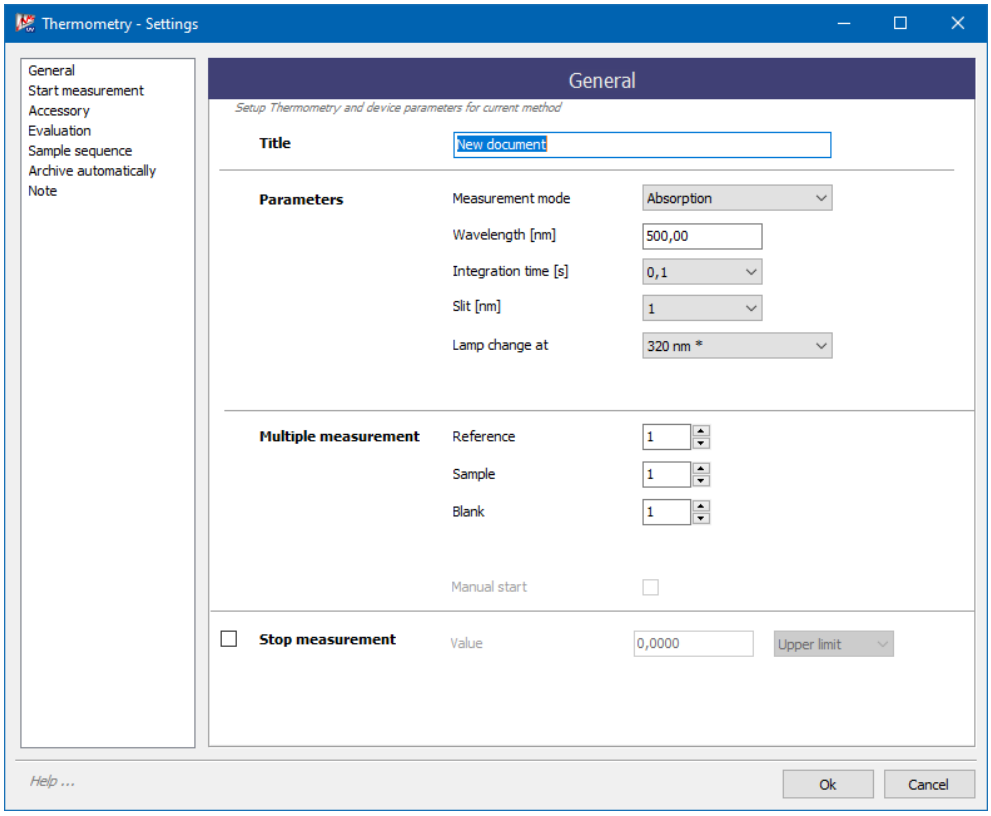
This section includes all configurations that can be made for a method in the **Thermometry** module.

Creating a method

- Click on **Method setup** in the document window to open the method window.
- Make the settings on the screens of the method window.
- Finish entering the parameters by clicking on **Ok**.
  - ✓ The method parameters are output on the left side of the document window on the **Method** tab. The icons for starting the measurement appear in the toolbar of the document window.

9.1.1 Thermometry - Settings | General

On the **General** screen, the basic measurement configurations are made.



Title

Enter the title of the document here, which is displayed in the document tab. You can edit the title later.

Parameters

In this area, select the parameters for the optical measurement.

Option	Description
Measurement mode	The following measurement modes can be selected: ■ **Transmittance** ■ **Absorption**
Wavelength [nm]	Enter wavelength for the analysis
Integration time [s]	Select the time for recording a measuring point
Slit [nm]	For SPECORD 210/250 PLUS Select spectral width (optical resolution): 0.2; 0.5; 1; 2; 4 nm **Note**: The 0.2 nm slit was not yet installed in older SPECORD 210/250 PLUS. It is not available for selection for these devices.
Lamp change	Select the wavelength of the change from UV lamp to Vis lamp The preset lamp change at 320 nm guarantees an optimal distribution of energy across the entire wavelength range of the spectrometer. If you are only working in UV or Vis range, you may also measure with the selected lamp using the options **UV only** or **Vis only**.

Multiple measurement

You can carry out a measurement several times in succession and use the mean for further calculations and analyses. For measurements with very little energy, e.g. samples with high absorbance, this procedure can improve the signal-to-noise ratio and increase the measurement accuracy.

Option	Description
Multiple measurement	If necessary, enter the number of measurement repetitions for the sample types **Reference**, **Blank**, **Sample** and **Standard**.

Option	Description
	If the **Manual start** option is enabled, a request to start is made for each individual measurement within a repetition.

Optionally, you can define a measured value that stops the measurement when it is reached.

Option	Description
Stop measurement	**Value** The measurement stops when this measured value is reached. The unit depends on the selected measurement mode. **Upper limit/Lower limit** Depending on the expected curve, one of the limit options must be selected.

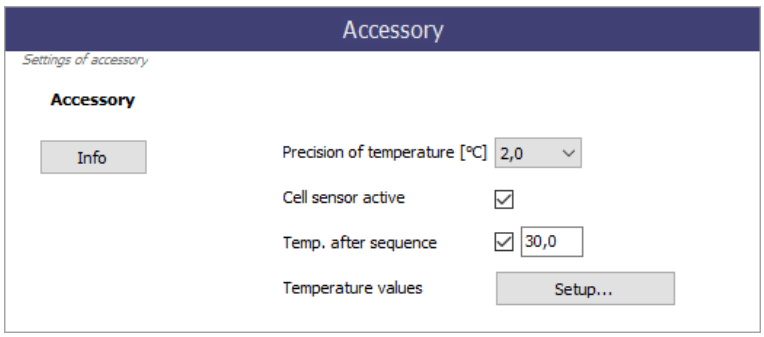
9.1.2 Thermometry - Settings | Start measurement

You define the measurement start of a sample on the **Start measurement** screen. The following start options are available:

Option	Description
Autom. without waiting time	The measurement starts immediately after you click on or .
Autom. with waiting time	After clicking on or , the measurement only starts after the wait time has elapsed.
Manually without waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the measurement starts immediately.
Manually with waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the wait time elapses first and then the measurement starts.
Waiting time	Time delay for start options with wait time

9.1.3 Thermometry - Settings | Accessory

On the **Accessory** screen, you parameterize the temperature curve approached by the accessories and set the operating mode when using two Peltier temperature controlled cell changers.



Setting the temperature control

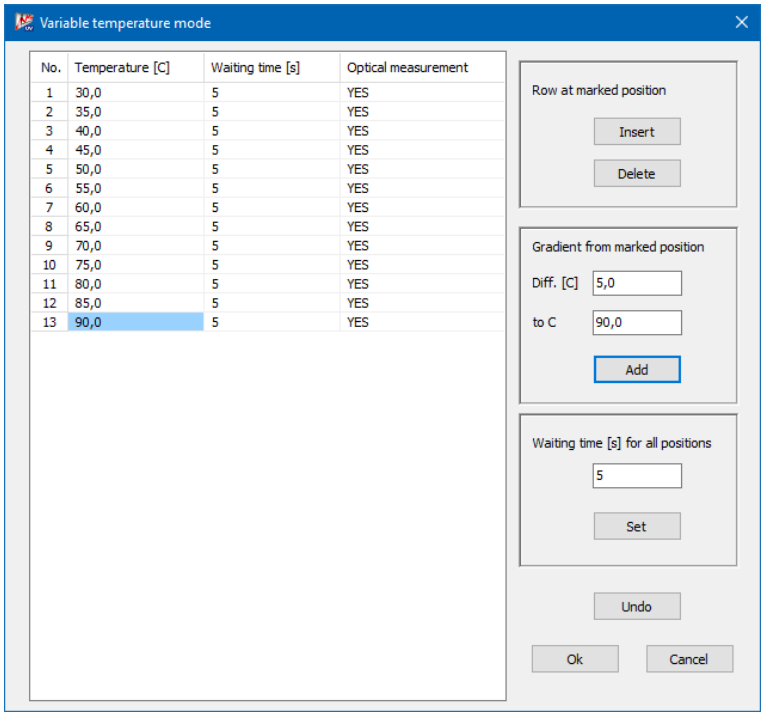
Option	Description
Precision of temperature [°C]	Select the accuracy of the temperature control

Option	Description
Cell sensor active	At the start of the measurement when the target temperature is reached, the registered cell temperature is recorded. The measured value (absorbance/%T) is assigned to the cell temperature. The temperature measurement is therefore more accurate than the sample block temperature. If the option is not enabled, the block temperature (standard temperature) is recorded and indicated as an abscissa value in the **Thermometry** module.
Temp. after sequence	Activate holding temperature after optical measurement This temperature is approached and held after the last optical measurement.
Info	Display information about the adjustable temperature range and the current temperatures in accessories

Entering the temperature progression

After clicking on **Setup**, the **Variable temperature mode** window appears. The parameters of the temperature stages can be edited individually in the table rows or defined automatically using the checkboxes and input fields.

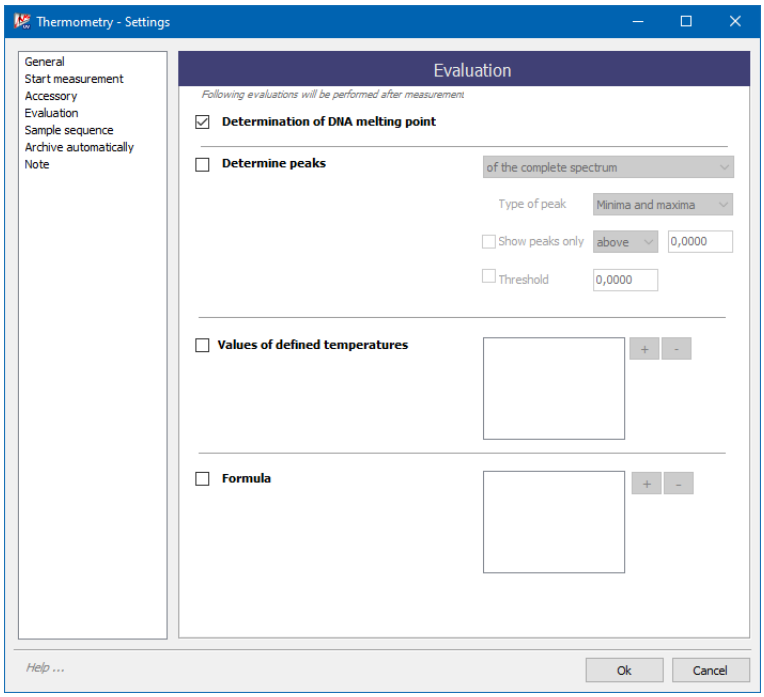
Option/button	Description
Paste	Enter a new temperature step after the highlighted table row
Delete	Delete the highlighted table row
Gradient from marked position	Automatically generate a temperature gradient from a highlighted table row. Starting with the start temperature of the highlighted table row further temperature stages are inserted into the table in steps until the final temperature has been reached. **Diff. [C]** Temperature difference of a temperature stage **to C** Final temperature of the gradient **Add** Append temperature gradient at the highlighted position
Waiting time [s] for all positions	Waiting time from reaching the setpoint temperature to the start of the optical measurement Click on **Set** to transfer the entered temperature to all temperature levels in the table. **Note**: Regardless of the set waiting time, the optical measurement is carried out no less than 5 s after reaching the temperature within the agreed temperature accuracy range in the block. The waiting time is added to this 5 s period.
Undo	Reverse the last action
Optical measurement	**Yes** Perform an optical measurement at temperature step **No** No optical measurement takes place at the temperature step.



9.1.4 Thermometry - Settings | Evaluation

You can choose the following analyses on the **Evaluation** page:

- Determination of DNA melting point
- Peak determination
- Output of measured values at selected temperatures
- Input of formulae



Determination of DNA melting point

When the **Determination of DNA melting point** option is activated, the melting point of the DNA melting curves is determined.

Determine peaks

By enabling the checkbox **Determine peaks** extreme values are automatically searched for based on specified criteria. The peaks are highlighted in the graphical display of the measurement curve and displayed on a separate tab in the analysis area.

Option	Description
Selection list	**of the complete spectrum** Search for all peaks in the measuring range **only in defined ranges of the spectrum** Search for peaks in defined spectral ranges
Type of peak	Select the type of peak: **Minima**, **Maxima** or **Minima and maxima**
Show peaks only	Absolute limit for the display of peaks Peaks are only displayed if they are above or below the entered ordinate value.
Threshold	Difference between peak height and the adjacent local maximum/minimum Peaks are only displayed if they exceed (maximum) or fall below (minimum) the entered threshold value.

Values of defined temperatures

You can determine measured values at selected temperatures of the measurement curve. These measured values are displayed in the sample table in the analyses of the document window and can be used to calculate a formula.

- Activate the **Values of defined temperatures** checkbox.
- Click on + , enter the temperature within the temperature range in the input field, and click on + again to transfer it to the list.

Formula

You can link the measured values of one or more samples in a formula.

See also

Using formulae [▶ 36]

9.1.5 Thermometry - Settings | Sample sequence

On the **Sample sequence** screen, you can specify the sequence of samples for a subsequent measurement, which you can start using the icon in the document window. You can also create a sample sequence directly before a measurement.

Requirements for the sample sequence

- Activating the calibration requires entering a sequence with standard samples.
- When using cell changers and autosamplers, the samples are assigned to the sample positions in the accessories.
- If the sample sequence is empty, the **Sequenz settings** window will first appear when starting the measurement of the sample sequence. This window may only be exited once there has been at least one sample defined.

See also

Sample sequences [▶ 29]

9.1.6 Thermometry - Settings | Archive automatically

You can automatically save, export, and print the measurement data and its analysis. This allows you to standardize your data archiving processes and ensure that data is not lost. Select the target files and report templates in the **Archive automatically** screen. Additionally, automatic archiving must be activated program-wide in the **Options** window and the times for the individual archiving functions must be selected.

See also

Automatically archive measurement data [▶ 28]

9.1.7 Thermometry - Settings | Note window

A note on the method may be optionally entered on the **Note** screen.

9.2 Performing measurements in the Thermometry module

The prerequisite for starting a measurement is that a new method has been created or loaded in the document window. The measurement can be started with a sample sequence stored in the method or as individual measurement.

The following icons are displayed for the measurements:

Icon	Description
Measure sequence	Start sample sequence If you have not saved any sample sequences to the measurement parameters, the **Sequenz settings** window will appear after you click on this icon. This window may only be exited once there has been at least one sample defined.
Measure sample	Start individual sample measurement independent of the sample sequence configured
Reference	Measure reference A separate reference measurement is required if the sample sequence does not start with a reference measurement or no reference is available that matches the current method parameters.
Stop	Stop current measurement and do not continue
Suspend sequence	Interrupt the measurement and continue at a later time The current sample measurement is completed. The pending sample sequence is then displayed and can be edited.
	Adjust the temperature in a Peltier temperature controlled accessory

Measure reference

If the sample sequence does not have a reference at the first location, the reference must be recorded separately.

- Place the reference into the sample space.
- Click on **Reference** and confirm the prompt about the reference measurement.
  - ✓ The reference measurement is run. All subsequent measurements are corrected with this reference until the measuring parameters are modified by a new method configuration or the next reference measurement takes place.

Start first sequence

With the start of the sample sequence the samples are processed in the order specified in the sample table.

- Place the first sample of the sequence in the sample space or fill cell changer/autosampler with samples.
- Click on **Measure sequence**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.

✓ The sample sequence is processed. The measured values and analyses are displayed in the document window.

Interrupting or stopping the sequence

An ongoing measurement may be interrupted and then continued or stopped completely.

- Click on **Stop** to stop the measurement.
  ✓ The measurement of the sequence is stopped and cannot be continued. Measurement data recorded up to this point remain intact and may be processed further.
- Click on **Suspend sequence** to interrupt a measurement and continue it later.
  ✓ The current sample measurement is ended and then the processing is interrupted. The measurement pause may be used to view and edit the ongoing sample sequence.

Start next sequence

After processing the first sample sequence, the sequence may be started again or re-edited on other occasions. This is also possible if the document has already been saved and re-opened to display the results.

- Click .
  The **Edit sequence** window appears with the sequence stored in the method.
- If necessary, compile a new sequence.
- Confirm the setting in the **Edit sequence** window by clicking on **Ok**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  ✓ The current sequence is processed and the data appended to the existing measurement table and analyses.

Performing single measurements

Regardless of the sequence configured, single samples of sample type **Sample** may be measured and appended to the measurement table and analyses.

- Place the sample into the sample space.
- Click on **Measure sample**.
- Follow further on-screen prompts for starting the measurement.
  ✓ The measurement is run and the data is appended to the existing measurement table and analyses.

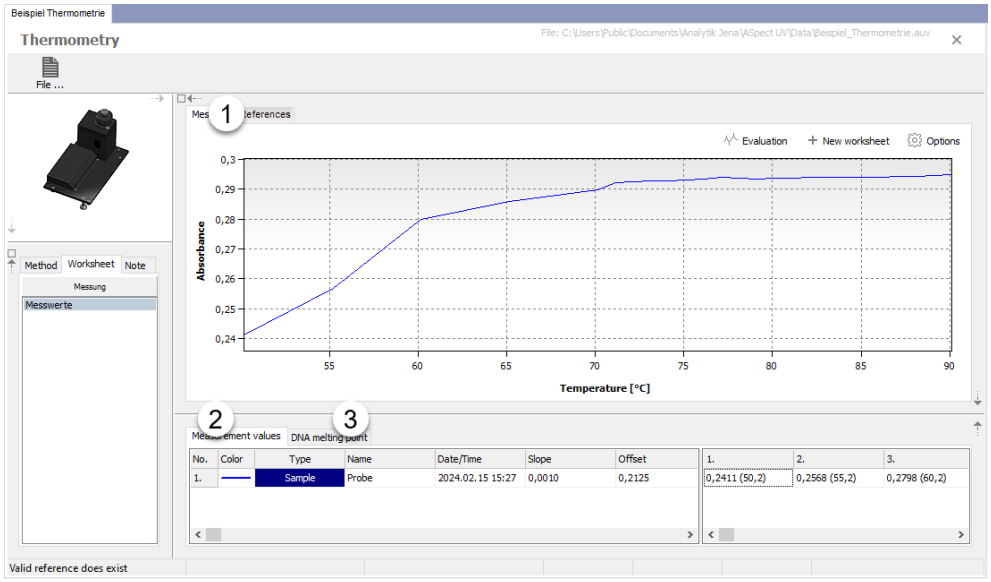
Tip

If measurements of other sample types are to be appended, click on **Measure sequence** and enter a sequence with the corresponding samples.

9.3 Displaying, evaluating, and processing results in the Thermometry module

This section explains the particularities of the results display in the Thermometry module window.

Document window in the Thermometry module



No.	Description
1	Worksheets showing the temperature curve, references
2	**Measurement values** tab with the individual measured values of the samples
3	Tab **DNA melting point**

Measurement worksheet

The **Measurement** worksheet contains the measurement data. The spectra are displayed in the upper half of the worksheet.

The **Measurement values** tab in the lower half of the worksheet contains the sample table in the order of the measurements and the table with the digital measured values. The other tabs contain data analyses that have already been defined in the method. You can add to and edit these analyses.

New worksheet

You can create additional worksheets in the document window and carry out further analyses on them. In this way, you can create different analyses side by side in one document (file). The **New worksheet** worksheet is created after clicking on + **New worksheet** in the **Measurement** worksheet. The unedited, original measurement data is first copied to the new worksheet and can then be edited.

Sample table

The display of the sample table can be configured freely. After right clicking on the table header the following parameters can be selected in the context menu:

- Number in the sequence
- Position in accessories when using cell changer or autosampler
- Batch when using cell changer or autosampler
- Sample name
- Sample type
- Slope
- Range limits of the slope
- R^2 adjust
- Sample-specific variables A – H for calculations in formulae

Via Drag&Drop the order of the table columns can be changed.

The individual measurements for each sample are listed adjacent in a separate table.

See also

Show spectra and measurement curves on the worksheet [▶ 19]

9.3.1 Display options for the results in the Thermometry module

The following functions are available for displaying the temperature curve:
- Scale curves
- Add text to curves (text box)
- Select curves/samples
- Change the color of curves
- Hide a curve (deactivate a sample)

See also

Show spectra and measurement curves on the worksheet [▶ 19]

9.3.2 Evaluating the temperature curves

The data analyses offered in this method can also be performed later. The functions have been compiled in the menu **Evaluation** that is available on every worksheet. The analyses always relate to the measured values of the respective worksheet. If the measured values are processed with mathematical functions, the analysis on this worksheet is adjusted accordingly.

The analyses are output in their own spreadsheet in the bottom part of the worksheet.

Edit analysis

The analysis parameters can be edited for existing analyses.

▶ Click on **Settings** in the spreadsheet of the analysis and change the analysis parameters in the dialog window.

✓ The analysis is updated.

Delete analysis

Analyses that are not required may be deleted.

▶ At the top right of the spreadsheet of the analyses click on ✕.

✓ The analysis is removed from the worksheet.

DNA melting point

You can determine the melting point in a DNA melting curve.

▶ On the worksheet, select the menu item **Evaluation** | **DNA melting point**.

✓ An overview of the determined melting points is displayed.

Peaks

An automatic peak search can be started with the **Peaks** function.

▶ On the worksheet, select the menu item **Evaluation** | **Peaks**.

▶ Select the following options in the **Settings peak list** window.

Option	Description
Selection list	**of the complete spectrum** Search for all peaks in the measuring range **only in defined ranges of the spectrum** Search for peaks in defined spectral ranges
Type of peak	Select the type of peak: **Minima**, **Maxima** or **Minima and maxima**
Show peaks only	Absolute limit for the display of peaks Peaks are only displayed if they are above or below the entered ordinate value.
Threshold	Difference between peak height and the adjacent local maximum/minimum Peaks are only displayed if they exceed (maximum) or fall below (minimum) the entered threshold value.

- Click **Ok** to confirm.
  - ✓ The peak list is displayed.

Values of def. temperatures

The **Values of def. temperatures** function compiles measured values at selected temperatures in a table. You can then use these measured values in a formula.

- On the worksheet, select the menu item **Evaluation | Values of def. temperatures**.
- Click on +, enter the temperature within the temperature range in the input field, and click on + again to transfer it to the list.
  - ✓ The value table is displayed.

Formula

Use the **Formula** function to link the measured values of one or more samples in a formula.

- On the worksheet, select the menu item **Evaluation | Formula**.
- Click on + and create the formula using the formula editor.
- If necessary, add further formulae in the same way.
  - ✓ The results are displayed on the **Formula** tab.

Range for slope calculation

The slope is initially calculated over the entire temperature curve. After the end of the measurement, you can limit this range and only use a section of the temperature curve, ideally the linear part, for the calculation.

- If the slope is only calculated for individual samples, highlight these samples on the worksheet.
- On the worksheet, select the menu item **Evaluation | Range for slope calculation**.
- Enter times for the start and end of the linear range.
- In the list select the samples for which the slope will be calculated.
  Set to all measurements: The calculation is performed for all samples
  Set only to marked measurements: The calculation is only performed for the previously highlighted samples.
  - ✓ The value of the **Slope** in the measured values table is updated. Any analyses are also re-calculated.

9.3.3 Processing temperature curves mathematically

You can apply mathematical functions, e.g. the addition of a constant, to the measurement data. The measurement data and existing analyses on a worksheet are then recalculated and updated. You can apply the mathematical operations consecutively in the same worksheet.

NOTE

If the measurement data in the **Measurement** worksheet is changed, e.g. due to re-measurement or by disabling a sample, the data in the other worksheets is not updated.

Reverse data editing

The operations report can be found on the left-hand side of the document on the **Worksheet** tab. Here, the operations are listed one after the other. By clicking on the corresponding operation, the editing step is displayed. You can undo operations on this tab.

- Right click on the last operation to be reversed.
- Select one of the two options in the context menu:

- **Copy to a new worksheet up to this step**
  A new worksheet is opened and the data is copied with the change history up to the selected operation. All operations remain intact in the previous worksheet.
- **Delete operation**
  All steps including the selected operation are deleted in the current work sheet.

✓ The operations are copied to a new worksheet or undone according to the selected option.

Cut out

Use this function to select a curve section for display and further processing/analysis. The values outside the selected range are no longer taken into account.

▶ On the worksheet, select the menu item **Evaluation** | **Cut out**.

✓ The cursor changes to a vertical line with the label "Range".

▶ Click on the left or right limit of the x-coordinate range to be cut out and with the mouse button held down move the cursor to the opposite limit. Then release the mouse button.

▶ Alternatively enter the range limits in the **Cut out** window in the **Start** and **End at X :** fields.

▶ Confirm the entry in the **Cut out** window by clicking on **Ok**.

✓ The curve display is updated. Now only the selected area of the measurement graph is visible.

Offset

This function is used to add a constant to the measured values. The value of the constant may be both positive or negative. This allows for interferences to be simulated or compensated.

▶ On a new worksheet, select the menu item **Evaluation** | **Offset**.

▶ Enter the value in the **Offset** field.

✓ The measured values and analyses are re-calculated and the displays updated.

Factor

This function is used to multiply the measured values by a constant. The multiplication of an absorbance value by a constant theoretically corresponds to a change in the pathlength or concentration of the sample.

▶ On a new worksheet, select the menu item **Evaluation** | **Factor**.

▶ Enter the value in the **Factor** field.

✓ The measured values and analyses are re-calculated and the displays updated.

Smooth

This function is used to smooth the curve using the Savitzky-Golay method.

▶ On the worksheet, select the menu item **Evaluation** | **Smooth**.

▶ In the dropdown list **Base points**, select the number of points to be considered for smoothing in accordance with Savitzky-Golay.

✓ The curve is recalculated and the display is updated.

Derivative

This function is used to calculate the derivative of the 1st to 4th order for the measurement curve with integrated constant smoothing over 5 points and a variable number of interpolation points for the Savitzky-Golay derivative filter (n points). The derived curve can suppress background signals that are superimposed on the measurement and emphasize the specific absorbances more clearly.

A curve can be derived several times. However, the algorithm is specifically adapted to the derivative type, therefore the fourth derivative does not result in the same y-coordinate values as four times the first derivative. Therefore, the same method should always be used for the quantitative analysis.

Especially the derivative of a higher order always results in the "coarsening" of the measurement graph. Therefore, dependent on the width of the measurement graph structure, always select the highest possible number of support points. Smoothing beforehand to suppress the statistical noise is sometimes also recommended. Note that the value range is reduced in accordance with the selected number of support points (n) by the number of values (n-1)/2+2 at both ends of the spectrum. To reduce this effect, you can carry out an interpolation beforehand.

- On the worksheet, select the menu item **Evaluation** | **Derivative**.
- In the **Derivative** list, select the order of the derivative.
- In the list **Base points** select the number of support points to be used for the derivative with integrated smoothing filter.
  - ✓ The derivative is calculated and the display updated. In the audit trail the order of the derivative and the number of support points are documented.

9.4 Example measurement in the Thermometry module

In the example, the melting point of a DNA sample is determined. A temperature curve in the range 25 ... 90 °C is run. The measurement requires Peltier-tempered accessories with a cell sensor. A suitable DNA sample or water can be used as sample.

The following steps must be carried out:

1. Create the document in the module.
2. Open method and enter parameter.
3. Start measurement.

Preparing a document

Select the menu item **Modules** | **Thermometry** or click on the icon in the task bar.

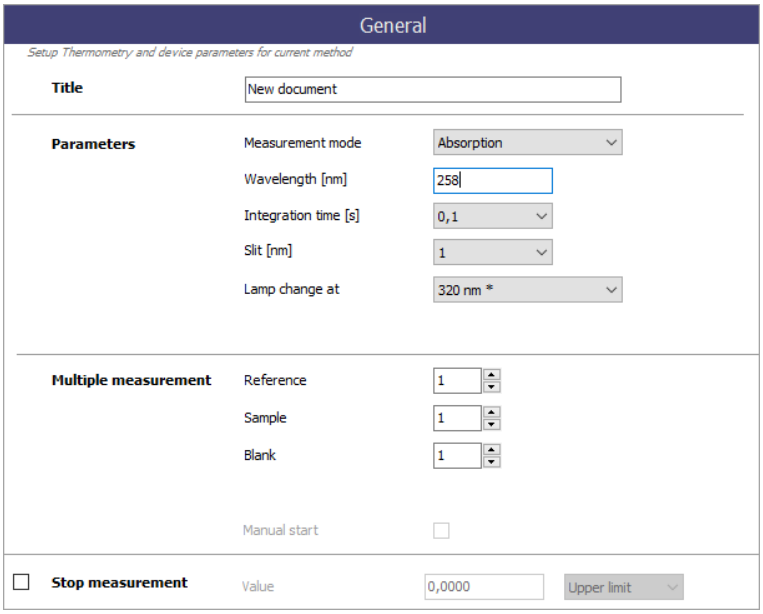
Defining method parameters

- Click on **Method setup** in the document window.
- Enter the parameters on the screen of the **Thermometry - Settings** method window (see below).
- Confirm the parameter input by clicking on **Ok** and return to the document window.

Entry of parameters

Configure the settings as shown in the screenshot.

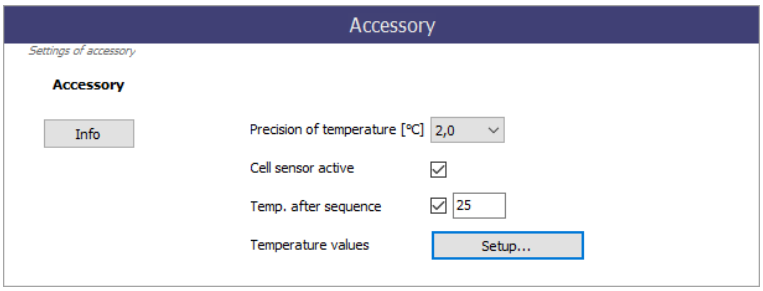
General screen



Start measurement screen

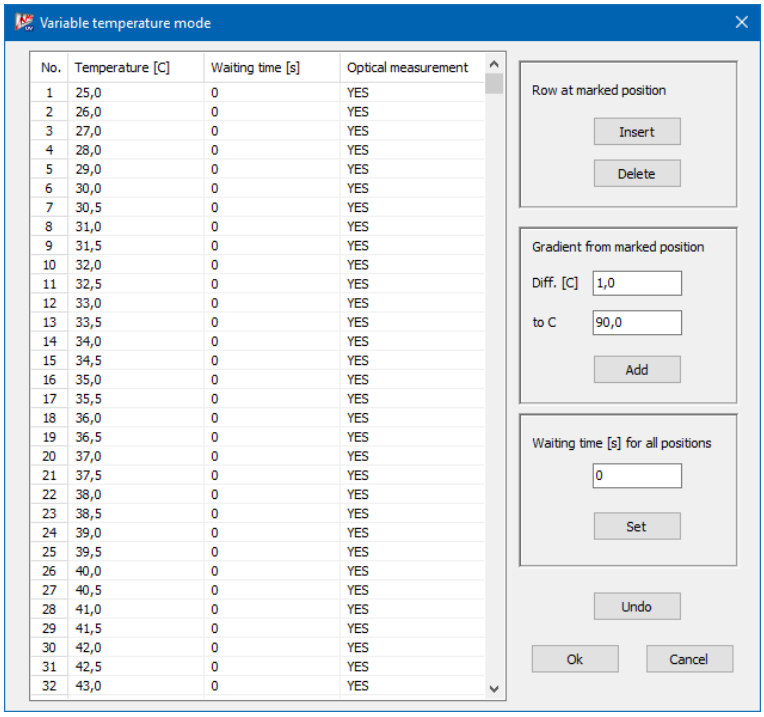
Make no entries.

Accessory screen

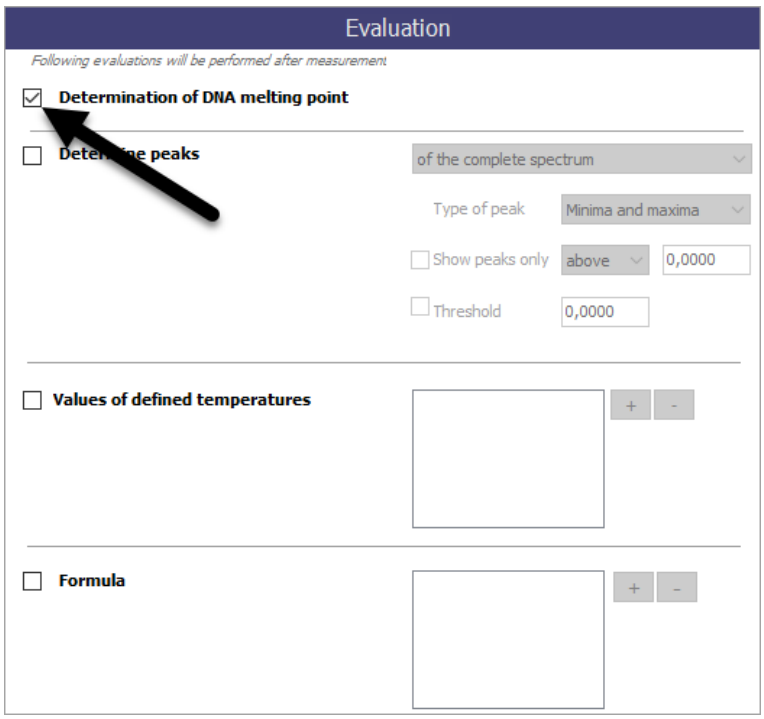


Setting the temperature curve parameters:

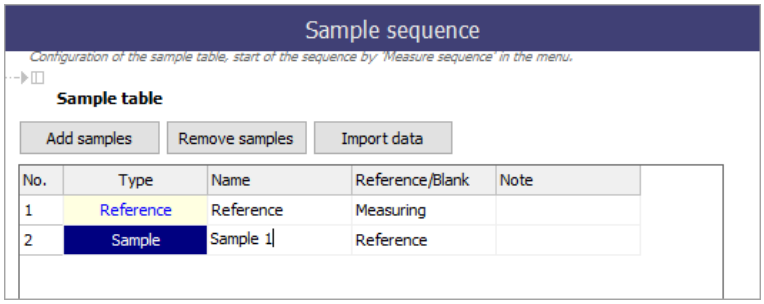
- Click on **Setup...** to open the **Variable temperature mode** window.
- Click on the **Temperature [°C]** column and enter the value "25".
- Enter the value "1" in input field **Diff. [C]** and the value "30" in field **to C**. Click **Add**.
- Repeat these entries for the value pairs "0.5 °C"/"80 °C" and "1 °C"/"90 °C".
- Click **Ok** to confirm the entries.



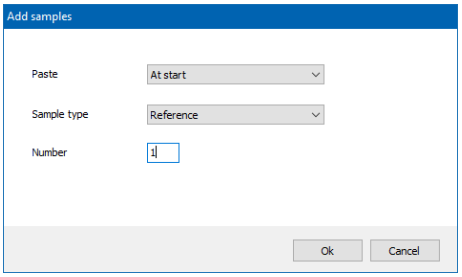
Evaluation screen



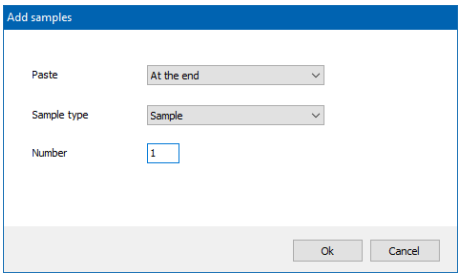
Sample sequence screen



▸ Click on **Add samples** and set a reference at the start of the sample table:



- Click on **Add samples** again and add a sample to the end of the sample table:



- Enter "Reference" as the name in the first row of the sample table and confirm with the Enter key.
- Enter "Sample 1" as the name in the second row of the sample table and confirm with the Enter key.

Archive automatically screen

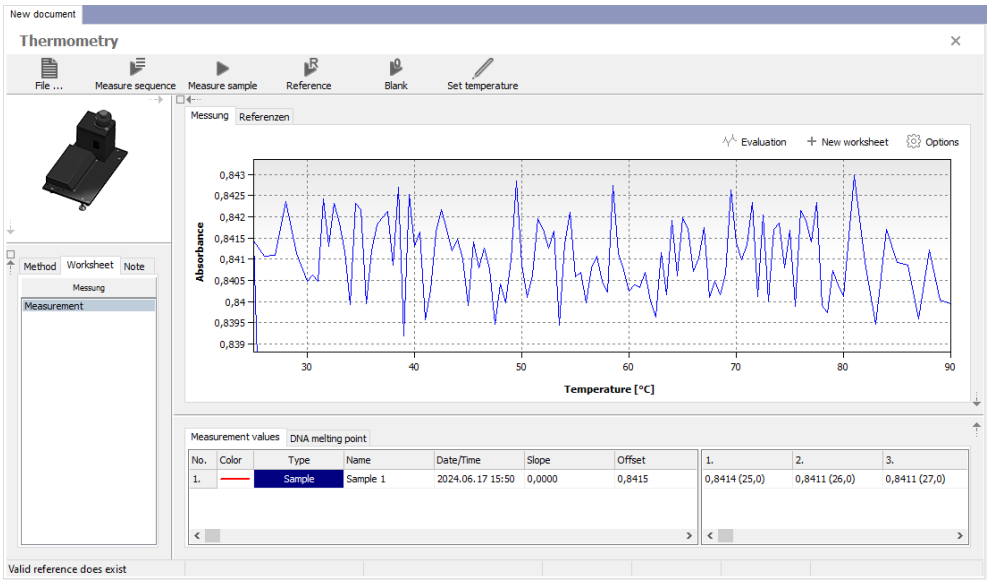
Make no entries.

Note screen

Make no entries.

Performing the measurement

- Click on in the document window.
  The start information for measuring the reference is displayed.
- Insert the reference sample and click on **Yes** to start the measurement.
- The reference measurement is performed. A prompt to measure sample 1 is displayed.
- Insert sample 1 and click on **Yes** to start the measurement.



10 Colormetric module

The **Colormetric** module performs the colorimetric analysis of transmittance spectra of transparent solid or liquid samples and reflectance spectra of non-transparent solid or powdery samples.

The following parameters can be determined in the Colorimetry module:

Color spaces/standard color values
- Tristimulus values X, Y, Z (as per EN ISO 11664)
- Tristimulus values x, y (as per EN ISO 11664)
- CIE lab, CIE luv (as per EN ISO 11664)
- Hunter lab

Observation angle/illuminants
- Viewing angle 2° and 10°
- CIE illuminant A and D65 according to EN ISO 11664
- CIE illuminant C

Color numbers
- White index, yellow index
- Platinum Cobalt according to ASTM D 5386-05 with linear regression via yellow index according to ASTM E313-15
- Iodine with calibration function via CIE lab values
- Gardner according to DIN ISO 4630
- Saybolt calculated from CIE lab values acc. to ASTM D156, D6045

Open Colormetric module

▶ Open the **Colormetric** module by clicking on the icon in the task bar.

▶ Alternatively, select the menu item **Modules** | **Colormetric**.

✓ A new document is opened in the workspace.

All functions of the document window of the **Colormetric** module are assigned to the measurement of spectra and their colorimetric analysis. You can now create a method and start a measurement with analyses based on it.

10.1 Method configuration in the Colormetric module

This chapter includes all configurations that can be made for a method in the **Colormetric** module.

Creating a method

▶ Click on **Method setup** in the document window to open the method window.

▶ Make the settings on the screens of the method window.

▶ Finish entering the parameters by clicking on **Ok**.

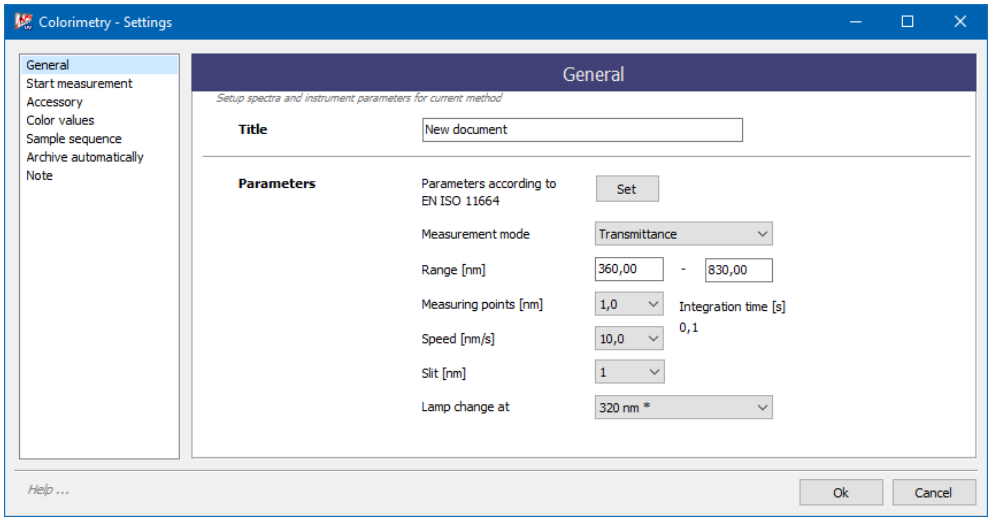
✓ The method parameters are output on the left side of the document window on the **Method** tab. The icons for starting the measurement appear in the toolbar of the document window.

See also

Basic structure and functions of ASpect UV [▶ 11]

10.1.1 Colorimetry - Settings | General

On the **General** screen, the basic measurement configurations are made.



Title

Enter the title of the document here, which is displayed in the document tab. You can edit the title later.

Parameters

In this area, select the parameters for the optical measurement.

Option	Description
Parameters EN ISO 11664	Click on **Set** to set the measurement parameters for the spectral range, the measuring point distance and the spectral width required by EN ISO 11664.
Measurement mode	The following measurement modes can be selected: ■ **Transmittance** ■ **Reflectance** (only for reflectance measuring attachments and integrating sphere)
Range [nm]	Enter the wavelength range for the measurement in the input fields For colorimetric analysis, at least the spectral range 380 ... 780 nm must be recorded.
Measuring points [nm]	Select distance between measuring points.
Speed [nm/s]	Select measuring speed
Integration time	Time for recording a measuring point This value is calculated automatically.
Slit [nm]	For SPECORD 210/250 PLUS Select spectral width (optical resolution): 0.2; 0.5; 1; 2; 4 nm **Note**: The 0.2 nm slit was not yet installed in older SPECORD 210/250 PLUS. It is not available for selection for these devices.
Lamp change	Select the wavelength of the change from UV lamp to Vis lamp The preset lamp change at 320 nm guarantees an optimal distribution of energy across the entire wavelength range of the spectrometer. If you are only working in UV or Vis range, you may also measure with the selected lamp using the options **UV only** or **Vis only**.

10.1.2 Colorimetry - Settings | Start measurement

You define the measurement start of a sample on the **Start measurement** screen. The following start options are available:

Option	Description
Autom. without waiting time	The measurement starts immediately after you click on or .
Autom. with waiting time	After clicking on or , the measurement only starts after the wait time has elapsed.
Manually without waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the measurement starts immediately.
Manually with waiting time	After clicking on or , a prompt appears to start the measurement. If you answer **Yes**, the wait time elapses first and then the measurement starts.
Waiting time	Time delay for start options with wait time

10.1.3 Colorimetry - Settings | Accessory

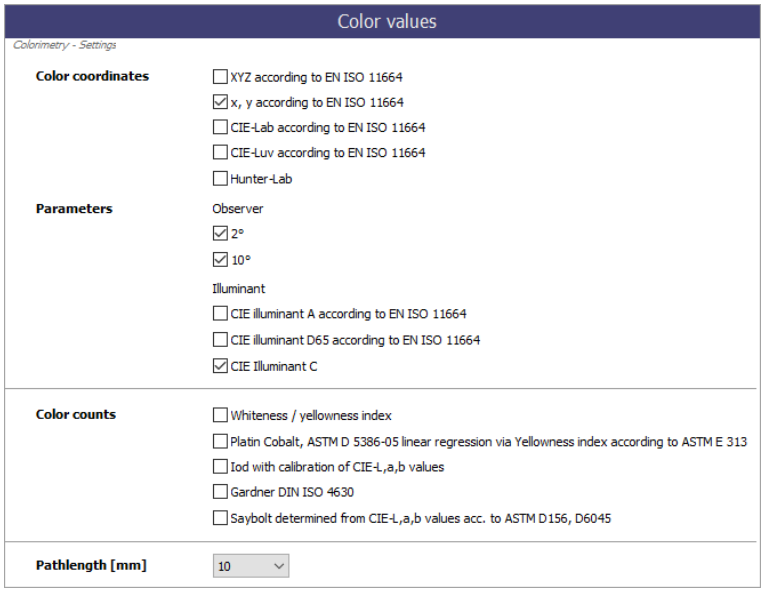
The parameters in the **Accessory** screen depend on the installed accessories.

See also

Using accessories [▶ 39]

10.1.4 Colorimetry - Settings | Color values

On the **Color values** screen, the color coordinates and color numbers to be calculated are selected.



Color coordinates

The following color coordinates can be selected for the calculation:

- XYZ according to EN ISO 11664
- x, y EN ISO 11664
- CIE-Lab EN ISO 11664
- CIE-Luv EN ISO 11664
- Hunter-Lab

Parameters

The color coordinates can be determined under two observation angles:
- 2°
- 10°

The following illuminants are available:
- CIE illuminant A according to EN ISO 11664
- CIE illuminant D65 according to EN ISO 11664
- CIE Illuminant C

Multiple color coordinates and parameters can be selected for the analysis of a measurement.

Color counts

The following color numbers can be calculated:
- Whiteness / yellowness index
- Platin Cobalt. ASTM D 5386-05 linear regression via Yellowness index according to ASTM E 313
- Iod with calibration of CIE-L.a.b values
- Gardner DIN ISO 4630
- Saybolt determined from CIE-L.a.b values acc. to ASTM D156. D6045

Thickness

To determine the color coordinates and the color numbers derived from them, a transmittance or reflectance value is required for the standardized pathlength of 10 mm.

- For transmittance measurements, select the active pathlength in the direction of the beam for the sample or cell used from the Thickness list or enter the value directly in the list field.
- For reflectance measurements of impermeable surfaces, the value must be set to 10 mm as standard.

NOTE

In the standards for determining the color numbers Platinum Cobalt (Hazen), Iodine and Gardner, it is important to remember that an application may only take place if the absorbance characteristics or the color value of the sample are similar to the corresponding standard. The color value is defined by its spectral color. To ensure the validity of a colorless standard, e.g. water, it is necessary to define an epsilon environment around the achromatic point. Both parameters are accordingly predefined in an Ini-file for the specified color values, taking both metrological and color-specific aspects into consideration. If these limits need to be changed, open the colcount.ini file in an editor at ProgramData\Analytik Jena\ASpect UV. Change the values to meet your requirements and save the file again.

10.1.5 Colorimetry - Settings | Sample sequence

On the **Sample sequence**, you can specify the sequence of samples for a subsequent measurement, which you can start using the icon in the document window. You can also create a sample sequence directly before a measurement.

Requirements for the sample sequence

- When using cell changers and autosamplers, the samples are assigned to the sample positions in the accessories.
- If the sample sequence is empty, the **Sequenz settings** window will first appear when starting the measurement of the sample sequence. This window may only be exited once there has been at least one sample defined.

10.1.6 Colorimetry - Settings | Archive automatically

You can automatically save, export, and print the measurement data and its analysis. This allows you to standardize your data archiving processes and ensure that data is not lost. Select the target files and report templates in the **Archive automatically** screen. Additionally, automatic archiving must be activated program-wide in the **Options** window and the times for the individual archiving functions must be selected.

See also

Automatically archive measurement data [▶ 28]

10.1.7 Colorimetry - Settings | Note

A note on the method may be optionally entered on the **Note** screen.

10.2 Performing measurements in the Colormetric module

The prerequisite for starting a measurement is that a new method has been created or loaded in the document window. The measurement can be started with a sample sequence stored in the method or as individual measurement.

The following icons are displayed for the measurements:

Icon	Description
Measure sequence	Start sample sequence If you have not saved any sample sequences to the measurement parameters, the **Sequenz settings** window will appear after you click on this icon. This window may only be exited once there has been at least one sample defined.
Measure sample	Start individual sample measurement independent of the sample sequence configured
Reference	Measure reference A separate reference measurement is required if the sample sequence does not start with a reference measurement or no reference is available that matches the current method parameters.
Stop	Stop current measurement and do not continue
Suspend sequence	Interrupt the measurement and continue at a later time The current sample measurement is completed. The pending sample sequence is then displayed and can be edited.
	Available for cartridge sipper system and APG sampler: Switch pump on or off and convey sample or stop conveying
	Available for APG sampler: Lower or raise sample cannula
	Available for APG sampler with stirring function: Switch stirrer on or off
	Adjust the temperature in a Peltier temperature controlled accessory

Measure reference

If the sample sequence does not have a reference at the first location, the reference must be recorded separately.

- Place the reference into the sample space.

- Click on **Reference** and confirm the prompt about the reference measurement.
  - ✓ The reference measurement is run. All subsequent measurements are corrected with this reference until the measuring parameters are modified by a new method configuration or the next reference measurement takes place.

Start first sequence

With the start of the sample sequence the samples are processed in the order specified in the sample table.

- Place the first sample of the sequence in the sample space or fill cell changer/autosampler with samples.
- Click on **Measure sequence**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  - ✓ The sample sequence is processed. The measured values and analyses are displayed in the document window.

Interrupting or stopping the sequence

An ongoing measurement may be interrupted and then continued or stopped completely.

- Click on **Stop** to stop the measurement.
  - ✓ The measurement of the sequence is stopped and cannot be continued. Measurement data recorded up to this point remain intact and may be processed further.
- Click on **Suspend sequence** to interrupt a measurement and continue it later.
  - ✓ The current sample measurement is ended and then the processing is interrupted. The measurement pause may be used to view and edit the ongoing sample sequence.

Start next sequence

After processing the first sample sequence, the sequence may be started again or re-edited on other occasions. This is also possible if the document has already been saved and re-opened to display the results.

- Click .
  The **Edit sequence** window appears with the sequence stored in the method.
- If necessary, compile a new sequence.
- Confirm the setting in the **Edit sequence** window by clicking on **Ok**.
- Follow the subsequent on-screen prompts for inserting the samples and starting sample measurements.
  - ✓ The current sequence is processed and the data appended to the existing measurement table and analyses.

Performing single measurements

Regardless of the sequence configured, single samples of sample type **Sample** may be measured and appended to the measurement table and analyses.

- Place the sample into the sample space.
- Click on **Measure sample**.
- Follow further on-screen prompts for starting the measurement.
  - ✓ The measurement is run and the data is appended to the existing measurement table and analyses.

Tip

If measurements of other sample types are to be appended, click on **Measure sequence** and enter a sequence with the corresponding samples.

Re-measuring samples

Outliers of a measurement may be re-measured and thus values from a measuring series that differ greatly replaced by new values. The re-measurement of samples is always recorded in the audit trail. For the re-measurement of a probe, you will need to switch to the **Measurement** worksheet.

- Place the sample in the sample space.
- Right click on the row of the sample to be re-measured. For multiple measurements, you can select a single value by clicking with the right mouse button.
- In the context menu, select **Remeasure sample**.
- Follow further on-screen prompts for starting the measurement.
  - ✓ The measurement is run and the measured value replaced in the sample table. The existing analyses are updated.

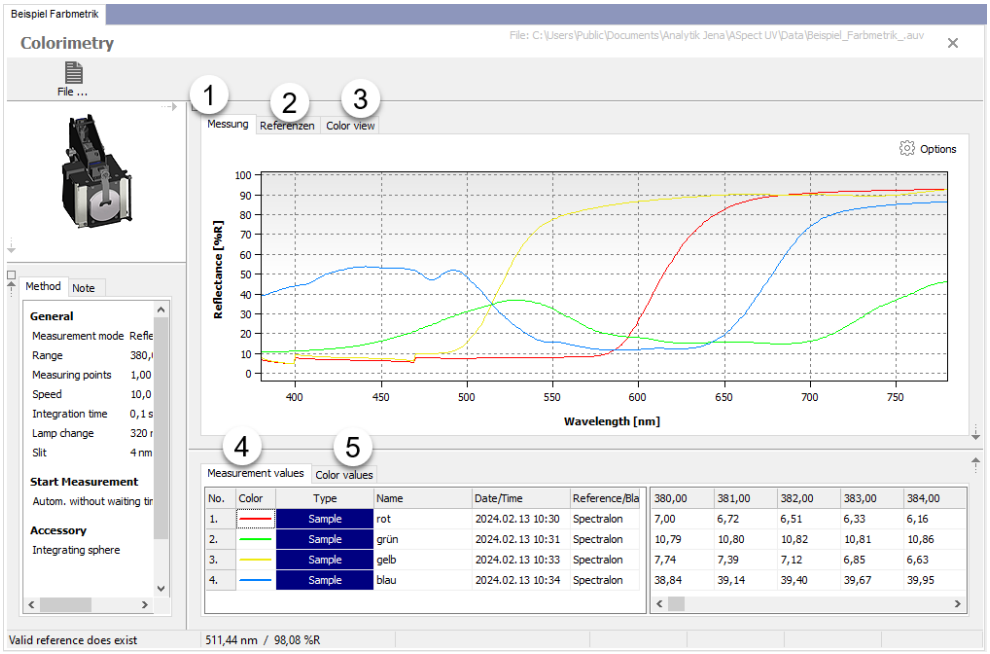
NOTE

If additional worksheets besides the **Measurement** worksheet are already available in the document, these are not updated during a re-measurement.
When using cell changers or APG the sample to be re-measured must be placed in the same position in the accessories. The position in the accessories can be displayed in the sample table on the worksheet.
Time-cyclical measurements cannot be re-measured.

10.3 Displaying and analyzing results in the Colormetric module

This section explains the particularities of the results display and analysis in the **Colormetric** module window.

Document window in the module **Colormetric**



1 Work sheet **Measurement**
2 Work sheet **References**
3 Work sheet **Color view**
4 Tab **Measurement values**
5 Tab **Color values**

Measurement worksheet

The **Measurement** worksheet contains the measurement data. The sample spectra are displayed in the upper half of the worksheet.

References worksheet

The w**References** orksheet shows the reference spectra and the measured values of the references.

Sample table

The **Measurement values** tab contains the sample table in the order of the measurements and the table with the digital measured values of the sample spectra. The sample table can be configured freely. After right clicking on the table header the following parameters can be selected in the context menu:

- Number in the sequence
- Color of the measurement curve in the chart
- Batch when using cell changer or autosampler
- Position in accessories when using cell changer or autosampler
- Sample type
- Sample name
- Date and time of the measurement
- Notes
- Temperature for methods with Peltier-tempered accessories

Via Drag&Drop the order of the table columns can be changed.

Analysis of the spectra

On the **Color values** tab, the data analyses already defined in the method are shown. You can add to and edit these analyses:

▶ On the **Color values** tab, click on **Settings**.

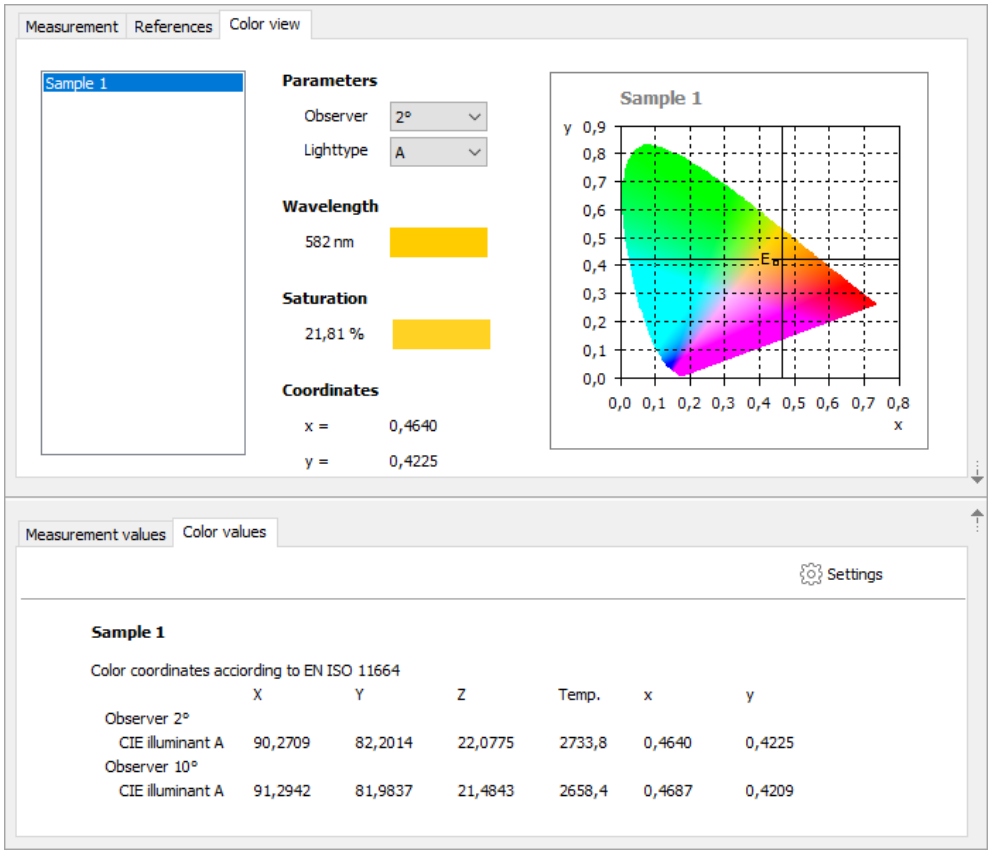
▶ In the **Settings - Color values** window, activate the desired color coordinates with the parameters or the color numbers to be calculated.

✓ The view on the Color values spreadsheet is adjusted depending on the selected parameters.

Color view worksheet

The **Color view** worksheet displays the chromaticity coordinates and their position in the coordinate system.

Option/value	Description
Parameters	Parameters for calculating the standard chromaticity coordinates: **Observer** Select observation angle **Illuminant** Select illuminant **Note**: The selection on this tab does not have an effect on the results output on the **Color values** tab. The pathlength is set at 1 cm, regardless of the pathlength agreed.
Wavelength	Dominant wavelength of the hue on the standard color value chart
Saturation	On the standard color value table, the saturation of the hue is the ratio of the distance of illuminant (achromatic point)/color coordinates (x, y) and illuminant/dominant wavelengths on the standard color value chart.
Coordinates	xy values of the hue on the standard color value chart



See also

- The document window [▶ 14]
- Show spectra and measurement curves on the worksheet [▶ 19]

10.3.1 Display options for the spectra in the Colorimetry module

The following functions are available for displaying the color spectrum:

- Scale curves
- Add text to curves (text box)
- Select curves/samples
- Change the color of curves

- Hide a curve (deactivate a sample)

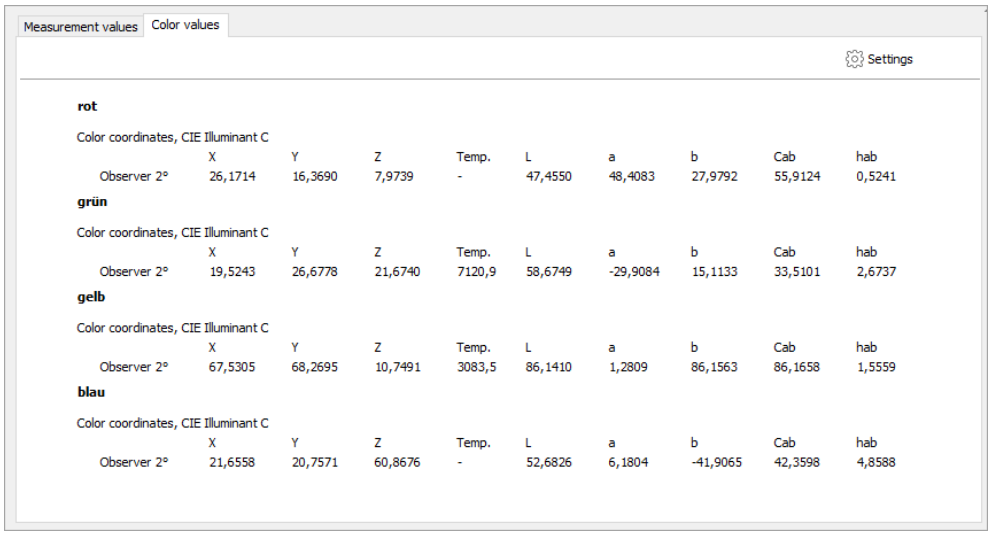
See also

Show spectra and measurement curves on the worksheet [▶ 19]

10.3.2 Analyzing spectra in the Colormetric module

The data analyses offered in this method can also be performed later. The analyses are output in their own spreadsheet in the bottom part of the worksheet on the **Color values** spreadsheet.

- On the **Color values** spreadsheet, click on **Settings**.
- In the **Settings** - **Color values** dialog window, activate the desired color coordinates with the parameters or the color numbers to be calculated.
  - ✓ The view on the **Color values** tab is adjusted depending on the selected parameters.



See also

Colorimetry - Settings | Color values [▶ 119]

10.4 Example measurement in the Colorimetry module

A determination of the tristimulus values at the observation angles of 2° and 10° with standard illuminant A serves as an example. An integrating sphere and single-color paper can be used for the measurement. If unavailable, a cell with water can be used as reference and a color solution as sample. For information on handling the integrating sphere, see the "SPECORD PLUS Accessories" operating instructions.

The following steps must be carried out:

1. Create the document in the module.
2. Open method and enter parameter.
3. Start measurement.

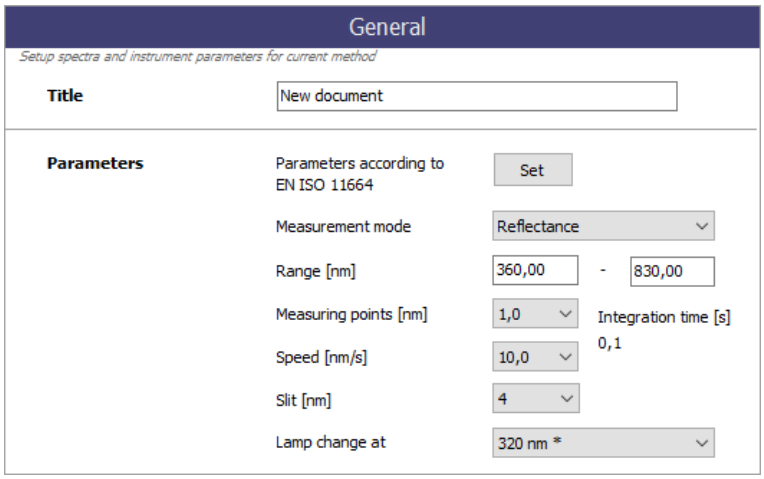
Preparing a document

- Click on in the task bar or select menu item **Modules** | **Colormetric**.
  - ✓ A new document is opened.

Defining method parameters

- Click on **Method setup** in the document window.
- Enter the parameters according to the screenshot on the screens of the **Colorimetry - Settings** method window (see below).
- Confirm the parameters in the method window by clicking on **Ok** and return to the document window.

General screen



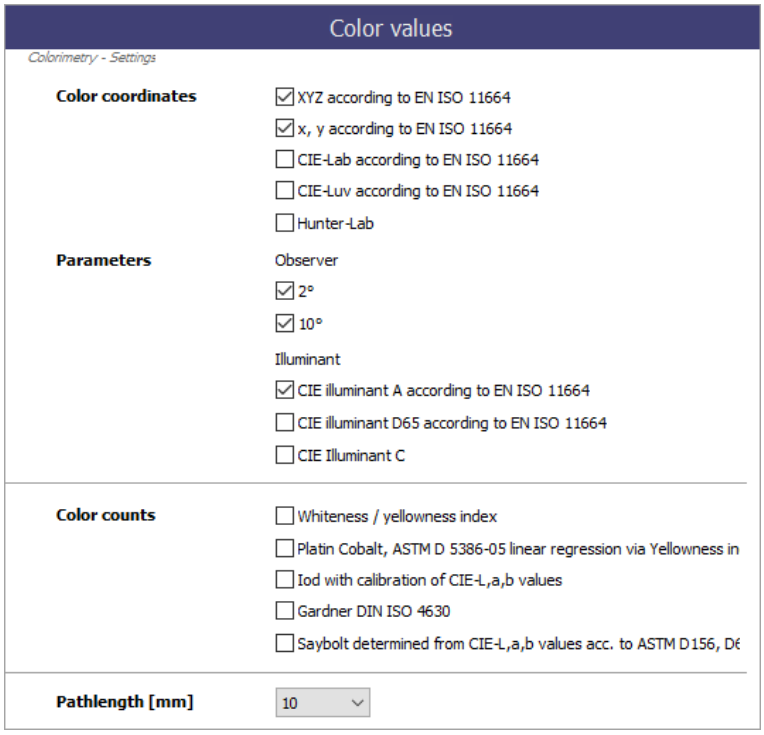
Start measurement screen

Make no entries.

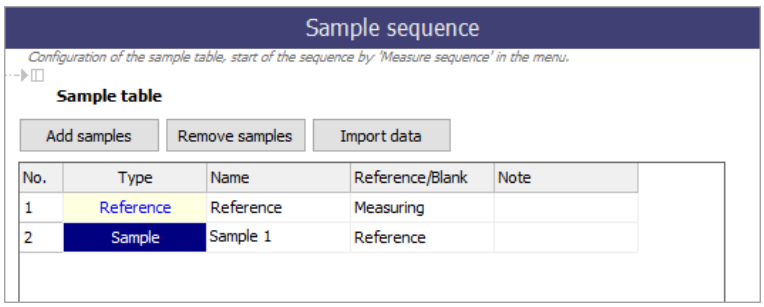
Accessory screen

Make no entries.

Color values screen



Sample sequence screen



Archive automatically screen

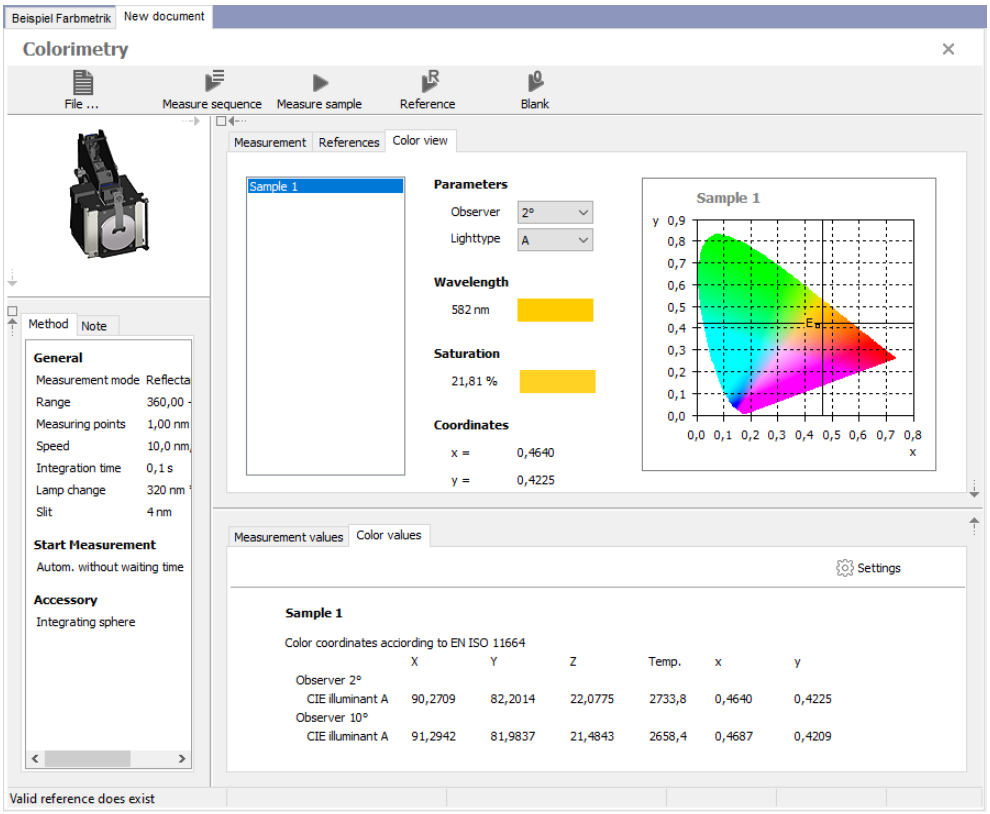
Make no entries.

Note screen

Make no entries.

Performing the measurement

- Click on in the document window.
  The start information for measuring the reference is displayed.
- Insert the reference sample, e.g. reflectance standard from integrating sphere accessory, and click **Yes** to start the measurement.
  - ✓ The reference measurement is performed. A prompt to measure sample 1 is displayed.
- Insert sample 1 and click on **Yes** to start the measurement.
  - ✓ The sample spectrum appears in the document window.



11 General device functions – Instrument menu

11.1 Show device status

After selecting menu item **Instrument** | **Info**, the device status of the SPECORD PLUS is displayed. After successful initialization, display information on the firmware version and on connected accessories.

If the SPECORD PLUS is not connected to the computer, the message "Simulation mode: SPECORD XXX PLUS" is shown, whereby XXX corresponds to the device configured in the window **Options** | **Start** | **Simulation** (**Settings** | **Options**).

See also

Configuring simulation mode [▶ 141]

11.2 Initializing the device and starting simulation mode

In accordance with the standard settings in the **Options** | **Start** | **Start ASpect UV** window, the device is initialized when the program is started and SPECORD PLUS is switched on, i.e. there is a connection established between the device and the computer. The SPECORD PLUS is then ready to perform measurements.

The ASpect UV program runs in simulation mode if it is not connected to the SPECORD PLUS. In this mode, existing measured values may be analyzed and processed. In addition measuring functions are simulated; the program can be explored without the device being switched on.

If the connection to the SPECORD PLUS fails while starting the ASpect UV, ASpect UV automatically starts in simulation mode. The device can be set to the ready-to-measure state by subsequent initialization.

Initialize SPECORD PLUS

- If necessary, install and connect the accessories in the SPECORD PLUS. Switch on the SPECORD PLUS.
- Close all documents in Aspect UV.
- Select the menu item **Instrument** | **Initialization** or click on the **Initialization** icon in the task bar.

  ✓ The monochromator of the SPECORD PLUS moves and the message **Initialization** is displayed on the monitor. If the options to switch on the lamps are not activated in the window **Options** | **Start** | **SPECORD PLUS**, a prompt relating to switching on the lamps will appear. At the end of the lamp switch-on phase, connected accessories are initialized and the SPECORD PLUS is ready to measure.

Start simulation mode

- Close all documents in Aspect UV
- Select the menu item **Instrument** | **Simulation**.
- The USB connection to the device is closed and the device and accessory chosen in the **Options** | **Start** | **Simulation mode** window are activated. If no further measurements are to take place, the SPECORD PLUS may be switched off at the power switch.

11.3 Correct SPECORD PLUS

Basic and grid correction

The SPECORD PLUS is fully adjusted and set up ex factory. Changes in the adjustment caused by transport, ambient temperature or change of lamps will be corrected by the ASpect UV program, without requiring mechanical intervention in the device.

The following parameters are checked during the basic correction and corrected if necessary:

- Offset (dark current)
- Zero order of the lamps
- Amplifier stages of the receivers
- Wavelength correction using internal holmium filter and UV lamp

In the SPECORD 250 PLUS, a mesh correction is additionally performed and the mesh of the pre-monochromator aligned with the mesh of the main monochromator.

NOTE

Only perform the basic correction after 2 hours warm-up time. During this period both lamps must be switched on.

In the SPECORD 250 PLUS, start the grid correction first and then the basic correction.

- ▶ Remove samples and accessories that influence the beam path (integration sphere, flow cell etc.) from the beam paths in the sample space.
- ▶ Only SPECORD 250 PLUS: Select the menu item **Instrument** | **Correction** | **Grid Correction**.
  - ✓ The grid correction starts immediately.
- ▶ Select the menu item **Instrument** | **Correction** | **Basic correction**.
  - ✓ The basic correction starts immediately.
- ▶ Optionally display the results of the correction.

At the end of the correction process, the new correction data is permanently saved in SPECORD PLUS and on the computer. The data remains in place until the correction values are next recorded and are used for the correction of all subsequent measurements.

Note: If measurements are carried out exclusively with accessories that are complex to install, such as Peltier temperature controlled changers, and if these were already installed during initialization, they can also remain in the sample chamber if the accessory detection was switched off before the correction. The samples must be removed from these accessories beforehand.

Correcting infinite absorbance

Correction of the infinite absorbance is only possible if the "Validation according to USP" module has been installed.

- ▶ Remove samples and accessories that influence the beam path (integration sphere, flow cell etc.) from the beam paths in the sample space.
- ▶ Carry out a mesh correction (with SPECORD 250 PLUS) and basic correction (see above).
- ▶ Select the menu item **Instrument** | **Correction** | **Correction of infinty absorbance**.
  - ✓ Recording of the correction spectra starts.

At the end of the correction process, the correction spectra are saved in Aspect UV on the computer. The data remain in place until the correction spectra are next recorded and are used for all subsequent measurements.

See also

Calculation of measured values and recording of the reference values [▶ 180]

11.4 Checking the measuring technology condition of the SPECORD PLUS.

ASpect UV provides functions for checking the measuring technology condition of SPECORD PLUS. This allows for validation of the correctness of the measured values and makes it easier to find device errors and faults. The functions for checking SPECORD PLUS are located in the **Instrument** menu.

11.4.1 Checking the lamp intensity

The halogen lamp for the Vis range and the deuterium lamp for the UV range are subject to normal wear. With aging, the beam properties deteriorate resulting in a worse signal-to-noise ratio and thus a lower photometric reproducibility and a reduced photometric range. The lamp test checks whether the energy of the lamps is still sufficient to meet the technical specification of the SPECORD PLUS.

If one or both lamps have been replaced, the device corrections must be carried out again.

- Remove samples and accessories that influence the beam path (integration sphere, flow cell etc.) from the beam paths in the sample space.
- Select the menu item **Instrument** | **Test** | **Lamp check**.
  - ✓ The energy measurement of the UV lamp followed by the Vis lamp takes place.

After the completion of both measurements the bar charts of the measured results of the tested lamps and the information about the lamp condition are displayed in the window **Lamp check**:

- The energy is within normal range
- The lamp approaches the end of its life.
- The lamp should be exchanged soon.

11.4.2 Checking the functionality

ASpect UV contains a diagnostic program with which the following device functions can be checked:

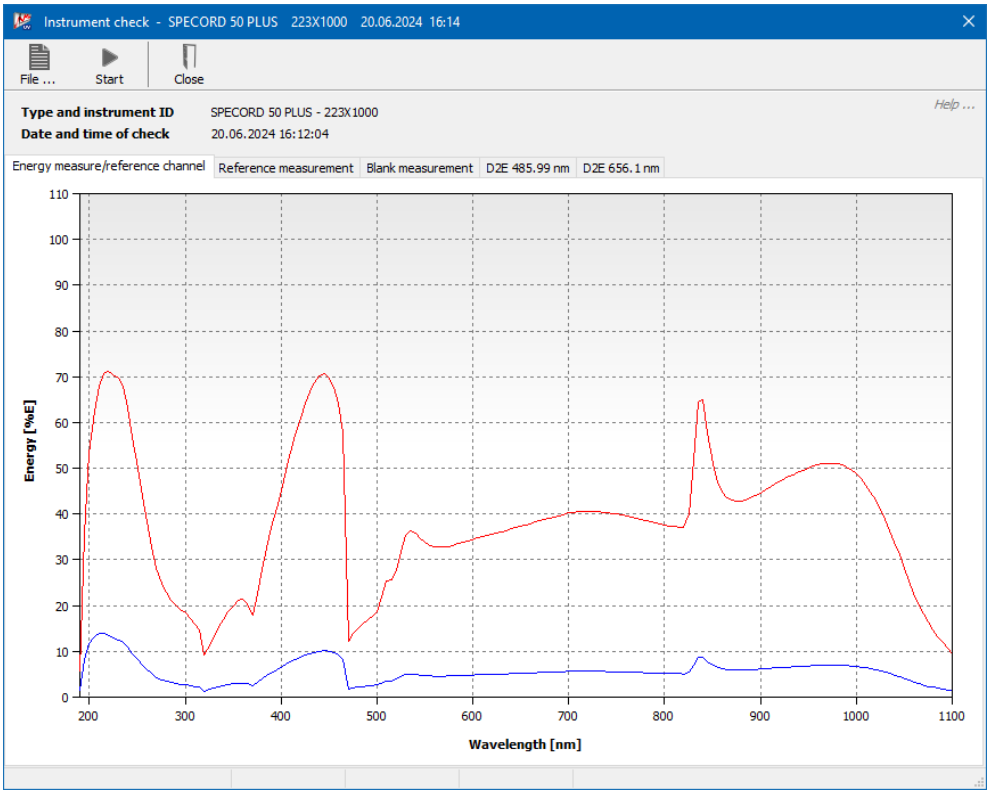
- Reference measurement as ratio of measuring and reference beam path in %T
- Energy in the measurement and reference beam path
- Blank measurement in %T as 100-percent base line
- Wavelength accuracy through registration of the spectral lines of the deuterium lamp at 485.9 nm and 656.1 nm

The diagnostic results can be printed and saved in a file.

- Remove samples and accessories that affect the beam path (integrating sphere, flow-through cell, etc.) from the beam paths in the sample chamber.
- In the main window, select menu item **Instrument** | **Test** | **Instrument check**.
- Click on ▶ **Start**.
  - ✓ The test items are processed automatically.

After completion of the test, the measuring graphs are displayed on the 4 tabs of the **Instrument check** window. In case of device errors, corresponding messages are output.

Display after device test



For the graph view, the graphical zoom function is available.

- With the mouse button held down, draw a frame around the area to be enlarged. The action is reversed by double clicking on the diagram.

The results of the device check may be saved, reopened and printed using the **File** menu.

11.4.3 Measuring energy

During the energy measurement, the energy progression is recorded separately in the reference and measurement beam paths and output as energy values. This function is mainly used by Service to evaluate the device condition and find faults.

After selecting **Instrument** | **Test** | **Energy measurement**, the window of the same name appears.

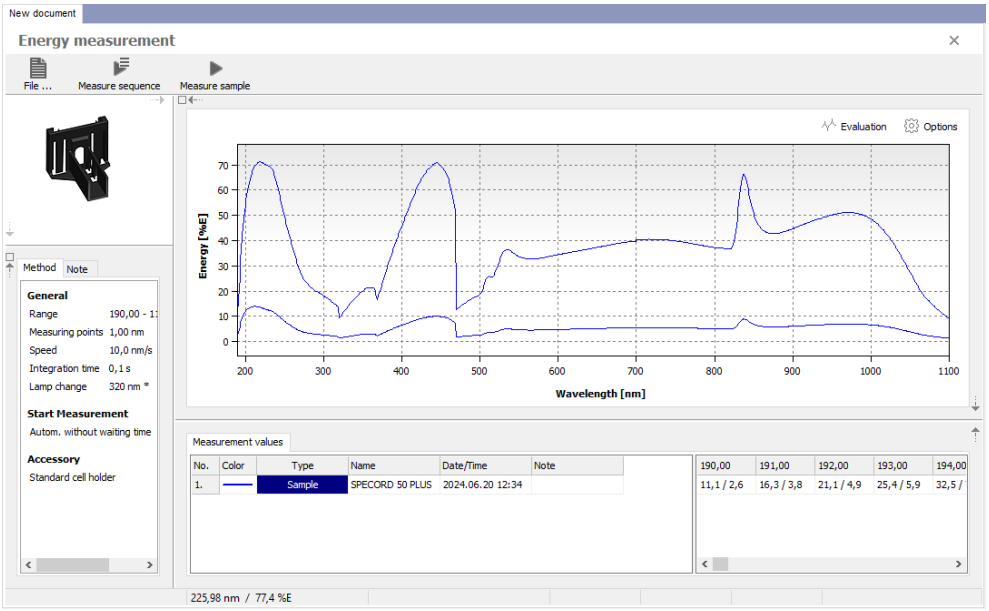
The measurement parameter configuration takes place in the same way as the configuration in the **Spectrum** module with the following limitations:

- Only the energy signal is recorded.
- No calibration is provided.
- There is only the sample type **Sample**.

Start/analyze energy measurement

After selecting the measurement parameters, the icons for starting the energy measurement are enabled.

- Start the measurement by clicking on **Measure sample**.
- Add further measurements if necessary.
- To analyze the data, the functions **Peaks**, **Values of def. wavelengths** and **Formula** can be applied.



11.4.4 Setting the zeroth order

With the **Zeroth order** function, the monochromator is rotated into a position where the light is not divided at the mesh but reflected like in a mirror. The undivided (white) light passes through the sample space and can be easily monitored due to its intensity. This is used to adjust accessories, e.g. microcells, in the beam path. The zeroth order may be separately set for the halogen lamp and the deuterium lamp.

- To configure the zeroth order of the deuterium lamp, select **Instrument** | **Zeroth order** | **UV lamp**.
- To configure the zeroth order of the deuterium lamp, select **Instrument** | **Zeroth order** | **Vis lamp**.
  - ✓ The lamp radiation not passes undivided through the monochromator and becomes visible in the sample space.

11.5 Additional functions for controlling accessories

The following functions for controlling accessories are available in the **Instrument** menu:

- Switching active accessory detection on and off
- Switch active accessories on and off electrically
- Move cell changers and samplers to individual positions
- Adjust cell changers
- Optimize pump times
- For Peltier temperature controlled accessories: Query the temperature range and the current temperatures

11.5.1 Switching accessories on and off

With this function, the electrically controlled accessory is switched off. The accessory is also moved to the parking position and the power supply interrupted. The accessory can then be easily removed from the sample chamber without risk of short circuit.

- In the main window, select menu item **Instrument** | **Accessory** | **Off**.

✓ The accessory is switched off and will not be displayed in the method parameters anymore. The accessory can then be removed from the sample chamber.

▶ To re-activate the accessory, select the menu item **Instrument** | **Accessory** | **On**.

✓ The accessory is initialized and available again for methods and measurements.

NOTE

If the accessory plug is not removed from the connection on the SPECORD PLUS, the accessory is automatically recognized again the next time the device is initialized.

11.5.2 Switching active accessory detection on and off

This function is only relevant for the cell carousel. The detection of active accessories can be switched off with software support without the identification plug having to be pulled. In the subsequently opened method parameters, the accessory is treated as a passive accessory, even though the accessory continues to be supplied with power. Use this function when you are using the cell carousel as a holder only. When the cell carousel is not powered, the tray moves freely and the cells cannot be positioned in a reproducible manner.

▶ Select the menu item **Instrument** | **Accessory** | **Accessory recognition off**.

✓ The accessory detection is switched off and no longer used for the subsequent measurements. The accessory continues to be supplied with power.

▶ To re-activate the accessory, select the menu item **Instrument** | **Accessory** | **Accessory recognition on**.

✓ The accessories are available again for methods and measurements.

11.5.3 Adjusting the cell changer and moving to individual positions

Moving to positions in the cell changer

The cell changer or cell carousel may be moved to a specific sample position.

▶ In the main window, select menu item **Instrument** | **Accessory** | **Sample position**.

▶ In the **Sample position** window, move to the desired position with the buttons.

✓ The cell changer moves to the specified position.

Button	Description
Pos. 1	Move the cell changer to position 1 and initialize
Pos. +1	Move the cell changer to the next position
Parking	Move the cell change to parking position In the parking position it is easier to assemble the cell changer in the sample space or pack it into its storage box.

Adjust cell changers

To position the cells optimally within the beam path the cell changer can be adjusted with the aid of a computer.

An adjustment is necessary in case of

- using the cell changer for the first time
- the use of special cells
- after a basic correction
- after transporting the SPECORD PLUS

▶ Assemble the empty cell changer in the sample space.

▶ Switch on the SPECORD PLUS and start ASpect UV.

- When using microcells: Fill the microcells with solvent, e.g. water, and place them in each position in the sample changer.
  When using standard or semi-microcells: Empty all spaces in the cell changer.
- Start adjustment by selecting **Instrument** | **Accessory** | **Adjust**.
  - ✓ The adjustment is carried out automatically and the corrected values saved to the device and the PC.

11.5.4 Optimizing the pump time of the cartridge sipper system

When determining the optimum pumping time, the measured value is continuously recorded while the sample or reference solution is pumped through the cell. The change in energy, absorbance and transmittance is displayed on the screen on 3 tabs over time. During the process the measured value increases or decreases and finally reaches a plateau. The optimum pumping time corresponds to the reaching of the plateau phase. At this time the cell has been flushed sufficiently with sample or reference and the carry-over is smallest.

Functions of the Optimization pumping time window

The following functions are available in the menu bar:

Function	Description
File ...	Menu for data administration **Save** Save optimization data **Load** Open optimization data **Close** End optimization of the pumping time
Start	Start optimization
Pump on / **Pump off**	Switch the pump on and off independently of the start of the measurement
Stop	Stop the measurement early

Enter the following parameters on the **Settings** tab:

Parameter	Description
Wavelength	Analysis wavelength of the sample
Measurement time	Total measuring time for the optimization
Integration time	Time for recording a measuring point, e.g. 0.1 s
Slit	Only SPECORD 210/250 PLUS: Slit setting, e.g. 1 nm
Pump start	Time during the measurement at which the pump starts
Pump stop	Time during the measurement at which the pump stops
Slow run	Reduce the pump speed to half of the normal speed to reduce degassing or segregation, or to be able to dose more accurately with small sample volumes
Energy, **Absorption**, **Transmittance**	Ordinate range for displaying the measured values on the corresponding tabs

Performing optimization

- Provide reference and sample solution.
- Start optimization by selecting **Instrument** | **Accessory** | **Optimization pumping time**.
- Remove the flow cells from the holder and fill them with reference solution:

- Submerge the aspiration hose into the reference solution and click on .
- Once the cell is filled without bubbles, stop the pump by clicking on .

▶ Place the flow cells in the holder and submerge the aspiration hose into the sample solution.

▶ Start the measurement by clicking on .

✓ To start, the reference is automatically determined and then the measured values are recorded.

▶ Observe the change of the measured value on one of the tabs **Energy**, **Absorption** or **Transmittance**:

- The time range in which the pump is running is highlighted in white. The range during which the pump was stopped is gray.
- The pumping time is optimal when the measured value is stable or has reached the required accuracy.
- In the time after switching off the pump, you can observe whether the sample remains stable or changes due to decaying turbulence.

11.5.5 Adjusting the APG autosampler, moving to individual positions, and optimizing the pump time

Moving to individual positions

Individual positions of the sampler can be moved to separately.

▶ Select the menu item **Instrument** | **Accessory** | **Sample position**.

▶ In the **APG 64 xyz autosampler** positioning window, move the autosampler arm to the desired position with the buttons.

Adjusting the autosampler

Depending on the size of the sample container opening, the sample positions may need to be readjusted.

▶ Place a sample container on the 4 corners of the sample tray.

▶ Click on one of the positions and move the autosampler arm over the position.

▶ Use the icon (down) in the positioning window to lower the cannula holder without the cannula. Then insert the cannula and position slightly over the edge of the container.

▶ Centrally position the cannula using **Offx** and **Offy**. Repeat the process at the other 3 corners and determine the values for Offx and Offy.

▶ Set the final immersion depth. To do this, move the sample intake tube in its guide with the sample arm lowered.

The following functions are available in the window for adjusting the autosampler:

Button	Description
Offx / **Offy**	Set the cannula in the x and y direction in the center of the container
	Adjust the Z-lift of the sampler arm
Factory default	Restore the factory settings
Pos. 0	Initialize APG and move to position 0 Position 0 can only be approached in the positioning window. The system can be pre-rinsed at this position with a separate purge cup in this position.

APG S sampler

With the APG S, the sample tray can be adapted to customer requirements. Additional functions are displayed in the positioning window for this purpose:

Function	Description
nx / **ny**	Set the number of sample containers via the number of table rows (nx) and columns (ny).
nx0 / **ny0**	Move position 1 in x/y direction
lx / **ly**	Set the sample position via the spacing of the sample tubes relative to each other. The graphic representation in ASpect UV is not adjusted.

Optimize pump time

The pump time of the cartridge sipper system must be optimized for the transport path of the sampler.

- Provide reference and sample solution.
- Start adjustment by selecting **Instrument** | **Accessory** | **Optimization pumping time**.
- Click on **Sample positions** and move to the position of the reference.
- Click on **Needle down** to lower the autosampler arm.

Continue as described for the pump time optimization of the cartridge sipper system.

Move to the positions on the APG with the buttons , and and lower or raise the autosampler arm.

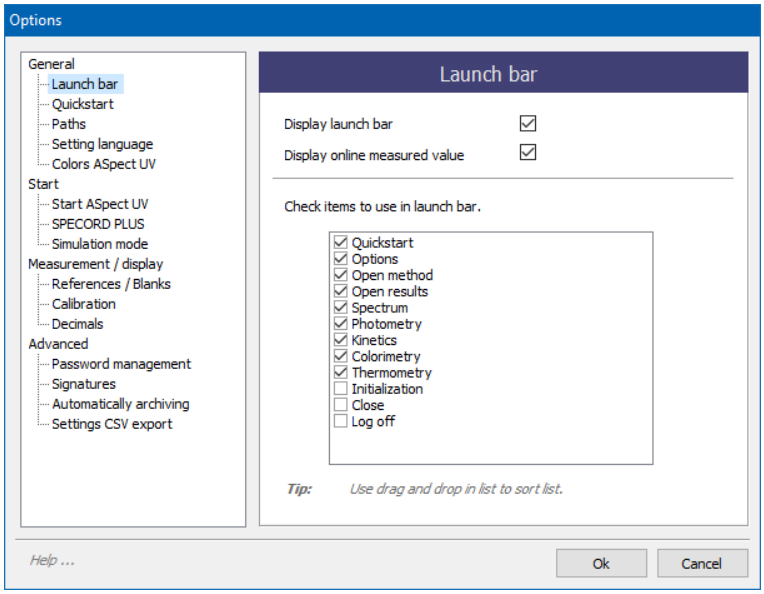
See also

Optimizing the pump time of the cartridge sipper system [▶ 135]

12 Set up ASpect UV in the Options window

A number of functions for setting the view, the start and the execution of the program are included in ASpect UV. For example, a quick start menu with your most used methods can be displayed at program start or the calibration in the individual modules can be preconfigured.

These settings are made in the **Options** window. For a better overview, the screens of the window are arranged thematically into the groups **General**, **Start**, **Measurement / display** and **Advanced**.



12.1 Configuring the launch bar

The task bar on the left-hand side of the desktop gives you quick access to individual modules and functions of ASpect UV.

- Open the **Options** | **General** | **Launch bar** window with the **Settings** | **Options** menu option.
- Activate the options for the desired elements and drag and drop the activated elements into the desired order (by holding down the mouse button).
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The elements are displayed in the selected order in the task bar of the main window.

12.2 Configuring quick start

Quick start is a collection of methods in which routine methods may be saved. When quick start is accessed, these methods are available for use and may be started immediately. For a better overview, you can arrange the methods in groups from ASpect UV 2.0 onwards. In the **Options** | **General** | **Quickstart** window there are two lists for this, one with the groups created and one with the methods assigned to a group.

Creating a new Quick Start element

First create a new group and then assign the methods (measurement parameter files) to the group.

- Open the **Options** | **General** | **Quickstart** window with the **Settings** | **Options** menu option.
- To create a new group, click on + next to **List of quickstart group items**.
- Enter a title in the **New item for quickstart** window and confirm with **Ok**.
  - ✓ The new group now appears in the group list.
- To assign a method, click on + next to **List of quickstart items**.
- In the **New item for quickstart** window, enter a title, select a group from the list and click on ... a method file to select it.
- Click **Ok** to confirm the entered data.
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ These settings are effective in the **Quickstart** window.

Sorting/editing elements in Quick Start

You can sort the order in which the groups and methods should appear in the **Quickstart** window.

- Select an element in one of the lists and move it to the desired position using the arrows next to **Group** or **Title**.
  Alternatively, hold down the mouse button and drag and drop an entry in the respective list to the desired position.
  - ✓ In the **Quickstart** window, the groups are arranged in consecutive tabs. The methods and their names are listed one below the other on the group tabs.

You can give the elements in a group a new title or assign a different method.

- To change a title, click on the title field twice in slow succession. If only the text is highlighted, enter the new title and confirm with the Enter key.
- To change a method, click on the method field and then click on ... Select the new method in the **Open** window.
  - ✓ The elements are edited accordingly.

Removing elements from the Quick Start

You can clean up the Quick Start and delete elements that are no longer required.

- To delete a method, first select the group to which the method is assigned and then select the method element in the list.
- Click on - next to **List of quickstart items**.
  - ✓ The method element is deleted from the list and no longer appears in the **Quickstart** window.

A group can only be removed if it does not contain any methods. The **Quickstart** window must contain at least one group.

- To delete a group, select the group in the list.
- Click on - next to **List of quickstart group items**.
  - ✓ The group is deleted from the list and no longer appears as a tab in the **Quickstart** window.

See also

- Configuring the start of ASpect UV with module or Quickstart [▶ 9]
- Using Quickstart [▶ 10]

12.3 Directory path presets

You can preset directories for loading or saving data (methods, results, calibrations, templates for printing and exporting, sample information data). You can make the settings separately for each module or for all modules in ASpect UV.

- Open the **Options** | **General** | **Paths** window with the **Settings** | **Options** menu option.
- In the **Module** list, select the module for which the directories are to be set. If the same directory is to be preset for all modules, select the **All modules** option.
- Select a function in the list, for example **Open method**, and select a directory option in the list next to it:
  - **Last used path**: The last path used will be used the next time the selected data is loaded/saved.
  - **Default path**: The path set here is displayed at next load/save.
- Click on ... and set the path in the **Select directory** window.

Note: If you select a file via **File** | **Open results** or **File** | **Open method**, then the last opened directory is displayed.

12.4 Setting the language

You can select different languages for the program interface in ASpect UV. To change the language, no document/module must be open.

- Close all documents in Aspect UV.
- Open the **Options** | **General** | **Setting language** window with the **Settings** | **Options** menu option.
- Select a language for the user interface in the **Language** list.
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The ASpect UV user interface is displayed in the selected language.

12.5 Setting the color scheme

You can change the colors of the program user interface.

- Open the **Options** | **General** | **Colors ASpect UV** window with the **Settings** | **Options** menu option.
- Select an object in the **Item** list and click on the color. Continue in this way until the colors have been assigned to all elements.
- Save the created color scheme with .
- Load with a saved color scheme with .
- Restore the default color settings with .
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The new color scheme is applied to the program interface.

12.6 Defining the start mode for ASpect UV

ASpect UV starts with an empty desktop by default. However, you can also start directly with a new document in a favorite module or with the Quick Start. You can also choose whether the SPECORD PLUS is connected and initialized with ASpect UV at startup or whether initialization should take place later.

- Open the **Options** | **Start** | **Start ASpect UV** window with the **Settings** | **Options** menu option.
- If the device is to connect to ASpect UV at startup, enable the **Initialize instrument** option.
  Note: First switch on SPECORD PLUS and wait until the alignment of the monochromator drives is complete. Then start ASpect UV.
- If ASpect UV is to be started with a specific module or the Quick Start, select this in the **Item** list.
- Confirm the settings with **Ok** and close the **Options** window.
  ✓ The settings will take effect the next time ASpect UV is started.

12.7 Switching on the lamps and recording monitor files

When initializing the device, you can have the two lamps switched on automatically. If automatic activation is deactivated, a dialog will open asking whether to switch on the lamps during initialization and start of a method. The lamps are only switched on when this is answered with **Yes**. You can also switch the lamps off when they are no longer required. Please note, however, that switching the lamps on frequently reduces their service life.

In a service case, you may be asked to activate the monitor file during remote maintenance. The monitor file records the data traffic between the device and the software and can provide the service department with information about a possible error.

- Open the **Options** | **Start** | **SPECORD PLUS** window with the **Settings** | **Options** menu option.
- To switch the lamps on automatically during initialization, enable the options **Switch on the UV lamp** or **Switch on the Vis lamp**.
- Activate the **Monitoring file** option to record the monitor file.
  The next time a measurement is started, the data traffic is recorded.
- To switch off the two lamps, enable the corresponding option **UV off** or **Vis off**.
- To switch the lamps on manually, select **UV on** or **Vis on**.
- Confirm the settings with **Ok** and close the **Options** window.
  ✓ The settings for automatically switching on the lamp will take effect the next time the program is started.

12.8 Configuring simulation mode

You can use ASpect UV without the device being switched on to analyze data or create methods for routine measurements. To do this, ASpect UV is operated in a mode that simulates a switched-on device and the accessories used. This is particularly necessary

for creating methods because the configurable parameters depend on the device and accessories. Measurements are also simulated in simulation mode. You can therefore use this mode to explore ASpect UV without a device.

- Open the **Options** | **Start** | **Simulation mode** window with the **Settings** | **Options** menu option.
- In the **Instrument** list, select the device type.
- In the **Accessory** list, select the accessory.
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The settings are applied in simulation mode.

12.9 Define temporal validity of references and blanks

As of ASpect UV 2.0, you can load saved references and blanks and use them for further sample measurements. You can limit the validity of these reference spectra or reference values in terms of time. If you do not want to use saved references or blanks, you do not need to configure these settings.

- Open the **Options** | **Measurement / display** | **References / Blanks** window with the **Settings** | **Options** menu option.
- Activate the **Period of validity** option for both **References** and **Blanks** and enter the number of days in the **days** field.
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The validity period for references and blanks is adopted.

12.10 Defining settings for calibrations

You can define the validity for calibrations based on the coefficient of determination to be achieved or the duration. If the coefficient of determination is not achieved, the calibration is discarded and must be recreated. Calibrations whose validity period has been exceeded are also discarded. You can also define default settings for the method parameters of the calibration.

- Open the **Options** | **Measurement / display** | **Calibration** window with the **Settings** | **Options** menu option.
- If the calibration must generally achieve a coefficient of determination, enable the **R^2 adjust** option and enter the value in the field next to it.
- If the calibration is only to be used for a specific time, enable the **Period of validity** option and enter the value in the field next to it.
- Select the default settings for the method parameters if required:
  - **Regression**: Calculation model for the calibration curves
  - **Unit** : Concentration unit
  - **Thickness**: Pathlength of the cells
  - **Upper limit value** and **Lower limit value**: Concentration limits between which the calibration is valid. Measured sample concentrations beyond a limit value are marked.
- Confirm the settings with **Ok** and close the **Options** window.

✓ The settings are applied to the following measurements and calculations of the calibrations.

12.11 Set decimal places for output values

You can define the number of decimal places displayed and used for the export for all numerical values in ASpect UV.

- Open the **Options** | **Measurement / display** | **Decimals** window with the **Settings** | **Options** menu option.
- Select an application or module from the **Choice category** list.
- Increase or decrease the number of decimal places with the arrow keys next to the measuring units.
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The settings are applied to the next measurements and calculations.

Note: The internal calculation accuracy for floating-point numbers is double. When exporting, make sure the necessary number of decimal places is set in order to reduce calculation inaccuracies.

12.12 Configuring password properties

If you are using the FDA 21 CFR Part 11 Compliance module with user management, you can set the criteria for the validity of passwords. This screen in the **Options** window should only be activated for administrators.

- Select the **Options** | **Advanced** | **Password management** window with the **Settings** | **Options** menu option.
- Activate the options if required.
- Confirm the settings with **Ok** and close the **Options** window.

Settings for the passwords

Option	Description
Check minimum length	Minimum number of characters for the password
Large and lower case	Password must contain upper and lower case letters
Special character (? *#/\^°)	Password must contain at least one special character
Digits	Password must contain at least one digit
the last passwords must not be used	When a new password is created, the system checks whether the user has used it before. If a password has already been used under the last passwords (number), it will be rejected.

12.13 Creating signatures

If the additional FDA 21 CFR Part 11 Compliance module is used, Aspect UV files can be signed. A signature limits further editing options for a document. The limits can be freely selected for every created signature. Optionally, the signature sequence to apply to a document can be defined.

In the **Options** | **Advanced** | **Signatures** window, you manage the signatures and their properties. On the **List of signatures** tab, existing signatures with their stored functions are displayed, and signatures are created and deleted. A required signature sequence can be defined in the **Sequence of signatures** tab.

Adding, editing and deleting signatures

- Open the **Options** | **Advanced** | **Signatures** window with the **Settings** | **Options** menu option.
- Open the **List of signatures** tab.
- To add a signature, click on + to open the **Signature append** window.
  - Enter the signature name in the **Name** input field and an additional description in the **Description** field.
  - In the **Document**, **Measurement procedure** and **Worksheet** tabs, activate the functions that can still be carried out with the file after the signature is applied.
- To edit an existing signature, double-click on the relevant signature in the list.
- Mark a signature that is no longer required in the list and click - to delete it.
  Only signatures not included in the signature sequence can be deleted.

NOTE

Functions that can no longer be carried out after application of a signature will remain disabled after the application of further signatures. A signature cannot remove the restrictions of a previous signature.

Defining a signature sequence

If a signature sequence is defined, signatures included in the sequence can only be applied in the indicated sequence. A document is considered fully signed when all signatures have been applied. For incompletely signed documents, a message that the file has not been completely signed appears when saving and opening the file.

Signatures in the **Available signatures** list are not included in the signature sequence. They can be used on a document at any time and in any sequence.

- In the **Options** | **Advanced** | **Signatures** window, select the **Sequence of signatures** tab.
- Select a signature in the **Available signatures** list and move it to the **The order to be followed when signing** using the arrow button.
- Transfer all further required signatures to the **The order to be followed when signing** list in the same manner.
- Sort the collected signatures in a sequence. Mark each signature and move it to its required position with the arrow keys to the right of the list.
  Work downward from the top of the signatures list to the bottom
- Mark the signatures not required in the sequence and transfer them back to the **Available signatures** list with the arrow key in the middle.
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The documents can now be signed.

NOTE

Permission to use a specific signature must be assigned to each user in their user profile.

See also

Electronic signatures [▶ 173]

12.14 Activating automatic archiving

Automatic archiving of documents can be set in ASpect UV. You must activate this function in the **Options** window and select the time for each archiving function. Define the file name and the report options for automatic archiving in the method.

- Open the **Options** | **Advanced** | **Automatically archiving** window with the **Settings** | **Options** menu option.
- If automatic archiving is to take place throughout the program, enable the **Automatically archiving** option.
  If the option is disabled, automatic archiving is switched off program-wide, regardless of whether this function is enabled in a method.
- Select a function, for example **Save**, in the **Archiving function** list.
- Activate the options to carry out the selected archiving function, e.g., **When closing the document**.
- Define all further archiving functions in the same manner.
- If you want to protect the data against loss caused by connection problems during automatic archiving, activate the **Save locally after connection issues** function. In this case, the data is saved in the defined folder and can be restored from there.
- Confirm the settings with **Ok** and close the **Options** window.
  - ✓ The settings are taken into account when the next method is created.

12.15 Configuring the CSV export

For the CSV export, make program-wide settings in the **Options** window.

- Open the **Options** | **Advanced** | **Settings CSV export** window with the **Settings** | **Options** menu option.
- Configure the settings and click on **Ok** to confirm.
  - ✓ The settings will be used for the next CSV export.

Settings for CSV export

Option	Description
Transposed	Rotate output of columns and rows in CSV export For example, in the **Spectrum** module, the default is that the wavelength is written continuously in one row, and the corresponding measured values in the next row. In the transposed display, output is by column: one column with the wavelengths, and the corresponding measured values in the next.
Column separator	The following column separators can be selected: ■ **Space** ■ **Semicolon ";"** ■ **Coma ','** ■ **Tab**

13 Validating the SPECORD PLUS (optional)

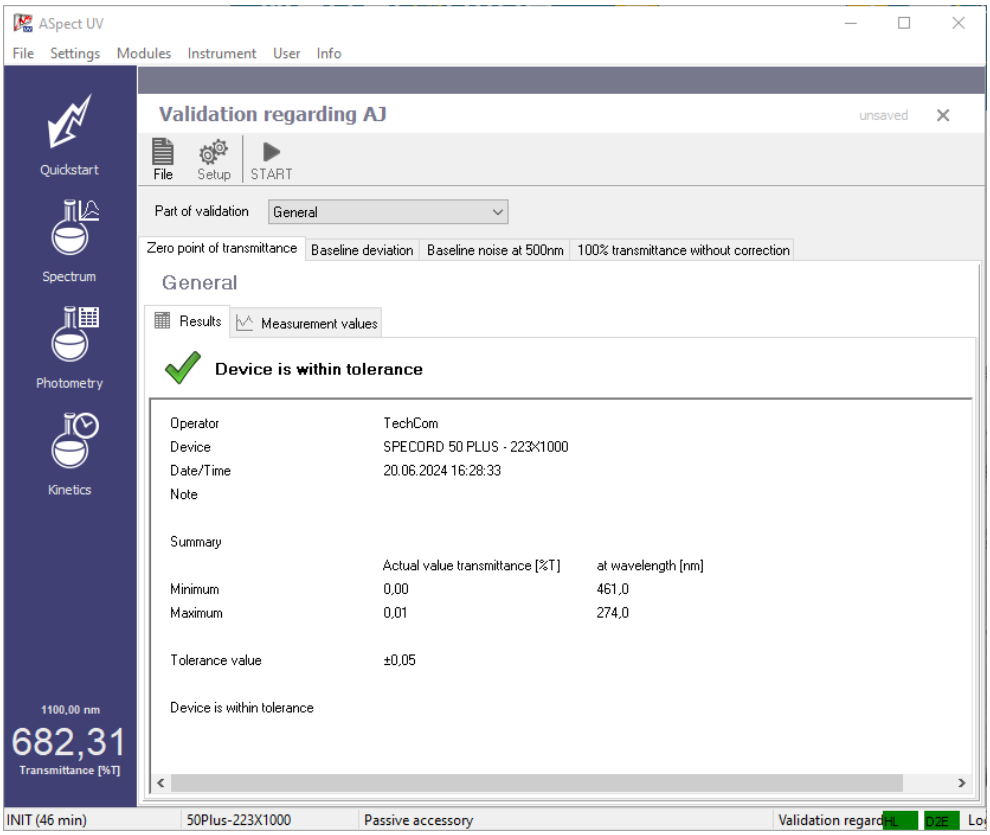
For quality assurance when working with the SPECORD PLUS, performing a validation at regular intervals is recommended. The following modules are optionally available for the various requirements in the individual labs:

- **Validation regarding AJ**: Comprehensive validation of the metrological properties according to the manufacturer's technical data
- **Validation regarding Standard Ph. Eur.**: Validation according to the requirements of the European Pharmacopoeia
- **Validation regarding USP**: Validation in accordance with the requirements of the Pharmacopoeia of the United States of America
- **Economic maintenance**: Validation as part of a service agreement

13.1 Validation regarding AJ

Validation regarding AJ is a comprehensive validation of the measuring technology properties in accordance with the technical data of the manufacturer (see Technical Data in the "SPECORD PLUS UV/Vis Spectrophotometer" instructions). Furthermore, personal limit values may be determined for the validation in order to validate the device for a specific measurement task.

Validation regarding AJ module window



The **Validation regarding AJ** module window appears after you select the **Instrument** | **Test** | **Validation** | **AJ** menu item.

The scope of the parameters to be verified is determined under **Settings**. The results of the validation are displayed on a separate tab for each test parameter. The **Results** tab outputs the digital test results in each case and the **Measurement values** tab shows a graphical representation of the measured spectra. In the list field **Part of validation** a parameter group for the display can be selected in each case.

An audit trail is recorded during validation.

The results of the validation may be saved, exported, printed and opened again.

NOTE

To achieve optimum results observe the following notes:

- Start the validation after a device warm-up period of 2 hours. During this period both lamps of the SPECORD PLUS must be switched on.
- Perform a basic correction directly before opening the window Validation or, for the SPECORD 250 PLUS, a mesh and basic correction.

13.1.1 Test parameters and required equipment

Test parameters

The following parameters can be checked using the device validation:

Parameter	Description
Transmittance zero point	Measurement with covered measurement beam path and open reference beam path in the range of 200 ... 1000 nm The minimum and maximum of the zero point transmittance of the device are calculated from the result.
Baseline deviation	Recording of the baseline in the absorbance mode in the range of 200 – 510 nm
Baseline noise	Recording of 30 measuring cycles of the baseline in the range 490 – 1000 nm Determination of the RMS noise (standard deviation) at 500 nm
100% transmittance uncorrected	Measurement of the baseline in transmittance without correction Determining the minimum and maximum transmittance
Photometric accuracy Vis range	Test with a certified standard filter Determination of difference between measured absorbances and specified target values of the standard filter set at 5 wavelengths
Photometric accuracy in the VIS and NIR range	For SPECORD 210 PLUS with extended measuring range Test with a certified standard filter Determination of difference between measured absorbances and specified target values of the standard filter set at 10 wavelengths
Photometric accuracy UV range	Measurement of the absorbance of a potassium dichromate solution at four wavelengths in the range 235 ... 350 nm Determination of the difference between the measured absorbances and the specified target values of the potassium dichromate solution
Photometric accuracy at 430 nm	Measurement of the absorbance of a potassium dichromate solution at a wavelength of 430 nm Determination of the difference between the measured absorbance and the specified target value of the potassium dichromate solution

Parameter	Description
Wavelength accuracy	Measurement of the wavelength positions of the peaks of a holmium glass filter or a holmium oxide solution with known nominal values for the wavelength in the 5 ranges 270 ... 285 nm, 350 ... 370 nm, 450 ... 485 nm, 530 ... 545 nm and 630 ... 645 nm.
Wavelength accuracy at 486 nm and 656 nm/UV lamp	Measurement of the wavelength position of the D2E lines (485.99 nm and 656.1 nm) at the wavelengths 486 nm and 656.1 nm
Wavelength reproducibility	Performance of ten measurement cycles at 358 - 365 nm for determining the standard deviation of the wavelength position of the holmium oxide peak
Stray light	Determination of the maximum value of the scattered light in transmittance mode with different edge filters in the following ranges: KCl filter cell: 198 nm NaJ filter cell: 220 nm – 240 nm $NaNO_2$ filter cell: 340 nm
Spectral resolution	Test of the spectral resolution capability with a toluene solution in n-hexane by determining the absorbance ratio of the wavelength 269 nm to the wavelength 266 nm (A_{269}/A_{266})
Longterm stability	Repeated measurement of the baseline over an hour and calculation of the gradient of the measured values at 500 nm

Test equipment

For the validation of the SPECORD PLUS, the following filters and certified standards are required:

- Certified filter set for photometric measurement of the Vis spectral range and certified holmium oxide glass filter for wavelength accuracy
- Holmium oxide standard solution in perchloric acid for wavelength accuracy (as an alternative to the holmium oxide glass filter)
- Potassium dichromate standard solution for the UV photometry and for 430 nm
- Sodium nitrite standard solution for the stray light measurement
- Sodium iodide standard solution for the stray light measurement
- Potassium chloride standard solution for the stray light measurement
- Referenced water cell or bidistilled water (free from gas bubbles)
- 0.02% standard solution of toluene in hexane and hexane as a reference for the spectral resolution test

NOTE

For the certified standards, the manufacturers specify a temperature range for use on the certificates. You must comply with this temperature range during validation. A validation outside the specified temperature tolerances can result in incorrect measurement results!

13.1.2 Entering validation parameters

At the start of the validation, the parameters to be validated need to be selected.

- Select the menu item **Instrument** | **Test** | **Validation** | **AJ**.
- Click on **Settings**.
- In the **Settings** window, select the test parameters and enter the details of the standards used.
- Confirm the settings with **Ok**.

✓ The **Settings** window closes. In the **Validation regarding AJ** window, the icon **Start** is enabled.

Selecting test parameters – General tab

The parameters to be tested can be selected as required so that you can define your own validation routine for the spectrometer.

Test parameters	Description
General	Transmittance zero point; baseline deviation; baseline noise; 100% T line, uncorrected
Photometric accuracy Vis	Photometric accuracy in the Vis range
Photometric accuracy Vis/NIR	Only for SPECORD 210 PLUS with extended measuring range Photometric accuracy in the Vis range and in NIR range (up to 1200 nm)
Photometric accuracy UV / 430 nm	Photometric accuracy in the range 235 – 350 and at the wavelength 430 nm
Wavelengths	Wavelength accuracy and wavelength reproducibility in the range 250 nm to 650 nm
Stray light	Scattered light at 198 nm, 220 nm, 240 nm and 340 nm
Spectral resolution	Spectral resolution with a toluene solution in n-hexane by determining the absorbance ratio of the wavelength 269 nm to the wavelength 266 nm (A269/A266)
Long-term stability	Measurement of the baseline over an hour and calculation of the gradient of the measured values at 500 nm

Selecting limit values – Acceptance criteria tab

The limit values for the device test can be set in accordance with the parameter limits and tolerances guaranteed by the manufacturer or within your own defined range limits. In the latter case it will be ensured that the spectrometer is suited for a specific measuring task.

Option	Description
Default values AJ	Use parameter limits and tolerances guaranteed by the manufacturer The data corresponding to the technical specification is displayed in the input fields of the table. They cannot be edited.
Values from file	Use own data record with parameter limits and tolerances **New** New limit values entered **Save** Save limit values The files are given the extension *.vat (validation tolerances). **Load** Load saved limit values and use for the validation

Enter key data of the standards used

Enter the identification numbers and target values of the resources used on the respective tabs if you have selected the corresponding test on the **General** tab.

Photometric accuracy Vis tab

Name/ID	Identification number of the certified standard filter kit (gray filter) in accordance with the datasheet
Fiter parameter	**5** test wavelengths and related filter absorbances by absorbance value 1

Photometric accuracy Vis/NIR tab

Only for SPECORD 210 PLUS with extended measuring range

Name/ID	Identification number of the certified standard filter kit (gray filter) in accordance with the datasheet

	Fiter parameter	**10** test wavelengths and related filter absorbances by absorbance value 1
Photometric accuracy UV / 430 nm tab	**Reference**	Identification number of the reference (0.01 N sulfuric acid or perchloric acid)
	60 mg/l potassium dichromate / 600 mg/l potassium dichromate	Enter the identification number of the potassium dichromate solutions with the concentration 60 mg/l and 600 mg/l.
	Test wavelengths and nominal absorbance values	Enter **Wavelengths [nm]** and **Nominal values [A]** for the test according to the data sheet.
Wavelengths tab	**Name/ID**	Identification number of the wavelength standard used: Holmium oxide filter or holmium perchlorate standard solution
	Test wavelengths	Target values of the spectral peak in accordance with the datasheet
Stray light tab	**Reference (H2O)**	Identification number of the reference
	Stray light KCl at 198 nm	Identification number of the potassium chloride standard solution
	Stray light NaI at 220, 240 nm	Identification number of the sodium iodide standard solution
	Stray light NaNO2 at 340 nm	Identification number of the sodium nitrite standard solution
Spectral resolution tab	**Reference (Hexane)**	Identification number of the hexane reference solution
	Toluene/Hexane	Identification number of the toluene standard solution

13.1.3 Running the validation

NOTE

To achieve optimum results observe the following notes:

- Start the validation after a device warm-up period of 2 hours. During this period both lamps of the SPECORD PLUS must be switched on.
- Perform a basic correction directly before opening the window Validation or, for the SPECORD 250 PLUS, a mesh and basic correction.

Place filters and cells

All filters and cells with standard solutions used, including references, must always be placed in the measurement beam path. The reference beam path remains empty for all measurements!

Running the validation

After entering the validation parameters in the window **Settings**, the icon ▶ **Start** is released. The validation runs assisted by the program. Dependent on your selection of test parameters in the **Settings** window, the measurements are performed consecutively.

- ▶ Start the validation by clicking on ▶
- ▶ Follow the subsequent instructions for the use of filters and cells in the windows.
- ▶ After each partial validation step the test results and defined tolerances are displayed in a window. The test result window offers the following options for the further validation procedure:

Option	Description
Retry	Repeat test point The measurements already recorded for the current test item are discarded. The repetition of a test item is documented in the audit trail.
Continue	Start measurement of the next test parameter
Abort	Cancel validation However, measured values recorded so far are saved temporarily and are displayed on the validation tabs.

Display validation results

After completing the validation, the results are displayed on the tabs of the **Validation regarding AJ** window.

In the list **Part of validation**, the group of the test parameters to be displayed is selected. The **Results** tab displays the digital measurement results in comparison to the permissible tolerances. The spectra are shown on the **Measurement values** tab. Select **File** | **Overview** to display a concise overview of the validation results.

Display the audit trail

- In the document window, select the menu item **File** | **Display Audit Trail**.
- Click on the **Audit Trail** tab.
  - ✓ The complete audit trail is displayed regardless of the validation section selected.

Note: The audit trail is also printed with the "Detailed.lst" template.

Export validation results

- In the document window, select the menu item **File** | **Export**.
- In the **ASCII-Export** window, enter the name of the export file and the decimal separator and confirm with **Ok**.
  - ✓ The data will be exported.

Print validation results

- In the document window, select the menu item **File** | **Print**.
- In the **Open** window in the folder \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports\Validierung AJ, select the "Compact.lst" or "Detailed.lst" print template.
- In the **LLPrint Preview** window, select the option **Print all pages**.
  - ✓ The protocol is printed.

NOTE

With an operational qualification, the printout is included in the OQ report.

13.2 Validation Standard Ph. Eur.

Standard Ph. Eur. validation validates measuring technology properties in accordance with the requirements of the European Pharmacopoeia (chapter 2.2.25). Standard Ph. Eur. validation is carried out in accordance with edition 12.3.

Standard Ph. Eur. validation module window

The **Standard Ph. Eur. validation** module window is displayed after selection of menu item **Instrument** | **Test** | **Validation** | **Standard Ph. Eur.**.

The scope of the parameters to verify is defined under **Setup**. The validation results are displayed on a separate tab for each test parameter. The digital test results are output in the **Results** tab and the measured spectra are displayed graphically in the **Measurement values** tab. In the **Part of validation** list, a parameter group to display can be selected for each case.

The audit trail may be shown in a separate window. The results of the validation may be saved, printed and opened again.

NOTE

To achieve optimum results observe the following notes:

- Start the validation after a device warm-up period of 2 hours. During this period both lamps of the SPECORD PLUS must be switched on.
- Perform a basic correction directly before opening the window Validation or, for the SPECORD 250 PLUS, a mesh and basic correction.

13.2.1 Test parameters and required equipment

Test parameters

The following parameters are checked using the device validation:

Parameter	Description
Wavelength accuracy	Measurement of up to five standard wavelengths optionally with the rare earth oxide filters holmium oxide, didymium glass filter and/or lower UV
Absorbance UV/Vis	Absorbance test with potassium dichromate solutions 60 mg/l at the wavelengths 235, 257, 313, 350 nm and 600 mg/L at 430 nm
Photometric linearity	Test of the photometric linearity at a standard wavelength with 3 ... 4 different absorbances or concentrations optionally with neutral density glass filter, potassium dichromate or niacin
Stray light at 198 nm	Stray light measurement at 198 nm with potassium chloride solution 12 g/L
Spectral resolution	Test of the spectral resolution capability with a toluene solution in n-hexane by determining the absorbance ratio of the wavelength 269 nm to the wavelength 266 nm (A_{269}/A_{266}) This test is optional and only required for the analysis of selected substances.

Test equipment

For the validation of the SPECORD PLUS, the following filters and certified standards are required:

- Standard solution holmium oxide in perchloric acid, holmium glass filter, didymium glass filter or rare earth metal oxide filter for wavelength control according to Ph.Eur. (selection according to the measuring range used)
- Potassium dichromate standard solutions for checking absorbance in the UV and for 430 nm according to Ph. Eur.
- Potassium chloride standard solutions for scattered light measurement according to Ph. Eur.
- Referenced water cell or bidistilled water (free from gas bubbles)
- 0.02% standard solution of toluene in hexane and hexane as a reference for the spectral resolution test
- CRM with 3 ... 4 different absorbances/concentrations at a standard wavelength optionally with the CRMs neutral density glass filter, potassium dichromate or niacin for testing the photometric linearity

NOTE

For the certified standards, the manufacturers specify a temperature range for use on the certificates. You must comply with this temperature range during validation. A validation outside the specified temperature tolerances can result in incorrect measurement results!

13.2.2 Entering validation parameters

At the start of the validation, the parameters need to be selected.

- Select the menu item **Instrument** | **Test** | **Validation** | **Standard Ph. Eur.**.
- Click on **Settings**.
- In the **Settings** window, select the test parameters and enter the details of the standards used.
- Confirm the settings with **Ok**.
  - ✓ The **Settings** window closes. In the **Validation regarding Standard Ph. Eur.** window, the icon **Start** is enabled.

Selecting test parameters – General tab

The parameters to be checked are defined in the European Pharmacopoeia. Activate the parameters you want to check.

View acceptance criteria – Acceptance criteria tab

On the Acceptance criteria tab, you will find the acceptance criteria to be achieved according to the European Pharmacopoeia.

Enter key data of the standards used

Enter the identification numbers and target values of the excipients used on the corresponding tabs.

Tab Wavelengths

Seldom earth metall oxide filter	Identification number of the rare earth metal oxide filter used ID number of the holmium oxide glass filter, didymium oxide glass filter or rare earth metal oxide filter Lower UV
Test wavelength 1 ... Test wavelength 5	Standard target values of the spectrum peaks according to data sheet

Absorbance UV/VIS tab

Reference	Identification number of the reference (0.01 N sulfuric acid or perchloric acid)
60 mg/l potassium dichromate	Identification number of the potassium dichromate solutions with a concentration of 60 mg/l
600 mg/l potassium dichromate	Identification number of the potassium dichromate solutions with a concentration of 600 mg/l
Test wavelengths and nominal absorbance values	Wavelengths and absorbances according to the data sheet

Linearity tab

Type of CRM	Select test equipment: Netural glass filter, Potassium dichromate or Niacin
Reference	Identification number of the reference
Wavelength	Test wavelength according to data sheet
CRM 1 ... CRM 4	Activate number of test devices (at least 3) In the first field enter the identification number and in the second enter the target absorbance value for the test equipment in the second field

Stray light tab

Reference (H2O)	Identification number of the reference
Stray light KCl at 198 nm	Identification number of the potassium chloride standard solution

Spectral resolution tab

Reference (Hexane)	Identification number of the hexane reference solution
Toluene/Hexane	Identification number of the toluene standard solution
Slit	For SPECORD 210 PLUS and SPECORD 250 PLUS The slit (spectral bandwidth) has an influence on the spectral resolution of the device. An overview of the spectral slit widths and the values to be achieved can also be found on this tab.

13.2.3 Running the validation

NOTE

To achieve optimum results observe the following notes:

- Start the validation after a device warm-up period of 2 hours. During this period both lamps of the SPECORD PLUS must be switched on.
- Perform a basic correction directly before opening the window Validation or, for the SPECORD 250 PLUS, a mesh and basic correction.

Place filters and cells

All filters and cells with standard solutions used, including references, must always be placed in the measurement beam path. The reference beam path remains empty for all measurements!

Running the validation

After entering the validation parameters in the window **Settings**, the icon **Start** is released. The validation runs assisted by the program. Dependent on your selection of test parameters in the **Settings** window, the measurements are performed consecutively.

- Start the validation by clicking on
- Follow the subsequent instructions for the use of filters and cells in the windows.
- After each sub-step of the validation, the test results and the tolerances according to the European Pharmacopoeia are displayed in a window. The test result window offers the following options for the further validation procedure:

Option	Description
Retry	Repeat test point The measurements already recorded for the current test item are discarded. The repetition of a test item is documented in the audit trail.
Continue	Start measurement of the next test parameter
Abort	Cancel validation However, measured values recorded so far are saved temporarily and are displayed on the validation tabs.

Display validation results

After completing the validation, the results are displayed on the tabs of the **Validation regarding Standard Ph. Eur.** window.

In the list **Part of validation**, the group of the test parameters to be displayed is selected. The **Results** tab displays the digital measurement results in comparison to the permissible tolerances. The spectra are shown on the **Measurement values** tab. Select **File** | **Overview** to display a concise overview of the validation results.

Display the audit trail

- In the document window, select the menu item **File** | **Display Audit Trail**.
- Click on the **Audit Trail** tab.
  - ✓ The complete audit trail is displayed regardless of the validation section selected.

Note: The audit trail is also printed with the "Detailed.lst" template.

Export validation results

- In the document window, select the menu item **File** | **Export**.
- In the **ASCII-Export** window, enter the name of the export file and the decimal separator and confirm with **Ok**.
  - ✓ The data will be exported.

Print validation results

- In the document window, select the menu item **File** | **Print**.
- In the **Open** window, select the "Compact.lst" or "Detailed.lst" print template in the folder \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports\Validierung\Standard Ph Eur.
- In the **LLPrint Preview** window, select the option **Print all pages**.
  - ✓ The protocol is printed.

NOTE

With an operational qualification, the printout is included in the OQ report.

13.3 Validation according to USP

The **Validation regarding USP** is a validation of the measuring technology properties in accordance with the acceptance criteria of the United States Pharmacopeia USP <857>.

The tests can be performed based on the following USP versions: USP 38, USP 40, USP 41, USP 42, USP-NF 2021, USP-NF 2022, USP-NF 2023, USP-NF 2024, USP-NF 2025 or USP-NF 2026.

The test parameters and acceptance criteria have been revised with USP 42. All subsequent USP versions correspond unchanged to USP 42.

Validation regarding USP module window

The **Validation regarding USP** module window is displayed after selecting menu item **Instrument** | **Test** | **Validation** | **USP**.

The scope of the parameters to test is defined under **Settings**. The results of the validation are displayed for each test item in the **Validation regarding USP** window. The audit trail may be shown on an additional tab. The results of the validation may be saved, exported, printed and opened again.

NOTE

To achieve optimum results observe the following notes:

- Start the validation after a device warm-up period of 2 hours. During this period both lamps of the SPECORD PLUS must be switched on.
- Perform a basic correction directly before opening the **Validation regarding USP** window or, for the SPECORD 250 PLUS, a mesh and basic correction, as well as a correction of the infinite absorbance.

13.3.1 Test parameters, acceptance criteria and required test equipment

Validation according to USP includes the following parameters:

- Accuracy and precision of the wavelength
- Accuracy and precision of the absorbance
- USP 42 and higher: Check of the photometric linearity
- Compliance with limit values for stray light
- Check of the resolution

The USP requires the validation of the spectrometer in the operating range, i.e. the wavelength and absorbance range the expected measured values lie in.

To cover a measurement range as large as possible, the use of several methods as well as certified reference materials (CRM) is recommended. The user is responsible for the selection of suitable CRMs and methods in accordance with the respective operating range.

In addition to the standards recommended by the USP, alternative CRMs may also be permissible if their certification is documented completely and comprehensively.

Wavelength

The USP requires proof of accuracy and precision of the wavelength.

Test equipment/CRM	Accuracy	Precision
■ Hg and D_2 emission lines ■ Rare-earth metal oxide solution (CRM) ■ Rare-earth metal oxide glass (CRM) ■ Alternative CRM	Minimum of 6 measured values Difference between the average value and certified value of the CRM: UV: ≤ 1 nm Vis: ≤ 2 nm	Minimum of 6 measured values Standard deviation from average: ≤ 0.5 nm

Absorbance

The USP requires proof of the accuracy and the precision of the absorbance.

USP 42 and higher: The photometric linearity requirements are met if the criteria for accuracy are satisfied at at least one wavelength in the UV and/or visual range and at three different absorbances.

Test equipment/CRM	Accuracy	Precision
$K_2Cr_2O_7$ solution (235; 257; 313; 350 nm)	≤ ±1% A above 1.0 A or ≤ ±0.010 A below 1.0 A	Minimum of 6 measured values
Neutral glass filter (440; 465; 546,1; 590 and 635 nm)	USP version 38, 40, 41: ≤ ±0.8% A above 1.0 A or ≤ ±0.0080 A below 1.0 A USP version 42 and higher: ≤ ±0.8% A above 1.0 A or ≤ ±0.008 A below 1.0 A	Standard deviation ≤ 0.5% A above 1.0 A ≤ 0.005 A below 1.0 A
Alternative CRM		

Stray light

To determine the stray light, filters with a sharply defined spectrum (cut-off filters) that do not transmit light below a defined wavelength are used. Ideally, the cut-off wavelength should be as close as possible above the wavelength to test.

The USP describes two methods for determining stray light:

The "10 mm vs. 5 mm" method

- Measurement of a 5 mm cell (filter solution) as a reference
- Measurement of a 10 mm cell (filter solution) as a sample
- Determination of the position and height of the absorption maximum and the stray light value S_λ

The "10 mm vs. 10 mm H_2O" method

- Measurement of a 10 mm cell (water) as a reference
- Measurement of a 10 mm cell (filter solution) as a sample
- The absorption measured at the certificate wavelength must be ≥ 2.0 A

USP version 38, 40, 41

Test equipment/CRM	Method	Requirement
12 g/l KCl (190 - 205 nm)	10 mm vs. 5 mm	$S_\lambda \leq 0.01$; $A_\lambda \geq 0.7$ A
10 g/L NaI (210 - 259 nm)	10 mm vs. 10 mm	$A_{\lambda max} \geq 2$ A
Acetone (250 - 320 nm)		
50 g/l $NaNO_2$ (300 - 385 nm)		

USP version 42 and higher

Test equipment/CRM	Method	Requirement
12 g/L KCl (190 - 210 mm)	10 mm vs. 5 mm	$S_\lambda \leq 0.01$; $A_\lambda \geq 0.7$ A
10 g/L NaI (210 - 270 nm)	10 mm vs. 10 mm	$A_{\lambda max} \geq 2$ A
Acetone (250 - 330 nm)		
50 g/l $NaNO_2$ (300 - 400 nm)		

$S_\lambda = 0.25 \times 10^{-2A_\lambda}$

S_λ – Stray light

A_λ – Absorption value of the longest wavelength maximum

Due to the lower stray light quotient of the SPECORD PLUS devices, the measuring range for NaI, Acetone and $NaNO_2$ is extended by a few nanometers when compared to the long-wave range given in table 3 of USP <857>.

USP <857> therefore specifies the following acceptance criteria for the two methods:

The "10 mm vs. 5 mm" method

- The wavelength of the longest wave maximum (λ) is greater than the certificate wavelength - measurement uncertainty
- $S_\lambda \leq 0.01$; $A_\lambda \geq 0.7$ A

The "10 mm vs. 10 mm H_2O" method

Based on the long-wave determination of the wavelength (λ), at which the absorption exceeds the 2.0 A value, the following applies:

- λ is greater than the certificate wavelength - measurement uncertainty
- Below the certificate wavelength - no measurement uncertainty, absorbance values < 2.0 A

Resolution

The USP requires that the spectral bandwidth used by the spectrometer must not exceed 1/8 of the natural half-width of the absorption of the substances.

UV-range verification

- Reference: Hexane
- Measurement of a 0.02% toluene solution in hexane
- Calculation of quotient A_{269}/A_{266}

For most pharmaceutical applications, a spectral resolution of 2 nm will suffice, which corresponds to the following acceptance criterion:

$A_{269}/A_{266} \geq 1.3$

The quotient is temperature-dependent, the temperature effect increases with rising spectral resolution.

Temperature dependency of quotients A_{269}/A_{266} for toluene in hexane:

Measurement temperature [°C]	Spectral bandwidth [nm] and A_{269}/A_{266}				
	0.5 ± 0.1	**1.0 ± 0.1**	**1.5 ± 0.1**	**2.0 ± 0.2**	**3.0 ± 0.2**
20 ± 1	2.4 – 2.5	2.0 – 2.1	1.6 – 1.7	1.3 – 1.4	1.0 – 1.1
25 ± 1	2.3 – 2.4	1.9 – 2.0	1.6 – 1.7	1.3 – 1.4	1.0 – 1.1
30 ± 1	2.1 – 2.2	1.8 – 1.9	1.5 – 1.6	1.3 – 1.4	1.0 – 1.1

Alternatively, suitable atomic emission lines can be used. The spectral bandwidth of the spectrometer corresponds to the half-width determined for the emission line.

- Deuterium emission lines: Suitable for visual range
- Mercury emission lines: Suitable for UV and visual range

The corresponding line tables are saved in the validation software of ASpect UV.

Test equipment/ CRM	Requirement
Hg and D_2 emission lines	The spectral bandwidth of the spectrometer must be ≤ 1/8 of the half-width of the absorption band of the substance (2 nm is sufficient for most pharmaceutical substances).
Toluene in hexane	$A_{269}/A_{266} \geq 1.3$

13.3.2 Entering validation parameters

At the start of the validation, the parameters and test equipment need to be selected.

- In the main window, select menu item **Instrument** | **Test** | **Validation** | **USP**.
- Click on **Settings**.
- In the **Settings** window, select the ranges and parameters to be checked and make the necessary settings for the test equipment entries (see below).
- Confirm the validation parameters with **Ok**.

  ✓ The **Settings** window is closed and the icon **Start** is enabled.

Tip

Once you have set all parameters and entered the required CRM data, save the data by selecting **File** | **Save** in the **Validation regarding USP** window. The data will then also be available for another validation, once the same CRM is used.

Selection of CRM and measuring ranges

The USP requires the validation of the spectrometer in the operating range. Not only must a suitable CRM be selected, often also the measuring range, e.g. the wavelengths when testing the wavelength accuracy/precision, must be determined. If this is required, the ... button appears after selecting the CRM.

- On the **General** screen, make the necessary entries and mark the test parameters to be validated with a tick.
- On the left side of the **Settings** window, select the test parameters.
- On the test parameter screen, mark the CRM with a tick.
- Click ....
- Mark the measured values in the selection window. If necessary, use **Settings** to open the **Settings CRM** window and transfer the CRM data from the certificate to the corresponding input fields. Several CRMs may be activated for a test parameter, thus covering your operating range.

Note: With CRM, on the screens **Stray light** and **Resolution** click immediately on **Settings**, there are no measured values to be selected here.

▶ Close the selection window with **x**.

General screen

On the **General** screen, determine the scope of the device validation and enter the general parameters.

Parameter	Description
Title	Title of the document The title is displayed in the document tab.
User	Name of the user If user administration is installed, the user logged into ASpect UV is displayed.
USP Version	Selection of USP version for the validation
Part	Selection of validation ranges
Slit	For SPECORD 210 PLUS and SPECORD 250 PLUS Spectral width (select spectral resolution of the spectrometer) Note: Select the spectral width that you will also be using for your measurements. The spectral resolution of the spectrometer should not exceed 1/8 of the half bandwidth of the analysis band.
Temperature	Ambient temperature of installation location Some CRMs are temperature-dependent.
Number of signs	Required number of signature fields for test reports Two signature fields are provided as standard (for the user and the service technician). It is possible to select up to 4 signature fields.
Note	Additional note for validation

Wavelength screen

On the **Wavelength** screen, select the parameters for checking the wavelengths (accuracy and precision). The filter wavelengths shown are only preset and give an approximate guide value. Target values are the values from the certificates entered in the **Settings CRM** window.

CRM	Wavelengths [nm]
Holmiumoxid (glass filter)	279; 360; 453; 536; 637
Didymium oxide (glass filter)	329; 472; 512; 681; 875
Holmium oxide solution	241; 249; 278; 287; 333; 345; 361; 385; 416; 451; 467; 536; 640
Didymium oxide solution	731; 740; 794; 801; 864
Rare earth metall oxide liquide filter - Lower UV	201; 211; 222; 239; 252
D2E lines	486; 656,1
Hg emission lines	194,2; 237,9; 248,2; 253,7*; 265,4; 289,4; 296,7; 302,15; 334,15; 365,0; 404,7; 407,8; 435,8; 546,1; 577,0; 579,1; 871,7; 1014,0; 1092,1 *Only possible with gap smaller than 2 nm
Alternate CRM	

Absorbance screen

On the **Absorbance** screen, select the parameters for determining the photometric accuracy and precision. Here, the wavelength and absorbance range of your analyses must be covered.

The following CRM may be selected:

CRM	Measuring range / Concentration	Wavelength range [nm]
Potassium dichromate	20 ... 200 mg/l in increments of 20 mg/l	235 ... 257
Niacin	6; 12; 18 and 24 mg/l	213 and 261
Neutral glass filter	0.04 ... 3.0 Abs	440 ... 635
Alternate CRM		

Typical absorbance of potassium dichromate at the wavelengths 235 nm and 237 nm:

Concentration [mg/l]	Absorbance [235 nm]	Absorbance [257 nm]
20	0.25	0.29
40	0.50	0.57
60	0.75	0.86
80	1.00	1.16
100	1.25	1.45
120	1.50	1.75
140	1.75	2.05
160	2.00	2.35
180	2.25	2.65
200	2.50	2.95

Average absorbance of niacin at the wavelengths 231 nm and 261 nm

Concentration [mg/l]	Absorbance (approx.)
6	0.25
12	0.50
18	0.75
24	1.00

Stray light screen

On the **Stray light** screen, select the CRM and the method for stray light measurement.

CRM	Measuring range [nm]
KCl (12 g/l)	190 ... 205
NaI (10 g/l)	210 ... 259
Aceton	250 ... 320
NaNO2 (50 g/l)	300 ... 380

The wavelength ranges specified for the filter correspond to the information given in table 3 of USP <857>. Due to the lower stray light quotient of the SPECORD PLUS devices, the measuring range for NaI, Acetone and $NaNO_2$ is extended by a few nanometers when compared to the long-wave range.

Resolution screen

On the **Resolution** screen, select the method and the corresponding CRM for determining the spectral resolution. In addition to the toluene/hexane method, the spectral resolution may also be determined using the half width for the atomic emission lines.

CRM	Measurement range
Toluol/Hexane	UV (ratio A_{269}/A_{266})

CRM	Measurement range
D2E lines	486 nm; 656.1 nm,
Hg emission lines	194.2 nm; 237.9 nm; 248.2 nm; 253.7 nm*; 265.4 nm; 289.4 nm; 296.7 nm; 302.15 nm; 334.15 nm; 365.0 nm; 404.7 nm; 407.8 nm; 435.8 nm; 546.1 nm; 577.0 nm*; 579.1 nm*

*Only possible with gap smaller than 2 nm

Archive automatically screen

On the **Archive automatically** screen, you can set the data to be automatically saved or exported during validation. The text format and PDF format can be selected for the export. The USP_komplett.lst report template must be selected.

See also

Test parameters, acceptance criteria and required test equipment [▶ 156]

13.3.3 Running the validation

Place filters and cells

All filters and cells with standard solutions used, including references, must always be placed in the measurement beam path. The reference beam path remains empty for all measurements!

Running the validation

After entering the validation parameters in the window **Settings**, the icon **Start** is released. The validation runs assisted by the program. Dependent on your selection of test parameters in the **Settings** window, the measurements are performed consecutively.

- Start the validation by clicking on
- Follow the subsequent instructions for the use of filters and cells in the windows.
- After each partial validation step, the test results and acceptance criteria in accordance with USP is shown in a window. The CRM measurement can be repeated and the test continued or interrupted.

Option	Description
Yes	Repeat CRM measurement The measurements already recorded for the current test item are discarded. An entry is made in the validation audit trail.
No	Accept measured values and continue with the validation
Cancel tests	Cancel validation Previously recorded and completed measurements are temporarily saved and displayed in the main window.

Display validation results

Once a measuring range for a test parameter/CRM has been fully processed and processing of the next range or a new test parameter/CRM starts, the results are shown on the corresponding tab below. In this way, measurement results from validation parts that have already been completed can be assessed while the validation is still running.

Display the audit trail

- In the document window, select the menu item **File** | **Display Audit Trail**.
- Click on the **Audit Trail** tab.
  - ✓ The complete audit trail is displayed regardless of the validation section selected.

Note: The audit trail is also printed with the "Detailed.lst" template.

Signing a document

- In the document window, select the menu item **File**|**Sign document**.
- Click **Login**.
- Select the signature.

- You have the option of entering a comment in the **Comment** field.
- Save the document with **File** | **Save**.
  ✓ The document is now signed.

Print validation results

- In the document window, select the menu item **File** | **Print**.
- Select the template USP_All_Data.lst for printing.
- In the **LLPrint Preview** window, select the option **Print all pages**.
  ✓ The protocol is printed.

NOTE

With an operational qualification, the printout is included in the OQ report.

13.4 Validation Maintenance Economic

The economic maintenance validation is carried out as part of maintenance if a maintenance contract has been concluded. With the conclusion of a service agreement, you acquire the **Economic maintenance** module with which the basic functions of SPECORD PLUS are tested.

Economic maintenance module window

The **Economic maintenance** module window appears after you select the **Instrument** | **Test** | **Validation** | **Economic maintenance** menu item.

Enter the parameters of the standard under **Settings**. The results of the validation are displayed on a separate tab for each test parameter. The **Results** tab outputs the digital test results in each case and the **Measurement values** tab shows a graphical representation of the measured spectra. In the **Part of validation** list, a parameter group for the display can be selected in each case.

The audit trail can be displayed in a separate window. The results of the validation may be saved, printed and opened again.

NOTE

To achieve optimum results observe the following notes:

- Start the validation after a device warm-up period of 2 hours. During this period both lamps of the SPECORD PLUS must be switched on.
- Perform a basic correction directly before opening the window Validation or, for the SPECORD 250 PLUS, a mesh and basic correction.

13.4.1 Test parameters and required equipment

Test parameters

The following parameters are validated in the **Economic maintenance**:

Parameter	Description
Zero point of transmittance	Measurement with covered measurement beam path and open reference beam path in the range of 200 – 1000 nm The minimum and maximum of the zero point transmittance of the device are calculated from the result.
Baseline deviation	Recording of the baseline in the absorbance mode in the range of 200 – 1000 nm
- Photometric accuracy (Absorbance at 465 nm)	Test with a certified standard filter Determination of the difference of the measured absorbance in comparison with the specified target values of the gray glass filter F2, F3 and F4 with 465 nm
Wavelengths with rare earth oxide filter	Measurement of the wavelength positions of the peaks of a holmium oxide glass filter with known target values for the wavelengths in the five ranges 270 – 285 nm, 350 – 370 nm, 450 – 485 nm, 530 – 545 nm and 630 – 645 nm
Spectral resolution	Determination of spectral half width at D_2E line at 656.1 nm The measurement is carried out using the UV lamp (D_2E lamp).

Test equipment

The following standards are required for the **Economic maintenance** validation:

- Certified filter set for the photometric measurement of the Vis spectral range and certified holmium oxide glass filter for the wavelength measurement (HELLMA standard filter set)

NOTE

For the certified standards, the manufacturers specify a temperature range for use on the certificates. You must comply with this temperature range during validation. A validation outside the specified temperature tolerances can result in incorrect measurement results!

13.4.2 Entering validation parameters

At the start of the validation, the certification data for the test equipment to be used must be selected.

- In the main window, select menu item **Instrument** | **Test** | **Validation** | **Economic maintenance**.
- Click on **Settings**.
- In the **Settings** window, configure the necessary settings for the test equipment (see below).
- Confirm the validation parameters with **Ok**.

  ✓ The **Settings** window is closed and the button **Start** is enabled.

General tab

On the **General** tab, you can enter a user name and a comment for the validation. You will also find an overview of the test parameters. The scope of testing is determined by the manufacturer.

Acceptance criteria tab

On the **Acceptance criteria** tab, you will find the values to be achieved according to the manufacturer's specifications.

Photometric accuracy at 465 nm tab

Enter the characteristics of the gray filter set here.

Filter parameter	Identification number of the filters according to the data sheet
Test wavelengths and nominal absorbance values	Enter wavelengths and target values for the test in accordance with the datasheet.

Tab Wavelengths

Enter the identification data of the holmium oxide glass filter here.

Name/ID	Identification number of the holmium oxide glass filter used
Test wavelengths	Target values of the spectral peak in accordance with the datasheet

Spectral resolution tab

This tab contains information on the measuring conditions of the test point.

13.4.3 Running the validation

NOTE

To achieve optimum results observe the following notes:

- Start the validation after a device warm-up period of 2 hours. During this period both lamps of the SPECORD PLUS must be switched on.
- Perform a basic correction directly before opening the window Validation or, for the SPECORD 250 PLUS, a mesh and basic correction.

Place filters and cells

All filters and cells with standard solutions used, including references, must always be placed in the measurement beam path. The reference beam path remains empty for all measurements!

Running the validation

After entering the validation parameters in the window **Settings**, the icon ▶ **Start** is released. The validation runs assisted by the program. Dependent on your selection of test parameters in the **Settings** window, the measurements are performed consecutively.

- Start the validation by clicking on ▶
- Follow the subsequent instructions for the use of filters and cells in the windows.
- After each partial validation step the test results and defined tolerances are displayed in a window. The test result window offers the following options for the further validation procedure:

Option	Description
Retry	Repeat test point The measurements already recorded for the current test item are discarded. The repetition of a test item is documented in the audit trail.
Continue	Start measurement of the next test parameter
Abort	Cancel validation However, measured values recorded so far are saved temporarily and are displayed on the validation tabs.

Display validation results

After completing the validation, the results are displayed on the tabs of the **Economic maintenance** window.

In the list **Part of validation**, the group of the test parameters to be displayed is selected. The **Results** tab displays the digital measurement results in comparison to the permissible tolerances. The spectra are shown on the **Measurement values** tab. Select **File** | **Overview** to display a concise overview of the validation results.

Display the audit trail

- In the document window, select the menu item **File** | **Display Audit Trail**.
- Click on the **Audit Trail** tab.
  - ✓ The complete audit trail is displayed regardless of the validation section selected.

Note: The audit trail is also printed with the "Detailed.lst" template.

Export validation results

- In the document window, select the menu item **File** | **Export**.
- In the **ASCII-Export** window, enter the name of the export file and the decimal separator and confirm with **Ok**.
  - ✓ The data will be exported.

Print validation results

- In the document window, select the menu item **File** | **Print**.
- In the **Open** window in the folder \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports\Economic Maintenance, select the "Compact.lst" or "Detailed.lst" print template.
- In the **LLPrint Preview** window, select the option **Print all pages**.
  - ✓ The protocol is printed.

14 User administration and electronic signatures

The optionally available FDA 21 CFR Part 11 Compliance module includes the user administration and provides an option for the electronic signing of measuring results.

14.1 User management

14.1.1 Pre-installed users

The ASpect UV user administration allows flexible assignment of user rights. Each user can be allowed or denied access to individual functions from the full range of ASpect UV functions.

Users created by default

Users with various access rights are created in the installation of the FDA 21 CFR Part 11 Compliance module, which can be used directly or as an example for your own rights management. Logins and passwords have already been assigned for registration of these users, they can however be edited or deactivated.

Tip

Deactivate these users in order to define templates for user profiles with different roles using the **Transfer permissions** function. These profiles may then be transferred to users that actually exist.

AJ Service

AJ Service is a user who has all permissions, i.e., a combination of Administrator and Researcher. This user is used by AJ Service staff for maintenance work and for tests during software qualification.

Administrator

The **Administrator** has full access to the user management and can create, edit and transfer user profiles. He does not have access to the measuring modules and cannot create methods or start measurements.

Login: Admin

Password: admin

User Level 1 (Researcher)

The **User Level 1 (Researcher)** has unrestricted access to the functions of ASpect UV. He can view the user administration but cannot create a new user profile or modify existing user profiles.

Login: User1

Password: user1

User Level 2 (TechAssistant)

The **User Level 2 (TechAssistant)** has access to the following functions:

- Open results
- Opening methods
- Open modules
- Start measurements
- Analyze measurements

He may not:

- Create methods
- Perform device corrections
- View the user administration

Login: User2

Password: user2

User Level 3 (Laboratory Supervisor)

User Level 3 (Laboratory Supervisor) has access to the following functions:

- Open results
- Opening methods
- Open modules
- Create methods
- Analyze measurements
- Start measurements in the quick measurement, from which results cannot be saved

He may not:

- Start measurements in the ASpect UV modules
- Test and correct SPECORD PLUS
- View the user administration

Login: User3

Password: user3

User Level 4 (Service)

The **User Level 4 (Service)** has been set up for Service. It has access to the following functions:

- Perform simple measurements
- Correct SPECORD PLUS
- Test SPECORD PLUS
- Start and analyze energy measurement
- View list of users

He may not:

- Open the photometry, spectrum, colorimetry, thermometry or kinetics modules
- Access methods and results of these modules

Login: User4

Password: user4

14.1.2 Functions in the user administration

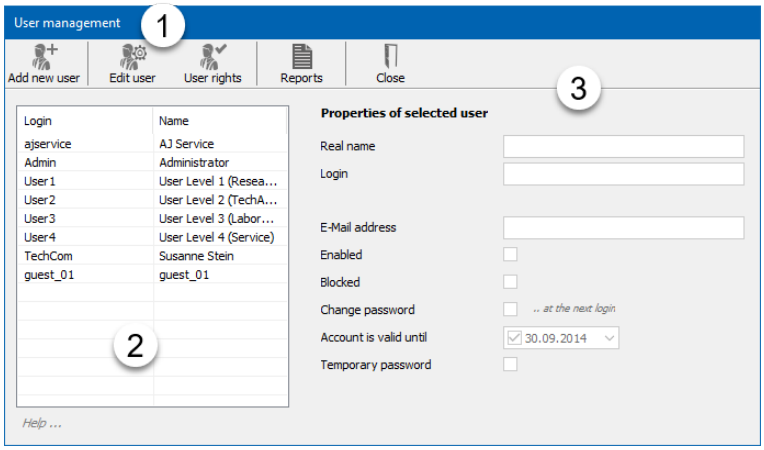
The user administration can only be organized by a user with the appropriate rights. The **Administrator** user is pre-installed in this case. The users **User Level 1 (Researcher)** and **User Level 4 (Service)** can view the entries in the user administration but cannot edit them.

Opening the user management

▶ In the main window, select menu item **User** | **User management**.

✓ The user administration is opened. Dependent on access rights, users can be created and edited or only the list of users can be viewed.

User management window



No.	Description
1	Menu bar

No.	Description
2	List of created user profiles
3	Properties of a selected user profile

All functions for creating and editing user profiles are arranged in the menu bar:

Icon	Description
Add new user	Create a new user profile
Edit user	Change properties of a user profile
User rights	Enable or disable access authorization to each function in ASpect UV for a selected user Transfer user profiles
Reports	Create reports on logins in ASpect UV and user administration
Close	Close user administration

14.1.3 Creating and editing users

Only users with full access rights to the user administration can create a new user. Use the pre-installed **Administrator** user, for example.

When you create a user in ASpect UV, you can decide whether you want to manage the user properties (e.g. login and password) in ASpect UV or use the properties of the existing Active Directory Domain Services.

Once a user has been created, you must then assign them the user rights in ASpect UV. This allows you to prohibit or allow a user to use each individual function in ASpect UV. You can create sample user profiles and transfer their rights to a user.

Creating and managing users in ASpect UV

- In the main window, select menu item **User** | **User management**.
- Click on **Add new user**.
- Configure the following settings in the **User** window.

Option	Description
Login	User login
Use management	**ASpect UV** Manage user properties within ASpect UV
Real name	Name of the user
E-Mail address	User email address
Enabled	Enable if the user profile is to be used.
Blocked	Enable if the user profile must not be used. With a locked user profile the user can no longer log in to the program.
Change password	Enable if the user is to create his own password after the first login with this profile. The option must also be enabled if the user has been reactivated following a lock/expiry of validity by Admin.

Option	Description
Account is valid until	Enable and configure an expiry date if the user profile is to be only valid for a specific time period. Validity up to and including expiry day 23:59
Password / **Change password**	Password and password repeat for the user login to the program

- Confirm user settings with **Ok**.
- Accept the rights of another user for the authorization settings in ASpect UV or set the rights manually afterwards.
  - ✓ The new user has been created. You can continue to edit the user rights in ASpect UV.

Manage users with Active Directory

- Click on **Add new user**.
- For the **Use management** parameters, select the option **Domain**.
- In the **Login** field, enter the login of the existing user in the Active Directory.
- In the **Domain** field, enter the domain name.
- Accept the rights of another user for the authorization settings in ASpect UV or set the rights manually afterwards.
  - ✓ The new user is created and can log in to ASpect UV with the login from the Active Directory. You can continue to edit the user rights in ASpect UV.

Edit user

You can subsequently change the properties of a user who is managed within ASpect UV. For example, you can block a user or reset their password. Properties of users managed in the Active Directory can only be changed there.

- Select the user from the list of users in the **User management** window.
- Click on **Edit user**.
- Change settings in the **User settings** window.
  - ✓ The user properties have been changed.

14.1.4 Assigning user rights

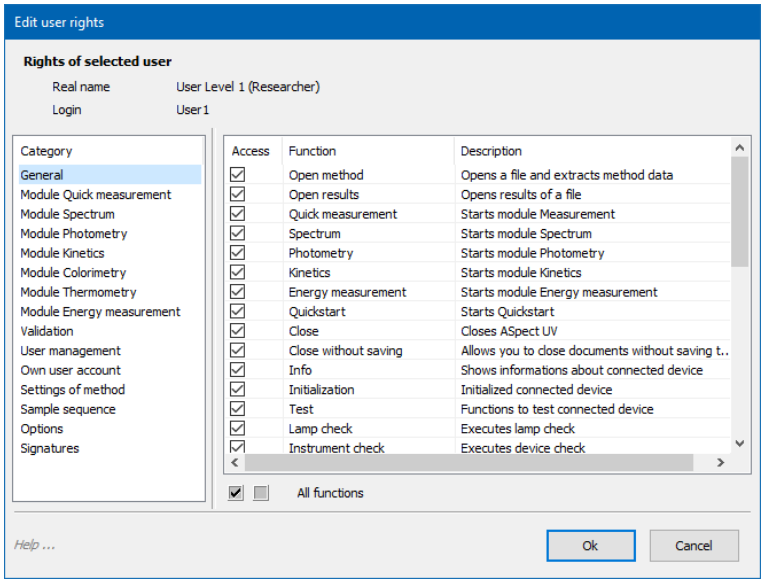
Assigning user rights

Each user can be granted individual access to the functions of ASpect UV.

Note: The options in the category **General** are related to the main window of ASpect UV. If you wish to withdraw or grant the right **Open method** or **Open results**, these options must be accordingly (de)activated in the individual modules.

- Select the user from the list of users in the **User management** window.
- Select the menu item **User rights** | **Edit user rights**.
- On the left side of the **Edit user rights** window, select the category in each case and on the right side enable all functions to which the user is to be given access.

  ✓ Individual rights are assigned to the user profile.



Transfer user rights

The user rights of a user profile may be transferred to another profile. In this way, you can create sample profiles/roles with different access authorizations and assign these to new user profiles. The default user profiles User 1 - User 4 may be used as a basis for these user profiles.

- Select the target profile in the **User management** window.
- Select the menu item **User rights** | **Transfer rights**.
- In the **Transfer rights** window, select the outbound/role profile for the user rights and confirm with **Ok**.

  ✓ The user rights of the profile selected are transferred to the target profile.

Special signature features

Permission to apply a signature to a document must be granted separately to each user. A distinction is made here between signatures that must be applied in a defined sequence and signatures with no sequence. The **Signatures** category is only visible if signatures have already been created in the **Options** | **Advanced** | **Signatures** window.

- Select the user from the list of users in the **User management** window.
- Select the menu item **User rights** | **Edit user rights**.
- Activate all signatures for the selected user in the **Signatures** category.

- If you activate a signature that is not in the signature sequence, the **Signing outside of the signature sequence** option must be activated in the **Own user account** category. Only then can the user use this signature. Otherwise, the signatures will not be available for this user, despite activation in the **Signatures** category.

See also

Creating signatures [▶ 143]

14.1.5 Creating reports on the user management screen

In the user management, various reports can be created and printed out.

- Audit trail of the user management
- List of registrations in ASpect UV
- List of all users
- Rights of selected user

The right to view reports must be enabled for a user in the user rights.

Audit trail

All changes to the user profiles are documented in the audit trail.

- In the **User management** window, select menu item **Reports** | **Audit Trail** | **View**.
- Using the filter settings, the entries may be sorted, filtered and printed according to **Admin**, changed user profile and date. To do this, change the settings and click on **Reload**.
- To print/export the entire audit trail, select the menu item **Reports** | **Audit Trail** | **Print** and the report "UM_Audit Trail.lst" in the path \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports\User Administration.

List of registrations

In the list of logins, all successful and unsuccessful user logins and logouts in ASpect UV are documented with the time.

- In the **User management** window, select menu item **Reports** | **List of logins** | **View**.
- Using the filter settings, the entries may be sorted, filtered and printed according to users, login times and registration status (**rejected**, **successfull** or **logged off**). To do this, change the settings and click on **Reload**.
- To print/export the entire list, select the menu item **Reports** | **List of logins** | **Print** and the report "UM_LoginList.lst" in the path \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports\User Administration.

List of all users

The list of all users includes the user profiles created with information on status, date created and the date of the last login in ASpect UV. The user list may only be printed/exported.

- In the **User management** window, select the menu item **Reports** | **List of all users** | **Print** and the report "UM_UserList.lst" in the path \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports\User Administration.

Rights of selected user

With the rights report, you can print/export an overview of the rights for a selected user.

- In the **User management** window, select a user profile.
- Select the menu item **Reports** | **Rights of selected user** | **Print** and the report "UM_UserRights.lst" in the path \\Users\Public\Documents\Analytik Jena\ASpect UV\Reports\User Administration.

14.1.6 Logging out a user

With the **Log off** function, a user can log out of the running ASpect UV program. Another user or the same user can then log in again. This right should be enabled for every user.

To log out, it is necessary to close all document windows of the modules beforehand.

- In the main window, select menu item **User** | **Log off**.
  - ✓ The main window of ASpect UV is locked.
- To log in again click on **Login** .
- Enter the login and corresponding password.
  - ✓ The ASpect UV program is released for further actions.

14.1.7 Lock ASpect UV

With the **Lock ASpect UV** function, the current ASpect UV program is locked until the same or another user logs in again. The permission to unlock by another user must be enabled for the corresponding user in the user administration beforehand

Ongoing measurements will be completed in the locked state.

- In the main window, select the menu item **User** | **Lock ASpect UV**.
- The main window of ASpect UV is locked.
  - ✓ To log in again click on **Login** .
- Enter the login and corresponding password.
  - ✓ The ASpect UV program is released for further actions.

14.1.8 Passwords in ASpect UV

Validity criteria for passwords

The password validity criteria can be configured in the **Options** | **Advanced** | **Password management** window once authorization has been granted in their user profile.

Login

After three incorrect login attempts the respective user account is blocked. The block can only be lifted by a user with administrator level access rights.

Changing the password

A user may change the password if this function has been released in his user profile.

- In the main window, select menu item **User** | **Change password**.
- In the **Password** and **Confirm password** fields, enter the new password.
  - ✓ The new password is accepted.

See also

Configuring password properties [▶ 143]

14.2 Electronic signatures

What is a signature?

Documents can be signed in the optional FDA 21 CFR Part 11 Compliance module.

Signing a file applies a digital signature (the login data of the signing user), and also restricts editing of the file. These editing restrictions affect data management, measurements or analyses on the worksheets, and can be defined for each signature. If the functionality of a file is restricted by a signature, these restrictions cannot be lifted by applying another signature. Optionally, a required sequence can be defined for signatures that must be maintained for the signing process.

The signature of a file affects a logged in user. This user can only use the file functions permitted by both the file signature and the user permissions.

Permission to apply a signature to a file must be granted to each user separately in the respective user profile. A user can be granted permission to use multiple signatures.

Creating signatures in the program

The signatures are managed in the **Options** | **Advanced** | **Signatures** window. Signatures can be created, edited and deleted here. The sequence to apply signatures can also be defined here.

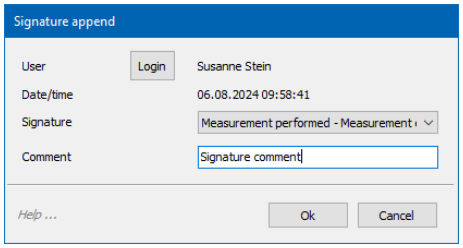
Assigning signature permissions

The permission to use one or more signatures must be assigned in the user profile.

Signing a document

The user must be logged into ASpect UV to apply signatures.

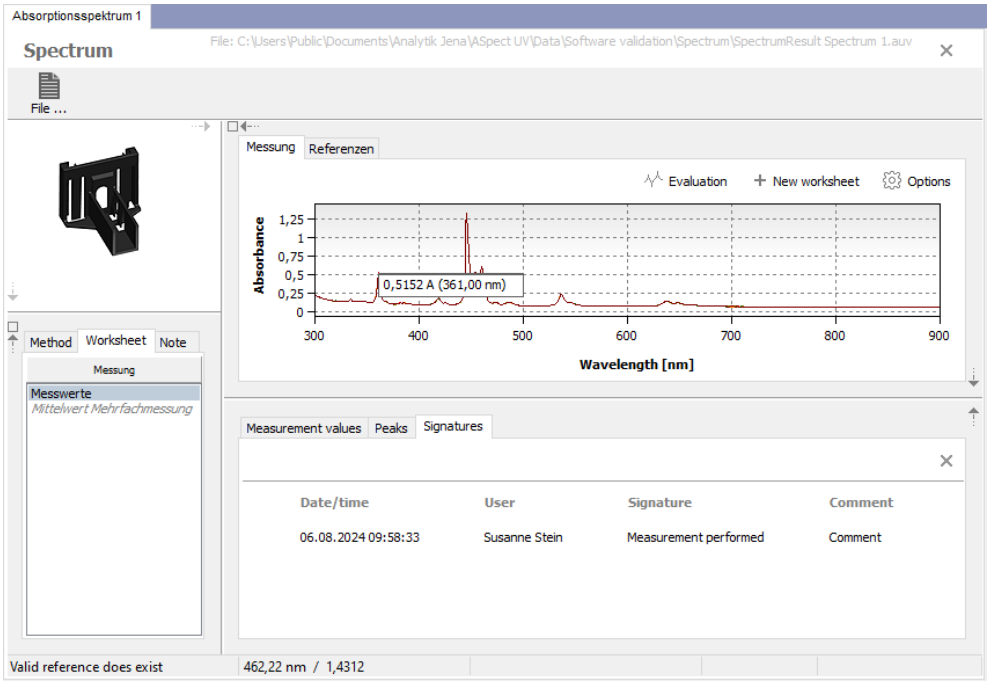
- In the document window, select the menu item **File** | **Sign document**.
- In the **Signature append** window, click on **Login** and log in with your own login details.
  - ✓ The user's signatures are displayed.
- Select the signature in the **Signatures** list.
- A comment can be added in the **Comment** field, which is confirmed with **Ok**.
- If any further saving of the document is restricted by the signature, a message appears that the file must now be saved for the last time. After confirming the message with **Yes** , save the file in the **Save as** window.
  - ✓ The document has now been signed by the user. All further editing of the document is restricted in accordance with the selected signature.



Displaying signatures

Signatures are displayed in the bottom part of the document window next to the tabs for data analysis.

- To display the signatures in the document window select the menu item **File** | **Display signatures**.
- To hide the signatures, click on ✕ in the **Signatures** tab, or select the **File** | **Hide signatures** menu item.


Absorptionsspektrum 1
Spectrum
File: C:\Users\Public\Documents\Analytik Jena\ASpect UV\Data\Software validation\Spectrum\SpectrumResult Spectrum 1.auv
File ...
Messung
Referenzen
Evaluation
New worksheet
Options
Absorbance
1,25
1
0,75
0,5
0,25
0
0,5152 A (361,00 nm)
300
400
500
600
700
800
900
Wavelength [nm]
Method
Worksheet
Note
Messung
Messwerte
Mittelwert Mehrfachmessung
Measurement values
Peaks
Signatures
Date/time
User
Signature
Comment
06.08.2024 09:58:33
Susanne Stein
Measurement performed
Comment
Valid reference does exist
462,22 nm / 1,4312

15 AJ File Protection

The optional software AJ File Protection protects data against intentional and unintentional data manipulation, e.g., deletion or modification of data. A filter driver allows directory access by authorized applications, access by other applications is blocked. The functionality of virus scanners and professional replication, synchronization or data backup software is not impaired if Microsoft standards are complied with.

AJ File Protection must be installed and configured by the system administrator. The installation requires administrator rights.

A detailed description of the installation and configuration of the software can be found on the installation CD.

In combination with the separate rights for automatically saving and exporting that can be configured in the optional "FDA 21 CFR Part 11 Compliance" module, the AJ File Protection software guarantees complete data privacy for method creation, data acquisition and evaluation, and archiving.

16 Optional SOAP module

With the optional SOAP module you can remotely control the SPECORD PLUS with ASpect UV. A web server is integrated in ASpect UV, which can be addressed with the SOAP network protocol. For this purpose, the PC on which ASpect UV is installed and which is connected to the SPECORD PLUS must be connected to the network.

Using the web server

- Switch on the SPECORD PLUS and start ASpect UV.
  - ✓ The SPECORD PLUS is initialized.
- Start the web server with **Modules** | **SOAP**.
- In the **SOAP Web Service** window, click on **Start**.
  - ✓ The web server in ASpect UV can now be addressed by the SOAP network protocol and initiate measurements with SPECORD PLUS.

If you are interested in this function, please contact your Analytik Jena sales partner.

17 Revision overview

Version	Changes
00.15	First edition
01.16	■ New: Thermometry module, Colorimetry module
02.16	■ Change colorimetry: Correction of the standards used Publication of the English version
03.19	■ New: Data export in CSV format ■ Change: Sample sequences ■ Change: Lamp change available in the measurement parameters ■ New: Validation of the SPECORD PLUS according to manufacturer specification, Ph. Eur., USP and economic maintenance ■ New: Correcting infinite absorbance ■ New: AJ File Protection ■ New: Reports in the user administration for audit trail, logins, user profiles and user rights
04.20	■ Change: Device validation according to Ph. Eur. Issue 10 ■ New: Device validation according to USP version 42 available
A (02/2021)	■ Extended functions in the user administration ■ Extended signatures and signature sequences ■ Automatic archiving ■ Device validation according to USP edition USP-NF 2021 is available
B (09/2023)	■ Change of legal form of the manufacturer
C (02/2024)	■ Device validations according to USP edition USP-NF 2022 and USP-NF 2023 are available
D (08/2024)	■ Saved references can be applied to other measurement data ■ References must be given a name ■ Time-cyclic measurements are possible in modules Photometry and Spectrum ■ Measurement repetitions can be configured for each sample type ■ Values of different samples can be linked together in formulas ■ The AREA, TIME and Y functions are available in the formula editor ■ For cyclical measurement, the dark current measurement can be carried out once before the first measurement or before each measurement within the cycle ■ Analyses and mathematical processing are possible in the document window on worksheet Measurement ■ This WebApp function is no longer available
E (03/2026)	■ Device validations according to USP edition USP-NF 2024, USP-NF 2025 and USP-NF 2026 are available ■ Device validation according to Ph. Eur. Edition 12.3

I Annex

I.1 Pre-installed methods

The installation of ASpect UV contains prepared methods for various applications. After a standard installation, these *.auv files are stored in the following folders

C:\Program Files (x86)\Analytik Jena\ASpect UV\Methods

and C:\Users\Public\Documents\Analytik Jena\ASpect UV\Methods

Dependent on the selected language the methods are installed in German or English during the installation.

Enzymology

The enzymology methods are suitable for analyses using test kits by R-Biopharm. The test kits can be ordered online at r-biopharm.com

The following accessories are intended for the measurements:

- 8-cell changer
- 15-cell carousel

The methods have been installed in the following folders:

- German
  \\Aspect UV\ Methods \Enzymatik\8xWechsler and
  \\Aspect UV\ Methods \Enzymatik\15xWechsler
- English
  \\ASpect UV\Methods\Enzymatic\8xcell changer and
  \\ASpect UV\Methods\Enzymatic\Cell carousel

The following methods have been installed:

No.	Method Ger	Method Eng	Order no.
1	Acetaldehyd	Acetaldehyde	Roche- Gelbe Linie 10668613035
2	Cholesterin	Cholesterol	Roche- Gelbe Linie 10139050035
3	Citronensäure	Citric acid	Enzytec Generic Line E1214
4	D-/L-Milchsäure	D-/L-Lactic acid	Enzytec Generic Line E1255
5	D-3-Hydroxybuttersäure	D-3-Hydroxybutyric acid	Roche- Gelbe Linie 10907979035
6	D-Äpfelsäure	L-Malic acid	Roche- Gelbe Linie 11215558035
7	D-Glucose	D-Glucose	Enzytec Generic Line E1210
8	D-Glucose/D-Fructose	D-Glucose/D-Fructose	Enzytec Generic Line E1245
9	D-Sorbit/Xylit	D-Sorbitol/Xylitol	Roche- Gelbe Linie 10670057035
10	Acetic acid	Acetic acid	Roche- Gelbe Linie 10148261035
11	Ethanol	Ethanol	Roche- Gelbe Linie

No.	Method Ger	Method Eng	Order no.
			10176290035
12	Glycerin	Glycerol	Enzytec Generic Line E1224
13	Harnstoff_Ammoniak	Urea/Ammonia	Roche- Gelbe Linie 10542946035
14	Lactose/D-Galactose	Lactose/D-Galactose	Enzytec Generic Line E1213
15	L-Äpfelsäure	L-Malic acid	Roche- Gelbe Linie 10139068035
16	L-Ascorbinsäure	L-Ascorbic acid	Enzytec Generic Line E1267
17	L-Glutaminsäure	Glutamic acid	Roche- Gelbe Linie 10139092035
18	L-Milchsäure	L-Lactic acid	Enzytec Generic Line E1254
19	Sucrose /D-glucose	Sucrose/ D-glucose	Enzytec Generic Line E1246
20	Saccharose/ D-Glucose/ D-Fructose	Saccharose/ D-Glucose/ D-Fructose	Enzytec Generic Line E1247
21	Stärke	Starch	Enzytec Generic Line E1268
22	Sulfit	Sulfite	Roche- Gelbe Linie 10725854035

Methods for biochemical analysis

The methods for biochemical analysis are intended for the use of passive accessories (adjustable holders for small microcells).

The methods have been installed in the following folders:

- German
  \\ASpect UV\ Methods \Bio
- English
  \\ASpect UV\ Methods \Life Science

The following methods have been installed:

No.	Method German	Method English
1	Absorption 205 nm, Faktor 31	Absorbance 205 nm, Factor 31
2	Absorption 215 nm, 225 nm	Absorbance 215 nm, 225 nm
3	Absorption 260 nm, Faktor 33	Absorbance 260 nm, Factor 33
4	Absorption 260 nm, Faktor 40	Absorbance 260 nm, Factor 40
5	Absorption 260 nm, Faktor 50	Absorbance 260 nm, Factor 50
6	Absorption 260 nm	Absorbance 260 nm
7	Absorption 280 nm, Faktor 1,38	Absorbance 280 nm, Factor 1.38
8	Absorption 280 nm	Absorbance 280 nm
9	DNS-Reinheit	DNA-purity
10	Kalb und Bernlohr	Kalb and Bernlohr
11	Kalckar und Shafran	Kalckar and Shafran
12	Scopes-Formel	Scopes-Formula

No.	Method German	Method English
13	Warburg-Christian-Formel (DNS)	Warburg-Christian formula (DNA)
14	Warburg-Christian-Formel (Eiweiß)	Warburg-Christian formula (protein)
15	Whitaker und Granum	Whitaker and Granum

Water analysis

The methods for water analysis are suited for analyses with Spectroquant test kits. The test kits can be ordered on the internet at http://www.merckmillipore.com/.

Passive accessories (standard cell holders) are intended for the measurements:

The methods have been installed in the following folders:

- German
  \\ASpect UV\Methoden\Wasseranalytik
- English
  \\ASpect UV\Methods\Water analysis

The following methods have been installed:

No.	Method Ger	Method Eng	Order no.	Area
1	Ammonium Test	Ammonia test	1.14752.	0.01 ... 3.00 mg/l NH4-N
2	Nitrat Test	Nitrate Test	1.09713.	0.1 ... 25.0 mg/l NO3-N
3	Phosphat Test	Phosphate Test	1.14848.	0.025 ... 5.00mg/l PO4-P
4	Sulfat Test	Sulfate test	1.14791.	25.0 ... 300mg/l SO42-
5	Sulfit Test	Sulfite test	1.01746.	1.0 ... 60.0mg/l SO32-

I.2 Calculation of measured values and recording of the reference values

This section provides a brief introduction to the calculation of measured values in the spectral photometer and the meaning of the baseline and its correction.

For an absorbance measurement the transmitted energy I_0 (reference value) and the energy I weakened by the sample is measured at each wavelength of interest. This takes place in arbitrary units, because only the ratio is of relevance. Quantitatively, the absorbance behavior is expressed in transmittance **T[%]** or absorbance:

$D = \frac{I}{I_0}$	D – Permeability I_0 – Energy without weakening (base value) I – Energy leaving the sample
$T[\%] = D * 100$	T[%] - Transmittance in percent
$A = -\lg D$	Absorbance

Calculation of measured values for a double-beam spectrometer

To reduce measurement errors through changes in energy during the measurement (drift), two beam devices have been designed. With the aid of a reference beam the lamp spectrum is being "monitored". The two compared energy values from the measurement and reference beam path compensate for the fluctuations of the lamp energy.

Calculation of the reference value (also baseline):

$D_R = \frac{I_{MR}}{I_{VR}}$	D_R – Permeability for the reference

	I_{VR} – Energy of the reference beam
	I_{MR} – Energy of the measurement beam

Calculation of the sample value

$D_P = \frac{I_{MP}}{I_{VP}}$	D_P – Permeability for the sample
	I_{VP} – Energy of the reference beam
	I_{MP} – Energy of the measurement beam

Calculation of the measured value

$D = \frac{D_P}{D_R}$	D – Permeability
	D_P – Permeability for the sample
	D_R – Permeability for the reference

What to do with the reference sample in double-beam devices?

In a single beam device the use of the reference sample is easy. Insert the reference sample into the beam path and perform the reference measurement. Replace the reference sample with the sample containing the analyte and perform the sample measurement.

In the double-beam device there exist, dependent on the subsequent sample measurement, various combinations for the use of the reference and therefore, unfortunately, also possible errors:

The following 3 combinations are possible and lead to correct results:

Combination	Reference measurement		Sample measurement	
	Measuring beam path	Comparison beam path	Measuring beam path	Comparison beam path
1	Reference	empty	Sample	empty
2	Reference	Reference	Sample	Reference
3	empty	empty	Sample	Reference

Correcting infinite absorbance

Correction of the infinite absorbance is important for samples with very low transmittance and may contribute toward better measuring results for the absorbance.

With very low transmittance values close to the 0% transmittance line, the signal noises cause a transmittance of 0 or a negative transmittance. As the absorbance is determined as a negative common logarithm from the transmittance (see above), and this is only defined for values greater than zero, absorbance is generally set to the calculation accuracy figure for these transmittance values. In ASpect UV, this absorbance value is 9.

Depending on the energy (spectral width and wavelength of the radiation source) and the sensitivity curve of the recipient (photodiode), the lower noise threshold in absorbance is considerably lower. This results in high, unstable absorbance values, not caused by the absorbance of the sample but by the signal noises and calculation accuracy. Peaks or edges are poorly identified and evaluated here in these noisy spectra.

In order to correct this, the software is used to determine correction spectra, with which the effect of the signal noise on the extent of the lower noise threshold is minimized. In this way, it is possible to create absorbance spectra that are more easily analyzed, even with very high absorbance values (5 - 7).

The correction of the infinite absorbance is required, in particular, for the stray light tests according to USP. When evaluating the stray light using the "10 mm versus 5 mm" method, a positive effect is achieved here as there are two strongly absorbing samples, as well as a reference and a sample.

I.3 Data format for importing sample information

Sample information data is imported in the method configuration dialog on the **Sample sequence** tab.

Import file formats

Data in the formats *.csv and *.txt. can be imported.

Keywords

If the first row of the sample information files contains column information (separated by a semicolon) all of the following rows will be assigned to the corresponding columns by column. Keywords are not case sensitive.

The following keywords are valid for the columns:

Keyword	Meaning
type	Sample type
name	Sample name
nomvalue	standard concentration
notes	sample note
initweight	sample weight
dilution	Dilution
varA, varB, ... , varH	Variable A, variable B, ... , variable H

The following keywords are assigned to the sample types. Once again, the keywords are not case sensitive:

Keyword	Sample type
meas	Measurement
ref	reference sample
wash	flushing sample
calib	calibration standard
nomeas	no measurement
blank	blank sample

Example

type;name;nomvalue;notes;initweight;dilution;varA;varB;varH;
ref;probe1a;0;note44;55;66;1;2;
calib;Standard1;55;note66;77;88;3;4;
calib;Standard2;75;note66;77;88;3;4;
meas;probe2b;0;note55;66;77;2;3;
blank;Leerwert;0;note66;77;88;4;5;
wash;Waschloesung;0;note66;77;88;5;6;

Importing sample names only

If no keywords can be identified in the first row, all rows (incl. the first) are interpreted as sample names and assigned to the sample table in sequential order

Example

Sample 0815

Sample 0816

Sample 0817

Sample 0818

Sample 0819