analytikjena
An Endress+Hauser Company

Operating Manual

ASpect CS
Software for HR-CS AAS

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For a proper and safe use of this product follow the instructions. Keep the operating manual for future reference.

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

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Table of contents

1 ASpect CS Software

ASpect CS is the control and analysis software for Analytik Jena atomic absorption spectrometers. The software supports AAS devices from the contrAA series.

The method parameters for the measurement procedures can be optimized to the specific demands of the sample to be analyzed. The obtained data can be recalculated, exported to various file formats and printed out.

Software version described

This document is based on the version ASpect CS 2.3.

Intended use

ASpect CS is used exclusively to control the above mentioned devices and to analyze the data obtained with these devices. The manufacturer does not assume any liability for problems or damage caused by the non-intended use of ASpect CS. ASpect CS and the device to be controlled by it may only be operated by appropriately qualified and instructed personnel. The operator must be familiar with the information given herein and in the user manual of the devices.

1.1 Starting ASpect CS

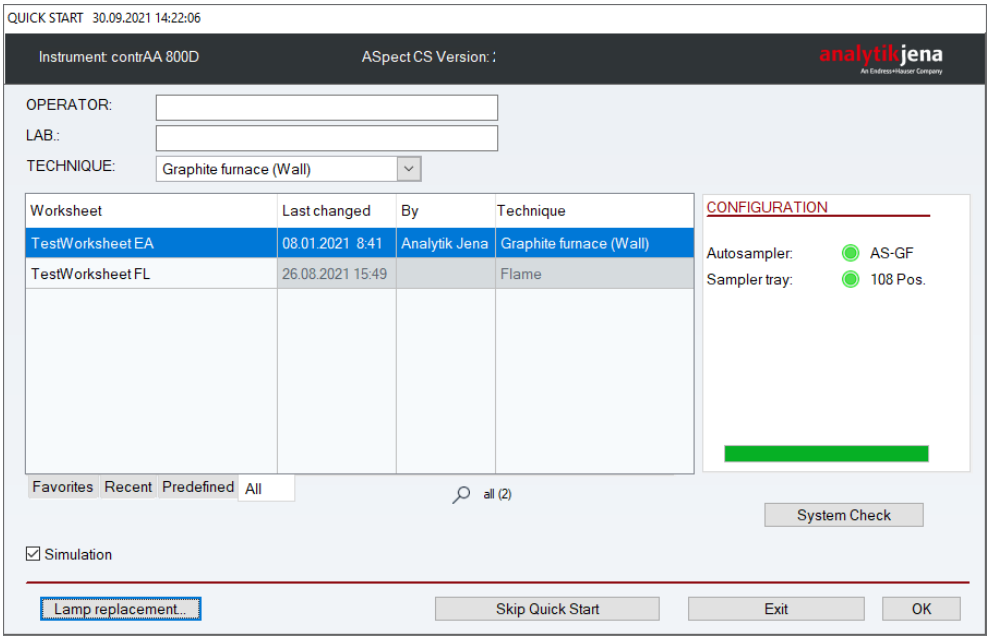
Start ASpect CS together with the AAS device. This procedure connects the device to the PC and initializes it in the software.

- Switch on the AAS device and the autosampler.
- Click on the ASpect CS icon on the Windows desktop.
  ASpect CS starts.
- If the user management option has been installed, you will be prompted to enter a user name and password. The ASpect CS program will only be accessible after successful entry of these data.

The Quick Start opens after the software has been launched. This gives you the option of selecting worksheets with preset methods and sequences to quickly start a measurement or switching directly to the ASpect CS interface.

1.1.1 Quick Start window

After the software has been started and an operator logged in (only if user administration is installed), the **Quick Start** window appears. From here you can load a worksheet, or switch to the main window of the software without any further default settings. You can also open the **Quick Start** window from the main window, via the menu item **File** | **Quick Start**.



Settings in the Quick Start window

The following options and buttons are available in the **Quick Start** window.

Option / button	Description
Operator	If using the optionally installable user management, this input field shows the user currently logged in. If user privilege management is not being used, you can enter an operator name manually.
Lab.	You can enter up to 30 characters. The name entered last is saved and issued as information on result reports.
Technique	You can select different atomization techniques depending on the configuration of the AAS device. **Graphite furnace (Wall)** Electrothermal atomization (EA) in the standard graphite tube The sample is in liquid form. Atomization of sample matter occurs at the wall of the graphite tube. **Graphite furnace (Platform)** Electrothermal atomization (EA) in a graphite tube with platform The sample is in liquid form. Atomization of the sample occurs on the platform of the graphite tube. **Flame** Atomization in the flame with burner/nebulizer system **Hydride** Determination of hydride-forming metals and mercury in a quartz cell, if necessary in combination with mercury enrichment. **HydrEA** Determination of hydride-forming metals and mercury with enrichment in the coated graphite tube **Graphite furnace solid** Electrothermal atomization (EA) in a graphite tube for solids The samples are transferred to the graphite tube on sample platforms using a solids autosampler (SSA 600 or SSA 6z).
Simulation	For training and demonstration purposes, it is possible to operate the software without an analyzer connected. When enabled, all device functions (including data acquisition and analysis) are run in simulation mode.

Option / button	Description
System Check	Establish connection between AAS device and PC (software) Click this button to detect the spectrometer and accessories and configure them according to the selected atomization technique.
Lamp replacement	Software assisted replacement of the xenon lamp Click this button to start instructions for replacing the lamp.
Skip Quick Start	Switch to the main window without selecting a worksheet
Exit	Close the **Quick Start** window and exit the software
OK	After selecting a worksheet, switch to the main window and start a measurement

Worksheet table

The worksheet table displays the currently available worksheets. The four tabs make it easier for you to find a worksheet:

Tab	Content
Favorites	Worksheets marked as **Favorite**
Recent	Recently used worksheets
Predefined	Worksheets from Analytik Jena, which are installed at the same time as the software
All	All worksheets
	Use the magnifying glass icon to filter the worksheets by elements. When you click the icon, an element list will be displayed from where you can select an element. You can repeat the selection if you want to search for more than one element. If you have selected multiple elements, all worksheets that contain at least one of the elements will be displayed (OR logic). The software searches both methods directly linked to a worksheet and methods that are loaded within a linked sequence.

1.1.2 Starting with a worksheet

A worksheet is a folder that contains a method and a sequence. Optionally, worksheets can also contain settings for the sample ID and for saving the result file. With a worksheet selected, you can start a measurement straight away. If there are several versions of the method and sequence, the latest (current) versions are always used for the measurement.

- Install accessories on the analyzer and then switch on the accessories and the device.
- Start the software.
  The **Quick Start** window appears.
- Enter the necessary details in the **Operator** and **Lab.** fields.
- Select the atomization technique from the **Technique** list.
- Click on **System Check**.
  The device and accessories are initialized and connected to the PC/software. The device configuration is displayed in the field above. The system also checks whether the installed accessories match the selected technique.
- Select the required worksheet in the worksheet table.
- Click on **OK**.
  - ✓ The main window of the software appears. The method and sequence are already loaded.

Depending on the worksheet configuration, you can now link the method and sequence loaded along with the worksheet to a sample ID file or start the measurement directly.

See also

Quick Start window [▶ 7]

1.1.3 Starting without a worksheet

Without a prepared worksheet, you have to load or configure the method, sequence and sample ID for the measurement.

- Install accessories on the analyzer and then switch on the accessories and the device.
- Start the software.
  The **Quick Start** window appears.
- Enter the necessary details in the **Operator** and **Lab.** fields.
- Select the atomization technique from the **Technique** list.
- Click on **System Check**.
  The device and accessories are initialized and connected to the PC/software. The device configuration is displayed in the field above. The system also checks whether the installed accessories match the selected technique.
- Click on **Skip Quick Start**.
  The main window of the software appears.

General sequence of a measurement routine

Specify a method and a sequence for your analysis task and start the measurement routine.

The following actions are necessary for a manual or an automatic measurement procedure:

- Specify the **method parameters** (method development).
- Create a **sequence**. The sequence contains the information on the samples and actions in their order of processing. Some sample describing data, such as the name of the sample and its position on the autosampler may be entered directly and are saved with the sequence.
- For routine analysis it is useful to create a **sample information file** (sample ID). This file contains sample-related data such as sample name, dilution factor and autosampler position. These data are needed if the concentration is to be back-calculated to the original sample. Sample information files are text files and can be created with external applications.
- Start the **measurement**.

The results are instantly written to the result database during the measurement. This central results file is accessed by the integrated data management functions (e.g. export, print, etc.).

After the measurement routine has been started, the result data are entered in the results list. You can access a detailed view (e.g. individual values, spectra) by selecting the corresponding sample row. The results obtained last are always appended to the end of the table; overwriting of results is not possible.

Further data analysis is possible by the Reprocessing function. Measured data can be prepared for printing the report or exported.

1.1.4 Opening a second instance of the application

If the application is already running, another program instance of this application will be opened in offline mode. In this mode, there is no communication with the device. However, all other functions such as developing methods or loading and analyzing results can be used parallel to the running measurements in the first program instance.

Start the program in the second instance using the menu item **File** | **Start Offline Program Instance**.

See also

Evaluating measurements parallel to running analyses [▶ 81]

1.2 Closing ASpect CS and switching off the analyzer

Always switch off the analyzer through the software by exiting ASpect CS.

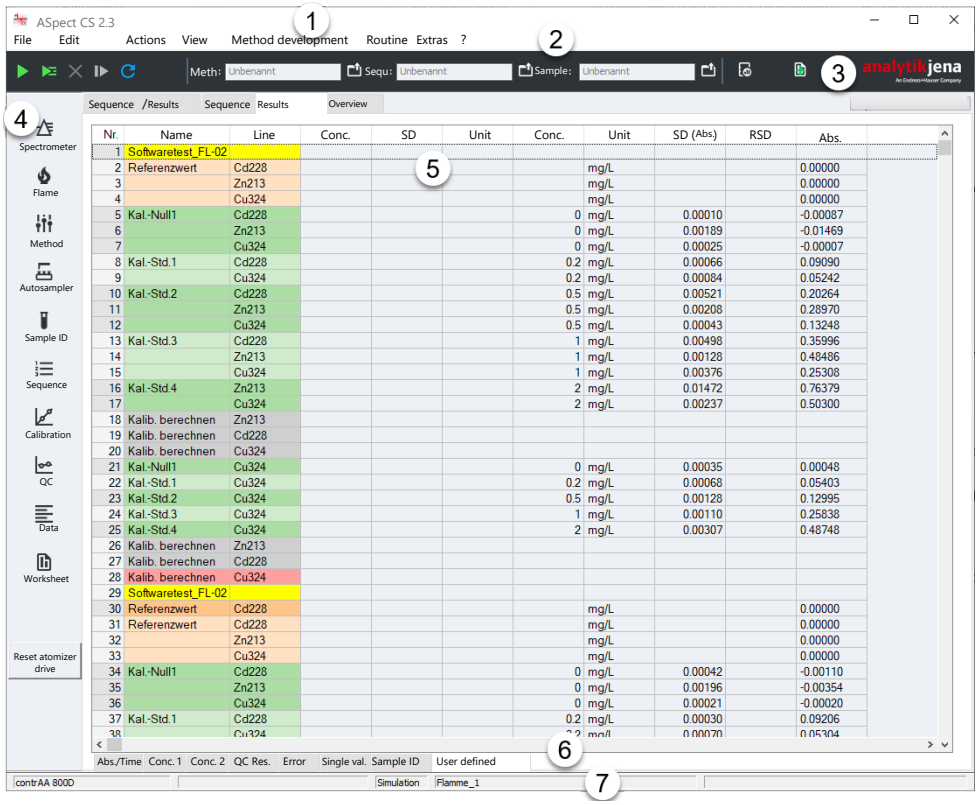
- Select the menu item **File** | **Exit**.
- If, at this time, method, sequence or sample information data have not yet been saved, you will be prompted to save the data.
- Depending on the accessories installed and the atomization technique used, further notifications about software-based actions will be given:
  - Flame: Extinguish burning flame
  - Hydride system: Flush hydride system
  - Xenon lamp: Switch off the xenon lamp
    Note: After you have switched off the lamp, you must wait 30 seconds before switching off the contrAA. A countdown of the wait time is displayed graphically on the screen.
- contrAA 800 only: If the optical flush is running, a prompt appears asking whether to switch off the flushing process.

✓ After processing the actions, ASpect CS is closed and the analyzer is switched off.

1.3 General information on operation

1.3.1 The workspace

After the software is started, first the **Quick Start** window opens. From here, you can access the workspace.



Main components of the workspace

No.	Description
1	The **title bar** provides information about the software version, the connected device, the technique, and the worksheet (if loaded).
2	The **menu bar** is used to access all program functions of the software.
3	The **toolbar** contains the buttons for starting and pausing measurement sequences, and displays the currently loaded method, sequence and sample ID file. Click the button behind the fields to load the data record. You will also find the button, which is used to create a new worksheet.
4	This icon toolbar gives you access to the most important windows (functions) of the software. When one of the windows is opened, the corresponding icon turns red. If several windows are open, clicking on the icon again brings that window to the front.
5	The main window shows the sequence and the measurement results on different tabs.
6	Some main tabs have additional **sub-tabs** found in the bottom area of the window.
7	The **status bar** at the bottom displays information about the connected device, the logged-in user, and the name of the currently displayed result file.

1.3.2 Using help

Help on the operation of the program is available via the menu item **?** | **Help topics**. While working with Aspect CS windows and dialogs, you can activate context-sensitive help by pressing the function key **F1**.

The program displays brief information (tooltips) about buttons when you move the mouse pointer over them.

1.3.3 Overview of the menu bar, toolbar and icon bar

Functions in the menu bar

The menu bar is arranged at the top edge of the workspace. It is used to start all operating actions of the software. Menus and buttons not accessible for the current contents of the workspace appear grayed out. Some menu items, such as the print function, are displayed dependent on other windows being open.

Menu item	Description
File	■ Create, open and save methods, sequences and sample information data ■ Open results data ■ Delete methods and sequences ■ Export spectrum data ■ Print active window or report ■ Open report design mode ■ Start offline or online program instances ■ Open Quick Start ■ Create worksheets ■ Exit the application ■ Directly open the last opened methods and sequences
Edit	■ Copy and insert content of text and input fields ■ Copy selected rows of the results list to the clipboard ■ Delete the content of the results list
Actions	■ Open/close, bake out, and format the furnace ■ Extinguish the flame ■ Activate scraper ■ Flush system (hydride system, autosampler, or burner system) ■ contrAA 800: Initialize atomizer drive
Display	■ Open and close windows showing graphs and information during the analysis process e.g. signal curves ■ Select the scale of the signal axis for graphs ■ Display individual sample values
Method Development	■ Open windows required for method development ■ Edit worksheets ■ Open the cookbook
Routine	■ Start, pause or abort an analysis ■ Start single sequence rows ■ Reprocess results
Extras	■ Open **Data** and **Options** windows ■ Find samples ■ Activate Scientific Mode for method development ■ Activate Monitor Mode to document diagnostics data (only for diagnostics measures requested by authorized service personnel)
System	Available if the optional module "21 CFR Part 11 Compliance ASpect CS" is installed ■ Configure user management ■ Change a password ■ View audit trail ■ Sign the results
?	■ View help and version information

Toolbar

The buttons in the toolbar are mainly used to start/pause and continue the measurement routine. The toolbar fields display the currently loaded methods, sequences and sample IDs.

Tool	Description
	Start sequence measurement
	Measure selected rows in the sequence
	Cancel running measurement routine immediately
	Stop measurement routine after processing the running measurement Any cleaning steps of the atomization unit are still executed.
	Reprocess results
	Open file Saved methods, sequences or sample IDs can be loaded into the program and used for the current analysis.
	Open the cookbook
	Create new worksheet
	Only in second program instance: Refresh the results list

Icon bar

The icon bar provides quick access to the main functions of the software. Clicking on the button opens the window with the corresponding program function. After installation, the icon bar is located at the left-hand side of the screen, but it can be moved as desired by holding down the mouse button.

Button	Description
	Check spectrometer functions
	Open flame window
	Open furnace window
	Open **Hydride system** window
	Open method window
	Specify autosampler
	Open sample information data window
	Open sequence window
	Open window with calibration
	Open window with quality control data
	Open data management
	Manage worksheets, open saved worksheets

Button	Description
Reset atomizer drive	contrAA 800 only The device automatically monitors the correct positioning of the atomizer. You can also click on this button to move the atomizer back to its original position, for example after a mechanical impact against the burner head.

1.3.4 Frequently used control elements

Various button, mouse and keyboard functions are used in the software, which have the same or very similar meanings. These control elements are described here in general. Specific information is given, where necessary, in the description of the respective windows.

General buttons

The function of icon buttons is indicated by means of tooltips displayed when the mouse pointer hovers over the corresponding button.

Button	Description
OK	Close window and apply settings
Cancel	Close window, discard changes
Accept	Apply settings without closing the window
Close	Close window, settings cannot be saved permanently
Open	Open a selection window to load a file or a data record
Save	Open a selection window to save a file or a data record
	Open a selection dialog box, e.g. path selection dialog box
	Open the **Print** window. From this window, you can print out the contents of the active document window or export it to a file.

Tables

In some of the windows, values are entered directly into a table. Depending on the type of entry, the table cell behaves like an input field, a selection list, or an input field for a restricted numerical value range with arrow keys.

- To select a row of a table, click on the corresponding row in the first table column highlighted by a gray background. You can then move the selection bar using the arrow buttons on the keyboard.
- To change the column width, move the mouse pointer to the boundary line between two columns until a double arrow appears. Then press and hold the left mouse button and adjust the column width.

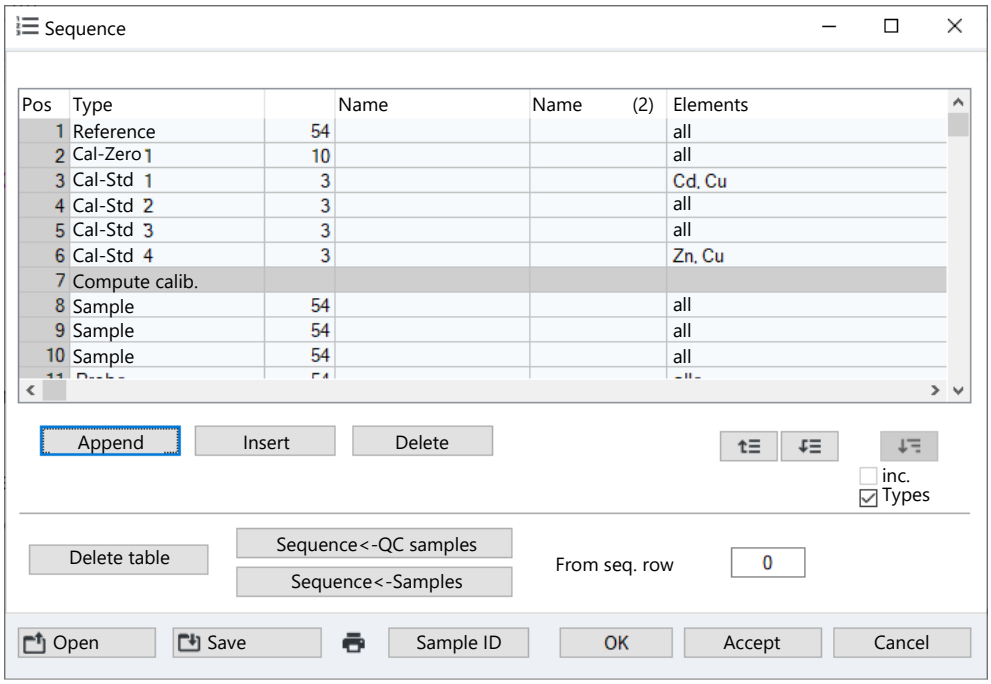
In input fields, the following functions are additionally available:

- The function key **F2** activates the editing mode. In this mode, the arrow keys are used for editing character by character. Pressing **F2** again reactivates the standard mode where the arrow keys are used to navigate between the cells.
- Text can be copied to the Windows clipboard via the menu item **Edit** | **Copy** or the key combination **Ctrl+C** and inserted via the menu item **Edit** | **Insert** or the key combination **Ctrl+V**.

Buttons accessible in tables

Button	Description
Append	Appends a new table row to the end of the list
Insert	Inserts a new table row before the selected row
Delete	Deletes the selected table row

Button	Description
	Moves the selected table row up by one position **Note**: A table row must be completely selected in order to move it. To do this, click on the number of the relevant row in the first column of the table.
	Moves the selected table row down by one position
	Transfers the value of the selected cell to all following table rows of the same sample type If the **inc.** checkbox is ticked (inc. stands for increment) this value will be incremented automatically, e.g. Sample001, Sample002, etc.



Graphs

In graphs, you can open a context menu by clicking the right mouse button. This menu provides options for copying either the graph or the entire window to the Windows clipboard. In several graphic windows, additional icon buttons are accessible:

Symbol	Description
	Activates the zoom mode After activating the button, press and hold the left mouse button to drag a frame around the area of the graph you want to zoom in and then release the mouse button.
	Deactivates the zoom mode and resets the graph to the original scale
	Activates the text mode After activating the button, press and hold the left mouse button to drag a frame in the graph and then enter the text. Double-clicking on existing text opens the window where you can edit or delete the text. Hold Ctrl and the right mouse button to move existing text.
	Activates the selection mode in signal or spectral plots Clicking the left mouse button adds labels to the measuring points.

Function keys

Key	Function
F1	Open the context-sensitive help
F2	Edit table cells
F6	Measure selected row of the sequence
F7	Open additional display windows during a measurement routine (e.g. signal curve)
F8	Close display windows
F10	Switch between the menu bar of the workspace and result window for operation via keyboard
F11	Continue stopped measurement routine
F12	Start and stop measurement routine

Using the printer

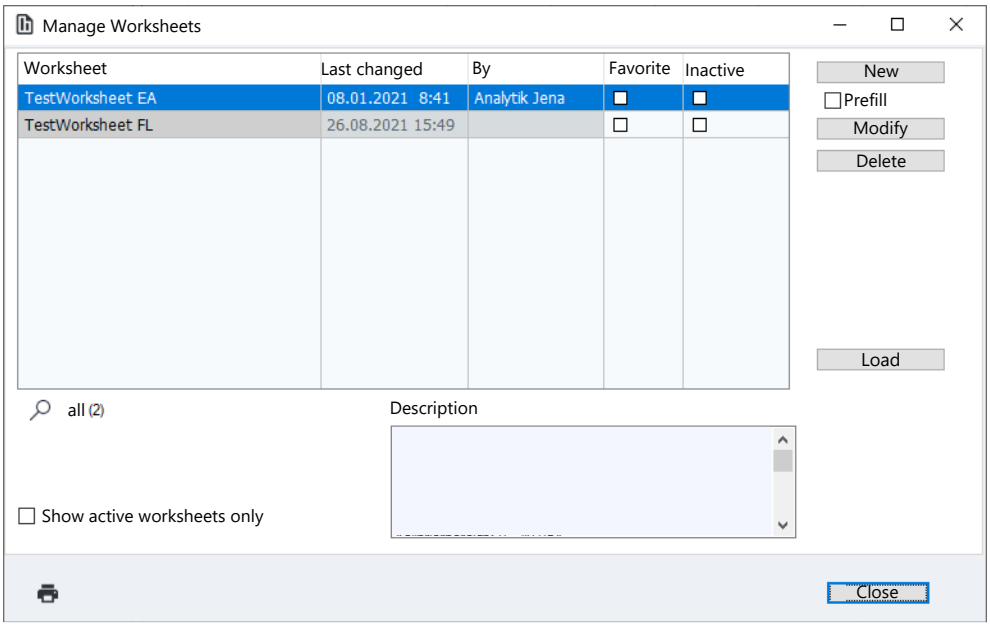
The software uses the default printer set up under Windows.

2 Managing worksheets

A worksheet is a folder that summarizes a method and a sequence. It is also possible to store settings for a sample ID and for results data in a worksheet. If a worksheet is loaded, you can start the measurement routine directly.

You can create, modify, delete, deactivate or load worksheets. The functions for this can be found in the **Manage Worksheets** window.

The **Manage Worksheets** window is opened by clicking on in the icon bar.



Elements in the Manage Worksheets window

Option/button	Description
New	Create new worksheet
Prefill	Apply the active sequence and method as the default setting
Modify	Edit selected worksheet
Delete	Delete selected worksheet
Load	Load selected worksheet for a measurement
Show active worksheets only	Hide all worksheets marked as inactive in the table
Description	Description of the selected worksheet This information is stored when the worksheet is created.

The table shows the following information about the worksheet:

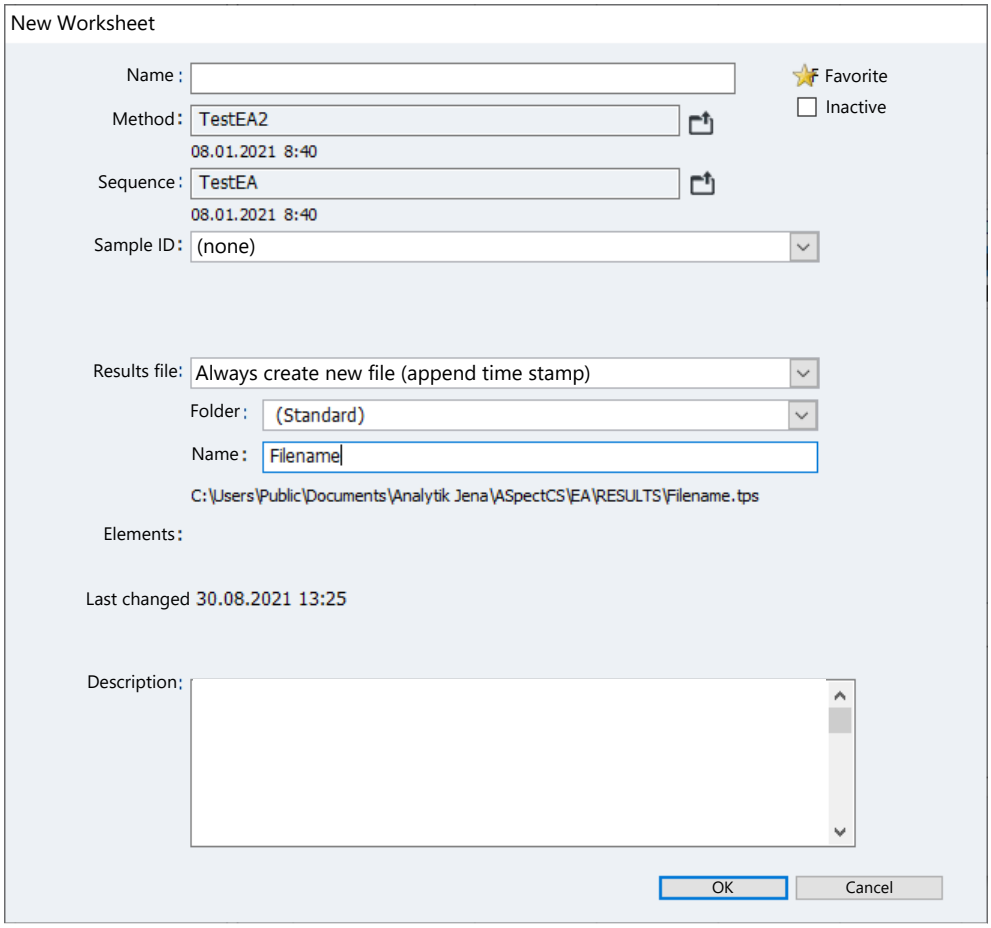
Table column	Description
Worksheet	Name of the worksheet
Last changed	Date of the last change to the worksheet
By	This operator made the last change. The name of the operator is taken from the Quick Start.
Favorite	Displays the worksheet on the **Favorites** tab in the **Quick Start** window.
Inactive	The worksheet is not displayed in the **Quick Start** window. However, a worksheet marked as inactive can be loaded in the **Manage Worksheets** window.

See also

Starting with a worksheet [▶ 9]

2.1 Creating a new worksheet

You can create a worksheet in the **New Worksheet** window.



Elements in the New Worksheet window

Option	Description
Name	Enter the name of the worksheet
Method	Method stored in the worksheet Click on Open database window and select the method.
Sequence	Sequence stored in the worksheet Click on Open database window and select the sequence.
Sample ID	Optional settings for loading a sample ID file **(none)** No settings are stored for the sample ID file. **Open folder containing Sample ID files** After loading the worksheet, the folder containing the sample ID file is opened. Click on and select the folder. **Load Sample ID file** A sample ID file is automatically loaded when the worksheet is loaded. Click on and select the file. You can also define a file mask using the "*" and "?" wildcards.

Option	Description
Results file	Optional settings for saving the results **(none)** Measurement routine starts with the **Start** window in which the name of the results file and the storage location are specified. **Always create new file (append time stamp)** Results of a measurement routine are saved in a new file each time. The file name is composed of a fixed component (name) and the time stamp for the measurement. Select a folder where the file will be saved and enter a name. **Create and append to file** A results file is created when started for the first time. At each subsequent start, the results will be appended to this file.
Description	The **Description** field initially displays by default some analysis parameters extracted from the method. You can freely edit these entries to give concrete information on how to use the worksheet. The entries appear in **Quick Start** and in the **Manage Worksheets** window for a selected worksheet.
Favorite	Click on the star to mark the worksheet as a favorite: Yellow star: Favorite Gray star: Not a favorite
Inactive	If activated, the worksheet will not be displayed in the Quick Start.

Specifying a worksheet

- To create a new worksheet, click on  in the icon bar to open the **Manage Worksheets** window and then click on **New**.
  Alternatively, click on  in the toolbar.
  The **New Worksheet** window appears.
- Select a method and a sequence.
  Note: In a sequence, you can load further methods as actions.
- Optionally specify the saving of the result file and the use of a sample ID file and edit the description.
- Close the window by clicking on **OK**.
  ✓ The new worksheet appears in the **Manage Worksheets** window and can be loaded.

See also

Starting a measurement routine [▶ 76]

2.2 Editing a worksheet

You can edit all settings in an existing worksheet.

- Click on  in the icon bar to open the **Manage Worksheets** window.
- Select the worksheet and click on **Modify**.
- The**Edit Worksheet** window appears.
- Make changes in the same way as when creating a new worksheet.
- Close the **Edit Worksheet** window by clicking on **OK**.
  ✓ The data record of the worksheet is updated.

2.3 Deleting a worksheet

You can delete a worksheet that is not needed.

- Click on  in the icon bar to open the **Manage Worksheets** window.
- Select the worksheet and click on **Delete**.
  - ✓ The worksheet is deleted after you confirm the query.

2.4 Loading a worksheet

You can select a worksheet in **Quick Start** or load it in the **Manage Worksheets** window.

- Open the **Manage Worksheets** window by clicking on  in the icon bar.
- Select the worksheet in the table and click **Load**.
  - ✓ The worksheet is loaded and the corresponding sequence is displayed in the main window.

Depending on the worksheet configuration, you can now link the method and sequence loaded along with the worksheet to a sample ID file or start the measurement directly.

Note:

When loading a worksheet, the current versions of the method and sequence are always used. If you load a method or sequence that differs from the worksheet, the settings for the results file and the sample IDs in the worksheet are reset.

3 Methods

Methods store the parameters required for an analysis.

- Selection of analysis lines
- Parameters for line analysis
- Spectrometer settings
- Atomizer settings
- Type of sample supply
- Calibration parameters
- Statistical analyses
- Settings for quality control and assurance
- Settings for measurement output

Measurement sequences can be created based on a method. The order of sample measurements and other actions within an analysis are defined in sequences. Saved methods can thus be used for analyses with different sequences.

The **Method** window is opened by clicking on in the icon bar. The last active method is displayed. If no method has been loaded since program start, the window displays contain the main settings are empty.

3.1 Creating, saving and loading methods

Methods are saved in a database. If the method parameters of an existing method are changed and these changes saved under the same name, a new version of the method is created. The existing method can therefore not be overwritten or be unintentionally deleted in this way. You can create, modify, save and load methods. Further functions for managing methods can be found in the **Data** / **Data management** window.

See also

Managing methods and sequences [▶ 155]

3.1.1 Creating a new method

When creating a new method you can make use of default settings, parameters of a saved method or current method parameters.

- Select the menu item **File** | **New Method**.

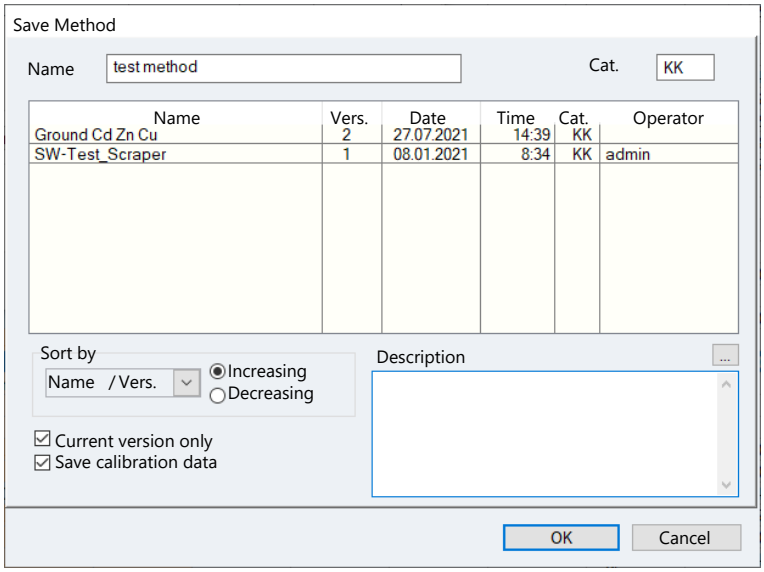
  Alternatively, click on if no method is activated.
- Select one of the three options in the **New Method** window:
  - **Based on default parameters**: Open the **Method** window with default settings for calibration and statistics only.
  - **Based on current parameters**: Open the **Method** window with the currently set method parameters.
  - **Based on saved method**: Select a method in the **Open Method** database window.
- Confirm the selection with **[OK]**.
  The **Open Method** window with the selected default settings appears.
- Specify the method on the various tabs and make the necessary optimizations.
- Activate the method parameters with the **[OK]** or **[Accept]** buttons.

✓ You can now save the method or use it for the next analysis. For the analysis, create a sequence based on the method and optionally fill in a sample ID table. Then start the measurement.

3.1.2 Saving a method

After entering the method parameters, save the method to the database. This allows you to load the method at a later time for further measurements or to include it in a worksheet. Methods are saved in the database in the **Save Method** window. You can save additional data with the method to categorize the methods and make them easier to find.

Elements in the Save Method window



Option	Description
Name	Method name
Cat.	Category (three characters) for further identification and sorting the methods This entry is optional.
Table	Overview of existing methods
Sort by	The options in this group allow you to sort the methods list. If the **Current version only** option is enabled, only the latest version is displayed for methods with the same name.
Save calibration data	Save any available calibration curves with the method The calibration curves can be used for further analyses.
Description	Optionally enter further explanations for the method Click on ••• to open a list with predefined comments. You manage these comments in the **Data** / **Pre-defined descriptions** window.

Saving a method

- In the **Method** window, click on **Save** and open the **Save Method** window. Alternatively, select the menu item **File** | **Save** | **Method**.
- Select the name of the method and other parameters in the **Save Method** window.
- Confirm the settings with **OK**.

  ✓ The method is saved to the database. If you use the same name as an existing method, a new version of the method is created in the database.

Note: The method is also saved in the results file of the measurement. After opening the results file, you can also restore the method. Further management functions for methods are available in the **Data** / **Data** window.

See also

- Creating predefined notes [▶ 162]
- Managing methods and sequences [▶ 155]

3.1.3 Loading a method

You can load saved methods and start a measurement based on them together with a sequence. Method parameters can be loaded from the methods database or from an existing results file.

Loading from the database

- Open the database window with one of the following alternatives:
  - In the toolbar, click on the folder icon next to the **Method** field.
  - Select the menu item **File** | **Open Method**.
  - Open the **Method** window by clicking on and then click on **Open**.
- Optionally, you can limit the displayed methods by selecting a category in the **Cat.** field. To display all methods, clear the **Cat.** field.
- Optionally, you can activate the **Current version only** option if you want to display only the latest version of a method.
- Select the method in the list and click on **OK**.
  - ✓ The **Method** window with saved parameters appears.

Loading from a results file

The method can be extracted from a results file displayed in the main window. This happens automatically when the sample individual values are displayed.

- Double-click on any sample in the results list or right-click on a sample and select **Single values** in the context menu.
- Click **Yes** to confirm the prompt asking if you want to load the method parameters.
  - ✓ The method can now be opened by clicking on .

3.2 Specifying method parameters

You can specify the measurement parameters for an analysis and the parameters for the results evaluation in the **Method** window.

Open the **Method** window by clicking on .

Buttons in the Method window

The bottom part of the window contains buttons that are available at all times.

Button	Description
Open	Open a saved method
Save	Save the current method parameters
	Print method parameters

Button	Description
	View properties of the method
OK	Accept parameters in the window and close the window
Accept	Accept parameters in the window but leave the window open
Cancel	Do not accept changed parameters and close the window

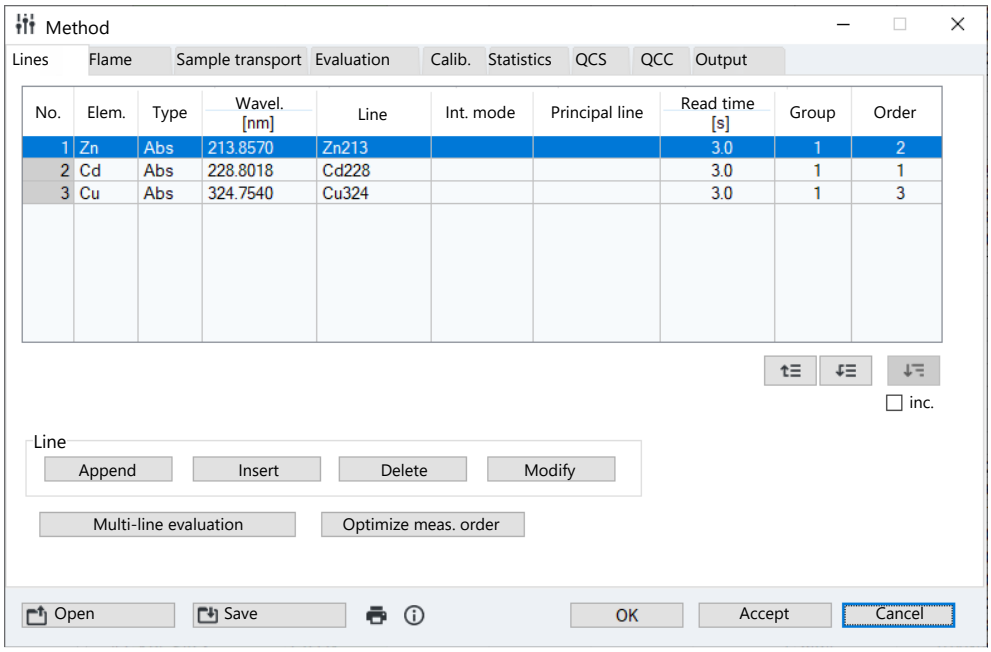
See also

- Frequently used control elements [▶ 15]
- Specifying sample information and QC samples [▶ 75]

3.2.1 Method / Lines window – Specifying analysis lines

In the **Method** / **Lines** window, select the analysis lines of the method. This selection loads the data from the cookbook with the default settings for atomization of the elements.

Elements in the Method / Lines window



Line table parameters

Table column	Description
No.	Sequence of selected lines in the table
Elem.	Element icon of the element to be analyzed
Type	Selection of measurement mode **Abs**: Absorption mode **Ems**: Emission mode
Wavelength	Wavelength of analysis line in nm
Line	Name of the analysis line In the main settings the name of the line consists of the element symbol and the wavelength. However, the name can be edited freely and must be unique.
Int. mode	Selection of the signal evaluation **Mean**: Signal averaging over the integration time **Area**: Peak area of absorbance over the integration time

Table column	Description
	Height: Peak height of absorbance over the integration time Use the **Mean** evaluation when using sufficient sample quantities, i.e. with flame technique and sometimes with the hydride technique. The **Area** and **Height** evaluations are used when atomizing defined sample quantities. Select these signal evaluations when using the graphite furnace technique, hydride technique or flame technique in connection with an injection module.
Principal line	Indication with which analysis line the current line is simultaneously measured (simultaneous measurement) The total duration of the analysis can be shortened by recording adjacent lines with a spectrometer configuration. Click on **Multi-line evaluation** to display the possible combinations.
Read time	Total measuring time for an analysis line
Group	Only flame technique Analysis lines with the same group number are measured with continuous sample flow, i.e. while starting the next analysis line and adjusting the burner, the autosampler's cannula remains immersed in the sample. This shortens the delay time between the analyses of the individual element lines and thus also the total measurement time. The autosampler emerges from the sample between different groups. The sample flow to the burner is interrupted. Elements should be assigned to different groups if the fuel gas flow and burner height change significantly. Then the delay time between analyses is used to stabilize the flame settings.
Order	Analysis order The measuring order can be freely defined. Only flame technique You can click on **Optimize meas. order** to define the order automatically, in ascending order by fuel gas flow.

Buttons in the Lines group

Use the **Append**, **Insert** and **Modify** buttons to add additional analysis lines to the line table or to edit a selected line. After clicking on one of these buttons the **Select Element/Line** window opens, where you can make further entries. Use the **Delete** button to delete one or more selected analysis lines from the method.

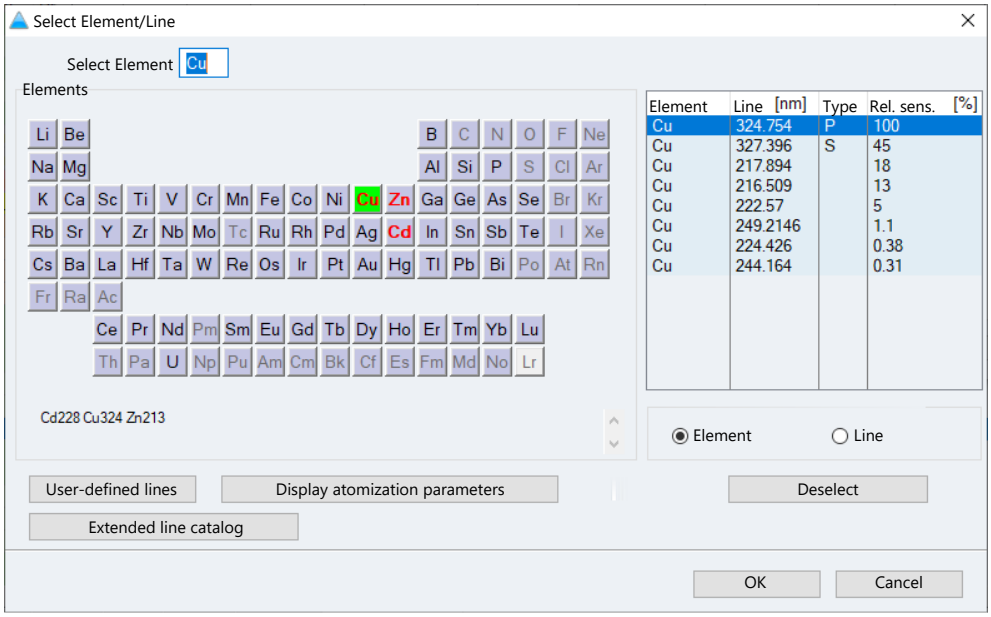
Additional buttons

Button	Description
Multi-line evaluation	Lines that can be recorded in one spectrometer setting can be measured simultaneously. This shortens the measurement time.
Optimize meas. order	Only flame technique Arrange lines in ascending order according to fuel gas flows

3.2.1.1 Inserting analysis lines into the line table

The analysis lines are selected in the **Select Element/Line** window.

The **Select Element/Line** window appears when you click on **Append** in the **Method** / **Lines** window.



Elements in the Select Element/Line window

The periodic table shows all elements that can be analyzed with the AAS technique (dark gray buttons and black element symbols). Any elements that are grayed out cannot be analyzed with the AAS technique.

The line table contains all selectable lines with the following information:

Table column	Description
Elem.	Element
Wavel.	Analysis wavelengths in nm
Type	Line type **P**: Primary wavelength. This wavelength is the most sensitive line with the relative sensitivity of 100%. **S**: Secondary wavelength. The secondary wavelength has the second highest sensitivity. **Note**: The primary wavelength is not always the recommended line for the measurement. For further information see in the **Cookbook** under **Remarks**.
Rel. sens.	Relative sensitivity compared to the primary wavelength **P**
Element / **Wavelength**	Sort the line table in ascending order by chemical symbol or wavelength
	Open cookbook with recommended analysis settings

Selecting lines

- In the **Method** / **Lines** window, click on **Append** or **Insert**.
  The**Select Element/Line** window appears.
- Click on an element symbol in the periodic table. The dark gray buttons are selectable elements. This only displays the lines of the selected element in the line table.
  Alternatively, enter the element symbol in the **Select Element** field.
  Clear the **Select Element** field to display the full list of elements in the line table.
- Select the lines in the line table.
- Continue until you have selected the lines for each analyte. Exit the window with **OK**.
  ✓ The selected lines are transferred to **Method** / **Lines** window.

Note:
When working through the methods, select several lines for each analyte. The primary line is not always the most appropriate one. Refer to the cookbook for recommended atomization parameters and possible interferences.

Checking flame parameters

When using the flame technique, click on **Display atomization parameters** to check the atomization parameters of the selected lines. If possible, combine only elements in a method for which the same flame type is recommended, i.e., either air/acetylene flame or nitrous oxide/acetylene flame. When you return to the Lines method page, you can click on Optimize meas. order to automatically sort the lines in ascending order by fuel gas flow.

Extended line catalog

After installation the line list contains a preselection of analysis lines. This can be supplemented by analysis lines from the extended line catalog.

- Click on **Extended line catalog.**
- Select the lines in the list by clicking with the mouse.
  Click again on a single line to remove the selection. Click on **Deselect** to remove all selections.
- Click on **Add** to transfer the selection to the line list.

NOTICE

The lines added from the extended line catalog cannot be removed from the standard catalog.

Creating and editing own analysis lines

You can create your own analysis lines and use them for the analysis.

- Click on **User-defined lines**.
- Enter the data for the new line in the **Edit lines** window: **Element**, **Wavelength** and **Type**.
- Transfer the entries to your own line list by clicking on **Add**.
- Click on **Close** to transfer your own lines to the line list of the **Select Element/Line** window.

You can edit and delete your own lines from the line list.

- Edit line: Select the line in the list of the **Edit lines** window, enter the new line data, and then click on **Modify**.
- Delete line: Select the line and click on **Delete**.

3.2.1.2 Measuring lines simultaneously

When combining lines, a search is performed in the current measuring program for lines that can be recorded together with the same monochromator configuration by the detector, and therefore also be measured simultaneously.

- In the **Method** / **Lines** window, click on **Multi-line evaluation .**
  The window of the same name appears with an overview of possible line combinations.

Elements in the window Multi-line evaluation

The possible line combinations are listed in the **Multi-line evaluation** window. A bar graph shows the position of the lines on the detector for the selected list row.

Table columns / button	Content
Checkbox	If enabled the respective line combination is measured simultaneously in the method.
Principal line	The measurement parameters of the **Principal line** are used to measure the line combination. **Line** Line name of the principal line **Wavel.** Wavelength in nm of the principal line
Additional line	**Line** Line name of the additional line to be analyzed **Wavel.** Wavelength in nm of the additional line to be analyzed
Meas.wavel.	Measuring wavelength in nm (center of the detector row)
Action status	Remarks
No combined lines	Delete all selections. No lines in the method are measured together.
Swap line priority	Swaps the principal line and additional line in a line combination.

For a line combination, a principal line and the additional line are automatically determined. The additional lines take the analysis time and the atomization parameters from the principal line. This assignment can be reversed by clicking on **Swap line priority**.

3.2.2 Method / Flame window – Specifying flame parameters

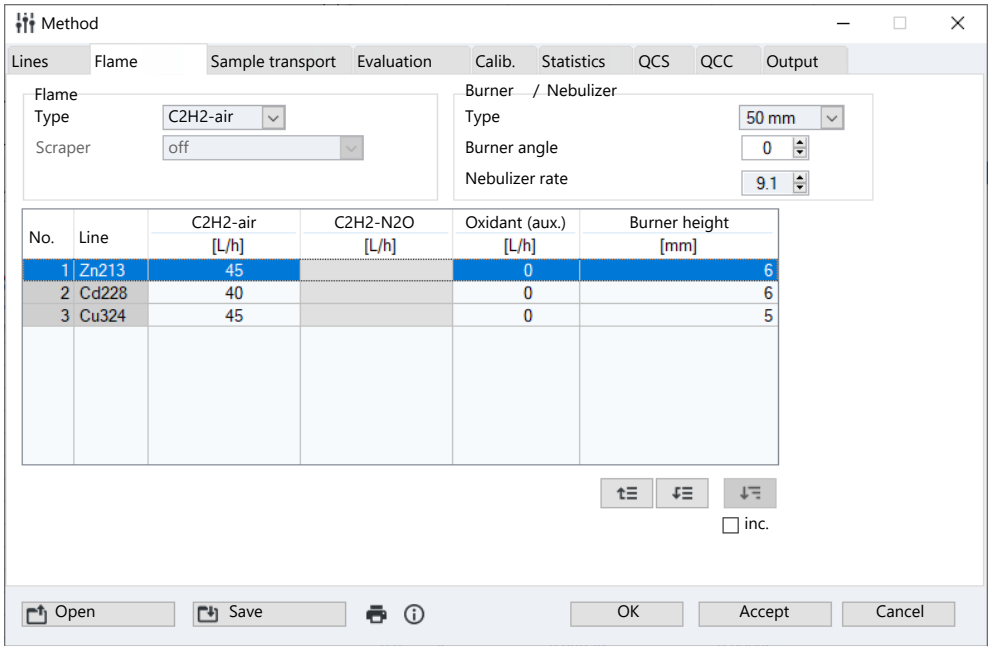
Only flame technique

In the **Method** / **Flame** window, specify the following parameters for atomization in the flame:

- Parameters for burner and nebulizer
- Flame type
- Gas flows
- Use of a scraper

The data from the cookbook is loaded first as default settings.

Click on  to open the **Method** / **Flame** window.



Line-independent settings

The line-independent parameters are the same for all element analyses with the current method. First set the parameters that apply to the entire method and cannot be varied for the individual analysis lines.

Option	Description
Flame / Type	Selection of the flame type **C2H2-air**: Acetylene-air flame, fuel gas flow = 40 – 120 L/h **C2H2-N2O**: Acetylene-nitrous oxide flame, fuel gas flow = 120 – 180 L/h This flame type can only be selected when using the 50 mm burner.
Scraper	The scraper is activated for the automatic analysis process with the 50-mm burner and acetylene/nitrous oxide flame. This automatically cleans the burner head. Cleaning can be performed before each sample, before each group, before each line, before each measurement or before each 2nd/3rd measurement.
Burner / Type	Display of the burner type used The device automatically recognizes the burner via the burner sensor.
Burner angle	Angular position of the burner relative to the optical axis The burner angle must be set manually on the burner (normally it is set to 0°). The entry of the value is optional. It only serves to complete analysis method and report data. Manually rotating the burner changes the sensitivity. As a rule of thumb: If the burner is rotated by 10°, the sensitivity decreases by a factor of 2 to 3. If the burner is rotated by 90°, the sensitivity decreases by a factor of 10.
Nebulizer rate	Aspiration rate of the nebulizer This rate is a nebulizer-specific value. The entry of the value is optional. It only serves to complete analysis method and report data.

Line-dependent parameters

The table lists the line-dependent parameters of the fuel gas flows and burner heights. The values can be searched for manually or automatically in the flame optimization program and transferred to this table of line-dependent flame parameters. If you are using an auxiliary oxidant, you can only optimize the flame manually. Alternatively, you can edit the values manually.

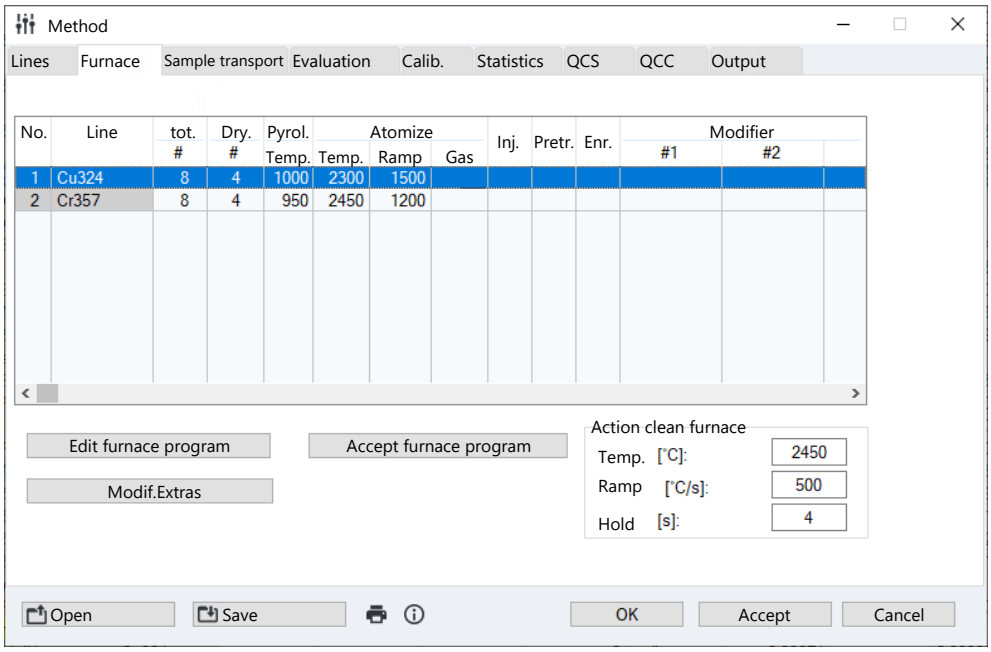
See also

Optimizing the flame [▶ 119]

3.2.3 Method / Furnace window – Specifying parameters for atomization in the graphite furnace

The **Method** / **Furnace** window contains an overview of the most important parameters of the furnace programs for the atomization of the elements being analyzed. The data of the furnace programs from the cookbook are entered as default settings for atomization of the individual elements using the graphite furnace technique. You can edit the furnace program for each analysis line in the **Furnace** window.

Click on  to open the **Method** / **Furnace** window.



You can use the table to see for which graphite furnace type (wall or platform) the method was created. If this type differs from the initialized type, this fact is also displayed.

The following furnace program parameters are listed:

Option	Description
Line	Name of the analysis line
tot.	Total number of furnace program steps
Dry.	Number of drying steps in a furnace program
Pyrol. Temp.	Pyrolysis temperature in °C
Atomize	Detailed display of temperature data during atomization phase **Temp.** End temperature of atomization phase **Ramp** Temperature variance during atomization phase in °C/s **Gas** Feed of inert gas
Inj.	Not selected Sample is injected before start of furnace program.

Option	Description
	"*" Sample is injected at a later point in time.
Pretr.	Thermal pretreatment If selected, sample or modifiers are thermally prepared.
Enr.	Enriches the sample if selected.
Modifier	Additionally used modifiers For each measurement, a maximum of five additional modifiers can be selected.

Buttons

Button	Description
Edit furnace program	Open the **Furnace** / **Furnace program** window that provides a full display of the furnace program. Furnace parameters can be adapted for any element line being analyzed. Alternatively you can also open the **Furnace** / **Furnace program** window by double-clicking on the row of the analysis line in the line table.
Accept furnace program	Applies the parameters of a selected analysis line to all subsequent lines in the list.
Modif.Extras	The **Furnace** / **Modif.Extras** window for specifying the modifiers used

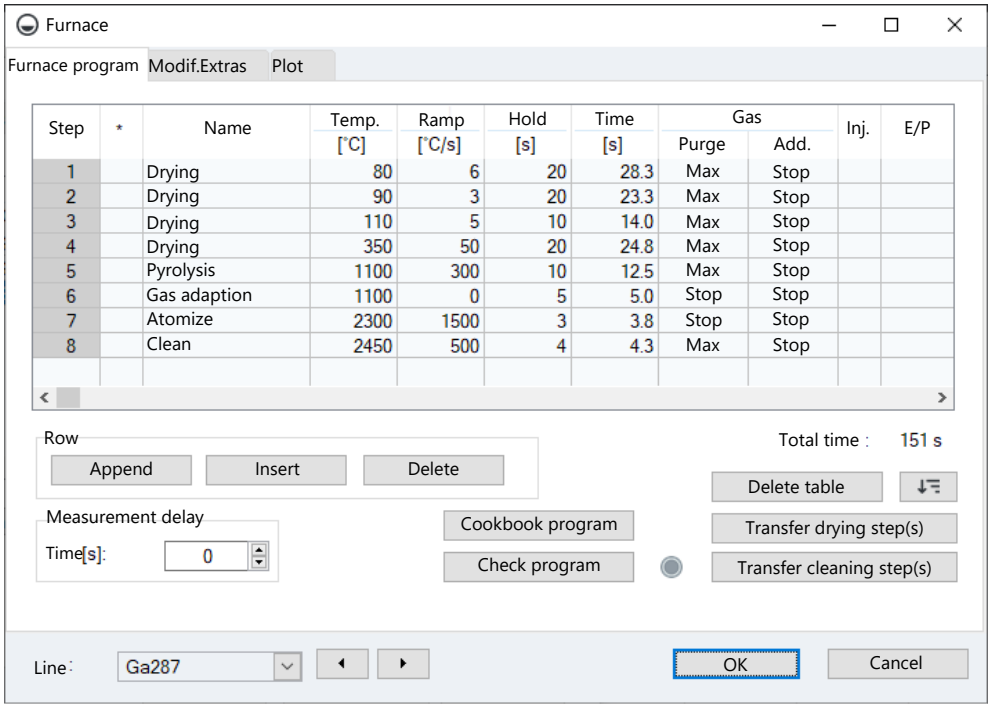
"Clean furnace" as an additional sequence action

The furnace will be cleaned by baking out on completion of a furnace program for a given element line in all cases. In addition, a further cleaning step can be defined in the sequence by selecting the **Clean furnace** special action The parameters for this action are entered in **Action clean furnace**.

Option	Description
Temp.	Specified end temperature for baking (cleaning) process.
Ramp	Rate of temperature change
Hold	Holding time at end temperature

3.2.3.1 Editing a furnace program

In the **Method** / **Furnace** window, click on the **Edit furnace program** button to open the **Furnace** / **Furnace program** window in edit mode.



Tabular display

For each analysis line, the table lists all steps belonging to the current furnace program with the associated settings for temperature, holding time, gas supply, use of modifiers, and enrichment/thermal pretreatment. After selecting an analysis line, the default settings for the cookbook are loaded first.

Control buttons and input fields

Option	Description
Append	Insert a new row at the end of the list
Insert	Insert a new row before a selected list place
Delete	Delete selected rows
Delete table	Delete entire furnace program table
	Copy the parameters of the selected row to all subsequent rows
Measurement delay	Enter a time delay for acquisition of the measuring signal if required By default, acquisition of the measuring signal will begin as the **Atomize** furnace program step starts. A time setting will delay the starting point of signal acquisition by the preset amount of time. This function is used to start the measurement only after the atomization temperature has been reached on the temperature plateau.
Cookbook program	Load furnace program from the cookbook for the selected analysis line
Check program	Check furnace program If the furnace program is found to contain errors of a kind that renders program execution impossible, the faulty step will be displayed in a message box. The program cannot be launched in this case. Correct the faulty step or change the furnace program that precedes this step. When the program starts, the furnace will be checked for potential thermal overheat situations if all basic conditions are known. If the temperatures or times selected are too high, the error message appears after the program start.
Transfer drying step(s)	Apply drying parameters of the selected analysis line for all analysis lines

Option	Description
Transfer cleaning step(s)	Apply parameters of the selected analysis line for cleaning the graphite furnace for all analysis lines

Specifying parameters for individual furnace program steps

On selection of an analytical line, a suitable furnace program will initially be loaded from the cookbook.

- Use the **Append**, **Insert** or **Delete** buttons to insert further steps into the furnace program or to delete steps.
- Click in a table cell to edit it.
  A list will open in this cell if preselections are limited. Numbers must be edited directly in the field.

Program steps

The following steps can be programmed in a furnace program:

Step	Description
Drying	Evaporation of solvent in the sample
Pyrolysis	Thermal pretreatment in which the sample is thermally decomposed without administration of oxygen
Ash	Thermal pretreatment in which the sample is thermally decomposed using an appropriately selected additive gas (for example, oxygen)
Atomize	Release of analyte atoms
Clean	Removal of residual sample matter
Cooling	
Gas adaption	Adaptation of gas flow to the atomization conditions

Temperature parameters

Option	Description
Temp.	End temperature of this step Value range: Maximum temperature up to 3000 °C in steps of 1 °C Minimum temperature not less than 20 °C above cooling water temperature (preferably 35 °C) of circulation cooler
Ramp	Heating rate to reach the target temperature Value range: 1 to 3000 °C/s in steps of 1 °C/s; FP (Full Power), NP (No Power) are possible limit rates
Hold	Hold time of the target temperature Value range: 0 to 999 s less heating time
Time	The total duration of the step (sum of heat time and hold time) is automatically calculated.

Gas supply

Option	Description
Purge	Flow of protective gas **Stop** No inflow, effective 2 s before step change **Min** Minimum inflow rate (0.1 L/min Ar) **Max** Maximum inflow rate (2.0 L/min Ar)
Add.	Flow of additive gas, e.g. air, nitrogen, etc.

Option	Description
	Stop No inflow, effective 2 s before step change **Max** Maximum inflow rate (0.5 L/min)

Injection step/thermal pre-treatment

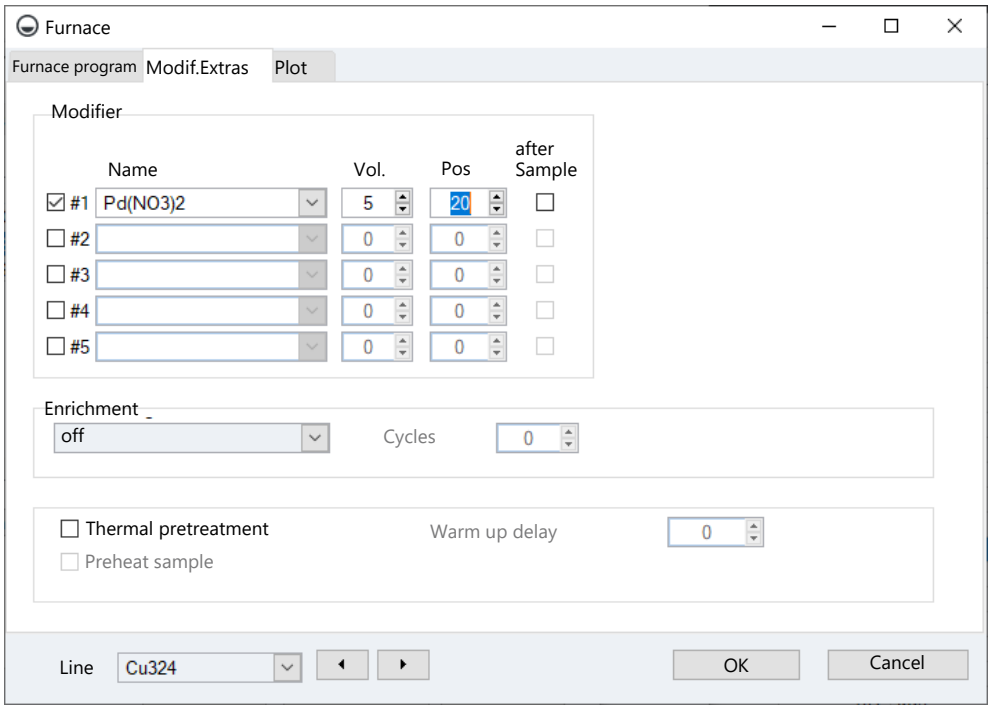
Option	Description
Inj.	If marked with a "*", the sample (gas in the HydrEA technique) will not be introduced into the graphite tube before completion of this step (pipetting into preheated tube).
E/P	Only solution analysis Enrichment/thermal pretreatment With enrichment, the sample is pretreated during the measurement cycle until the enrichment step, the tube is then cooled back to room temperature and the next sample volume is injected. With thermal pretreatment of analyte solution and/or modifiers, this pretreatment is performed up to the specified step. At the end of this step the graphite tube has to been cooled down and the sample injected. The number of enrichment cycles, the use of modifiers and the type of thermal pretreatment can be specified in the **Furnace** / **Modif.Extras** window.

You can optimize a furnace program for an analysis line using the software in the **Furnace** / **Optimization** window.

3.2.3.2 Specifying matrix modifiers, enrichment, and pretreatment

In the **Method** / **Furnace** window, click on the **Modif.Extras** button to open the **Furnace** / **Modif.Extras** window in edit mode. You can specify the following parameters:

- Use and volume of matrix modifiers
- Enrichment in the graphite tube through repeated pipetting and drying
- Thermal pretreatment of the sample



Selections for modifiers for matrix delimitation and thermal pretreatment must be made for each specific line.

Matrix modifiers

Up to five modifiers can be specified for analysis of a given element line. These can be activated by clicking on the relevant modifier checkbox. In order to prevent errors due to carryover effects, analytical components are recorded in the following standard order:

- Blank (in case of dilution)
- Modifier 1
- Further modifiers (if specified)
- Sample solution

Outputs to the graphite tube occur in reverse order, i.e. the sample is the first to be injected. As the other components are being supplied, residual sample matter is flushed from the dosing tube and injected into the graphite tube. This standard order of sample and modifiers can be modified if necessary.

Enter the following parameters for the modifiers:

Option	Description
Checkbox	Activate modifier for the analysis
Name	This list field contains the names of typically used modifiers. Select a name from this list or enter it directly in the input field.
Vol.	Volume to be taken (1 to 50 µL)
Pos	Position of the modifier on the sample changer
after Sample	Autosampler will pick up the modifier after the sample, i.e. before the sample is injected into the graphite tube.
Pretr.	Thermal pretreatment of modifier

Enrichment

For enrichment, the furnace program is repeatedly performed until the specified step is reached (column E/P). As part of each cycle, the sample quantity which is specified per sample table is injected and pretreated, the tube is then cooled to room temperature and the next sample volume is injected. This procedure allows greater sample volumes to be placed into the furnace. Modifier volume is injected only once.

The following enrichment modes can be specified:

Option	Description
off	No enrichment.
permanent (only samples)	Enrichment with each sample (without special samples such as standards, etc.)
permanent (incl. calibration)	Enrichment with each sample, including standards, QC samples and additive standards
if conc. too low	Enrichment only with samples whose concentration is lower than that of the detection limit
Cycles	Number of enrichment cycles (2 to 100) **Note**: The number of enrichment steps for real samples should be limited since the element being measured as well as all residue contamination in the tube are enriched.

Thermal pretreatment

For thermal pretreatment of analyte solution and/or modifiers, this option is performed up to the specified step in the furnace program. At the end of this step, the remaining components are injected into the tube.

Option	Description
Thermal pretreatment	Thermal pretreatment of modifiers or sample. In the **Modifier** area, the **Pretr.** checkboxes must be ticked for the modifiers to be pretreated. **Note**: The pretreatment temperature of the modifier can be higher than the pyrolysis temperature of the sample.
Preheat sample	Pretreat analyte solution, then add modifiers and other components.
Warm up delay	Define waiting time from addition of components to undergo thermal pretreatment to next components

NOTICE

Cool down the furnace after thermal pretreatment higher than 300 °C!

If the temperature of the thermal pretreatment is higher than 300 °C, the graphite furnace must be cooled to below 300 °C in an additional step before the remaining components are added. Pipetting into the hot furnace (above 300 °C) will destroy the tip of the tube! There will be no error message with higher temperatures!

Solid analytics using the SSA 600 solids autosampler

With solid analytics, only matrix modifiers may be specified for addition. Once a modifier has been activated, its name and volume can be defined (same as above).

For SSA 600 without liquid dosing, the modifiers must be pipetted to the sample by hand. The supply occurs immediately before the platform is brought into the furnace or as the final step of a complete sample preparation with the help of SSA 600.

For SSA 600 with liquid dosing, the modifier or the liquid samples are pipetted automatically.

In the thermal pretreatment in the solid analysis, the platforms are first pretreated with the modifiers (e.g. palladium). The furnace program is run through to step **E/P**. Then the tare is determined from the coated platform and the sample is dosed. The furnace program is then continued from step **E/P**.

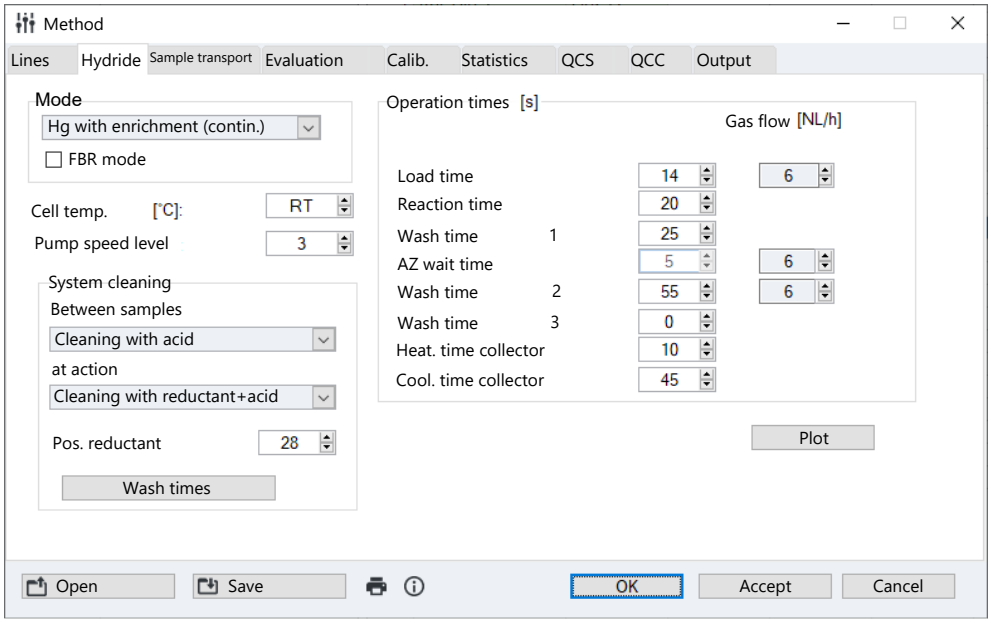
3.2.4 Method / Hydride window

The **Method** / **Hydride** window is used to set the parameters for the following hydride systems:

- HS60A/HS60
- HS55A/HS55
- HS 60 modular
- HS 55 modular

The hydride system connected is detected during device initialization. The parameters for the hydride injector HS50 are specified in the **Method** / **Sample transport** window. The commands for additional washing or loading of the hydride system are specified in the **Hydride system** window.

Click on  to open the **Method** / **Hydride** window.



Mode

You can choose among different modes depending on the equipment of the hydride system.

Option	Description
Hydride (continuous)	HS 60 A / HS 60 / HS 60 modular The reaction takes place in the reactor under continuous conditions. The sample can be fed with an autosampler or manually.
Hydride (batch)	HS 55 A / HS 55 / HS 55 modular The sample is pipetted into the reaction beaker (max. 30 mL). The beaker is clamped gas-tight to the head of the batch module. With the first channel of the 4-channel peristaltic pump, the reductant is pumped into the reaction beaker. The fast and partly vigorous reaction releases gaseous metal hydride or atomic Hg vapor.
FBR mode	Only Hg analytics in continuous operation Fast Baseline Return, FBR After the maximum absorption has been reached, the direct argon gas flow purges the cell during Wash Time 2 thus causing a fast return of the signal to baseline level.

Cell temperature / Pump speed level

Option	Description
Cell temp.	Only hydride technique For the hydride formers As, Se, Sn, Sb, Te and Bi, the cell temperature can be selected in the range between 600 °C and 1000 °C. For Hg analyses, you can choose between RT (room temperature < 60 °C) or 150 °C. The cell is heated to the selected cell temperature at the start of the analysis process, or you can start it in the **Hydride system**.
Pump speed level	Four speed levels (1 to 4) are available for the transport of the sample in continuous mode and the components. In continuous mode, the supplied sample volume is determined on the basis of this together with the reaction time.

System cleaning

For continuous operation

System cleaning may be selected optionally after every sample measurement and/or arranged as an action.

Option	Description
Between samples	System cleaning after each sample measurement **off** System is not cleaned. **Cleaning with acid** System is rinsed after every sample with diluted acid. The time is specified under **Wash time acid**. When half of the wash time is over, the sample path is switched to the reactor. **Cleaning with reductant+acid** This cleaning method is recommended if the system is heavily contaminated (samples with high element contents). First, the system is cleaned with reductant for the time **Wash time reductant**. This process is followed by a wait time (**Soak time**) to allow the reductant to take effect onto the deposits on the tube walls. Finally, the system is rinsed with diluted acid (**Wash time acid**).
at action	The system cleaning can be set as a programmable special action. This additional cleaning step can be inserted after samples with high analyte content. The options **Cleaning with acid** and **Cleaning with reductant+acid** are available for the action in the sequence (see above).
Pos. reductant	Position of reductant on the sample tray
Wash time	A window is opened for the definition of three wash times: **Wash time acid**, **Wash time reductant**, **Soak time**. Set the times according to the cleaning options.

Operation times

The operation times must be adjusted depending on the selected operating mode. All operation times are entered in seconds.

Option	Description
Load time	The sample pump requires this time to fill the sample hose upstream of the two-valve group with sample. This time is needed only for the first measurement of a new sample.
AZ wait time	Time directly preceding the baseline (auto zero) adjustment.
Prewash time	Time for cleaning the beaker with argon before the reaction (for hydride former) The pre-wash time is used to expel air to prevent an oxyhydrogen reaction during the subsequent reaction.
Reaction time	During this time, the sample pump pumps the sample into the reactor. This time is the crucial parameter for the supplied sample volume and the measuring sensitivity.
Pump time	In this time, the reductant is pumped into the beaker in order to start a reaction.
Wash time 1 ... 3	Times for the transport of the reaction gas with the argon flow. The transport paths are different in the individual phases for the various operating modes and can be presented graphically.
Heat. time collector	During this time, the heater runs to release the enriched mercury from the gold collector.
Cool. time collector	During this time, the gold collector is cooled to make it ready for the next enrichment.

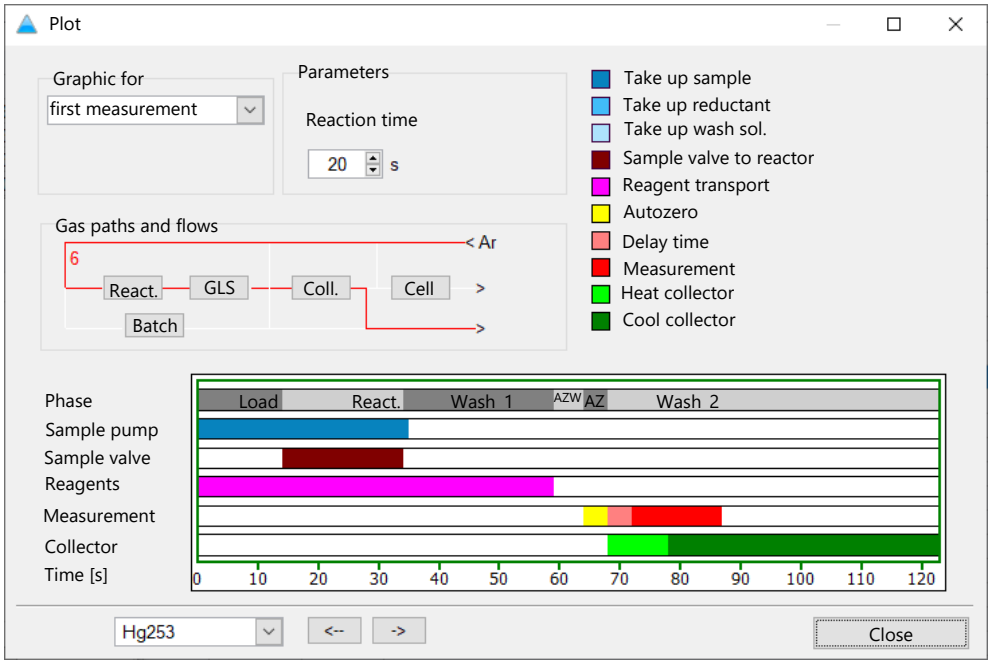
Option	Description
Gas flow	The argon flows into the associated phases with this value. The argon gas flow applies until a new gas flow can be entered. The gas flow can be switched over with varying frequency for the different operating modes. The gas paths for the individual phases are illustrated in the graphic of the analysis process on the hydride system. The gas flows are adjustable in three steps from 5 to 15 liters/hour.

Batch parameters

Option	Description
Sample volume	Volumes of the sample in the beaker
Enrichment cycles	For the batch operation with Hg enrichment on the collector Number of beakers whose content is enriched

Present gas flows and analysis procedures of the hydride/HydrEA system graphically

Click on **Plot** to open the graphic presentation of the gas paths for the individual phases of the analysis process. This window shows a graphic presentation of the programmed analysis process.



The individual phases of the analysis process are shown in colors in the process chart. Clicking on a particular phase shown by a colored field shows the corresponding parameters in the **Parameters** area and the set gas flow in the **Gas paths and flows** area. The process is determined by the operating mode selected.

Option	Description
Graphic for	If sample statistics has been activated (**Method** / **Statistics** window) the different processes can be displayed for the first, the next and the last measurement.
Gas paths and flows	This flow diagram shows the gas paths of the hydride system. The **React.** (reactor), **GLS** (gas/liquid separator), **Coll.** (gold collector), **Batch** (batch module) and **Cell** (cell) **Furnace** modules are shown with their connecting hoses (for argon and reaction gas). In the process graph, click on the phase whose gas flow you want displayed. The gas path is marked in red and the argon flow displayed numerically in L/h.

Option	Description
Parameters	Display and edit the operation times, measuring times and the corresponding gas flows of a selected phase Click on the corresponding phase. The name and the numerical value of the operation or measuring time / gas flow is displayed and can be changed. The process graph will be updated accordingly when you change a parameter.
Line	Selected analysis line

See also

Specifying measurements and actions in a sequence [▶ 68]

3.2.5 Method / Sample transport window – Specifying sample transport

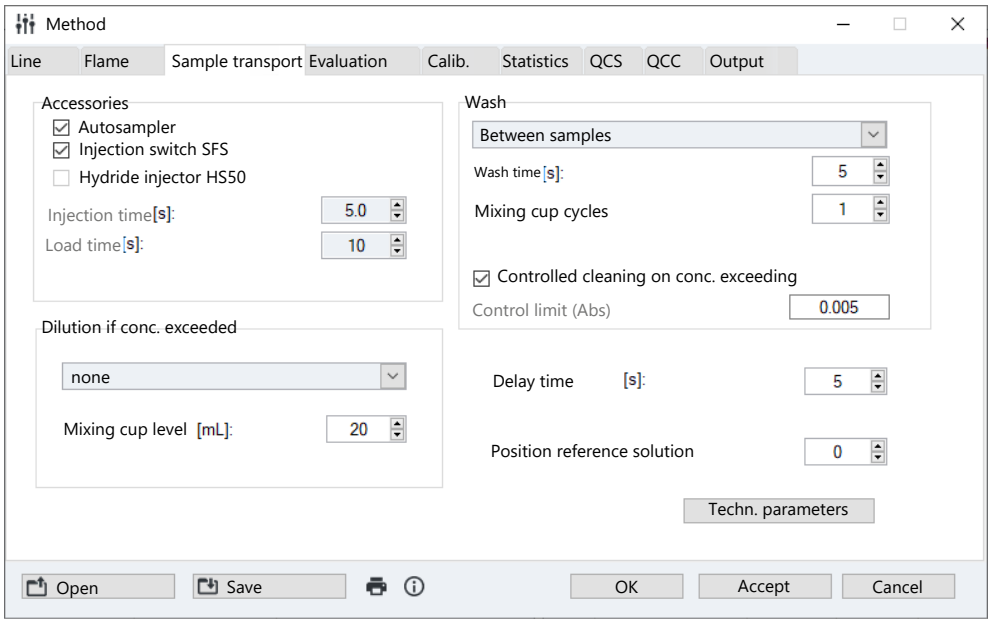
The display in the **Method** / **Sample transport** window differs depending on the atomization technique used.

3.2.5.1 Method parameters for autosamplers for flame and hydride technique

The following autosamplers are available for the flame technique:
- AS 52s / AS 51s
- AS-FD / AS-F

In the **Method** / **Sample transport** window, specify the following parameters:
- Use of the autosampler
- Wash mode and controlled cleaning
- Automatic dilution during the analysis
- Use of SFS 6 injection switch or HS 50 hydride injector

Open the **Method** / **Sample transport** window by clicking on  .



Using accessories

Option	Description
Autosampler	Use the connected and initialized autosampler. If deactivated the sample is supplied manually without autosampler.

Option	Description
Injection switch SFS	The SFS 6 injection module can be used in combination with an autosampler or in manual mode. The SFS 6 ensures reproducible conditions in the flame. It permanently draws in purging and carrier solution, which allows the burner to be kept at a constant temperature. Small sample volumes can be measured in a reproducible manner and gaged against a carrier solution. The following parameters are active if the **Area** or **Height** options have been selected as signal evaluation in the **Method** / **Lines** window. **Injection time** During this time, the valve of the SFS 6 opens the sample path to atomize the sample and transport the aerosol to the burner. The time depends on the highest expected concentration. Typical values: 0.5 to 2.0 s. **Load time** During this time, the sample aspiration path between the sample and the injection module is filled with new sample. The SFS 6 can also be used for processing time constant signals (mean integration).
Hydride injector HS50	The hydride injector HS 50 is a purely pneumatic batch system for manual operation. It consists of batch installation and cell holder with quartz cell. The reductant solution is transported pneumatically from the supply bottle into the reaction tank. The quartz cell is heated by the flame. The HS 50 works with the **Area** or **Height** signal evaluations. The measurement procedure is divided into the following parts: Prewash – Autozero – Reaction/Integration. **Reaction time** During the reaction phase reactant is transferred to the reaction beaker. The measurement signal acquisition starts at the same time the reaction time starts. The integration time has to be set in a way to acquire the total signal. **Prewash time** During the prewash time, the reaction beaker is purged of air. The prewash phase is omitted for the determination of Hg because the argon flow is necessary in order to transport the Hg out of the sample. **Sample volume**: Sample volume used

Dilution if concentration exceeded

If using the AS-FD and AS 52s autosamplers, you can dilute samples automatically. Here in the method, you can define the fill level in the mixing cup and activate automatic dilution when the concentration is exceeded.

Dilution if concentration exceeded checks the measured concentration of the samples. If the concentration exceeds the measuring range of the calibration curve by more than 10%, the sample is diluted in the mixing cup. Required volumes are mathematically determined as part of a program sequence, depending on the absorbance value for undiluted solution state. The calculated analyte volume is added to the mixing cup and the mixing cup is filled up to the defined fill level with diluent from the supply bottle.

Option	Description
Dilution if conc. exceeded	**none** Automatic dilution is disabled. **in mixing cup** Dilution is performed as described above.

Option	Description
Mixing cup level	The mixing cup is filled with diluent to this fill level. The value entered here is also used for the individual dilution of samples.

Note: You define the individual dilution of samples in the **Sample ID** window.

Washing and controlled cleaning

While a measurement sequence is running, you can specify washing steps to clean the various sample paths inside the system and its accessory units.

If the concentration of the sample exceeds the measuring range of the calibration curve by more than 10%, the burner/nebulizer system (flame technique) or the hydride system (hydride technique) can be washed to remove contamination from the previous measurement. During the wash, the absorbance/emission is measured in order to check the cleaning results. The automatic controlled cleaning is recommended after measuring highly concentrated samples, especially when the **Dilution if conc. exceeded** mode is activated.

Option	Description
Wash mode	**off** Automatic washing is disabled. **Between samples** Washing takes place after each sample, but not within a statistical series.
Wash time	During this time, rinsing agent is aspirated from the mixing cup. Includes washing of tube path and burner-nebulizer system.
Mixing cup cycles	Number of rinse cycles for the mixing cup In a rinse cycle the mixing cup is filled with wash liquid / diluent and then emptied again.
Controlled cleaning	If the concentration is exceeded, controlled cleaning takes place automatically.
Control limit (Abs)	The signal level must have returned to this value during the rinsing cycle before the diluted samples or samples with lower concentrations are measured.

Note: Controlled cleaning can also be defined in the sequence.

Autosampler wash sequence

To perform washing of the sample aspiration path and the burner-nebulizer system, the autosampler arm dips the cannula into the wash cup of the autosampler. A membrane pump provides wash liquid from a storage bottle for the duration of the dipping. Its pump rate is greater than the aspiration rate of the nebulizer or the pump rate of the hydride system. The complete sample path is cleaned (cannula, sample tube, injection module SFS6 and the burner-nebulizer system). Surplus amounts of wash liquid will flow off into the waste bottle.

The mixing cup of the AS 52s or AS-FD is cleaned by filling with wash liquid/diluent and draining it again in one single cycle.

Delay time

The delay time is required to transport the sample to the atomization unit (e.g. flame or reaction chamber in the hydride system). The measurement delay time must be adapted depending on the aspiration length between sample and nebulizer.

- Set the time in the **Delay time** field. If you define a pseudo measurement in the **Method**/ **Statistics** window, use the following times. If you do not activate a pseudo measurement, extend the specified times by 3 s.

Accessories / with activated pseudo measurement	Time
Short aspiration capillary, working manually	8 s
Standard aspiration capillary, working manually	12 s

Accessories / with activated pseudo measurement	Time
Injection module SFS, working manually	18 s
Autosampler without injection module	18 s
Autosampler with injection module	20 s

Other buttons / options

Option / button	Description
Position reference solution	Position of reference solution on the autosampler tray **Note**: You define all other sample positions in the sequence or the sample ID.
Techn. parameters	Open the **Autosampler** / **Techn. parameters** window Here you can specify further parameters for the autosampler, such as the immersion depth in the sample cups and the dosing speed.

See also

- Technical parameters of the autosampler for the flame technique [▶ 135]
- Specifying sample information and QC samples [▶ 75]
- Specifying measurements and actions in a sequence [▶ 68]

3.2.5.2 Method parameters for autosampler for graphite furnace technique (solution analytics)

For sample transport into the graphite furnace, one of the following autosamplers must be used:

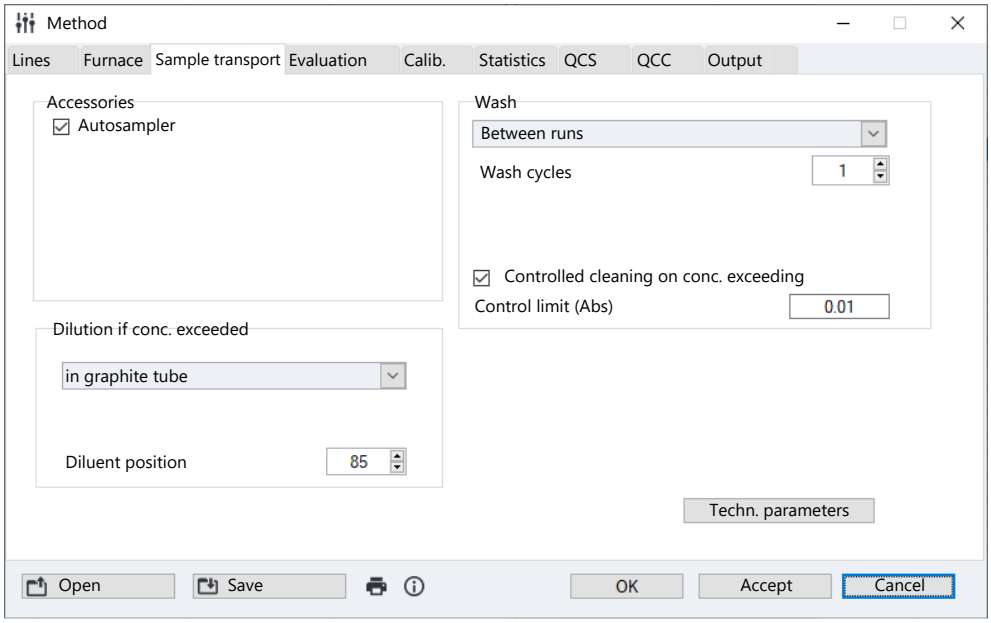
- MPE 60 or MPE 60/2
- AS-GF

In the **Method** / **Sample transport** window, specify the following parameters for these autosamplers:

- Use of the autosampler
- Wash mode
- Automatic dilution during analysis

The **Autosampler** option must always be activated for the graphite furnace technique for solution analytics.

Click on  to open the **Method** / **Sample transport** window.



Use autosampler for automatic dilution

In connection with the MPE 60 an automatic sample dilution can be carried out. Individual dilution factors can be set for each sample in the sample ID window. Method is available for general parameter settings (mode and position of the dilution agent) to achieve dilution.

You can also specify parameters for automatic dilution when the concentration exceeds the limit. If the concentration of the sample exceeds the measuring range of the calibration curve by more than 10%, the sample is diluted. The maximum dilution factor is limited by the smallest volume to be injected reliably (2 µL).

Dilution in the mixing cup is only possible with the MPE 60. For the MPE 60/2 and AS-GF autosamplers, an analyte reduction takes place directly in the graphite tube. In addition, unused sample cups can be used for dilution if the concentration is exceeded.

Option	Description
none	The samples is not diluted.
in graphite tube	The sample volume is reduced in accordance with the dilution factor and placed into the graphite tube. The remaining balance missing from the original sample volume is supplemented by dilution liquid.
reduced volume	The sample volume is reduced in accordance with the dilution factor and placed into the graphite tube. The remaining balance against the initial sample volume is not replaced.
in mixing cup	Only MPE 60 Dilution takes place in the mixing cup. The volume is always filled up to 500 µl.
in sample cups	Dilution is performed in unused sample cups, whose number and starting position on the tray are selected under **No. mixing cups**. The top up volume is specified under **Level in mix. positions**. The positions used must be reset after replacing the sample cups for further use in the **Autosampler** / **Techn. parameters** window using the **empty mixing cups** option.
Diluent position	Selects position of diluent on the sample tray.

Specify washing steps

While a measurement sequence is running, you can specify washing steps to clean the sample paths in the accessories.

Option	Description
Wash mode	**off** Wash mode switched off. No washing performed automatically. **Between runs** Washing after each statistic run **Between components** Washing after transfer of each component (modifier, standard, sample, etc.) into the graphite tube
Wash cycles	Number of wash cycles per wash, 1 to 5
Mixing cup cycles	Only MPE 60 Number of wash cycles for the mixing cup In a wash cycle the mixing cup is filled with wash liquid / diluent and then emptied again.

Controlled cleaning

If samples are analyzed that result in the working range of the calibration curve being exceeded by more than 10%, then the graphite furnace can be baked out to remove contamination from the previous measurement. During cleaning, the absorbance is measured to check the cleaning result. The automatic cleaning check is recommended after measuring highly concentrated samples and when the **Dilution if conc. exceeded** option is activated.

Option	Description
Controlled cleaning on conc. exceeding	If the concentration is exceeded, controlled cleaning takes place automatically.
Control limit (Abs)	The signal level must have returned to this value during cleaning before the diluted samples or samples with lower concentrations are measured.

Note
Controlled cleaning can also be defined as part of a sequence, independently of a concentration exceeded situation.

Washing the autosampler

After receiving the samples or other liquids, the pipettor tube is automatically cleaned with the washing liquid in the diluent cup (deionized water, slightly acidified with 0.1 N HNO_3). Here the cleaning liquid is pumped from the storage bottle through the dosing tube and into the wash cup of the autosampler.

Parameters for dipping depth and dosing speed

The parameters of the autosampler regarding the immersion depth in the various cups and dosing speeds are selected in the **Autosampler** / **Techn. parameters** window. Click on **Techn. parameters** to open the window.

See also

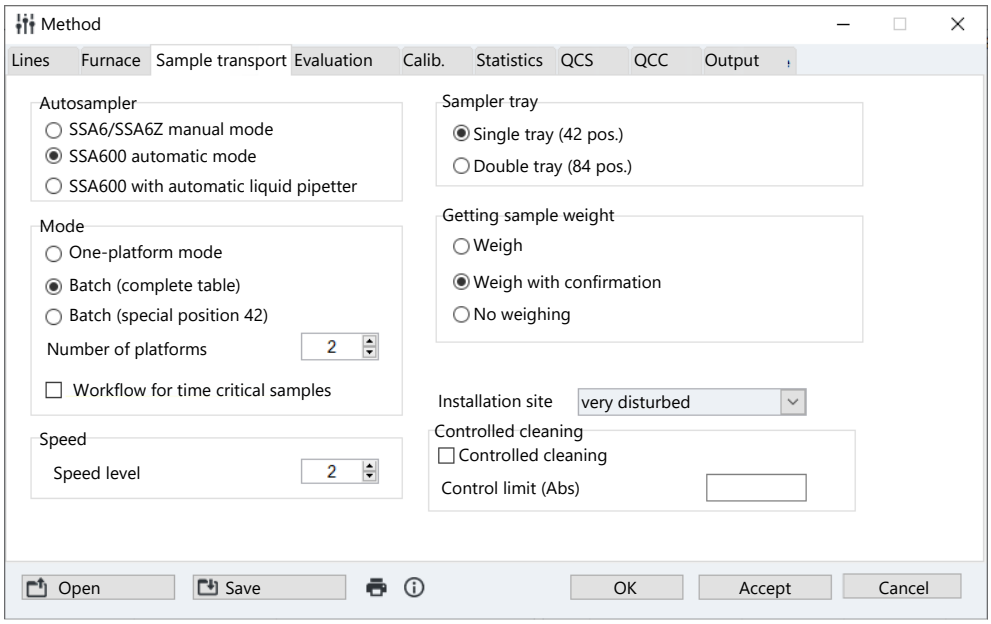
- Technical parameters of the autosampler for the graphite furnace technique [▶ 142]
- Specifying sample information and QC samples [▶ 75]
- Specifying measurements and actions in a sequence [▶ 68]

3.2.5.3 Method parameters for autosampler for solids analysis

In the **Method** / **Sample transport** window, specify the following parameters:

- Use of SSA 600 or SSA 6 (z) solids autosampler
- Operating mode – analysis procedure
- Autosampler modifications

Click on  to open the **Method** / **Sample transport** window.



Autosampler

Option	Description
SSA6/SSA6Z manual mode	Manual autosampler SSA 6 (z) If using the manual SSA 6 autosampler, no further sample transportation options need to be specified. All samples must be individually weighed and their sample mass values entered in the main window on the **Solid** tab.
SSA600 automatic mode	Automatic solids autosampler SSA 600
SSA600 with automatic liquid pipetter	Automatic solids autosampler SSA 600 with integrated dosing automatics for liquid components (standards and/or modifiers)

For working with the SSA 600 autosampler, you will specify the sequence of sample transportation in more detail in this window.

Option	Description
Mode	**One-platform mode** The analysis is performed with only one platform, which is always reloaded. This platform is located in tray position 1. During the analysis procedure, all necessary steps (taring, dosing, weighing, liquid dosing) are performed with this platform. **Batch (complete table)** Several platforms are used during the analysis. Analysis may run automatically, depending on your pre-settings. **Batch (special position 42)** Several platforms are used during the analysis. Analysis may run automatically, depending on your pre-settings. For samples requiring no

Option	Description
	weighing, for example Cal-Zero or liquid standards, position 42 on the sample tray is used. For this reason, an empty platform must be placed in this position as pipetting destination of sample is necessary. **Number of platforms** For **Batch (complete table)** and **Batch (special position 42)** Number of platforms used and available number of sample positions
Workflow for time critical samples	Behavior of the autosampler during sample preparation and dosing If activated, the platforms are only loaded with samples directly before the measurement. This prevents samples from volatilizing during longer waiting periods on the sample tray or from "creeping" across the platform due to high adhesion, as is the case with oils for example. This mode requires the operator to be present at all times. When deactivated, all available platforms are prepared before the start of the measurement. All actions that require the user's presence (sample loading or manual pipetting of modifiers) are performed in combination. The AAS device can measure in this mode without the constant presence of the operator.
Speed	The speed of the SSA600 movements can be set in three levels. Recommended level: 2
Sampler tray	Number of trays placed one on top of the other.
Getting sample weight	**Weigh** Once a dosed solid substance has been weighed, the weighed portion value is adopted without a preliminary query for acceptance of this weight. **Weigh with confirmation** The weighing result is displayed after each weighing of the solid. The operator can signal acceptance of the initial sample weight by pressing the green key (key on the autosampler or **OK** in the weighing window on the screen). Pressing the orange key (key on the autosampler or **Repeat** in the weighing window) returns the platform to the dosing position, changes the dosing and then weighs again. **No weighing** No concentration measurements are possible in this weighing mode. It is only intended for qualitative analysis of solid samples.
Installation site	Depending on the interfering factors (especially vibrations), set the precision of the built-in microbalance If the weighing time seems too long, you can shorten it by changing the setting for place of installation. This will be at the expense of precision.
Controlled cleaning	If the concentration is exceeded, controlled cleaning is performed automatically. If samples are analyzed that cause the working range of the calibration curve to be exceeded by more than 10%, the graphite furnace and sample platform are baked out to remove contamination from the previous measurement. During cleaning, the absorbance is measured to check the cleaning result. **Note**: Controlled cleaning can also be defined as part of a sequence, independently of a concentration exceeded situation.
Control limit (Abs)	The signal level must have returned to this value during cleaning before samples with lower concentrations are measured.

3.2.6 Method / Evaluation window – Specifying spectral range and background correction

In the **Method** / **Evaluation** window, define the line-specific evaluation parameters for determining the measurement results from the spectrum.

Open the **Method** / **Evaluation** window by clicking on  .

Line-specific parameters for signal evaluation

Option	Description
Line	Name of element line
Signal / **Smooth**	Not for flame technique **off**: Signals are not smoothed. **weak**: Signals are lightly smoothed, e.g. for noise suppression. **strong** : Signals are heavily smoothed.
Spectr.range	Number of pixels for recording a spectrum (max. 200) Only the specified number of pixels of the CCD row is read out and stored. This optimizes the computing time in the evaluation and the volume of stored data.
Eval.Pixels	**1 to 19 pixels** Number of pixels used for the evaluation of the absorbance signal and from which the measured values are ultimately formed. The absorbance values of the evaluation pixels are summed. This makes it possible to eliminate analysis inaccuracies which would be caused by a peak position between two pixels. Therefore, theoretically an absorbance of up to 9 could also appear as a measurement result. Recommended number of evaluation pixels: 3 **Height** Interpolation of the peak maximum **User defined** Free selection of the evaluation pixels, e.g. for evaluating multiplets. Example: 50,120-130 computes the sum of the measured values of pixels 50 and 120 to 130.
BGC mode	**IBC** Iterative baseline correction. This background correction requires a reference spectrum in the sequence. **IBC-m** Iterative baseline correction for broadband structures (molecular absorptions). This background correction requires a reference spectrum in the sequence. **without reference** The background correction does not require a reference spectrum. **with reference** The background correction requires a reference spectrum in the sequence.
Perm.Struct.	Eliminate permanent structures The procedure requires a reference spectrum. Permanent structures are bands that may be present in the reference and sample spectra at different intensities, but are not caused by the element being analyzed. Usually these structures are caused by molecular vibrations, e.g. from the nitrous oxide flame. **off**: Do not correct permanent structures. **on**: Correct permanent structures.
BGC fit	Adjust pixels for background correction

Option	Description
	dynam. The pixels for background correction are found automatically by the software. **static** The pixels for the background correction are specified by the user in the **BGC pixels** column.
BGC pixels	Position of the pixels for static adjustment of the background correction Enter the pixel numbers for the background correction. An example can be found in the status line.

Buttons

Button	Description
Spectral corrections	The**Spectral corrections** window appears. Existing correction models can be selected or new models can be created. **Note**: In the line spectra display, you can select pixels for background correction based on the graphical display and transfer them to the method.
Attenuation	The**Attenuation** window appears. For signal attenuation, only pixels to the left and right of the peak maximum are considered for signal generation. The signal of the peak pixel and, depending on the attenuation level, its adjacent pixels is "clipped out". The higher the level of signal attenuation selected, the further away the evaluated signal areas are from the peak pixel. Signal attenuation can extend the working range of the calibration. The edge pixels used for the evaluation are displayed in the **Evaluation pixels** column. Example: If the middle level is selected, two pixels at a distance of 3 pixels from the peak pixel are taken into account when forming the measured value.
Signal integration	Not for flame technique The**Signal integration** window appears. For the area evaluation of transient signals, the integration range can be limited to the range between 'from' and 'to'. This is especially useful for simultaneous multi-line evaluation; in other cases the range should already be limited during the measurement, e.g. by selecting a suitable measurement time. The limits for signal integration can also be set in the **Single values** window in the spectrum graph. Click on **Reset** to set the range of the selected table row to the entire measurement time. If no row is selected, the integration limits of all lines are reset.

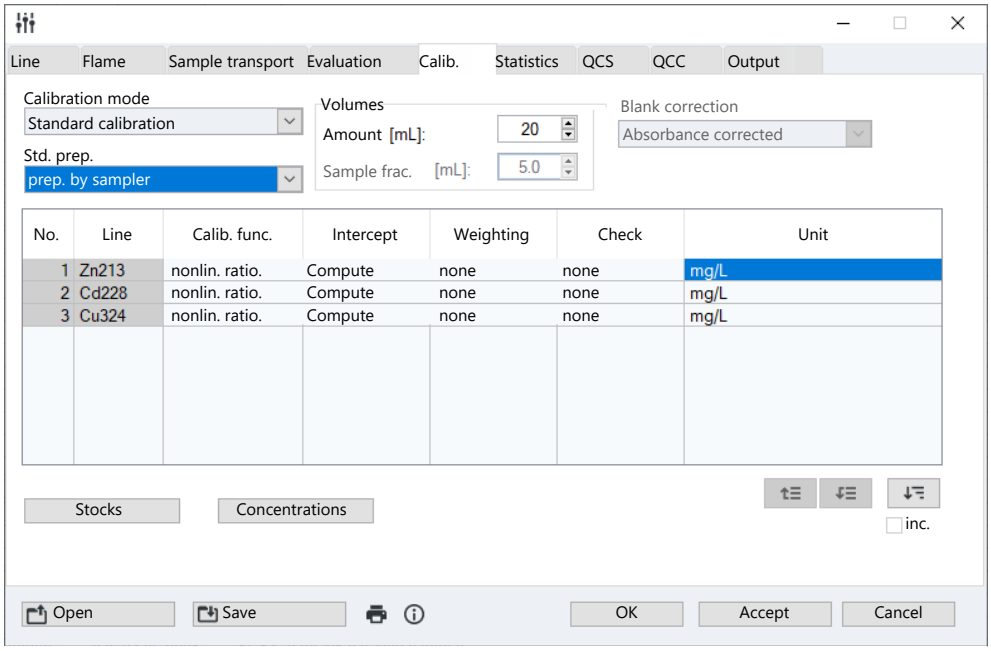
See also

- Creating a correction model for spectral corrections [▶ 94]
- Description of the algorithms used for spectral background correction [▶ 180]
- Displaying sample single values [▶ 88]

3.2.7 Method / Calibration window – Specifying calibration

In the **Method** / **Calibration** window you define the type of calibration and enter the concentration table of the standards. You can use multi-element standards for the calibration, which you specify as stock.

Click on  to open the **Method** / **Calibration** window.



Selecting the calibration method

Select the method from the **Calibration mode** list:

Calibration method	Description
No calibration	The sample results are presented exclusively as intensity. Calibration is not necessary for these measurements.
Standard calibration	The calibration takes place with samples of known concentration in the analytes (standards). Samples of unknown concentration are measured against this calibration.
Method of additions	Different concentrations of a standard are added to the unknown sample, which is then measured. The concentration of the analyte results from the comparison.
Method of additions calib.	The calibration curve, by means of which other concentrations can be determined, is set up by the method of standard addition. At the same time, the concentration of the first sample is found by this method.

Agreeing blank value corrections

Standard addition methods and addition calibrations require a blank value correction. Select the method from the **Blank correction** list:

Correction	Description
Absorbance corrected	In every standard addition procedure, the blank is measured too and the measured intensity value subtracted from all measured values before the regression line is calculated. This method was customary for a long time; with many real samples however, it leads to incorrect results.
Concentration corrected	First, a separate standard addition is carried out for the blank solution using the same concentration additions as for the sample. The resulting concentration is automatically subtracted from all other concentrations (conc. 2) determined by standard addition.

Standard preparation

Method	Description
manually	The reference solutions are prepared by the operator.
prep. by sampler	Only when using the autosampler AS-FD or AS 52s The reference solutions are prepared in the mixing cup of the autosampler by mixing different proportions of stock standards and diluent.

Method	Description
	In this case, under **Volumes** set the following for preparing the reference solutions: **Amount**: Total filling volume in the mixing cup (value range: 1 to 20 mL) **Sample frac.**: **only with addition method** Proportionate sample volume (increments of 0.5 mL) With the addition method, the fraction of the sample solution of a measurement series is always the same. The proportionate sample solution must be smaller than the total fill volume. The volume difference is filled up with stock solution and diluent. The sample volume/total volume ratio is the correction factor for the concentration to be computed.
by variation of volume	Only graphite furnace technique Different volumes of the stock solution or quantities of the reference sample are brought to atomization, thereby achieving a concentration gradation (based on the sample volume/weight).
by dilution	Only graphite furnace technique Defined volumes of the stock solution and the volume of diluent missing from the sample volume are transported into the graphite furnace in one transport step, thereby achieving a concentration gradation (based on the sample volume).

Line-specific calibration parameters

The line-specific parameters are set in the table:

Table column	Description
No.	Sequence of selected lines in the table
Line	Name of the analysis line
Calib. func.	Only for calibration using the standard method **linear** Linear progression of the calibration function $y = a + bx$ **nonlin. ratio.** Non-linear progression of the calibration function described by a rational function $y = \frac{a + bx}{1 + cx}$ **nonlin. quadr.** Non-linear progression of the calibration function described by a quadratic function $y = a + bx + cx^2$ **automatically** A linear and a non-linear function are calculated for the calibration. The sums of the squared residuals are compared (Mandel test). If the sum for the nonlinear function is significantly lower than that for the linear function, the nonlinear calibration curve will be selected. Otherwise, the linear calibration curve will be used. The non-linear function is selected in the **Options** / **Analysis sequence** window. As default setting the broken ratio function has been provided. **Note:** Only linear curve progressions are permitted for the standard addition method and the addition calibration.
Intercept	**Set zero** The calibration curve exactly intercepts the measured zero value point.

Table column	Description
	calculate The zero value is included in the calculation like any other calibration point.
Weighting	**none** All calibration points are taken into account with the same weighting. **1/conc** Give greater consideration to calibration points with smaller concentrations. **1/SD** Give greater consideration to points with smaller deviations within the multiple repeated measurements of a standard (requires: activated mean statistics option). **1/(SD*conc)** Combination of the calculation methods **1/conc** and **1/SD**
Check	The software allows automatic checking of determined calibration curves against a prediction range calculated on the basis of a manually selected statistical certainty. **none** All measured and non-deleted calibration points are used to calculate the curve. Calibration points are neither labeled nor eliminated. **Elim. outliers** If calibration points are outside the calculated prediction range, outliers are eliminated by means of an F-test (test to ascertain whether the exclusion of a point leads to a significant improvement of the residual scattering): ■ An F test is carried out for the calibration point which lies furthest outside the forecast range. If excluding this point does not lead to a significant improvement of the residual scattering, the point is included and the calibration curve is not optimized further. ■ If the exclusion of this point results in a significant improvement, the calibration point will be defined as outlier (marked in the table by "!", in the graph marked by red color) and the calibration recalculated without this point. ■ An F-test is performed again for the point that now deviates the most from the prediction range. This procedure is repeated until all outliers are removed. ■ All calibration points outside the new prediction range that have not been eliminated as outliers are marked with a "?" in the table and in blue in the graph.
Unit	Enter units for the concentration separately for each element.

Use  to transfer the value of the active cell to all subsequent cells in the table column.
Use the **Calibration Table** button to open the table for entering the standard concentration.

3.2.7.1 Specifying stock standards

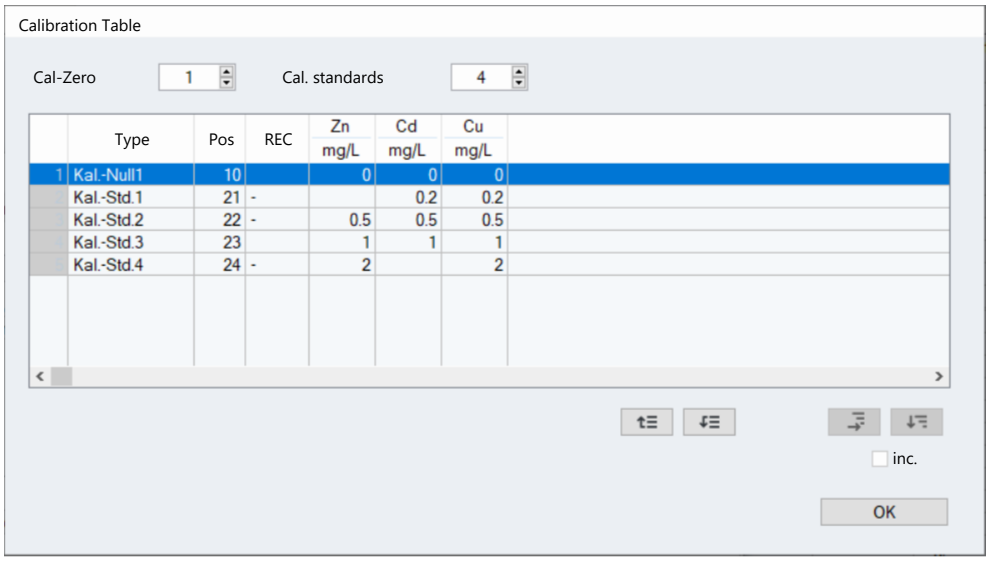
If you produce the standard concentrations automatically with an autosampler, you must specify stock standards from which the individual standards are then generated by dilution. To do this, you must specify the stock standards before completing the calibration table, and you can use multiple stock standards with different elements and concentrations. If you use stock standards more often, you can manage these in the database in the **Data** / **Stock std/QC samples** window.

- In the **Method** / **Calib.** window, click on **Stocks**.
  The list of stock standards appears. A maximum of 20 standards can be defined for one analysis.
- Click on **Append** or on **Insert** to add a new row to the stock list.
  The **Insert stock standard** window opens with two options:
  - Select the **From stock database** option if you want to use existing standards from the database. Select stock standards in the list.
  - Select the **manually** option if you want to enter the stock standards manually.
- Click **OK** to confirm.
- In the **Stock standard** window, enter the position of the standard on the autosampler in the **Pos** column and select the unit in the **Unit** column.
- For manual input, in the **Stock standard** window, click on **Concentrations** and enter the concentration for each element in the **Concentration entry** window.
- Finish the input by clicking on **Close**.

3.2.7.2 Entry of concentrations for manually prepared standards

In the **Calibration Table** window, specify the calibration standards with their element concentrations.

Calibration table for standard methods with manually prepared standards



Standard types

The following standard types must be specified for the different calibration methods:

Calibration method	Standard types
Standard calibration	**Cal-Zero**: Calibration zero standards without analytes Multiple calibration zero standards can be entered, e.g., if the elements being analyzed are present in different solvents. In this case the concentration of the respective element line must be set to "0", the other columns remain blank. **Cal-Std**: Calibration standards
Method of additions	**Cal-Std**: Calibration standard **Samp+Add**: Addition standards
Method of additions calib.	**Samp+Add**: Addition standards

Standard table

Column	Description
Type	Standard type The standards are numbered according to the selected number.
Pos	When using the autosampler Enter the position of the standard on the sample tray of the autosampler
REC	Only for standard methods Define standard as recalibration standard
Elements	Concentration of the individual elements in the standard

Completing the calibration table

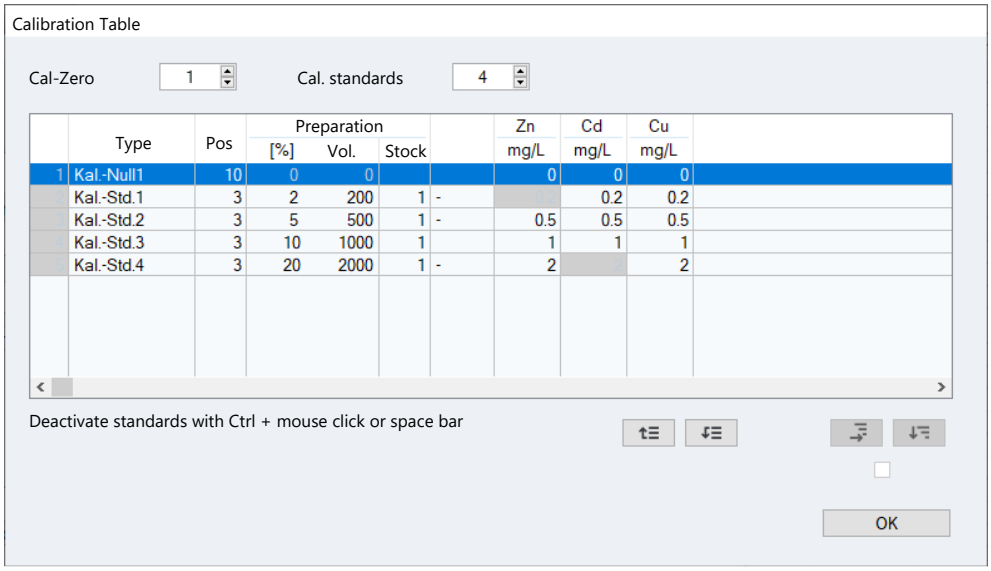
- In the **Method** / **Calib.** window, click on **Concentrations**.
  The**Calibration Table** window appears.
- Select the number of standards in the fields above the table.
- Enter the concentration of the elements in the table for each standard.
- Optionally enter the position of the standards on the autosampler. This setting is transferred to the sequence as a default setting and can be changed there.
- Click **OK** to confirm the settings.

3.2.7.3 Entry of concentrations for automatically prepared standards

With the flame technique, the calibration standards are prepared automatically by mixing with the autosampler. With the graphite furnace technique, a calibration series is created by volume graduation or dilution in the graphite furnace.

Stock standards are required for the automatic preparation of calibration standards.

Calibration table for standard methods with automatically prepared standards (flame technique)



Standard types

The following standard types must be specified for the different calibration methods:

Calibration method	Standard types
Standard calibration	**Cal-Zero**: Calibration zero standards without analytes Multiple calibration zero standards can be entered, e.g., if the elements being analyzed are present in different solvents. In this case the concentration of the respective element line must be set to "0", the other columns remain blank.

Calibration method	Standard types
	Cal-Std: Calibration standards
Method of additions	**Cal-Std**: Calibration standard **Samp+Add**: Addition standards
Method of additions calib.	**Samp+Add**: Addition standards

Standard table

Column	Description
Type	Standard type The standards are numbered according to the selected number.
Pos	Position of the stock standard on the sample tray
Preparation	**%**: For flame technique Percent by volume of the stock component in the solution **Vol.**: For flame technique Volume of the stock component in µL. The value is calculated from the % value entered and the total volume in the mixing cup **Amount** defined in the **Method** / **Calib.** window. **Vol.**: For graphite furnace technique This volume is injected into the graphite furnace. **Stock** Number of the stock standard in the stock table
REC	Only for standard methods Define standard as recalibration standard
Element lines	Calculated concentration of the individual elements in the standard

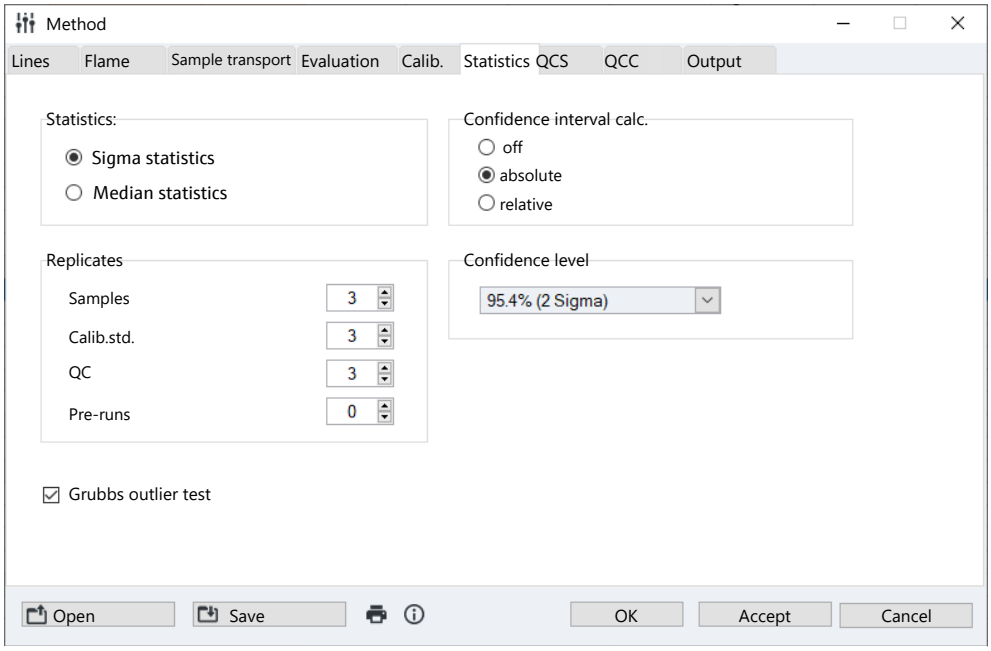
Completing the calibration table

- In the **Method** / **Calib.** window, click on **Concentrations**.
  The**Calibration Table** window appears.
- Select the number of standards in the fields above the table.
- Flame technique: For each standard, enter the percent by volume of the standard in the table.
- For graphite furnace technique: For each standard, enter the volume that will be injected into the graphite furnace.
- For each standard, enter the number of the stock standard.
- If lines in a standard are not to be used for calibration, deactivate them:
  To do this, click on the line field and then press the space bar. To reactivate, repeat the procedure.
- Click **OK** to confirm the settings.

3.2.8 Method / Statistics window – Specifying statistics parameters

In the **Method** / **Statistics** window, select the statistical methods to be applied to the calibration and sample measurement. The settings selected here are independent of the chosen calibration method and remain set at every method change.

Open the **Method** / **Statistics** window by clicking on  .



Statistics:

Option	Description
Sigma statistics	Calculate mean value and standard deviation Error statistics according to the arithmetic mean: Sample is measured several times after the blank cycles. Based on the measurement results, the arithmetic mean, the standard deviation and the relative standard deviation are calculated.
Median statistics	Calculate median and range (R) Error statistics according to the median method: The sample is measured repeatedly after the blank cycles. The measured values are sorted by size. The median value is the following value: ■ The value in the middle of the sorted list, if the number of measurement cycles is odd. ■ For an even number of measurement cycles, the mean of the two measurement values in the middle of the sorted list. As the smallest and largest individual measured values do not influence the measurement result, the median statistics are suitable for the elimination of outliers.

Replicates

Option	Description
Samples	Number of repeat measurements per sample
Calib.std.	Number of repeat measurements per calibration sample
QC	Number of measurement repetitions per QC measurement
Pre-runs	This number of measurements with sample (blank cycles) is inserted before the statistical series, e.g. to stabilize the flame. The values are not used to calculate the result.

Grubbs outlier test

For mean value statistics with at least three repeat measurements per sample

Option	Description
Deactivated	All values of the statistics series are used to determine the mean value.

Option	Description
Activated	Outliers are eliminated and are not used in the calculation of the statistics. The thus found mean values in the result table are marked by "!".

Confidence interval calc.

The calculation of the confidence interval is based on the chosen statistical certainty (see below). In addition to the error in the sample measurement, the confidence interval mainly includes the error in the calibration, so that a value is also presented even if the statistics function is switched off.

Option	Description
off	Confidence interval is not calculated
absolute	Show the confidence interval in absolute values (in concentration units)
relative	Show the confidence interval in relative values (in percent of the concentration value)

Confidence level

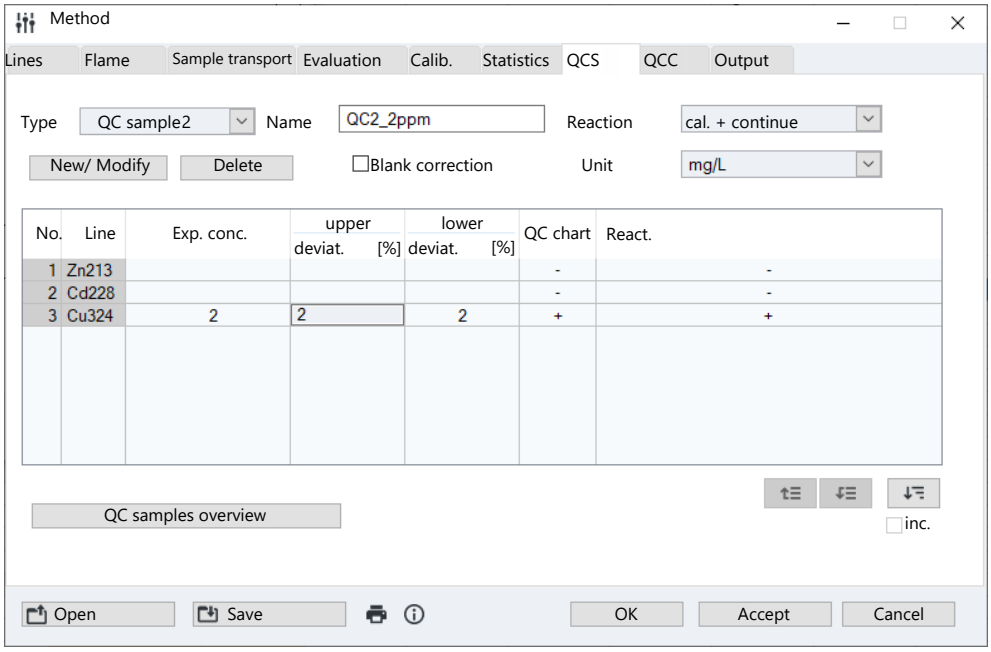
The confidence level can be selected between 68.3 and 99.9%. It is used to calculate the confidence interval of the samples and the prediction bands of the calibration curves.

3.2.9 Method / QCS window – Specifying quality control samples

In the **Method** / **QCS** window, you can specify the quality control (QC) samples. This involves the insertion of control measurements, with samples in predetermined positions during measurement. These control measurements should yield known results. It is either the absolute value (absorbance/concentration) or the concentration difference from the previous sample which is known. You can define different sample types for the quality control.

The results of the control measurements are automatically documented on quality control cards (QC cards, also called quality rule cards or control charts). The tabs are saved with the method and continued for any further measurement with the method. The system of QC control charts is therefore used for quality monitoring over a longer period of time.

Open the **Method** / **QCS** window by clicking on  .



Elements in the Method / QCS window

Option	Description
Type	This QC sample is displayed in the line table. You can edit the parameters of the QC sample here.
Name	Name of the displayed QC sample
Reaction	What to do if the results of the QC sample exceed or fall below the specified limits.
New/Modify	Define a new QC sample or modify an existing QC sample
Delete	Delete selected QC sample
Unit	Concentration unit of the QC sample
New/Modify	Define a new QC sample or modify an existing QC sample
QC samples overview	Open a list with line-specific parameters of all QC samples
Line table	The table displays the parameters of the QC sample selected in the **Type** list box.

Types of QC samples

You can specify the following QC sample types:

Option	Description
QC sample	Define a sample as a QC sample The concentrations of the QC sample may either be loaded from the database or typed in directly. **from database** Select the relevant QC sample in the adjacent list box. You can manage the database of QC samples in the **Data** / **Stock std/QC samples** window. **manually** Enter the concentrations of the QC sample directly into the line table Max. number of QC samples: 50
QC std.	Define a standard as QC sample Any standard defined in the calibration table can be used as a QC standard.

Option	Description
	Possible number of QC standards = number of standards in the calibration table (max. 65)
QC blank	Define the blank sample as a QC sample
QC spike	Define a spiked sample as a QC sample In recovery/addition, the measurement results of a defined concentration addition to one or several samples are checked. To this end, a QC stock sample is to be defined after any sample in the sample table (QC-Stock sample = sample + addition with a solution of known concentration). After measuring the sample and QC spike, the concentration difference of both is compared with the "Expected concentration increase" specified here and the recovery rate is calculated. For the flame technique, the spiked solution must already be premixed.

If certified control samples are not available, quality control can also be performed using duplicate determinations:

Option	Description
QC trend	The measured concentration value is stored when the quality control sample appears for the first time in the analytical procedure. When the QC sample appears the next time, the concentration difference is formed and evaluated. It is advisable to measure these control samples at the beginning and end of a sample series.
QC matrix	A sample to be analyzed is split before preparing the sample. The two parts pass separately through all steps of sample preparation and are placed separately on the autosampler as QC trend and QC matrix. The difference between the determined concentrations is evaluated.

Procedure if error limit is exceeded

For the QC sample types, you can select different procedures to be followed when the error limits are exceeded:

QC sample type	Procedure
QC sample **QC std.** **QC spike**	**flag** The measured value is marked in the sample table. The measuring program continues with the next sample. **recal. + continue** A recalibration is performed. The QC sample is then measured again. If the QC sample is now within the range, the measurement is continued with the next sample, otherwise the measuring program is stopped. **cal. + continue** A new calibration is performed. The QC sample is then measured again. If the QC sample is now within the range, the measurement is continued with the next sample, otherwise the measuring program is stopped. **recal. + rerun** A recalibration is performed. The QC sample is then measured again. If the QC sample is outside the range, the measuring program is stopped. If it is within the range, all samples are measured again after the last QC sample or the last (re)calibration. If the QC sample is again outside the permissible error limits, the measurement program will be stopped. **cal. + rerun** A new calibration is performed. The QC sample is then measured again. If the QC sample is outside the range, the measuring program

QC sample type	Procedure
	is stopped. If it is within the range, all samples are measured again after the last QC sample or the last (re)calibration. If the QC sample is again outside the permissible error limits, the measurement program will be stopped. **next method** The current measuring program is aborted and the measuring program of the next method is started. **Stop** The current measuring program is aborted.
QC blank	**flag** **next method** **Stop**
QC trend **QC matrix**	No reaction

Line-specific parameters of the QC sample types

Enter the line-specific parameters of the QC sample types in the line table.

Column	Description
Line	Name of the analysis line
Exp. conc.	For QC sample and QC std. Expected concentration in the QC sample
Exp. conc. increase	For QC spike Expected concentration increase from sample to spiked sample Enter the value corresponding to the spiked amount and concentration of the stock solution.
Exp. abs.	For QC blank Expected absorbance
lower lim.	Lower range of the error limit in percent (concentrations) or absorbance
upper lim.	Upper range of the error limit in percent or absorbance
QC chart	If marked with "+", the result of the quality control for this line will be presented on the QC tab in the result list.
React.	This procedure should be used if the error range limit is exceeded. If several lines are marked with "+", only one of these lines needs to have exceeded the error limits for the reaction to be triggered (OR logic).
Unit	Only **QC std.** Unit of the expected concentration

Entering parameters of QC samples

- In the **Method** / **QCS** window, click on **New**/**Modify** and create a new parameter set for a QC sample or edit the selected parameter set.
  The**Add/modify QC sample type** window appears.
- Select the QC sample type in the **Type** list.
- Only **QC samples**: If several **QC samples** are defined, define a consecutive number in the adjacent list box.
- Only **QC std.**: Select the number of the standard in the list box according to the order in the calibration table.

- Enter the line-specific parameters in the table.
  - ✓ Define further QC samples in the same way.

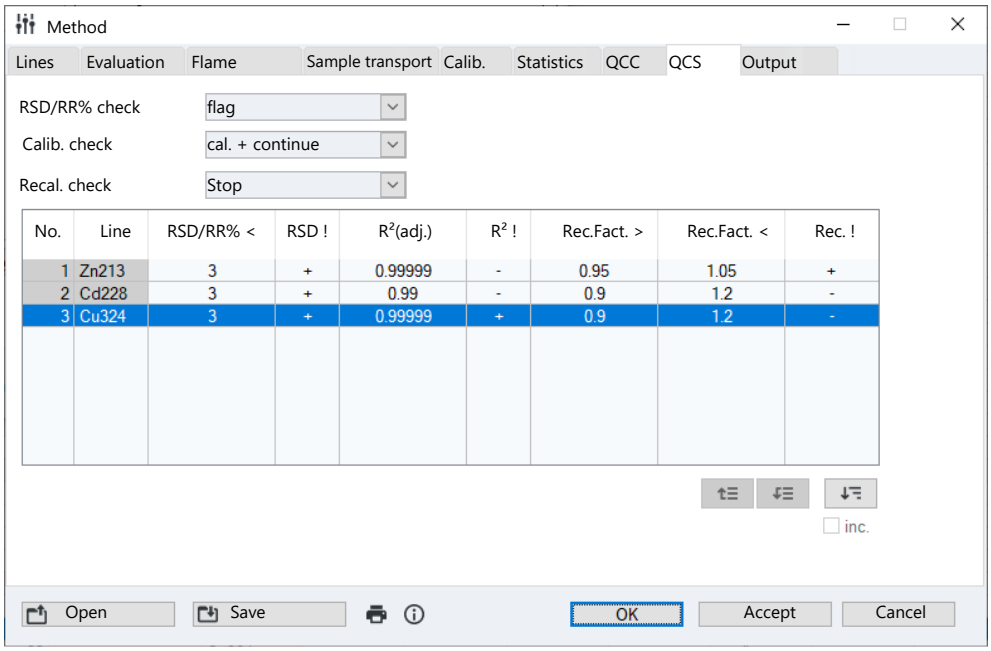
3.2.10 Method / QCC window

In the **Method** / **QCC** window, specify the following parameters for quality control during a sequence:

- Relative standard deviation (mean statistics) or relative range (median statistics)
- Calibration control
- Recalibration control
- Procedure if error limits are exceeded

You may choose various control options with different reactions simultaneously.

Open the **Method** / **QCC** window by clicking on  .



Types of quality control

Option	Description
RSD/RR% check	Control of the relative standard deviation or relative range
Calib. check	Calibration control
Recal. check	Control of recalibration factor

Reactions if error limits are exceeded

Option	Description
none	Do not perform the control in question
flag	Marks the corresponding sample, calibration or recalibration in the sample table, if the error limits are exceeded.
repeat + continue	Only **RSD/RR% check** Repeats the measurement of the respective sample, if the serial precision limit was exceeded, before the next sample is measured.
calib.+cont.	Only **Calib. check** and **Recal. check** If the error limits for the calibration or the recalibration factor are exceeded, perform a new calibration and then continue the measurement with the next sample.

Option	Description
next method	Only **Calib. check** and **Recal. check** Stops the measurement of the currently running method and starts the next method, if the error limits were exceeded.
Stop	Only **Calib. check** and **Recal. check** Stops the measurement of the currently running method, if the error limits were exceeded.

Control of the graphite furnace

Only graphite furnace technique

If a graphite furnace tube is used for too long, the analytical quality will decrease. You can monitor the graphite furnace tube usage time and will be alerted when a certain number of heating cycles is exceeded.

Option	Description
Max. heating cycles	Enter the number of measurements with the tube The current value of heating cycles is displayed in the adjacent field.
Reaction	Select reaction when maximum number of measurements is reached **no react.** Graphite furnace tube usage is not monitored. **flag** If the limit value is exceeded, mark the measurement in the sample table. **Stop** If the limit value is exceeded, stop the analysis process.

Line-specific parameters of quality checks

In the table, enter the line-specific parameters of the various quality checks. You may define for every analysis line, whether it shall be considered for the check. The reaction is triggered if one or more of the monitored lines exceed the error limits.

3.2.11 Method / Output window – Specifying output of results and memory content

In the **Method** / **Output** window, you can specify memory contents, number of decimal places of the results on screen and in the printout, as well as the order of lines in the printout.

We recommend saving the spectra when developing methods. This will give you important information about potential matrix and interference problems. Without saved spectra, any recalculation with changed method parameters is only possible starting from the calculated absorbance values. For example, the grid points of the background correction can no longer be changed because the spectra information for the individual pixels is missing. With a retracted routine method, saving the spectra is usually not necessary.

Click on  to open the **Method** / **Output** window.

- By activating the corresponding option, you also cause the method and the spectra to be saved with the analysis results.
- In the table below, define the number of decimal places for the display and printout of absorbance and concentration values, and the order in which the analysis lines shall appear on the printout.

Note
If the **Always save spectra** option is activated in the **Options** / **Analysis sequence** window, the spectra are always saved as well, regardless of the settings in the method parameters.

See also

Options for analysis sequence [▶ 167]

4 Sequences

The sequence defines in which order samples and actions are processed within a measuring routine. Some sample describing data such as sample name and position on the sample tray may also be entered directly. For permanent storage, however, the sample describing data must be saved as a sample information file.

A sequence is based on a loaded method, which contains the information about type of calibration, statistical evaluations, quality controls etc.

4.1 Creating, saving and loading sequences

Like methods, sequences are saved to a common database. You can create, modify, save and load sequences. You can find further functions for managing sequences in the **Data** / **Data management** window.

See also

Managing methods and sequences [▶ 155]

4.1.1 Creating a new sequence

First create or load a method. You can specify a new sequence of sample measurements and actions based on this method.

- Select the menu item **File** | **New Sequence**.
- Alternatively, open the window with the current sequence parameters by clicking on  or using the menu item **Method Development** | **Sequence**.
  - ✓ The **Sequence** window appears. You can now define measurements and successive actions.

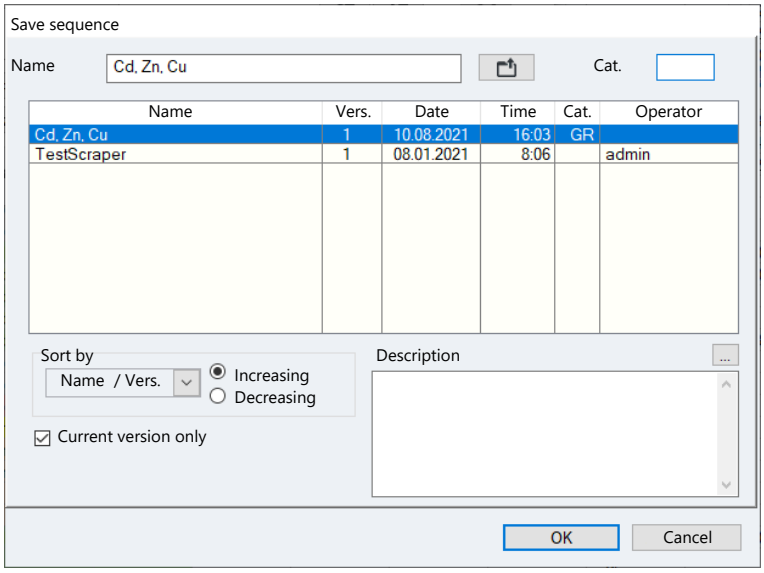
See also

Specifying measurements and actions in a sequence [▶ 68]

4.1.2 Saving a sequence

After entering the measurements and actions, save the sequence in the database. This allows you to reuse the sequence for later measurements. Sequences are saved in the database in the **Save sequence** window. You can save additional data with the sequence to categorize sequences and make them easier to find.

Elements in the Save sequence window



Option	Description
Name	Sequence name
Cat.	Category (three characters) for further identification and sorting the methods This entry is optional.
Table	Overview of existing sequences
Sort by	The options in this group allow you to sort the sequence list. If the **Current version only** option is enabled, only the latest version is displayed for sequences with the same name.
Description	Optionally enter further explanations for the sequence Click on ••• to open a list with predefined comments. You manage these comments in the **Data** / **Pre-defined descriptions** window.

Saving a sequence

- In the **Sequence** window, click on **Save** and open the **Save sequence** window. Alternatively, select the menu item **File**|**Save** | **Sequence**.
- Enter the name of the sequence and select other parameters in the **Save sequence** window.
- Confirm the settings with **OK**.
  - ✓ On doing so, the sequence will be saved to the database. If you use the same name as an existing sequence, a new version of the sequence is created in the database.

See also

Creating predefined notes [▶ 162]

4.1.3 Loading a sequence

You can load saved sequences and start a measurement routine based on them together with a method.

- Open the sequence database window with one of the following alternatives:
  - In the toolbar, click on the folder icon next to the **Sequ** field.
  - Select the menu item **File** | **Load analysis sequence**.

– Open the **Sequence** window by clicking on and then click on **Open**.

- Optionally, you can limit the displayed sequences by selecting a category in the **Cat.** field. To display all sequences, clear the **Cat.** field.
- Optionally, you can activate the **Current version only** option if you want to display only the latest version of a sequence.
- Select the sequence in the list and click on **OK**.

  ✓ The **Sequence** window with saved parameters appears.

4.2 Sequence window

In the **Sequence** window, you can specify the order of measurements and other actions of an analysis.

Open the **Sequence** window by clicking on .

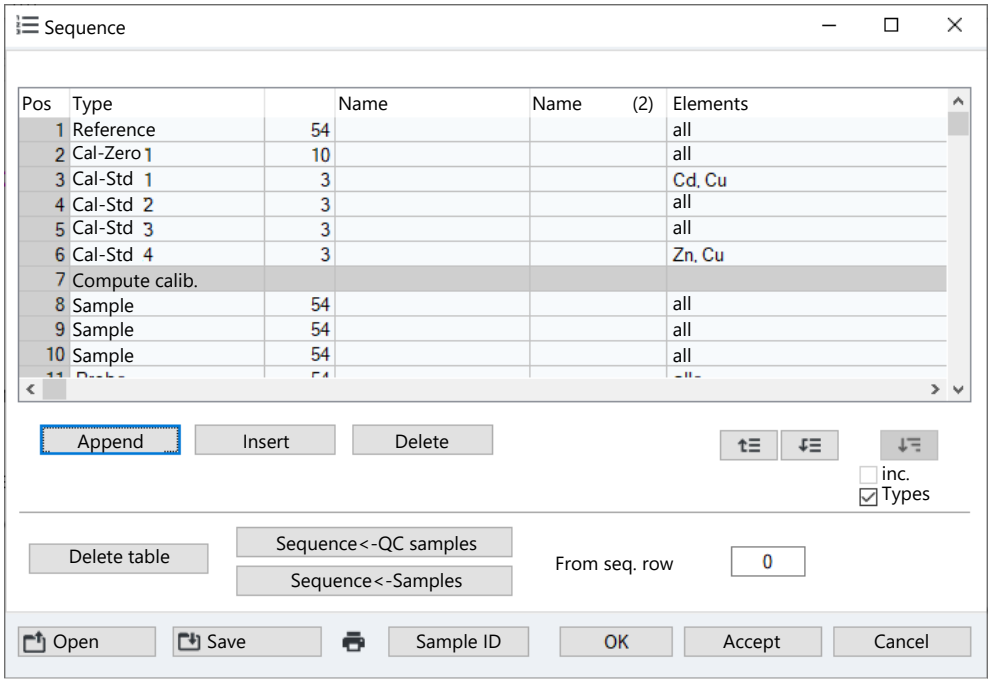


Table of sample and action sequences

The table shows the selected sample and action sequences in the order of processing.

Table column	Description
Type	Sample type or analysis step.
Pos	Sample position on autosampler tray (if used).
Name	Sample name This entry is optional. For calibration and QC samples this sample name is transferred from the method if a sample name was specified there. For analysis samples, the names can be transferred from the sample information file.
Name**(2)**	Additional name for sample identification (optional)
Elements	Only multi-element methods Elements or element lines that are analyzed in a sample or for which special actions are performed.

Table column	Description
	all All elements/element lines specified in the method are determined (default setting). Element symbol Only the named elements are determined, e.g. Cu, Pb. Element symbol + index (when analyzing several lines of an element) Only the named element lines are determined, e.g. Cu1, Cu2. **not** element symbol The named elements are not determined, e.g. not Cu, Pb. **not** element symbol + index The named element lines are not determined, e.g. not Cu1, Pb2.

Buttons

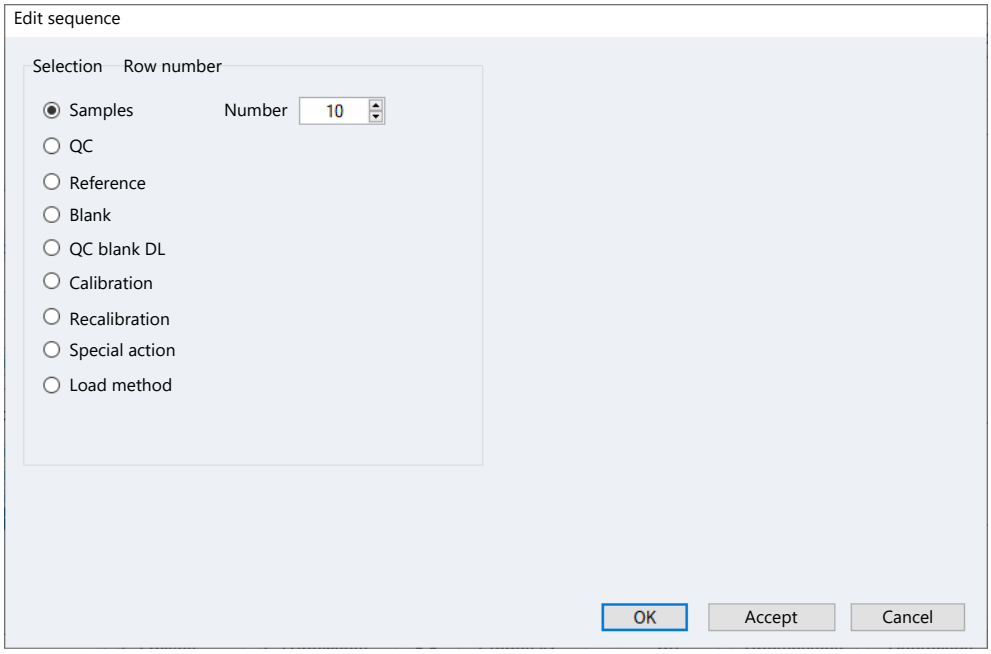
You can use the buttons to add measurements and actions to the sequence list, delete them or transfer existing sample information data.

Button	Description
Append	Add new row at the end of the list and open the **Edit sequence** window
Insert	Insert a new row above the selected list place
Delete	Delete selected rows
Delete table	Delete entire sequence table
Sequence<-QC samples	Transfer information about names of QC samples and their place in the autosampler from the **Sample ID** / **QC sample information** window. The information from the QC sample ID table are entered in the sequence table. The first row with new sample identification is defined in the **From seq. row** field.
Sequence<-Samples	Transfer information about sample names and place in autosampler from the **Sample ID** window The information from the sample ID table is entered into the sequence table. The first row with new sample identification is defined in the **From seq. row** field.

Further buttons and input options can be found in the overview of frequently used controls.

4.3 Specifying measurements and actions in a sequence

In the **Edit sequence** window, you can specify the order of measurements and actions for an analysis. The window appears when you click on **Append** or **Insert** in the **Sequence** window.



Possible measurements and actions

You can specify different measurements and actions for an analysis depending on the atomization technique used and the settings in the method.

Option	Description
Samples	Measure the number of samples specified under **Number**.
QC	Measure a QC sample and evaluate it as specified in the method After activating the option in the list, select one of the QC samples specified in the **Method** / **QCS** window. The parameters of the QC sample are displayed in the opposite field.
Reference	Only flame technique Always define the reference sample as the first measurement in the sequence. Distilled water is used as the reference.
Blank	Measure the blank sample without analytes
QC blank DL	Measure a blank sample to determine the limits of detection and quantitation according to the blank method
Calibration	Measure the standard samples with known concentration of the analyte and calculate the calibration according to the specification in the method
Recalibration	Measure the standard sample intended for recalibration and calculate a recalibration
Sample addition	
Blank addition	
Special action	These actions do not directly affect the measurement of the samples (see below).
Load method	Load a saved method to start another analysis within a sequence

Special actions

The following special actions can also be inserted in the measurement process:

Option	Description
Flame on / **Flame off**	Only flame technique Extinguish/ignite flame
Clean furnace	Only graphite furnace technique

Option	Description
	Additional bake-out step to clean the graphite furnace. The graphite tube is heated to a predefined temperature once. The parameters for this bake-out step are specified in the **Method** / **Furnace** window.
Format tube	Only graphite furnace technique Formatting the graphite tube
Clean system	For hydride technique Also clean system The parameters for this step are specified in the **Method** / **Hydride** window.
Load system	For hydride technique After reinstalling or cleaning the hydride system, as should be done daily after work is completed, the tubes must be loaded with reagents before starting the analyses. Therefore this action should occur in the sequence before the first measurement.
Lamp off	Switch off xenon lamp
Standby	Switch the xenon lamp to standby mode
Waiting time	Wait for the entered time and then continue with the analysis
Pause	Stop the analysis The sequence can then be continued by clicking on  .
Beep	Generate a beep from the PC, e.g. to indicate the end of the calibration (requires a sound card, speakers and activated Windows system sounds)
Repeat / **While**	Repeat a part of the sequence up to the While special action As an abort criterion a number of loop cycles or a time in minutes can be specified. The entries in the results file are supplemented with a counter or date and time according to the abort criterion. For an online measurement, the **autom.** option must be activated. This prevents the prompt for sample metering during the manual mode.
Show calib. plots	Display the calibration curve during the running sequence
Compute calib.	Recalculate the calibration function
Clean collector	For hydride/hydrEA technique Heat gold collector to remove analyte residues
Clean system	For flame technique Washing the sample path
Clean	Perform controlled cleaning for solution analysis The parameters are specified in the **Method** / **Sample transport** window.
Optics purging	For contrAA 800 Switch off optics purging or switch on purging with air or argon The action is skipped if purging is already completed. The purging times are taken from the **Options** / **Optics purging** window.

Specifying a sequence

- Click on  to open the **Sequence** window.
- Then click on **Append**.
  The **Edit sequence** window with the measurements and actions available for the current method.

- Activate the options one after the other and transfer them to the sequence table with **Accept**.
- Confirm the last option with **OK** and return to the **Sequence** window.
  The sequence table contains all measurements and actions in the order of selection.
- Optional: Enter the elements to be examined in the **Elements** table column.
- When using the autosampler:
  Specify the position of the samples on the autosampler. The positions of standard samples and QC samples are taken as a default setting from the method. The positions can be changed here.

Note: It is best to enter the names and positions of the samples to be analyzed in the **Sample ID** window and then transfer them to the sequence table.

Usual sequence for a measurement routine

A usual sequence contains the measurements in the order:

1. For flame technique: Reference measurement
2. Calibration
3. Number of samples

Optionally, QC samples, recalibration or measurement of the recovery rate can be inserted between or after the sample measurements.

See also

- Method / Hydride window [▶ 37]
- Method / Furnace window – Specifying parameters for atomization in the graphite furnace [▶ 31]
- Method parameters for autosamplers for flame and hydride technique [▶ 41]
- Method parameters for autosampler for graphite furnace technique (solution analytics) [▶ 44]
- Sequence window [▶ 67]
- Sample ID window [▶ 72]

5 Sample information data (sample ID)

The sample information data (sample IDs) include the specific data for the current analysis samples and QC samples, such as sample name, position on the autosampler, weight, dilution or concentration unit. Sample names and positions can be transferred to the sequence table by mouse click. The sample information data is saved as a table in CSV format and can also be edited in a spreadsheet program such as Excel. The reverse is also possible: externally created sample tables can be imported to ASpect PQ.

Open the **Sample ID** window by clicking on in the toolbar or via the menu item **Method development** / **Sample ID**.

5.1 Creating, saving and opening sample information data

Creating a new sample ID set

- Click on in the toolbar.
  Alternatively, open the **Sample ID** window with the menu commands **Method Development** | **Sample ID** or **File** | **New Sample Information File**.
  The **Sample ID** window appears.
- Specify the settings for samples and QC samples.
- Click on OK or Accept to activate the data set.
  - ✓ The sample IDs are activated and will be used for the next analysis. You can also save the sample ID for a later analysis.

Saving sample IDs

- In the **Sample ID** window, click on **Save**.
  Alternatively, select the menu item **File**|**Save** | **Sample information**.
  The standard **Save as** window appears.
- Enter the name for the data set in the **File name** field.
- Click on **Save** to save the sample ID.
  - ✓ The sample IDs are saved in CSV format. You can load the data for further analyses or edit it in a spreadsheet program or text editor.

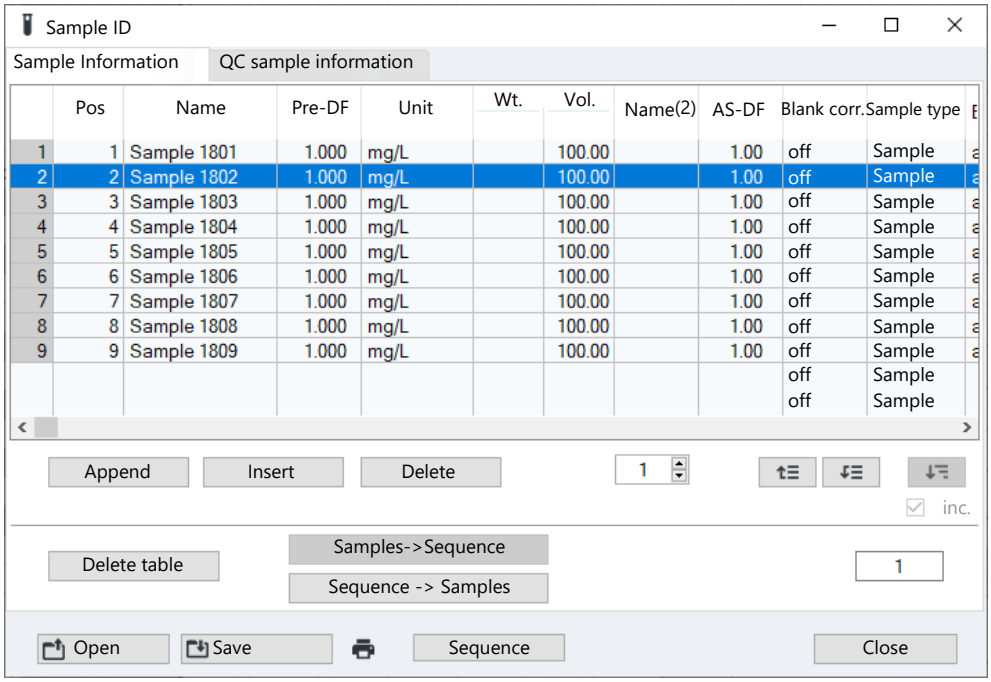
Open sample information data

- Open the sample ID with one of the following alternatives:
  - In the toolbar, click on the icon next to the **Samples** field.
  - Select the menu item **File** | **Open Sample Information File.**
  - In the **Sample ID** window, click on **Open**.
    The standard **Open** window appears.
- Select the file in the list and click **Open**.
  - ✓ The sample ID is displayed in the **Sample ID** window and can be used for the next analysis.

5.2 Sample ID window

In the **Sample ID** window, you can specify the samples and QC samples. In addition to the name and position on the autosampler, you can enter parameters important for the analysis.

Open the **Sample ID** window by clicking on  .



Sample information page

This page contains the list of sample properties.

Table column	Description
Pos	Position of sample on autosampler
Name	Sample name This entry is optional. Maximum number of characters: 20
Pre-DF	The predilution factor is the factor by which the original sample has been diluted before it is placed in the autosampler or fed to the atomization unit when working without autosampler. The factor is necessary to calculate the concentration of the original sample (**Conc.2** on the results table).
Unit	Concentration unit of sample.
Wt.	Initial weight in grams (solution analysis only) This mass of the original sample was brought into solution in the sample pretreatment. The initial weight is necessary to calculate the concentration of the original sample (**Conc.2**). **Note**: For solids analysis, known initial sample weights are entered or in the results window / **Solid** or weighed.
Vol.	The initial weight was dissolved in this volume (in mL) of the solvent. The value is necessary to calculate the concentration of the original sample (**Conc.2** on the results table).
Name(2)	Additional sample name. This entry is optional. Maximum number of characters: 20
AS-DF	Dilution factor of the autosampler. **Note**: The dilution mode used here is defined in the **Method** / **Sample transport** window.
Blank corr.	Blank correction **off** No blank correction is performed.

Table column	Description
	on For calculating the concentration of the original sample, the blank value measured last in the sequence is subtracted. **Note**: You specify the procedure for blank correction in the **Options** / **Calibration** window.
Sample type	Selection of the sample type **Blank** or **Sample type** The sample data of the sample ID is assigned to the sample order in the sequence according to the sample type, i.e. 1st blank value in sample ID = 1st blank value in sequence 2nd blank value in sample ID = 2nd blank value in sequence 1st sample in sample ID = 1st sample in sequence 2nd sample in sample ID = 2nd sample in sequence etc.
Elements	Only multi-element methods Elements or element lines that are analyzed in a sample or for which special actions are performed. **all** All elements/element lines specified in the method are determined (default setting). Element symbol Only the named elements are determined, e.g. Cu, Pb. Element symbol + index (when analyzing several lines of an element) Only the named element lines are determined, e.g. Cu1, Cu2. **not** element symbol The named elements are not determined, e.g. not Cu, Pb. **not** element symbol + index The named element lines are not determined, e.g. not Cu1, Pb2.

Buttons

Option	Description
Append	Insert number of new rows at the end of the list
Insert	Insert number of new rows before the selected list position
Delete	Delete the selected row
Number	Input field for the number of rows to be inserted or deleted
Delete table	Delete the entire table of sample information
QC samples->Sequence	Transfer sample names and positions in the autosampler to the sequence list Define the first row of the information to be transferred in the sequence list in the **From seq. row** input field.
Sequence -> Samples	Transfer sample names and positions in the autosampler from the sequence list to the sample information table Define the first row of the information to be transferred in the sequence list in the **From seq. row** input field.

QC sample information page

The QC samples are listed on this page in the same way as the **Sample information** page.

The table of QC samples is structured in a similar way to the sample table. In addition, the **Type** column contains information about the QC type. The **Unit** column is omitted because the unit is already defined in the method. Blank correction is not available for QC samples.

Button

Option	Description
QC samples->Sequence	Transfer QC sample names and positions on the autosampler to the sequence list

Further buttons and input options can be found in the overview of frequently used controls.

See also

- Method / Sample transport window – Specifying sample transport [▶ 41]
- Calibration and blank correction options [▶ 169]
- Frequently used control elements [▶ 15]

5.3 Specifying sample information and QC samples

If you require further data on samples or QC samples for the analysis, such as the initial weight or the predilution factor, you must specify the data in the **Sample ID** window. You can transfer the data entered there to the sequence.

- Click on  to accept the **Sample ID** / **Sample information** window.
- Enter the number of samples to be analyzed in the **Number** field. Then click on **Append** to insert the rows into the table.
- Enter the information required for each sample in the table.
- If the entries in all rows are the same, you can click on  to copy the entry of a selected cell to all subsequent cells of the column.
  If the **inc.** (increment) option is activated, the value is increased by 1 each time the information is transferred to the next row. This makes it easy to fill spaces in the autosampler or to number sample names consecutively.
- Text from input fields can be copied to the clipboard and pasted again. To do this, use the usual keyboard commands or right-click to open the context menu.
- When all information has been entered, in the **From seq. row** field enter the row of the sequence from which the sample information is transferred to the sequence. Transfer the information by clicking on **Samples->Sequence**.
- Specify the QC sample information analogously in the **Sample ID** / **QC sample information** window.

  ✓ The sample information will now be used for the next analysis.

6 Performing analyses and calculating results

6.1 Overview of the menu commands and buttons for starting the analyses in the main window

Measurements are started with the toolbar icons or via the Routine menu.

Symbol	Menu item	Function
	**Routine** | **Run sequence**	Start an analysis process
	**Routine** | **Run Selected Sequence Row...**	Execute the selected row or rows in the sequence. Several rows can be marked using the mouse in combination with the Ctrl- and/or Shift-Key.
	**Routine** | **Stop**	Stop the analysis process immediately The stop function should be used only with the flame technique. For hydride-/hydrEA technique and graphite tube technique sample residue remains in the system or graphite tube with direct stop and it can lead to contamination.
	**Routine** | **Break**	For hydride/hydrEA technique and graphite furnace technique During the execution of a hydride process or furnace program, a program break can be requested with this button. After this request was detected, the button is grayed out. The procedure will be executed to the end. Then, the analysis process will be stopped.
	**Routine** | **Continue**	Continues a stopped routine.
	**Routine** | **Reprocess**	Causes the reprocessing of the results, if the original data, e.g. the calibration function or the method, have changed.

6.2 Starting a measurement routine

After selecting the method, the sequence and, if necessary, the sample information data, all information is available to start the measurement routine.

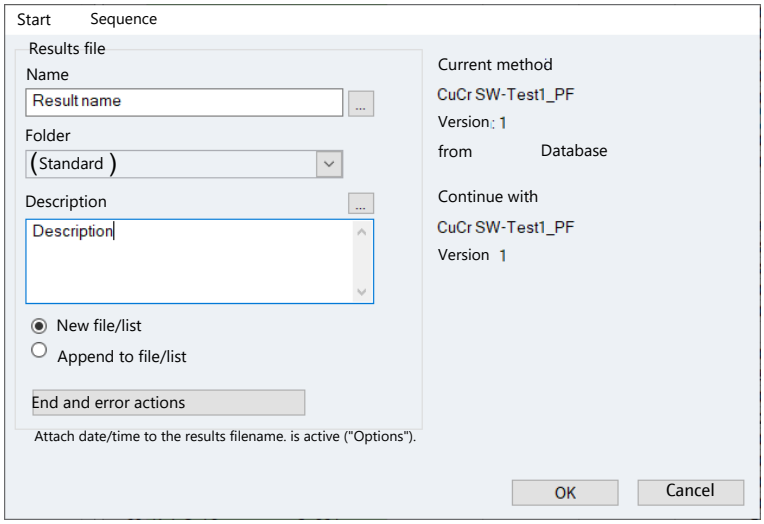
The contrAA must be prepared for the measurement according to the technique used:

- Xenon lamp is switched on.
- Flame technique: The flame has been ignited and burns longer than the specified warm-up time.
- Graphite technique: The graphite tube is inserted and the furnace is formatted.
- Hydride technique: The cell is pre-heated.
- Autosampler: Samples have been prepared and placed onto the tray.

Saving results during the analysis

The results of the analysis are saved to a database in the default folder or a user-defined subfolder directly during the measurement. They may be optionally saved to a new database or appended to an existing database. However, it is not possible to overwrite a result database by selection of the same name.

The target for result storage will be requested automatically at the start of a measurement routine. The **Start Sequence window opens for this purpose: Sequence name** with the following options for the results file:



Option	Description
Name	File name of the results database
Folder	Storage path of the results file The default folder for saving the files is displayed in the **Options** / **Folder** window.
Description	This note is saved with the analysis results. Entry is optional. You can click on ••• to select user-defined descriptions. You can configure these descriptions in the **Data** / **Pre-defined descriptions** window.
New file/list	When activated, a new file name must be entered. The program checks if the file name exists already. Existing files cannot be overwritten.
Append to file/list	New results are appended to an existing results file. Click ••• to open the selection dialog. Choose an existing results file from the displayed list.
End and error actions	Opens an option window with actions that are executed at the end or if the measurements are aborted early. The available options depend on the atomization technique. **Note**: The options can also be activated while a sequence is still running.
OK	Starting a measurement

The file contains the measurement and evaluation results, the sample ID information and the method. In addition, you can specify in the method if you want to save the calibration data. In this case, the method parameters are saved in the results database. Spectra are saved in a separate file with the same file name and different extension. The results database is saved with the extension TPS. Spectra files have the extension SPK.

Starting a measurement routine

- Prepare the device according to the atomization technique and ready the samples.
- Open the measurement routine by clicking on or via the menu item **Routine** | **Start Sequence...** in the **Start Sequence** window.
- Select a file name for the results file. You may optionally save the result to a new file or append it to an existing file. Overwriting of an existing file is not possible.

- Click on to **OK** to start the measurement routine according to the settings in the method and sequence.
  - ✓ If you use an automatic sampler, the measurement runs automatically. In case of manual sample supply without autosampler, the instructions for providing samples are displayed on the screen.

Displays during the analysis process

During the measurement, the results are displayed in real time in the process and results window. In addition, the following display windows can be opened:

- **Signal Plot**: Measurement signal curve
- **Spectrum Plot**: Absorption line of the analyte and the simultaneously recorded spectral environment
- **Bar graph**: Measured values in a bar graph
- **Report window**: Current flame status or furnace status
- **Sample conc. in calibration curve**: Position of the determined sample concentration in the calibration curve

You can preset the display of these windows in the **Options** / **Analysis sequence** window. The display windows can also be hidden or opened during the measurement:

- Click on **Sequence options** to open the **Results windows** window. Then activate the window options there and click on **Results windows**.
- Open all display windows via the menu item **Display** | **Open Results Windows** or the function key F7.
- Close all display windows via the menu item **Display** | **Close Results Windows** or the function key F8.

The measurement progress is documented in the sequence list of the results window. The rows with the successive actions are marked by the following symbols in the table column:

Symbol	Description
-	Not yet measured / executed
O	Currently being measured
+	Already measured / executed

In addition, buttons are displayed in the toolbar on the side during the measurement:

Button	Description
Sequence options	■ Define further options for the end of the sequence or in case of error ■ Open display window
Show method	Open method window The method can only be read, but not edited.
Sequence Samples	Open sequence window The sequence can be extended while the measurement is running. The sequence window contains the **Sample ID**, which is used to edit the sample ID.
Activate scraper	The scraper cleans the burner head between two measurements within a statistics series of a sample.
Extinguish flame	Extinguish the flame immediately

See also

- Creating predefined notes [▶ 162]
- Options for analysis sequence [▶ 167]

6.3 Interrupting, continuing or stopping a measurement routine

A running measurement routine can be interrupted and then resumed. In the graphite furnace technique and hydride technique, however, the running sample measurement should be continued to the end and only then interrupted. This procedure is to prevent sample residues from being deposited in the graphite tube or hydride system. In the flame technique, the measurement can be stopped at any time without restriction.

Stopping/interrupting the measurement routine

- Stop the measurement routine immediately by clicking on  or via the menu item **Routine** | **Stop**.
- Declare a break in the measurement routine by clicking on  or via the menu item **Routine** | **Break**. After this request was detected, the button is grayed out. The currently running hydride program or furnace program will be finished first. Then, the analysis process will be stopped.

Continuing the measurement routine

- Continue a stopped/interrupted measurement routine by clicking on  or via the menu item **Routine** | **Continue**.
  The **Continue sequence** dialog box with the action status before the break appears.
- Select one of the options to continue the measurement.
- If the method is changed, activate the **Continue with modified method** option. This results in a new method entry in the results file and another version of the method is saved.
- Click on **OK**.
  - ✓ The measurement routine is continued with the selected option and the results are updated in the results database.

6.4 Repeating actions of the sequence

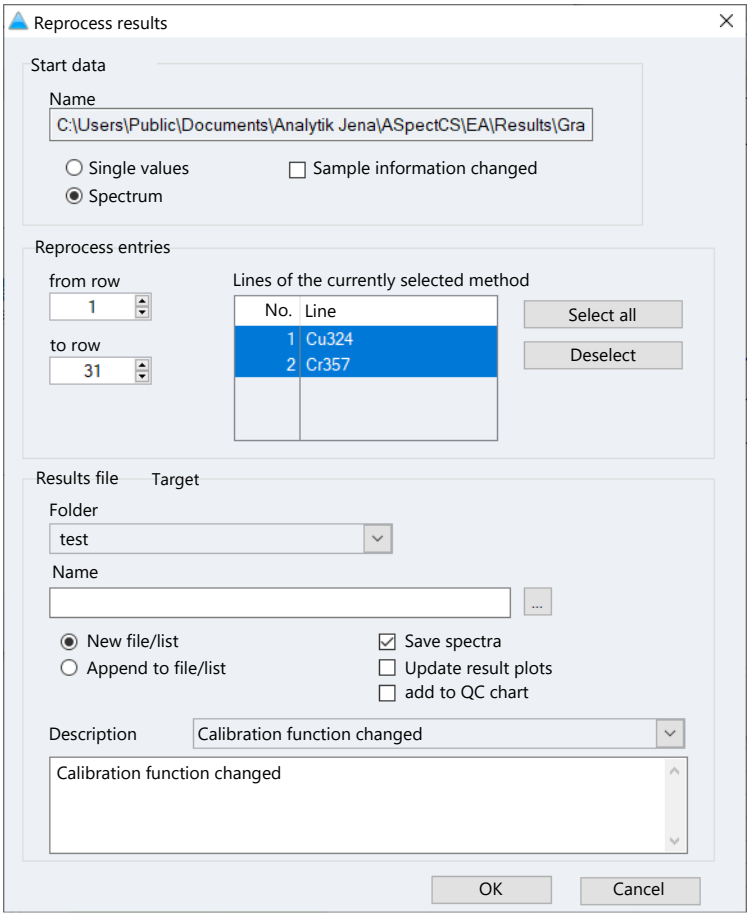
Single actions in a sequence, single measurements in statistic runs or special actions can be repeated.

- In the main window on the **Sequence** or **Sequence/Results** tab, select the row(s) with the action to be repeated.
- Start the measurement routine by clicking on  or via the menu item **Routine** | **Run Selected Sequence Row...**.
- In the **Start Sequence** window, select a file name under which you want to save the results for the repeat measurement.
  You may optionally save the result to a new file or append it to an existing file. Overwriting of existing results by selection of the same file name is not possible.
- Click on **OK**.
  - ✓ Repetition of the selected sequence lines starts.

When repeating the sequence or the measurement of individual rows, a new version of the method is saved. No check for changes in the method takes place in this case.

6.5 Reprocessing analysis results

Each time the evaluation conditions are changed, e.g. change of the calibration function or method changes, the results must be reprocessed to let the changes take effect. Similarly, the sample information data, e.g. sample names or dilution factors, can be changed and reprocessed in the output of the analysis results. The options for the reprocessing are specified in the **Reprocess results** window.



Options in the Reprocess results window

Option	Description
group **Start data**	
Name	Name of original file with analysis results.
Single values	Measurement results of sample single values were saved in the original file. Reprocessing is performed based on the single values.
Modified sample information data	The sample information data has been changed and should be taken into account in the reprocessing.
group **Reprocess entries**	
to row	Starting row in the results list
from row	End row in the results list
Lines of the currently selected method	Reprocess the selected lines
Results file (Target) group	
Folder	Storage path for the results file
Name	File name for the results file

Option	Description
	New file/list If activated, a new file name must be entered. The program checks if the file name exists already. Existing files cannot be overwritten. **Append to file/list** If activated, the reprocessed values are appended to the existing file.
Save spectra	Save spectra of the sample single values with the new analysis results This option is only active if spectra are stored in the source file.
Update result plots	Update the display windows during reprocessing
add to QC chart	Enter reprocessed values on the QC charts if QC charts are specified in the method
Description	This additional note is saved with the reprocessed analysis results. The entry is required if the user administration option is installed. User-defined descriptions can be selected from the list.

Performing reprocessing

- Click on  or select the menu item **Routine** | **Reprocess**.
  The**Reprocess results** window appears.
- Specify options and select a file name.
- Click on **OK**.
  - ✓ The reprocessing is performed.

Note: Reprocessed values can optionally be saved in a new file or appended to an existing results file. Manipulation of the original data is ruled out. The original results always remain as long as the original file is not deleted.

See also

Creating predefined notes [▶ 162]

6.6 Evaluating measurements parallel to running analyses

While measurements are running, it is impossible to evaluate results in the same program instance. However, it is possible to start a second program instance of the application in offline mode, while measurements are running in the first instance. In this mode, there is no communication with the device. However, all other functions such as developing methods or loading and analyzing results can be used parallel to the running measurements of the first program instance.

- Select the menu item **File** | **Start Offline Program Instance**.
  The second program instance starts.
- Open the results file of the currently running measurement with the menu command **File** | **Open Results**.
  The results measured so far are loaded to the results window.
- Load further results from the running measurement by clicking on  or via the menu item **View** | **Update results list**.
  - ✓ The results can be further processed, e.g. by opening the sample details or the calibration function.

Note: When reprocessing, the reprocessed results are saved in a new file. Accessing the original file requires reopening the results data.

6.7 Displaying results and analysis progress

Note: Depending on the selected operating mode, the measured values are determined in absorbance or emission. In the following, only absorbance values will be mentioned. The same specifications and information, however, also apply to emission values. The abbreviation **Abs.** is used for absorbance values in the value outputs, and the abbreviation **Ems** is used for emission values.

The measurement results and the sequence are displayed on a large scale in the background of the workplace in the results window.

The display on different tabs in the results window provides a good overview of the measurement results and statistical evaluations.

The following tabs are selectable:
- **Sequence/Results**: Content of the sequence and results tabs on one tab
- **Sequence**: Display of the current sequence
- **Results**: Presentation of measurement results
- **Overview**: Summary of the measurement results
- **Solid**

The status bar of the result window shows the file name of the current results file.

6.7.1 Sequence/Results tab

The **Sequence/Results** tab contains data from both the **Sequence** tab and the **Results** tab.

6.7.2 Sequence tab

The **Sequence** tab lists the active sequence and selected parameters from the sample ID. During the analysis, you can monitor the progress of the measurement routine here. The following symbols are used:

Symbol	Description
-	Not yet measured / executed
O	Currently being measured
+	Already measured / executed

6.7.3 Results tab

All measurement results and statistical evaluations are listed on the **Results** tab. For a better overview the values are distributed in tables. The index tabs for these tables are arranged at the bottom edge of the window.

The values are sorted by the order of sample measurement. For every sample, the analyzed elements are listed.

Abs./Time table

The table contains the absorbance values and the statistical evaluations according to the specified method (**Method** / **Statistics** window).

Table column	Description
No.	Number in analysis sequence
Name	Sample name
Line	Analytical line

Table column	Description
Abs.	Mean or median of the measured single absorbance values For solid analysis: normalized absorbance
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)
RSD%	Relative standard deviation (mean value statistics)
Date / **Time**	Measuring time
Single values(Abs.)	Single values of absorbance measurements

Solid table

Table column	Description
No.	Number in analysis sequence
Name	Sample name
Norm.Abs.	Mean value of the normalized absorbance (absorbance/initial weight)
SD	Standard deviation of **Conc. 1** (mean statistics)
RSD%	Relative standard deviation of **Conc. 1** (mean statistics)
Mass	Mean absolute analyte mass
Unit	Absolute unit of the analyte
Hum.[%]	Relative moisture of the sample
Wt.[%]	Weights for all individual amounts
Date / **Time**	Measuring time
Single values(Abs.)	Single values of absorbance measurements

Conc.1 table

The **Conc.1** table shows the analyzed concentration of the sample as it was fed to the AAS.

Table column	Description
No.	Number in analysis sequence
Name	Sample name
Line	Analytical line
Unit	Concentration unit
Conc.1	Analyzed concentration of sample
SD	Standard deviation of **Conc. 1** (mean statistics)
RSD%	Relative standard deviation of **Conc. 1** (mean statistics)
R	Range of Conc. 1 (median statistics)
R%	Relative range of Conc. 1 (median statistics)
Cf	Confidence interval
Rem.	Remarks on events during the measurement routine
DF	Dilution factor if concentration is exceeded If the concentration is exceeded, you can activate automatic dilution with the sample changer in the **Method** / **Sample transport** window. The dilution factor of this automatic dilution by the autosampler is taken into account in the calculation of Conc. 1.
Abs.	Mean or median of the measured single absorbance values For solid analysis: normalized absorbance
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)
Date / **Time**	Measuring time

Table column	Description
Single values(Abs.)	Single values of absorbance measurements

Conc.2 table

The **Conc. 2** table shows the concentration of the original sample. The sample information data is taken into account in the calculation of **Conc.** 2:

- Pre-dilution
- Weighed portion of solids
- Conversion factors for other units

Option	Description
No.	Number in analysis sequence
Name	Sample name
Line	Analytical line
Unit	Concentration unit
Conc. 2	Concentration of original sample taking sample information data into account
SD 2	Standard deviation of Conc. 2 (mean statistics)
RSD%	Relative standard deviation of Conc. 2 (mean statistics)
Cf	Confidence interval
Rem.	Remarks on events during the measurement routine
Abs.	Mean or median of the measured single absorbance values For solid analysis: normalized absorbance
Date / **Time**	Measuring time
Single values(Abs.)	Single values of absorbance measurements

QC Res. table

The **QC Res.** table shows the results of the QC samples: Setpoint and actual concentration, recovery rates (not for blank value), reactions to possible deviations (all types except blank value).

Table column	Description
No.	Number in analysis sequence
Name	Sample name
Line	Analytical line
QC for calibration functions	**R^2(adj.)** **Slope** **Char.conc.**: Characteristic concentration
QC for QC samples, not for QC blank	**Conc. 1** **Nominal val.**: Rated value **Recovery**: Recovery rate For QC samples and QC std., the recovery rate of the concentration is determined. For QC-Stock, QC-Trend and QC-Matrix, the recovery rate of the concentration increase caused by the spiking is determined.
QC for blank detection limit	**SD**: Standard deviation of the blank measurements **LOD**: Detection limit **LOQ**: Limit of quantitation
Rem.	Remarks on events during the measurement routine
Abs.	Mean or median of the measured single absorbance values For solid analysis: normalized absorbance

Table column	Description
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)
Date / **Time**	Measuring time
Single values(Abs.)	Single values of absorbance measurements

Error table

If errors occur during the measurements, the corresponding measurements are marked in red in all tables. The measurement error that has occurred is documented in writing in the **Error** table.

Single values table

The **Single values** table contains the measured single values of the absorbance.

Sample ID table

The **Sample ID** table contains the sample information data.

Table column	Description
No.	Number in analysis sequence
Name	Sample name
Line	Analytical line
Pos	Position of sample on autosampler
Pre-DF	The predilution factor is the factor by which the original sample has been diluted before it is placed in the autosampler or fed to the atomization unit when working without autosampler. The factor is necessary to calculate the concentration of the original sample (**Conc.2** on the results table).
Wt.	Initial weight in grams (solution analysis only) This mass of the original sample was brought into solution in the sample pretreatment. The initial weight is necessary to calculate the concentration of the original sample (**Conc.2**). **Note**: For solids analysis, known initial sample weights are entered or in the results window / **Solid** or weighed.
Vol.	The initial weight was dissolved in this volume (in mL) of the solvent. The value is necessary to calculate the concentration of the original sample (**Conc.2** on the results table).
Name(2)	Additional sample name.
AS-DF	Dilution factor of the autosampler. **Note**: The dilution mode used here is defined in the **Method** / **Sample transport** window.
Blank corr.	Blank correction **off** No blank correction is performed. **on** For calculating the concentration of the original sample, the blank value measured last in the sequence is subtracted. **Note**: You specify the procedure for blank correction in the **Options** / **Calibration** window.

User defined table

On the **User defined** table, you can select the parameters for the results output and their order in the table itself.

- Click the **Select columns** button in the top right corner of the table.
- Click with the mouse to select the parameters in the **Select columns** window.

- To change the order in the display, select the parameter and move it in the list using the arrow keys on the keyboard. Several simultaneously selected parameters are moved as a block.
  - ✓ After returning to the main window the results are displayed. You can change the width of the table columns by moving the mouse pointer to the table line in the table header (the pointer changes to a double arrow) and dragging the table column to the desired width with the mouse button held down.

Note: The column width is saved in this view. For the other tables in the main window changes of the column width are reset after exiting.

See also

Overview of markings used in the display of values [▶ 180]

6.7.4 Overview tab

The results of the analysis are summarized on the **Overview** tab. You can choose between different output options.

Option	Description
Conc.1	Analyzed concentration of sample
Conc. 2	Concentration of original sample taking sample information data into account
Abs.	Mean or median of the measured single absorbance values For solid analysis: normalized absorbance
Abs.(RSD / R)	Relative standard deviation or range of absorbance
SD	Standard deviation of **Conc. 1** (mean statistics)
RSD%	Relative standard deviation of **Conc. 1** (mean statistics)
LOD	Detection limit
LOQ	Limit of quantitation
Recovery(Nominal val.)	Recovery rate (setpoint)
R^2(adj.)	Correlation of the calibration curve

By activation of the respective check boxes, the following sample types can be displayed:
- **Samples**
- **QC samples**
- **Cal-Std**
- **Other**

Click on to open the **Print Overview** window, from which you can start the printout after specifying the lines and parameters to be printed. In addition to the printout on the connected printer, the data can also be saved as a TXT, HTML or PDF file and displayed in the corresponding application.

See also

Printing results data [▶ 151]

6.7.5 Solid tab

The **Solid** tab lists the order of the individual measurements of the solids analysis.

The order of calibration and sample measurements defined in the sequence is split into individual measurements and their initial weights, tare and dosing status are displayed and entered.

See also

Solid analysis with graphite furnace technique [▶ 99]

6.8 Opening results files or deleting them from the display

You can open saved analysis results to view them again.

Opening results file

The results files are stored in defined folders according to the atomization technique. Therefore, you can only open files that match the atomization technique selected in the **Quick Start** window. Line spectra are only accessible if a file with the spectra was saved with the results file.

- Select the menu item **File** | **Open Results**.
- Select the file in the standard **Open** window.
  The **Load results** window opens. In addition to the file names, the device name and number, the analysis technique used, the software version and the optional description are also output here.
- If the sample information data is required in later work steps, activate the **Extract sample information** option.
  The sample information is required, for example, for reprocessing with a changed sample ID.
- Click on **OK**.
  - ✓ The results file is loaded and displayed in the results window. The name of the currently loaded results file is displayed in the ASpect CS status bar.

You can reprocess or print the file. It is also possible to extract the method from the results file and use it for further measurements. If you extracted the sample ID when loading, this data is displayed in the **Sample ID** window.

Deleting the display of the current results list

A displayed results list is always deleted when you load another results file and replaced by the new results list. You can also explicitly delete the current display of the results list.

- Select the menu item **Edit** | **Delete results list**.
  - ✓ The results list is deleted and an empty main window is available for further work steps.

Note: The software has extensive reporting functions for printing the results. You can also import or export results. Results of individual samples can be found in the **Data** | **Data management** window.

See also

Printing results data [▶ 151]
Managing results data [▶ 157]

6.9 Sample details and spectra

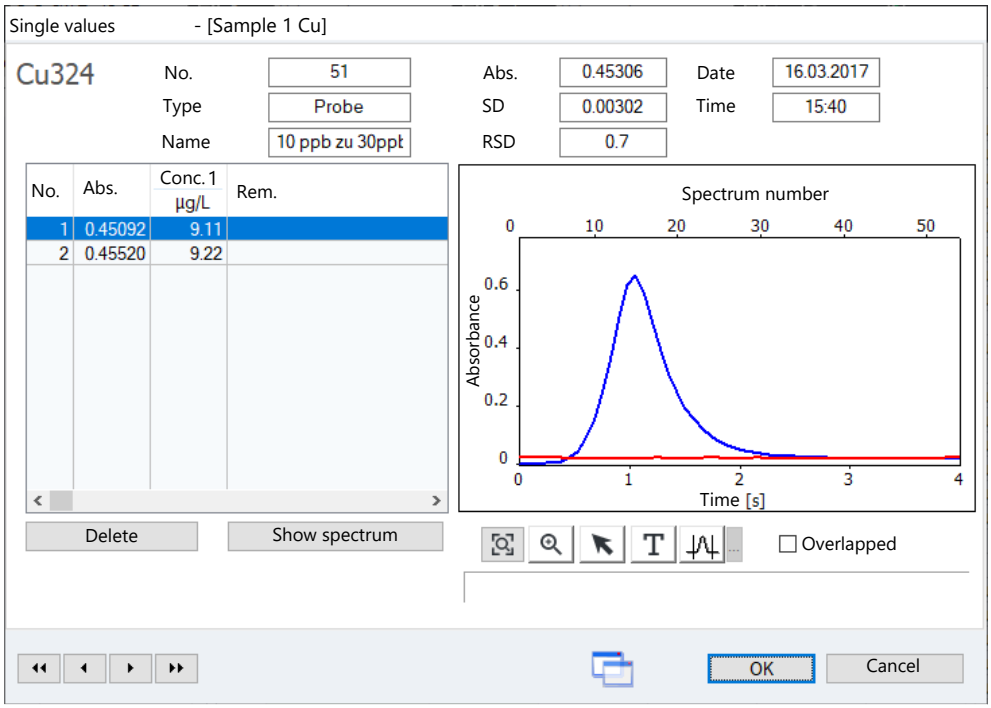
For each measurement in the results window, the individual values (statistics runs) of the measurement and, if also saved, the spectra can be displayed in the **Single values** window. If the spectra were saved with the analysis results, you can retrieve and edit the individual spectra in the **Spectra** window.

6.9.1 Displaying sample single values

You can display more detailed information on the individual values (statistics runs) and the signal curves of a sample measurement in the **Single values** window. The following functions are also available in this window:

- Display spectra of the single measurement
- Activate/deactivate single measurements in the calculation of the analysis value
- Adapt integration limits for the evaluation of signal areas

Open the **Single values** window by double-clicking on the corresponding sample row in the results table. Alternatively, you can select the row and choose the menu item **View** | **Detail results**.



Sample data

Field	Description
Line	Analytical line
No.	Number of measurement in the result table
Type	Sample type
Name	Sample name
Abs. / **Ems**	Absorbance value / emission value averaged over all single values
SD	Standard deviation (mean value statistics) This parameter is displayed independently of the statistical method chosen for the measurement (mean/median).
RSD	Relative standard deviation (mean value statistics)

Field	Description
	This parameter is displayed independently of the statistical method chosen for the measurement (mean/median).
Date / **Time**	Measurement time

Displaying / deleting single values

The determined sample single values are displayed in the table.

Table column	Description
No.	Number of single value within the sample measurement
Wt.	Only solids analysis Weighed portions of individual samples.
Abs.	Absorbance of the single value For solid analysis: normalized absorbance
Rem.	None The single value is included in the calculation of the sample mean. **MAN** The value was manually excluded from the sample value calculation. **KOR** The value was automatically excluded from the sample value calculation due to the Grubbs outlier test.

Buttons and options

Buttons / Option	Description
Delete / **React.**	Remove the sample single value from the mean value calculation or reactivate it for the calculation
Show spectrum	Only if single spectra were saved with the measurement and the Scientific Mode (menu item **Extras** | **Scientific Mode**) is activated Display of the measured wavelength-dependent line spectra, which give the sample single value
Replace with entry number	Only calibration standards Current sample is to be replaced by the sample at position no. in the results table during reprocessing.
	Reset graph zoom
	Zoom graph Hold down the mouse button and drag a frame around the area you want to enlarge
	Display signal values in the signal curve
	Insert text field into the graph Hold down the mouse button and draw a frame and then enter the text.
	Set integration limits of the signal
	Switch between the lines of individual samples and from one sample to the next in the results table
Overlapped	Individual spectra are displayed superimposed in the graph. The selected individual spectrum is displayed in bold.

The graph to the right of the table shows the signal curve and, for the graphite furnace technique, also the curve of the non-specific background of the respective selected single value over time. The number of measuring points corresponds to the number of

measured spectra. This depends on the measuring time and is specifically defined in the **Method** / **Lines** window for each analysis line. Signal areas that lie outside the integration range are highlighted in gray. Areas in which the spectra contain strong specific structures are highlighted in yellow in the **with reference** correction procedure. In this case, check the spectral baseline using the **Show spectrum** button.

Excluding single sample values

If desired, you may manually exclude a single value from the calculation of the sample average.

- In the table, select the single value you want to exclude.
- Click on **Delete**.
  The single value has the **MAN** mark in the **Rem.** column.
- Click to start the reprocessing.
  - ✓ The data is reprocessed and appended to the existing results file or saved to a new file.

Click on **React.** to reactivate a selected single value for the mean value calculation.

Note: By activating the Grubbs outlier test option, outliers among single values can be detected and eliminated automatically during the analysis.

Resetting integration limits

In the case of simultaneous analysis of several analysis lines (multi-line evaluation), the analysis line parameters of the principal line are also used for the additional lines in the method. With integral signal evaluation (graphite furnace technique) it is useful to adapt the integration limits of the additional lines to the actual peak curve.

- Click on and then in the graph click on the time of the start of integration.
  A vertical line appears.
- Click on the narrow button **...** and in the context menu select **Set integration end**.
  Then click on the time of the end of integration in the graph.
- Click on **...** again and select **Copy values to current method**.
  The marginal areas of the signal that are not to be taken into account are highlighted in color in the graph.
- Close the **Single values** window by clicking on **OK**.
  A message is displayed indicating that the method can be reprocessed.
- Click to start the reprocessing.
  - ✓ The data is reprocessed and appended to the existing results file or saved to a new file. The current values have been transferred to the method and can be displayed in the **Method** / **Evaluation** window by clicking on **Signal integration**.

6.9.2 Displaying and evaluating spectra

This function is only available if single spectra were saved with the measurement and the Scientific Mode (menu item **Extras** | **Scientific Mode**) is activated

You can open the line spectra of a single value in the **Single values** window.

- Double-click on the sample line in the main window.
  The**Single values** window appears.
- Select the single value in the table and click **Show spectrum**.
  - ✓ The**Spectra** window appears.

You can perform the following functions in the **Spectra** window:

- Display single spectra
- Edit background correction
- Display spectra array in 3D view

- Correct peak offsets

In the **Spectra** window, the spectra of the sample single values are displayed in different views on the left-hand side. Since the measured values are recorded by means of a CCD line, a three-dimensional spectrum array of signal changes dependent on wavelength range and time is created. Sections are made through the spectra array and thus the measurement curves are viewed two-dimensionally:

- At a fixed wavelength (pixel) over time
- At a certain time over the wavelength range.

Both views can be displayed in the graph.

Buttons in the window Spectra

Button	Description
Line parameters	Load line parameters for background correction and spectral evaluation from the method or send them to the method
3D plot	Open spectra plots in another window
	Switch between the lines of individual samples and from one sample to the next in the results table

Graphical view on the left-hand side of the tabs

In the view over the wavelength range, **pixel** is given as the abscissa. Three red wavelength values indicate the upper and lower limits of the measured spectral range as well as the position of the measurement pixel (peaks of the element line). The support pixels for the background correction are highlighted with gray lines. The measurement pixel is highlighted by a solid red line. The area of the evaluation pixels is highlighted in light red.

When using the background correction methods IBC and IBC-m, areas with permanent structures (absorption bands in the reference spectrum) are automatically blocked when the correction of permanent structures is deactivated. These areas are grayed out in the spectrum display.

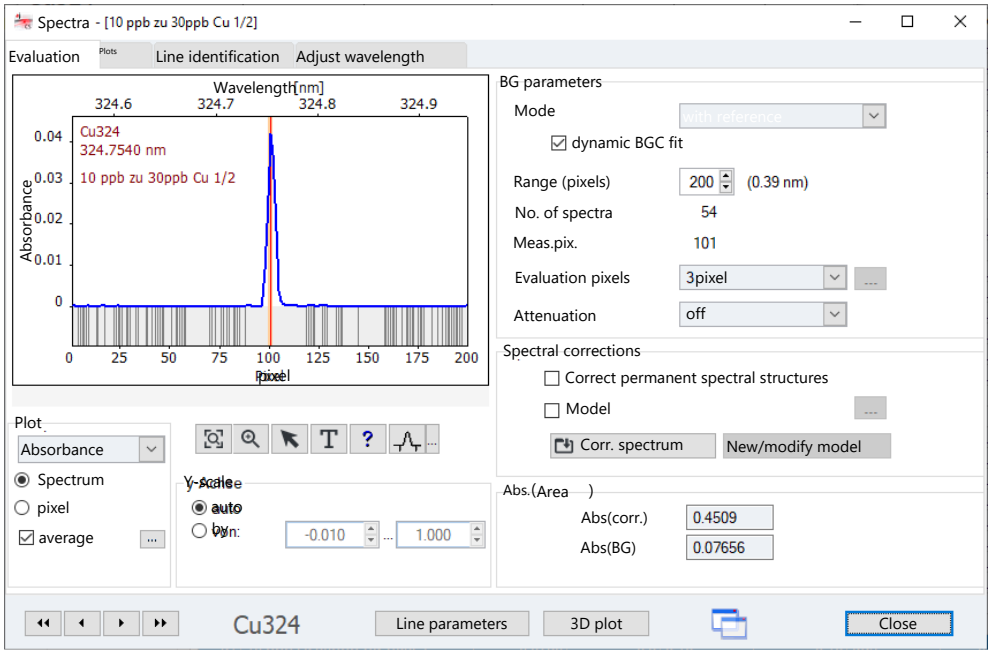
Option	Description
Selection list for graph display	**Absorbance | Reference energy | Sample energy** You can choose between displaying the absorbance spectrum of the sample, the energy spectrum of the reference value (mean only) and the energy spectrum of the sample.
Spectrum	Display the spectral curve of a selected measurement over the wavelength Use the arrow keys to select the number of the measurement to be displayed. **average** The mean spectral curve over all measurements is displayed. After clicking on ••• you can limit the range of spectra to be averaged. To do this, specify the start spectrum and the end spectrum of the range.
pixel	Display spectral curve at a selected pixel over time Use the arrow keys to select the number of pixels to be displayed. **Eff.** The integral over the evaluation pixels is displayed.
	Restore original coordinates after zoom
	Graph zoom After clicking select the spectral section to be enlarged with the left mouse button held down.

Option	Description
	Display pixel position on the graph curve If you move the mouse over the curve, the data for the measured value at which the mouse pointer is positioned is displayed below the graph.
	Insert text field into the graph Hold down the mouse button and draw a frame for the text box and then enter the text. You can edit text after double-clicking on an existing text field.
	Line identification After you click on the graph, the nearest line from the wavelength database is displayed.
	Set or delete support points for the background correction Background correction points can be set by clicking with the mouse. Clicking on an already selected pixel removes the background correction point. Areas of adjacent pixels can be selected by dragging the mouse. Areas that have already been selected are cleared again. Click on **...** to open the context menu: **Mark background correction points** Highlights the interpolation points in the spectrum display with vertical lines **Delete all background correction points** Deletes all selected support points **List of background correction points** Shows a list of the pixel numbers of the selected support points
Y-scale	Graph scaling **auto** Autoscaling: The spectrum is displayed with optimum ordinate expansion. **by** Manual scaling: The ordinate limits are entered in the fields.

6.9.2.1 Specifying background correction and evaluation pixels

You specify the background correction and the selection of the evaluation pixels in the **Spectra** / **Evaluation** window.

For the background correction (BGC) the supporting points can be selected again. Resulting changes in the signal curve are displayed simultaneously in the graph. The sample mean value is then recalculated either simultaneously or, in the case of a large data volume, on command. Found new support pixels can be transferred directly into the opened method. In this way, the ideal background correction is determined for a new method.



BG parameters area

Option	Description
Mode	Background correction method used **with reference** **without reference** **IBC** **IBC-m**
dynamic BGC fit	Only **with reference** Automatically find support pixels
Range (pixels)	Spectral range included in the evaluation The evaluation of the spectra can be carried out using a maximum of the stored number of pixels. If the evaluation range is restricted, the pixels to the left and right of the evaluation pixel are distributed symmetrically.
No. of spectra	Number of spectra (measurements) from which the sample single value was formed
Meas.pix.	Display of the measuring pixel The measuring pixel is pixel 101 in the middle of the receiver line.
Evaluation pixels	Number of pixels used to evaluate the measurement signal The integral representing the measurement result is calculated from the measured values of these pixels.
Attenuation	For signal attenuation, only pixels to the left and right of the peak maximum are considered for signal generation. The signal of the peak pixel and, depending on the attenuation level, its adjacent pixels is "clipped out". The higher the level of signal attenuation selected, the further away the evaluated signal areas are from the peak pixel. Signal attenuation can extend the working range of the calibration. The edge pixels used for the evaluation are displayed in the **Evaluation pixels** column. The evaluated areas are highlighted in color in the graph on the left.

Spectral corrections area

Option	Description
Correct permanent structures	Not for background correction **without reference** Automatic correction of permanent structures Permanent structures are spectral structures that occur in the reference and sample spectra, e.g. absorption bands of flame gases. This setting should be activated if these structures are not fully compensated.
Model	Selection of a model for spectral correction

Abs. (Mean) / Abs. (Area) area

The mean value of the absorbance **Abs(corr.)** is displayed in this area. When using the graphite furnace technique in connection with **with reference** background correction, the absorbance of the background **Abs(BG)** is also output.

Loading/sending line parameters

You can get the spectra evaluation settings for each analysis line from the method or send changes to the method from the **Spectra** window.

- In the **Spectra** window, click on **Line parameters**.
  The **Line parameters** / **Evaluation** window appears.
- In the line table, select the line whose parameter is to be sent to or fetched from the method.
- Activate the action option:
  copy from method/line – loads the original parameters from the method
  copy to method/line – updates the changed parameters
- Click on **OK**.
  - ✓ Depending on the setting, the changed parameters are sent to the method or the original parameters are loaded from the method.

See also

Description of the algorithms used for spectral background correction [▶ 180]

6.9.2.2 Creating a correction model for spectral corrections

In the routine, an attempt is made to select lines for analysis that are without interference or have a background that is easy to correct. If this is not possible, correction spectra can be used to eliminate the discontinuous interference, e.g. caused by line overlays with one or more matrix elements. The correction spectra of a matrix are each combined in a model and can then be linked to the line in the method.

To create and use a correction model for an analysis line, you must perform the following steps:

1. Identify possible interferences.
2. Create and save the correction spectra.
3. Create a correction model.
4. Transfer the parameters of the analysis line with correction model to the method.

Step 1: Identifying interferences

- Create a method with the analysis line. Select the following parameters in the method:

Method /	Activated options
Evaluation	**BGC mode**: **with reference** **BGC fit**: **dynam.**

Method /	Activated options
Output	**Save with results**: Activate the **Method** and **Spectra** options

- Measure analyte in the matrix.
- In the results window, double-click on the sample line.
  The**Single values** window appears.
- Then click on **Show spectrum**.
  The**Spectra** window appears.
- In the **Spectra** / **Line identification** window, identify the possible interferences of the analyte signal due to line overlays of matrix elements or molecular absorptions.

Note: Possible interfering elements or molecular bands can be found in Welz et. al: "High-Resolution Continuum Source AAS".

Step 2: Recording and saving correction spectra

Note: The concentrations of the matrix components do not need to match those in the samples but must be at least high enough for the spectra to have clear intensity values. For a correct spectra correction only measure one component at a time as a pure substance.

- Add the measurement of the interfering matrix components that cause spectral overlap to the sequence. Measure these components in single element solutions.
- Load the spectrum of a matrix component into the **Spectra** / **Evaluation** window (see step 1).
- Click on **Corr. spectrum**.
  The database window for saving the correction spectra opens.
- Enter a name for the spectrum and complete the process by clicking on **Save**.
- Save the spectra of the other matrix components in the same way.

Step 3: Creating a correction model

- Open the spectrum display of your sample with the analyte in the matrix (see step 1).
- In the **Spectra** / **Evaluation** window, tick the **Model** checkbox.
- Click on **New/modify model**.
  The**Spectral corrections** window appears.
- Click **Add** to open the selection of already saved correction spectra.
- Select the correction spectrum and click on **Load**.
  The spectrum is loaded into the **Spectral corrections** window.
- Load the other correction spectra in the same way.
- Activate the **Highlight corrected spectrum** option to check if the resulting sample spectrum is free of overlays.
- After clicking on **Mask.**, you can mask areas that are not to be used for the calculation of the correction model by holding down the mouse button.
  By default, the area of the analysis line (± 9 pixels) is already masked. It might be necessary to mask additional ranges if no pure substances were available for recording and these contaminations might be present in varying proportions.
- To save the correction model, click **Save** and enter a name for the model. Complete the process by clicking on **Save**.
- Close the **Spectral corrections** window by clicking on **Close** and return to the **Spectra** / **Evaluation** window.

Transferring analysis line with correction model to the method

You can copy the settings from the **Spectra** / **Evaluation** window to the method.

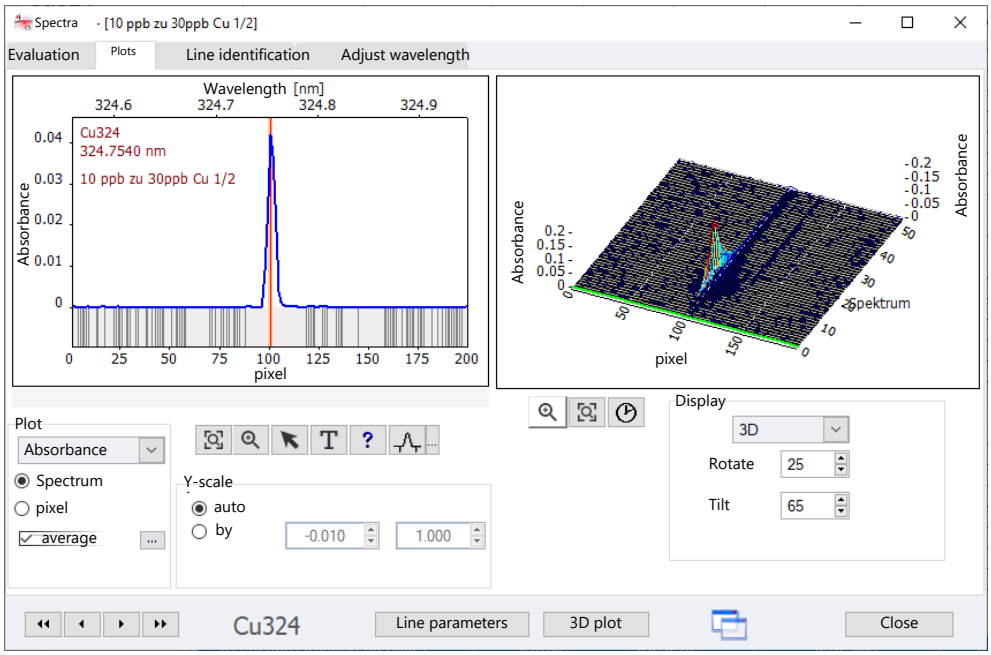
- In the **Spectra** / **Evaluation** window, click on **Line parameters**.
  The **Line parameters/Evaluation** window appears.
- Then activate the **copy to method/line** option there and click on **OK**.
  - ✓ In the **Method** / **Evaluation** window, the model is displayed next to the **Spectral corrections** button.

See also

- Method / Evaluation window – Specifying spectral range and background correction [▶ 49]
- Spectrum subtraction (correction of permanent structures) [▶ 182]

6.9.2.3 3D view of the spectra

The three-dimensional view of the spectra arrays of a sample single value is shown in the **Spectra** / **Plots** window.

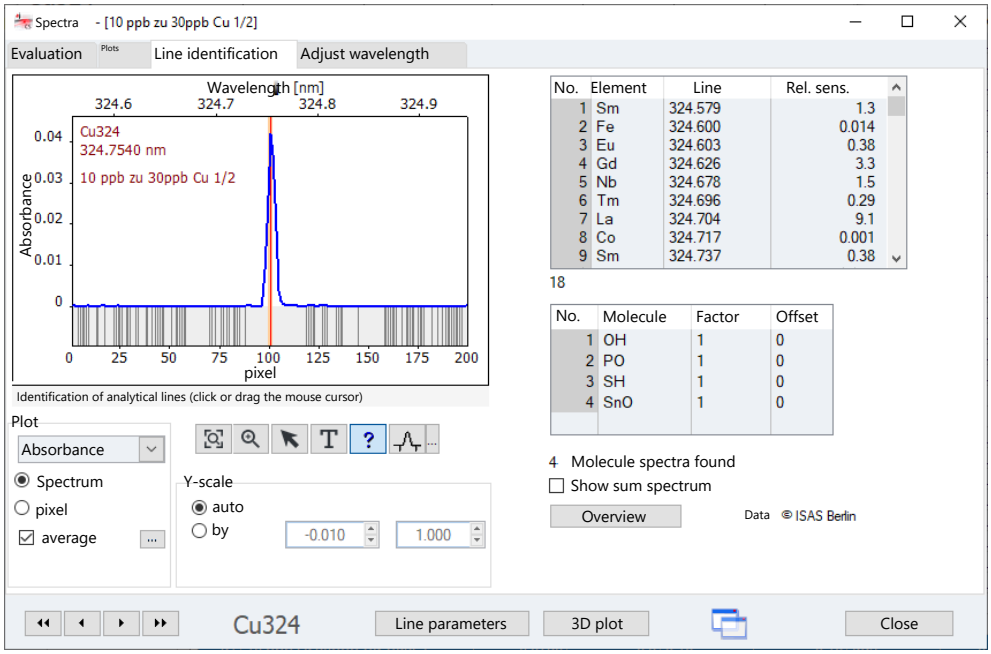


The plot of the spectra array is displayed three-dimensionally with variable gradients on the right-hand side of the window. The spectrum/pixel selected in the graph on the left is highlighted in light green in the plot.

Option	Description
	Zoom graph
	Reset graph
	Build a plot of the spectra array with different velocities
Display	Selection for the plot view

6.9.2.4 Line identification

Spectral peaks and molecular bands can be identified in the measured data based on a spectra and line database. This identification happens in the **Spectra** / **Line identification** window.



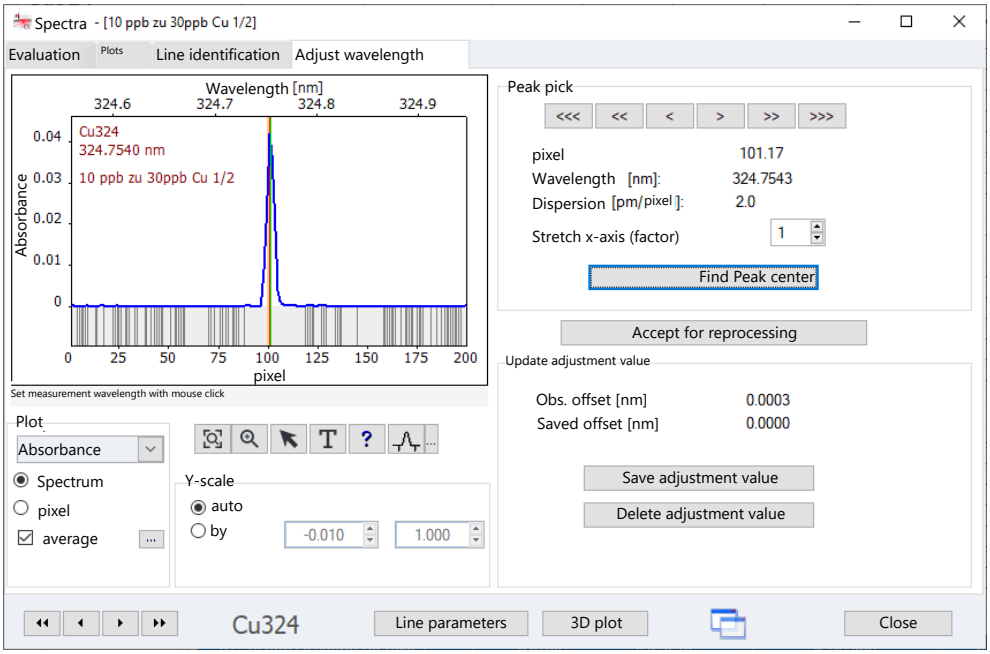
The top list shows the line database entries found in the current spectral range. Selecting a line sets the graph cursor to the wavelength of the line.

Clicking or dragging with the mouse searches the line database for element lines at the selected wavelength position. The element symbol is displayed next to the mouse pointer and the corresponding list entry is highlighted.

The bottom list shows the molecular bands found in the displayed spectral region. Selecting a line in the list displays the corresponding molecular spectrum. You can enter a value in the **Factor** table column by which the displayed spectrum is multiplied. The molecular band spectrum is compressed or stretched accordingly. An **Offset** shifts the spectrum by the value along the y-axis. The **Show sum spectrum** option activates an additional list column for displaying the sum of several spectra. This can also be used to explain complex background spectra.

6.9.2.5 Correcting peak offsets

The contrAA is pre-calibrated on delivery, i.e. frequently used analysis wavelengths have been checked and adjusted at the factory. If you use less common analysis wavelengths, you can check the correctness of the analysis wavelength in the **Spectra** / **Adjust wavelength** window. You can correct peak positions in the subpixel range, i.e. smaller than the pixel dispersion.



The determined correction factors are stored in the line/wavelength file and are valid for every further measurement. However, any correction factors entered can also be deleted from this file.

Peak pick

Option	Description
Arrow keys	Shift peak wavelength
pixel	Currently selected pixel
Wavelength	Current analysis wavelength
Dispersion	Spectral resolution in picometers per pixel
Stretch x-axis (factor)	Stretch spectrum
Find Peak center	Automatically search for peaks and correct offset
Accept for reprocessing	During reprocessing, the changed wavelength offset is taken into account when calculating the peak position.

Wavelength offset

Option	Description
Obs. offset [nm]	Newly determined offset
Saved offset [nm]	Previously saved offset
Save adjustment value	Save new offset in a line/wavelength file The values stored in this file are used for all subsequent measurements. **Note**: Only click the **Save adjustment value** button once.
Delete adjustment value	Delete the entry for the current analysis wavelength in the line/wavelength file.

Checking and remeasuring the peak offset

- Set the analysis wavelength in the **Spectrometer** / **Parameters** window and start measuring the peak.
  The measurement results are displayed in the **Spectra** / **Adjust wavelength** window.
- By entering a factor in the **Stretch x-axis (factor)** field, you can stretch the spectrum until the peak curve is clearly visible.

- If the peak is centered on the analysis pixel 101 (red line coincides with the peak), the peak is detected correctly. In this case, no further action is necessary.
- If the peak is next to the red line, click on **Find Peak center**.
  Alternatively, move the red line to the peak using the arrow keys.
- Click **Save adjustment value** to save the new peak offset. (Only click the button once!)
- Start a measurement at the analysis wavelength in the **Spectrometer** / **Parameters** window.
- In the **Spectra** / **Adjust wavelength** window view, the peak must now be centered on the analysis pixel 101.
  - ✓ The new data are stored in the line/wavelength file and are used for future analyses.

See also

- Exporting line/wavelength files [▶ 158]
- Measuring spectra peak at a selected wavelength [▶ 115]

6.10 Solid analysis with graphite furnace technique

In the solids analysis the fixed samples are introduced into the graphite tube on a graphite platform and atomized. Sample digestion can be omitted. In comparison to the settings for the solution analysis, for the solids analysis additional preparations or sample specifications are necessary:

- Dosing of the samples onto the platforms
- Pipetting of liquid components onto the sample platforms
- Establishment of the weighed portion
- Cleaning of the sample platforms by means of burning out
- Where appropriate establishing the tare of the platforms

These preparations for determining the weighed portion and loading the sample platforms can be carried out manually or processed automatically when using the SSA 600. When using an SSA 600 with liquid dosing unit the sampler pipettes modifiers and standards.

If the above actions have been performed before starting a sequence, the sequence will be executed automatically and without interruption.

6.10.1 Functions on the Solid tab

Sample preparation for the solids analysis occurs on the **Solid** tab in the main window. The tab shows a list with measurements to be carried out. The measurements of standard samples and samples defined in the sequence are broken down here into individual measurements (statistics runs) and the distribution of the samples on the platforms is defined.

Table elements

The table contains the following entries:

Option	Description
No.	Number of single measurement.
Seq/Row	Row number in the sequence

Option	Description
Depth at pos.	Positions of the sample platform on the SSA 600 tray From 1 to 42 for single-tray mode, from 1 to 84 for two-tray mode **Note**: Positions are assigned by the ASpect CS software! Samples must be distributed according to predefined positions.
Type	Sample type of the sample on this platform
Name	Sample scale
Line	Analytical line
#	Number of the statistics run
Wt.	Sample mass in mg If the entry "--------" is found in this column, the sample is not to be weighed and contains only liquid components (e.g. liquid standard). **Note**: Before determination of the weighed portion the tare of the sample platform must be established.
Tare	Mass of the empty platform in mg For samples that are not to be weighed, the entry "--------" is also shown here.
Dos.	Sample was dosed onto the platform, unless there is a "*" marker.
Std./Mod.	If marked with "*", this element indicates that liquid components (standards or modifiers) are dosed onto the platform.
Pretreat.	Only if thermal pretreatment is defined in the method If marked with "*", thermal pretreatment was carried out for the platform.

If known, the following settings can be directly entered at the sample table:
- Weighed portion if sample preparation occurred on external scales
- Deadweight (tare)
- Marking for completely dosed sample platform
- Marking for pipetted modifiers
- Marking for thermal pretreatment

Buttons for sample preparation

Buttons	Description
Tare	Determine the weight of the empty platforms for selected tray positions To do this, the platforms are transported to the scale and, after weighing, to their positions. The determined weight is entered in the **Tare** column.
Dosing	Move the platforms of the selected positions to the dosing position one after the other The dosing window appears with the information on which sample is to be dosed. Depending on what options were selected, more preparations can be made before or after this sample for marked positions. If a table already contains entries, related preparations will be skipped. Compliance with this order: Tare - Dosing - Weighing - (Dosing) - (Weighing) - Mod./Std Pipetting is compulsory. **with tare** Before dosing, the weight of the empty platform is determined. **with weighing** After dosing, the dosed sample is weighed. **with Mod./Std. pipetting** After weighing, the platform is taken to the liquid dosing station. If the **Weigh with confirmation** option is configured in the **Method** / **Sample transport** window, the "Dosing" and "Weighing" steps can be repeated as often as required.

Buttons	Description
	If all three options were set, this sequence may be used to run a complete sample preparation procedure. On completion of this sequence, the tray will contain filled platforms that are completely prepared for analysis. If one of the preparatory steps was not carried out, this step will be requested as part of the analytical procedure.
Weigh	Weigh dosed platforms
Load/Save	Save and reload weighing and dosing data of selected rows When changes are made to the sequence or method, the sample table is recreated on the **Solid** tab. The existing entries will be lost. This function can be used to recover and restore the data.
Std./Mod.	Successively transfers the platforms of selected positions into the position for dosing of liquid analytical constituents (liquid standards, modifiers) The window for liquid dosing appears. This screen shows the liquids to be dosed and the volumes to be dosed.
Prepare	Performs burning out or thermal pretreatment for platforms of the selected positions The platforms are placed in the furnace, the bake-out program is triggered and the platforms are returned to the tray as soon as the furnace has cooled down. During thermal pretreatment, the appropriate modifiers are first pipetted onto the platforms. Then the furnace program is run down to the "E/P" step. After the furnace has cooled down, the platforms are transported back to the tray. If the **Tare** option is activated, the empty platforms are weighed and their weight entered in the tare column.

Re-analyzing samples / correcting weight entries

Button	Description
Measure row(s)	Re-measure an element in a sample or measure a sequence row-by-row individually in method development When measuring the sample order row-by-row, the start must always be with statistics run 1 or the following run of the last measured statistics run.
Prepare re-measurement	Creates the current **Solid** tab of the statistics run to be remeasured from the entries for remeasuring selected in the results table. After this these sample platforms can be correspondingly dosed and weighed.
Re-measure single val.	Start measurement of the samples selected with the **Solid** function.
Delete entries	For selected table rows all entries in columns starting with column **Wt.** are deleted

6.10.2 Measuring solids samples

Manual solid analysis

If the samples are placed in the graphite tubes with the help of the manual autosampler SSA 6 (z), the weighed portion must be determined on a separate scale. In this case, enter the weights manually on the **Solid** tab.

Automatic solids analysis for non-time-critical samples

For non-time-critical samples, many preparation steps can be combined. The processing of non-time-critical samples is specified by deactivating the **Workflow for time critical samples** option in the **Method** / **Sample transport** window.

When using the SSA 600 with automatic liquid dosing, the dosing of modifiers and standards can take place during the processing of the sequence and does not have to be prepared manually. Up to four standards and three modifiers can be placed on the SSA 600. If more standards or modifiers are needed, they have to be pipetted manually. During thermal pretreatment, the modifiers are automatically applied to the platforms using the liquid dosing unit and then prepared for analysis in the graphite furnace.

Automatic analysis without operator intervention requires a sample platform for each individual measurement:

Total number of sample platforms = number of analysis samples x number of analysis lines x number of statistics runs

If the number of samples exceeds the number of platforms defined in the method, the platforms are re-dosed after processing.

- Create and activate a method and a sequence.
- Switch to the **Solid** tab in the main window.
  The **Pos** column shows the assignment of samples on the autosampler trays. The assignment is determined by the software and cannot be changed.
- Click on  in the toolbar to activate the method routine.
- Prepare the sample platforms according to the program instructions. Place the samples and pipette the liquid components.
  The measurement starts when all samples have been prepared or the number of sample platforms defined in the method have been filled.
- If there are still samples left after the first measuring run, select the corresponding sample rows in the sequence with the mouse. Hold down the Shift or Ctrl key to select several rows.
- Continue the measurement by clicking on  . Append the results to the existing ones by activating the **Append to file/list** option in the **Start Sequence** window.
- Prepare the sample platforms again according to the program instructions. Then the measurement starts automatically.

  ✓ The measurement results are displayed on the results tab of the main window.

Automatic solids analysis for time-critical samples

Samples that volatilize easily or "creep" out of the platform due to high adhesion and wet the edge and handle of the platform require rapid processing of the platform after sample application. The processing of time-critical samples is specified by activating the **Workflow for time critical samples** option in the **Method** / **Sample transport** window.

- Create and activate a method and a sequence.
- Switch to the **Solid** tab in the main window.
  The **Pos** column shows the assignment of samples on the autosampler trays. The assignment is determined by the software and cannot be changed.
- Click on  in the toolbar to activate the method routine.
- Follow the sample preparation instructions on the screen. A sample is prepared and measured. This is followed by a prompt to prepare the next sample platform until all samples have been processed.

The measurement procedure for time-critical samples requires the operator to be present at all times.

See also

Method parameters for autosampler for solids analysis [▷ 47]

6.10.3 Save data of previously prepared samples

When the sequence or method is modified the solid table is reconfigured and the samples are reassigned to the platforms. In order to prevent loss of existing weight data these data can be saved. These data can be stored to prevent this. Two storage areas for linked blocks are available for this purpose.

- Select the samples that have already been prepared.
  The samples must be in a contiguous block.
- Click on **Load/Save** on the **Solid** tab.
  The**Load/Save SSA600 table** window appears.
- Select one of the two storage locations there.
- Click on **Save selected entries** and confirm the subsequent message by clicking on **OK**.
- Close the **Load/Save SSA600 table** window by clicking on **Close**.
- After rebuilding the solids table, click on **Load/Save** again in the main window.
- Select the storage location in the **Load/Save SSA600 table** window.
- In the list field, enter the row number of the solids table from which the data block is to be inserted.
- Click on **Load entries starting from row number**.
  - ✓ The data block is inserted into the solids table starting from the specified row.

Then re-sort the platforms on the sample tray according to the solids table.

6.10.4 Re-analyze samples for solid analysis

Individual samples as well as individual elements can be re-analyzed when using solid analysis technique.

Repetition of single measurements (statistics runs)

When re-measuring, the solids table is restructured on the **Solid** tab. Existing dosing entries are deleted. If necessary, you should save the data of already prepared samples beforehand.

- Switch to the **Results** tab in the main window.
- Double-click on the sample with the outlier to open the **Single values** window.
- Mark the outlier in the table.
- Click on **Mark for re-measurement**.
- Close the **Single values** window.
- In the same way mark all additional outliers of other samples.
- Return to the **Solid** tab.
- Click on **Prepare re-measurement**.
  The solids table to be processed is created.
- Prepare the samples in accordance with the platform assignment for the analysis.
- Start the measurement by clicking on **Re-measure single val.**.
  - ✓ On the **Results** tab, sample results reprocessed based on the re-measured outliers are appended to the end of the table.

Re-analyze an element in a sample

- Select all individual measurements of the sample element in the solids table.
- Click on **Measure row(s)**.

- In the **Start Sequence** window, enter a new file name or activate the **Append to file/ list** option.
- Start the measurement by clicking on **OK**.

Measure the solid table by row (method processing)

In method development, the solids table can be processed row-by-row.

- Select the individual measurements of the sample element in the solids table.
- Click on **Measure row(s)**.
- In the **Start Sequence** window, enter a new file name or activate the **Append to file/ list** option.
- Start the measurement by clicking on **OK**.

Note: The measurement of an element of a sample must always be started with run #1 or the run that follows the last measured statistics run.

See also

Save data of previously prepared samples [▶ 103]

6.11 Washing the system

Wash steps are started for the various systems via the **Routine** | **Wash** menu item. In addition, rinse commands are accessible in the respective technique-specific windows such as for autosampler and hydride system.

Flame technique

The sampler tube is immersed in the rinse position and rinses the cannula. If the Injection Switch has been selected as accessory unit, the switch will open. This is to ensure that the sample path is rinsed, too. The rinse pump is continuously delivering fresh wash solution.

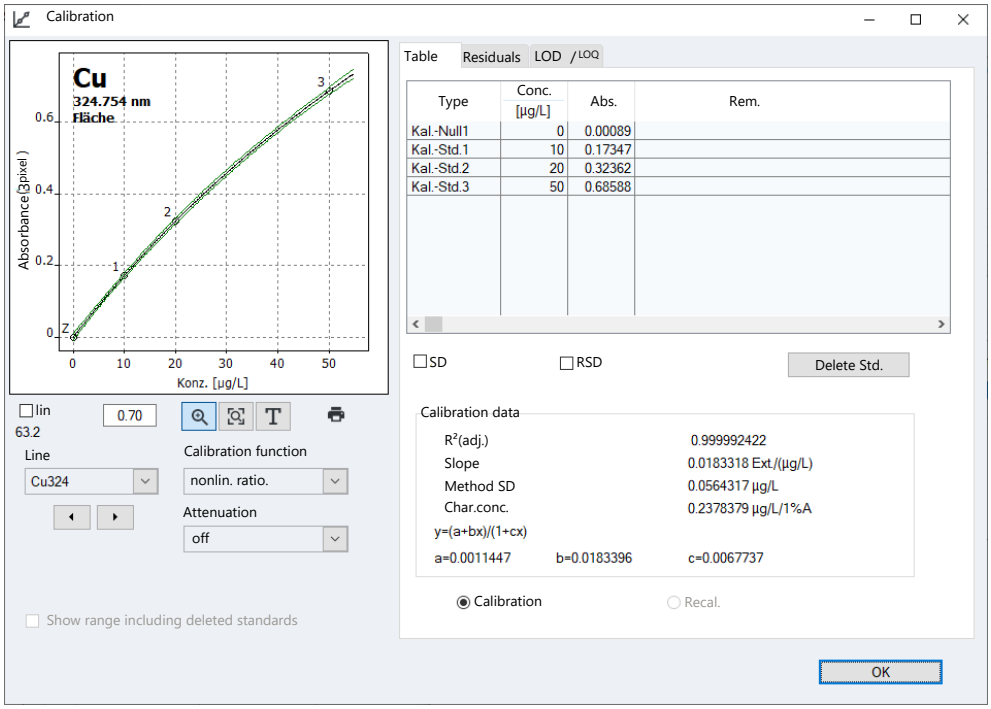
Hydride technique / HydrEA technique

The hydride system is rinsed with acid (or reductant, if necessary). The wash parameters for the hydride system are specified in the **Method** / **Hydride** window.

7 Calibration

Calibration is performed during the measurement according to the specified method parameters. The calibration curves and functions can be displayed and edited after the measurement.

Open the **Calibration** window by clicking on  or via the menu item **Method development** / **Calibration**.



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

- Graphical representation of the calibration curve
- Calibration table
- Parameter
- Residuals
- Limits of detection (LOD) and limits of quantitation (LOQ)

Selection fields in the Calibration window

Option	Description
Line	Select the analysis line whose calibration is displayed
Calibration function	Calibration function used The calibration function is set in the **Method** / **Calib.** window specifically for each element line. The function can be reselected in the list box and the results reprocessed accordingly.
Attenuation	Signal attenuation can extend the calibration range. The signal attenuation is defined in the **Method** / **Evaluation** window and can be varied here.
Show range including deleted standards	When standards are manually deleted, the calibration curve graph is adjusted to the new range. If the option is activated, the entire calibrated range is displayed.

See also

Method / Calibration window – Specifying calibration [▶ 50]

Method / Evaluation window – Specifying spectral range and background correction [▶ 49]

7.1 Showing the calibration curve

In the graph, the measuring points, the calculated calibration curve, and the residuals are displayed. The numbers at the measuring points correspond to those used on the Table tab. The calibration zero point has been identified with Z (Zero).

Color marking

Measuring points have been marked in the following manner:

Color	Meaning
Black	Normal measuring point
Light gray	Deleted/outlier (not included in calculation)
Blue	Suspected outlier (included in calculation)

The curves are also highlighted in color:

Graph color	Meaning
Black	Calibration curve within the valid calibration range
Blue	Calibration curve outside the valid calibration range
Green	Lower and upper limit of the prognosis range within the valid calibration range
Light gray	Lower and upper limit of the prognosis range outside the valid calibration range

Note on the prognosis or confidence range

The position of the prognosis range depends on the selected statistical certainty. It is a measure of the "quality" of the calibration, from which also the statistical certainty of the measurement of the analytical samples depends in the end. Besides, the prognosis range serves to identify suspected outliers among the calibration points. The confidence level is selected in the **Method** / **Statistics** window. The prediction or confidence band is selected in the **Options** / **Calibration** window.

Enlarge the calibration graph

After clicking on , you can enlarge a section of the calibration curve by holding down the left mouse button. Click on to reset the enlargement.

Insert remark

A text field for a remark can be inserted in the graph.

- Click on and hold to drag the frame for the text field on the graph.
- Enter the text in the input window and confirm with **OK**.
  - ✓ The text is displayed on the graph.

You can edit text after double-clicking on an existing text field.

Print calibration graph

Click to print the calibration curve and calibration data.

See also

Method / Statistics window – Specifying statistics parameters [▶ 56]
Calibration and blank correction options [▶ 169]

7.2 Displaying calibration results

The calibration results are displayed on the right-hand side of the **Calibration** window on three tabs.

Output of the measured values of the calibration standards – Table tab

The value pairs of the standards (entered concentration / measured value) are output on the **Table** tab of the **Calibration** window.

If a statistical evaluation has been specified in the method, the standard deviation (**SD**), relative standard deviation (**RSD**), the range (**R**) and the relative range (**R%**) can be output by activating the corresponding checkboxes.

To exclude individual calibration standards from the calculation, select the standard in the table with a mouse click and then click on **Delete Std.**. In multi-line methods, you are asked whether the standard should be deleted or reactivated for all lines or only for the current line.

The measurement is only marked as deleted and can be reactivated at any time.

This tab shows the calibration data as far as their calculation makes sense.

Parameter	Description
R^2(adj.)	Coefficient of determination
Slope	Slope of calibration curve
Method SD	Method standard deviation
Char.conc. / **Char.mass**	Characteristic concentration or mass (concentration or mass necessary to absorb 1% of the available light energy in the atomizer – equal to an absorbance value of approx. 0.0044)

Residuals tab

The graph on the **Residuals** tab shows the deviations of the calibration points from the calculated calibration curve and the limits of the prediction band.

Limits of detection and quantitation of the current calibration – LOD tab LOQ

The limits of detection and the limits of quantitation of the AAS can be determined based on the current calibration results. In this area, values of the blank method and the calibration curve method will be displayed only if the AAS has been calibrated already.

Parameter	Description
Limit of detection	The mass (concentration) of the element being analyzed that can be detected with a defined confidence level.
Limit of determination	The smallest mass (concentration) of the element being analyzed that can be determined with a defined confidence level.
SD Blank (DL)	Only blank method Measured standard deviation of the blank (IDL sample)
Compute	Start calculation of limits of detection and quantitation, e.g. after a change of the calibration curve

Calibration graph method

The calculation of the limits of detection and determination according to the calibration graph method necessitates a linear calibration graph. The calibration should be carried out in the lower concentration range. Calibration parameters that are essential for the result of computation include:

- Number and position of calibration points
- Number of repeat measurements per standard
- Quality of regression
- Slope of calibration curve
- Relative statistical certainty (probability level)

The values obtained from the calibration graph method can be considered useful only if the calibration was run in the lower concentration range.

Blank method

The standard deviation of the blank is determined within the sample measurement. For this purpose, the measurement of the blank (**QC blank DL**) is specified in the sequence.

Default calculation instructions for the blank method:

The blank is to be measured 11 x. From the obtained values, the absolute standard deviation SD of the blank is determined. The following formulas apply to the limits of detection and determination:

Limit of detection (LOD): LOD = 3 * SD / (slope of calibration curve)

Limit of quantitation (LOQ): LOQ = 9 * SD / (slope of calibration curve)

The number of measurement repetitions and the factors for calculating the limit of detection/limit of quantitation can be edited in the **Options** / **Calibration** window.

See also

- Specifying measurements and actions in a sequence [▶ 68]
- Calibration and blank correction options [▶ 169]

7.3 Modifying a calibration curve

You can modify an existing calibration curve in the Calibration window by:

- changing the calibration function used
- disabling/enabling standards

To change the calibration function, choose a new model from the calibration function list box.

To exclude a standard from the calculation, select it in the **Table** tab and then click on **Delete Std.**. The measurement is only marked as deleted and can be reactivated at any time.

The program recalculates the calibration curve and displays the modified curve. The changed calibration parameters are applied to the results when you start the reprocessing by clicking on  in the toolbar.

See also

- Reprocessing analysis results [▶ 80]

7.4 Replacing calibration standards by re-measurement

You can replace outliers in the calibration by measuring the sequence rows again, replacing the row in question and reprocessing the results:

- Provide the new standard to be measured. When using an autosampler, set the standard to the position specified in the sequence.
- Start the affected standard in the sequence and the measurement of the sequence row by clicking on  .
  The value of the newly measured standard appears at the end of the sample table.
- Double-click the standard you want to replace.
  The**Single values** window appears.

- Activate the **Replace with entry number** option and enter the row number of the re-measured value in the input field.
- Close the **Single values** window by clicking on **OK**.
- Start the recalculation by clicking on  and enter the rows that need to be recalculated.
  - ✓ When calculating the calibration, the affected standard is replaced by the new value. For all calculations following the recalculated calibration, the new calibration is applied.

8 Quality control

The Quality Control function serves to monitor the measurement results of a method over a longer period of time. For this purpose, specific QC samples of different types are chosen for a method and included in the measurement series. When evaluating the QC samples, the results are compared to those obtained with previous QC samples.

The evaluations are presented on quality control charts (QC charts) and saved along with the method. The QC charts are available after every loading of the method and will be updated at the next measurement start.

The type of QC samples and their parameters can be set in the **Method** / **QCS** window and in the sequence for carrying the QC sample within the measurement series.

You can view the QC charts of the loaded (active) method in the **QC** window. There, you can also define the parameters and the configuration of the QC charts.

Open the **QC** window by clicking on  or via the menu item **Method development** / **QC**.

8.1 Displaying QC charts

The QC charts are displayed in the **QC** / **QC chart** window. Separate charts are generated each for every QC sample type defined in the method and for every element line specified there.

Option	Description
Type	Select QC sample type to be displayed
Line	Select analysis line to be displayed
Displayed values	Number of displayed values and the date of the first and the last value displayed.
Entries	Total number of entries on the current QC chart and the date of the first and the last value.
x(max)	This number of entries is shown in the graph.
	Print QC graph including alphanumeric data and measured values

Graph area

Color	Description
Yellow field	Preparation period
Light gray horizontal line	Mean value calculated from preparation period
Red horizontal lines	Upper and lower control limit (C) calculated from preparation period (3 Sigma)
Green horizontal lines	Calculated warning limits (W; 2 Sigma).
Small black circles	Measuring points

If you click on a measured value in the graph, a window opens with the following information about this measured value:

Option	Description
Number	Number of the measured value in the QC series

Option	Description
Value	Measured value (converted according to the presentation type of the QC chart)
Date/ Time	Measuring time
Operator	Operator logged in at the time of the measurement
Version	Version of the method used
Delete entry / **Activate entry**	Select measured value as deleted or reactivate it
Add comment	Enter a comment for the measuring point, e.g. reason for deletion

8.2 Parameters of QC charts

The type and display of the QC charts is defined in the **QC** / **QC chart parameters** window.

Chart type

The following evaluations can be selected for the different QC sample types:

QC sample type	Type of QC evaluation
QC sample	**Mean chart**
QC std.	**Mean chart (norm.)**
	Recovery
QC trend	**Trend**
QC matrix	**Ranges**
	Precisions
QC blank	No selection provided. The absorbance of the blank is displayed.

For the **QC charts** chart type (process control chart), the target parameters and the control (C) and warning (W) limits are determined from the mean value and the scatter of the values of the previous period. For the **Target value chart** type, the target values and exclusion limits are determined from the expected values and limits of the quality control samples specified in the **Method** / **QCS** window.

Graphic setting

In this field, you can choose the point size used for the graph, and if the points shall be connected with each other by a line.

Option	Description
Point size	The individual points are displayed as circles. Choose a higher point size for larger circles.
Connect points	The graph points are connected with a polygon course.

8.3 Entries and limits of the QC charts

The content of the QC charts is defined in the **QC** / **Entries and Limits** window and can be adapted to the requirements of the respective laboratory with regard to the frequency of the entries.

Option	Description
Entry scheme	Selection of the values transferred to the QC charts

Option	Description
	all values Enter each QC check performed. **1 value/day** Enter only the last QC check of the day. **2 values/day** Enter only the first and last QC checks of the day. Definition of "day": One "day" corresponds to one day according to the PC clock. In the course of a day, any previous entry on the QC chart will be overwritten by a new QC value; however. When a new day begins, a new entry will be generated.
Number prep. period	Only **Control chart** (process control chart) The previous period is a number of QC chart entries used to calculate the control (**C**) and warning (**W**) limits. The preparation period always contains the older chart entries. If set to 0 (no prep. period), all entered QC data will be included in the calculation of control and error limits.
Factor	Only **Target value chart** The exclusion limits are calculated from the limits specified for the quality control samples multiplied by the factor (default is 1).

Renewing charts

When a displayed chart is (almost) full, i.e. the maximum number of entries has been reached, it can be renewed. There are several ways to renew the previous period for control charts.

Option	Description
Accept prep. period, delete remain	Accepts the preparation period of the old chart for application to the new chart and deletes remaining values.
Last values -> new prep. period	The values of the old chart measured last represent the preparation period of the new chart; all other values will be deleted from the chart. New measured values will be evaluated based on the newly created preparation period.
Delete all, new prep. period	All values will be deleted. New measured values will first fill the preparation period.
Process	Renew charts according to the selected option

9 Controlling and monitoring spectrometer and accessories

9.1 Spectrometer

In the **Spectrometer** window, you can check optical instrument functions and calibrate the spectrometer with software support (correct offsets). The following parameters can be set or output:

- Device data
- Switching the xenon lamp on and off
- Test of wavelength corrections
- Display of the readout parameters of the CCD line
- Start a measurement on a test wavelength
- Start continuous measurement for device optimizations
- Correct peak offsets

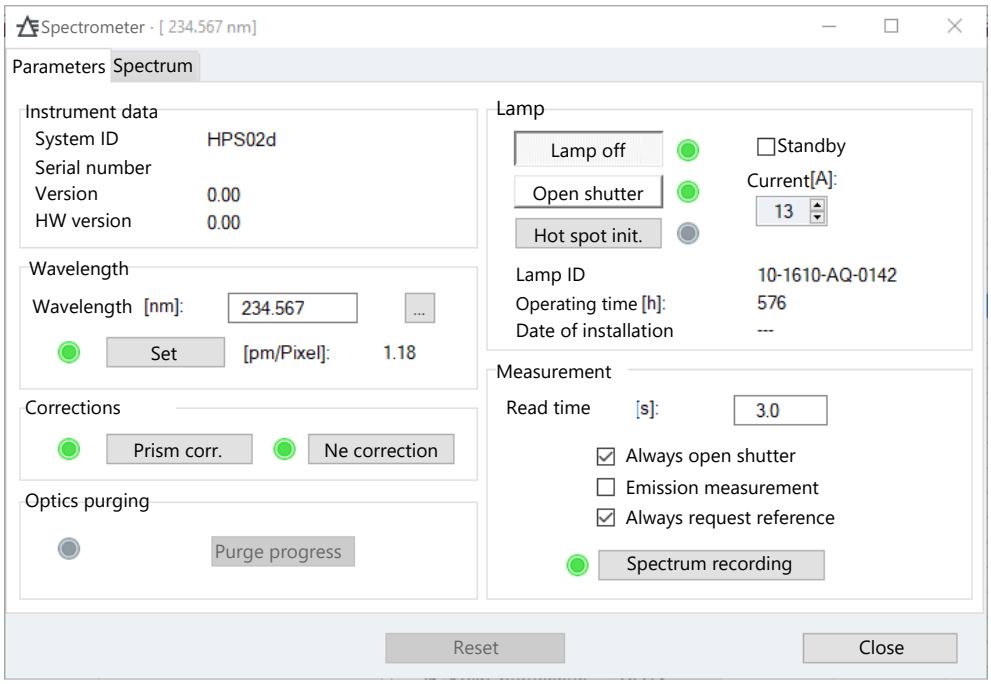
Open the **Spectrometer** window by clicking on  or via the menu item **Method Development** / **Spectrometer**.

9.1.1 Device function test on the contrAA

In the **Spectrometer** / **Parameters** window, you can check basic device functions and start a test measurement at a selected wavelength.

Essentially, when the contrAA is switched on and initialized, all indicator lamps must be active and green. Clicking on a button tests the corresponding device function. If the test is successful, the indicator light turns green.

Click on  to open the **Spectrometer** / **Parameters** window.



Instrument data

Display of the connected AAS and the installed software version.

Wavelength / Corrections

Option/button	Description
Wavelength	Display of the selected wavelength Click on ••• to open the **Select Element/Line** window for selecting the wavelength. Clicking on **Set** moves the monochromator to the selected wavelength.
Prism corr.	Check prism position and adjust automatically if necessary
Ne correction	Check wavelength correction with neon lines

Optics purging

contrAA 800 only

Click on **Purge progress** to check the status of the gas purging (air or argon purging). For reliable measurement results, purging must be completed (green status LED). This button is only active if optics purging is activated in the **Options** / **Optics purging** window.

Lamp

Option	Description
Lamp off / **Lamp on**	Switch xenon lamp off and on
Open shutter / **Close shutter**	Open and close shutter
Hot spot init.	Reinitialize system for hot spot tracking
Standby	When activated, the lamp current goes into standby mode. This extends the service life of the lamp.
Current	Change lamp current Only change this parameter after consulting the Service department. The default lamp current is optimized for ignition reliability and service life.
Lamp ID	Lamp identification code
Operating time	After the guaranteed 1000 h operating time has been exceeded, a corresponding message is displayed.
Date of installation	Date of the last lamp change If the lamp has not been changed, no date is displayed here.

Note: Information about the installed lamp is only displayed if the **Show lamp operating lifetime (spectrometer)** option is activated in the **Options** / **View** window.

Measurement

Option	Description
Read time	Total time for spectrum measurement
Always open shutter	When activated, the measurements in the **Spectrometer** window are always performed with the shutter open. If the system is to be tested with the shutter closed, e.g. when measuring the dark current, this option must be deactivated. **Note**: The shutter setting in this window does not affect the measurements outside this window. In all other cases, the shutter is controlled automatically.
Emission measurement	When activated, the intensity spectrum is measured. If this function is deactivated, the absorbance spectrum is displayed.
Always request reference	Perform a reference measurement before a spectrum measurement.
Spectrum recording	Start measurement of the spectrum with set parameters

See also

- Options for optics purging [▶ 169]
- View options [▶ 164]
- Inserting analysis lines into the line table [▶ 26]

9.1.2 Measuring spectra peak at a selected wavelength

You can start a test measurement at a selected wavelength in the **Spectrometer** / **Parameters** window.

- Provide a reference solution and a test solution with the analyte.
  Instructions for the test solution can be found in the cookbook.
- Click on  to open the **Spectrometer** / **Parameters** window.
- Under **Wavelength**, click on ••• and select the line in the **Select Element/Line** window.
  Alternatively, enter the value of the wavelength directly into the input field
- Click **Set** to set the wavelength.
  When the setting is completed successfully, the marker next to the setting turns green.
- Set the total measuring time in the **Read time** field.
- Activate the **Always request reference** option.
- Click on **Spectrum recording** and follow the instructions for the reference measurement and subsequent sample measurement.
  - ✓ The measurement results are displayed in the **Spectra** window.

In the **Spectra** / **Adjust wavelength** window, you can correct a peak offset.

See also

- Device function test on the contrAA [▶ 113]
- Correcting peak offsets [▶ 97]

9.1.3 Continuous measurement

In the **Spectrometer** / **Spectrum** window, start a continuous measurement at a specified wavelength. The continuous measurements are used for device optimization during service.

Open the **Spectrometer** / **Spectrum** window by clicking on  .

Graphical display and digital evaluation in the Spectrometer / Spectrum window

Option	Description
Display	Options for displaying the spectrum **Energy** Display of the energy spectrum, unit of measurement: cts (counts) In order to obtain measurement results with as little noise as possible, the integration times for the CCD line are selected so that the energy maximum is approx. 30000 cts. **Absorbance** Display of the absorbance spectrum

Option	Description
	Intensity Display of energy per time unit, unit of measurement: Mcts/s (mega-counts per second) With the output of the intensity, you can compare different peaks with regard to their absorption independent of the integration time.
Meas.pix.	The values of this pixel are displayed continuously according to the selected view. The **Maximum**, **Minimum**, **Mean** and **SD** fields display the results of the continuous measurement.
Burner height	For flame technique Burner height setting
Mark meas. pixels	Select the measuring pixel in the graph with a vertical red line
Mark mode	Select measured values for each pixel in the graph with a dot
Graph scaling	Enter values for the start and end points of the ordinate and abscissa directly in the input fields on the axes or, after activating zoom mode, select the area to be displayed by holding down the left mouse button. Undo scaling by activating the **auto** option
[Ref. spectrum]	Record reference spectrum
[Start]	Start continuous measurement

Starting a continuous measurement

The measurement is carried out manually without an autosampler. Attach the sample aspiration tube to the nebulizer cannula.

- Provide a reference solution and a test solution with the analyte.
  Instructions for the test solution can be found in the cookbook.
- Click on  to open the **Spectrometer** window.
- Set the wavelength on the **Parameters** tab.
- Switch to the **Spectrum** tab.
- Start the reference measurement with the reference solution by clicking on **[Ref. spectrum]**.
  If a reference spectrum is already present, the indicator lamp is green.
- Immerse the sample aspiration tube in the test solution. Click on **[Start]**.
  ✓ The measurement is performed continuously until you press **[Stop]**.

9.2 Flame

In the **Flame** window, you can check individual functions of the burner/mixing chamber/nebulizer system and set the parameters for the analysis of the individual elements individually.

Open the **Flame** window by clicking on  or via the menu item **Method Development** / **Flame**.

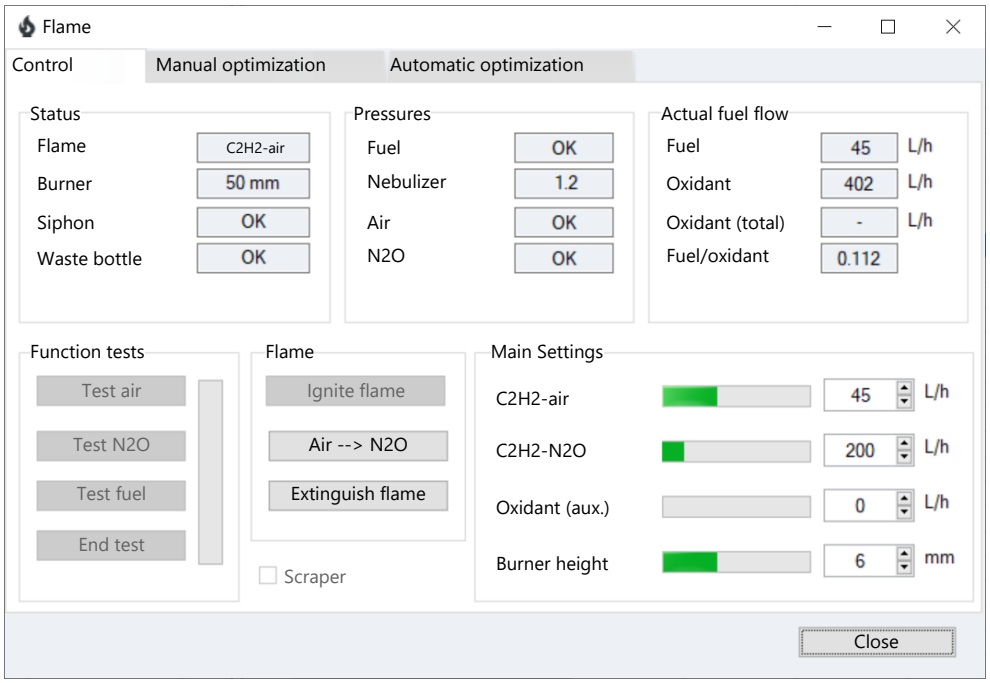
9.2.1 Testing flame functions

The **Flame** / **Control** window contains the following functions:

- Ignite/extinguish flame
- Switch air or nitrous oxide as oxidant

- Display of gas pressures and gas flows
- Activate scraper
- Setting the gas flows

Open the **Flame** / **Control** window by clicking on  .



Status

Option	Description
Flame	**off**: The flame is not burning. **C2H2-air**: The acetylene-air flame is burning. **C2H2-N2O**: The acetylene-nitrous oxide flame is burning.
Burner	Display of the installed burner **Error**: No burner is installed or the burner was not detected by the sensor.
Siphon	The level of the mixing chamber siphon, through which non-atomized liquid is discharged, is monitored. The siphon must always be sufficiently filled with liquid to prevent the flame from flashing back, especially the nitrous oxide flame. **OK**: The siphon is filled with liquid up to the overflow. **Error**: The level of the siphon is insufficient. Fill the siphon with deionized water up to the overflow. Remove the burner and carefully pour the water into the burner neck until it drains through the waste hose.

Pressures

Option	Description
Fuel	Status of the fuel gas pressure at the device inlet
Nebulizer	Operating pressure at nebulizer.
Air	Status of the air inlet pressure The status is only displayed when the air supply is open.
N2O	Status of nitrous oxide inlet pressure The status is only displayed when the nitrous oxide supply is open.

Actual fuel flow

Option	Description
Fuel	Fuel gas flow (C_2H_2)
Oxidant	Oxidant flow through nebulizer
Oxidant (total)	Total oxidant flow (oxidant + auxiliary oxidant) The value is only displayed if the auxiliary oxidant is activated.
Fuel/oxidant	Ratio of fuel flow to oxidant flow

Function tests

The test functions are accessible only if the flame is extinguished. The availability of the test functions depends on the context.

Button	Description
Test air	Open solenoid valve in air path Prerequisite: Air inlet pressure and fuel gas are present. The nebulizer pressure, oxidant flow and total oxidant are displayed if auxiliary oxidant is activated in the **Method** / **Flame** window.
Test N2O	Only acetylene nitrous oxide flame with 50 mm burner Open the solenoid valve in the nitrous oxide path Prerequisite: Nitrous oxide inlet pressure and fuel gas are present. Displays nebulizer pressure and oxidant flow and total oxidant (when the auxiliary oxidant is activated).
Test fuel	Set target gas flow (proportional valve) Displays fuel gas flow for the acetylene-air flame (with **Test air**) or the acetylene-nitrous oxide flame (with **Test N2O**). Either **Test air** or **Test N2O** must be activated before you click on **Test fuel**.
End test	Finishes the test function

Flame / Scraper

Option	Description
Ignite flame	Ignite acetylene-air flame ■ Ignition arm swings out; filament lights up. ■ Acetylene target gas flow (proportional valve) is adjusted when nebulizer pressure and oxidant flow have reached their setpoints. ■ If the flame does not ignite within 10 s, the ignition attempt is aborted. ■ If the flame is burning, **Extinguish flame** becomes active.
Air --> N2O	Switch from acetylene-air to acetylene-nitrous oxide flame. ■ Oxidant valve (3/2 solenoid valve) switches from air to nitrous oxide ■ Fuel gas flow for acetylene nitrous oxide flame (proportional valve) is set. ■ The button changes to **N2O --> air.**
N2O --> air	Switch from acetylene-nitrous oxide to acetylene-air flame ■ Fuel gas flow for acetylene-air flame (proportional valve) is set. ■ The button changes to **Air --> N2O.**
Extinguish flame	Extinguish the flame ■ When the acetylene-nitrous oxide flame is burning, switch to acetylene-air flame and wait a few seconds. ■ The fuel gas flow (proportional valve) is shut off. ■ After a few seconds of waiting (to expel the fuel gas from the mixing chamber and burner), air (solenoid valve) is shut off

Option	Description
Scraper	Only 50 mm burner with mounted scraper and acetylene-nitrous oxide flame Activate scraper for cleaning the burner head

Settings

You can edit the gas flows in the **Settings** group.

Option	Description
C2H2-air	Acetylene-air flame (fuel gas flow = 40–120 NL/h)
C2H2-N2O	Acetylene-nitrous oxide flame (fuel gas flow = 120–315 NL/h)
Oxidant (aux.)	Setting of the auxiliary oxidant flow
Burner height	Height of the burner relative the optical axis

Note: The attached burner is automatically detected by the burner sensor. Switching between C2H2-air and C2H2-N2O is only possible when the flame is burning and the 50 mm burner is installed.

See also

Method / Flame window – Specifying flame parameters [▶ 29]

9.2.2 Optimizing the flame

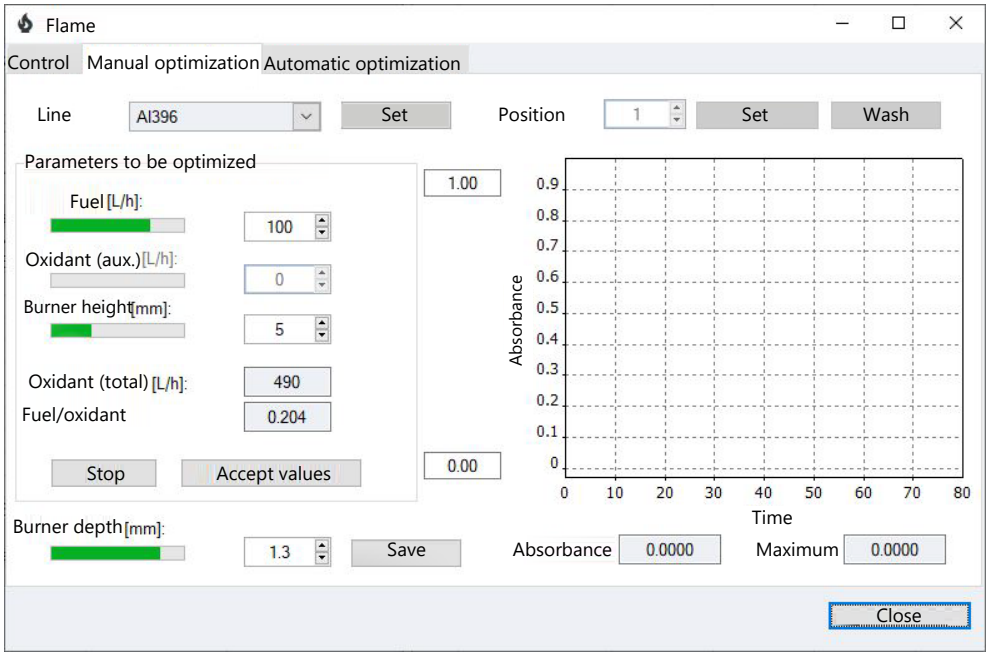
The optimum burner height as well as the gas composition of the flame strongly depend on the analyte. Therefore, you should fine-tune the values given from the cookbook once for each element. You can perform the optimization manually by changing the parameters and observing the signal curve. Use the manual optimization even if you have activated auxiliary oxidant in the method. If you are not use an auxiliary oxidant, you can have the flame parameters optimized automatically.

9.2.2.1 Manual flame optimization

You can perform manual flame optimization for an analysis line of the current method in the **Flame** / **Manual optimization** window. Manual optimization is required in the following situations:

- Use of auxiliary oxidant
- Optimization of the burner/mixing chamber/nebulizer system after cleaning the system

Click on  to open the **Flame** / **Manual optimization** window.



Option	Description
Line	Select analysis line of the method
Set	Set selected analysis line
Position	Position of the test sample on the autosampler
Set	Immerse the cannula of the autosampler in the test sample
Wash	Take up cleaning liquid from the wash cup
Fuel	Adjust the fuel gas flow
Burner height	Adjust the burner height relative to the optical axis of the beam path of the lamp
Oxidant (aux.)	Set auxiliary oxidant flow Air: 75 / 150 / 225 NL/h N_2O: 60 / 120 / 180 NL/h
Oxidant (total)	Display of the total oxidant flow
Fuel/oxidant	Display of the ratio of fuel gas flow to oxidant flow
Burner depth	Only contrAA 800 D Adjust burner depth
Start	Start measurement and record signal continuously
Stop	End the measurement
Accept values	Transfer determined flame parameters for the analysis line into the method
Graph	Display of signal curve
Absorbance	Current absorbance value
Maximum	Maximum absorbance value during the current measurement

Manual optimization with setting of auxiliary oxidant

- Ready the test solution.
  Instructions for the appropriate test solution can be found in the cookbook. The test concentration given there causes an absorbance of approx. 0.1. Use 2 to 3 times concentration for optimization.
- Select an analysis line from the **Line** list.
- Click on **Set** to move the monochromator to the wavelength of the line.

- Immerse the sample aspiration tube of the nebulizer in the test solution.
- If using the autosampler, place the sample on the autosampler and enter the position in the **Position** field. Then click on **Set**.
  The cannula is immersed in the test solution and the sample is aspirated.
- Start the measurement by clicking on **Start**.
- Perform optimization steps:
  Note: There is a small delay between the modification of the parameters and the signal response.
  - Use the arrow keys to change the fuel gas setting and observe the signal curve in the graph and in the **Absorbance** field. Set the maximum absorbance.
  - Change the burner height in the same way until the absorbance maximum is found.
  - If using auxiliary oxidant, change the **Oxidant (aux.)** parameter until the signal maximum is also set here.
  - Only contrAA 800 D: In addition, the depth setting of the burner can be optimized in the Burner depth field.
- Repeat the optimization steps until there is no relevant increase in the signal.
- End the measurement by clicking on **Stop**.
- Click on **Accept values**.
  ✓ The parameters for the selected analysis line are transferred to the method.

In the same way, find the appropriate parameters for all lines in the method.

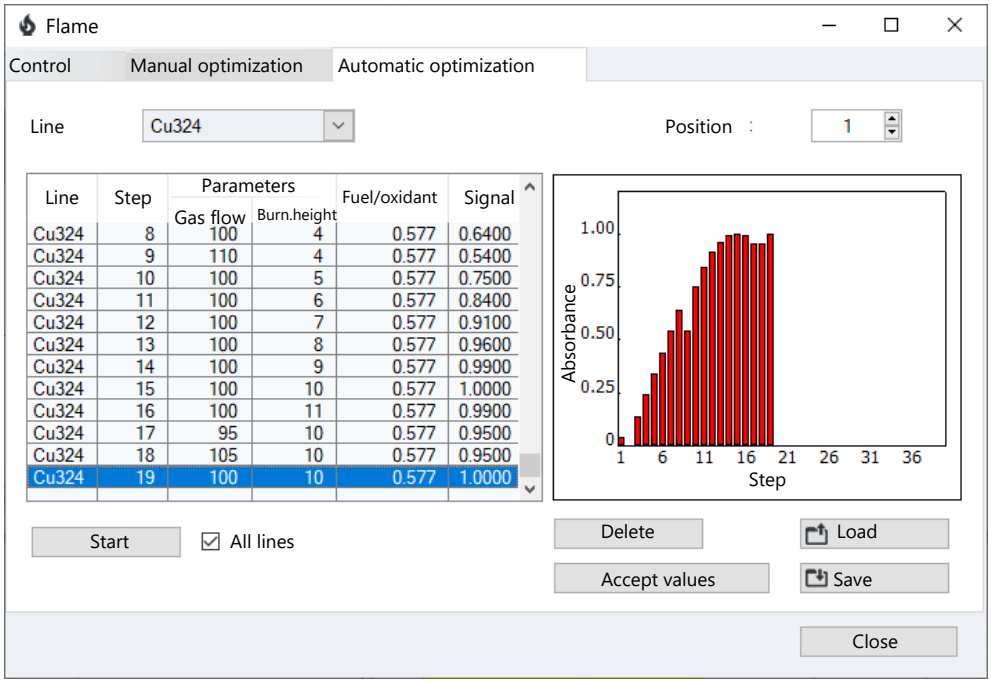
See also

Method / Flame window – Specifying flame parameters [▶ 29]

9.2.2.2 Automatic flame optimization

Automatic flame optimization is carried out in the **Flame** / **Automatic optimization** window. The optimization algorithm used changes the settings for fuel gas flow and burner height with the aim of gaining useful signal until a maximum is reached or a change in the parameters has no further effect on the useful signal. You can transfer the determined flame parameters to the method or save them and use them for other methods at a later time.

Open the **Flame** / **Automatic optimization** window by clicking on  .



Option	Description
Line	Select the analysis line of the method
Position	Position of the test sample on the sample changer
Start	Start measurement and record signal continuously
All lines / **all principal lines**	Perform optimization for all lines of the method with one sample solution In this case, the sample solution must contain all the elements of the method. If the method contains element lines that are measured simultaneously (principal lines specified in the **Method** / **Lines** window), the selection of lines to be optimized can be limited to **all principal lines**.
Delete	Delete determined values
Load	Load saved flame parameters
Save	Save optimized flame parameters
Accept values	Transfer the determined flame parameters for the set element line into the method
Table	Display of found parameters.
Graph	Display of signal curve

Procedure

- Ready the test solution.
  Instructions for the appropriate test solution can be found in the cookbook. The test concentration given there causes an absorbance of approx. 0.1. Use 2 to 3 times concentration for optimization. If you want to automatically optimize all analysis lines/principal lines, the test solution must contain these elements.
- Select an analysis line from the **Line** list or activate the **All lines** / **all principal lines** option.
- When using the autosampler: Place the test solution on the autosampler and enter the position on the sample tray in the **Position** field.
  For manual measurement: Immerse the sample aspiration tube of the nebulizer in the test solution.

- Click on **Start**.
  The**Automatic optimization** window appears.
- If required, activate the following option:
  Automatically save optimization data: If activated, enter the file name in the **File name** field.
  Measure additional lines: Only for multi-line evaluations. If the option is activated, the lines measured in addition to the principal line are also displayed. However, only the optimization parameters of the principal line can be transferred to the method.
  Set optimized values automatically for the current method.: With automatic optimization of all lines of the method, activate this option because only the data of the last line is available in the buffer after the optimization is completed.
- Confirm the settings with **OK**.
- For single line optimization: If not specified before the optimization, transfer the parameters for the line to the method after successful optimization by clicking on **Accept values**.
  ✓ The flame parameters are optimized and the determined values have been updated in the method. You can load saved values at a later time and transfer them to another method.

See also

Method / Flame window – Specifying flame parameters [▶ 29]

9.3 Furnace

The following parameters are set or furnace functions monitored in the **Furnace** window:

- Parameters of the furnace programs used in the method
- Selection of modifiers
- Optimization of the atomization and pyrolysis temperatures during method development
- Coating of the graphite tube for the hydrEA technique
- Graphical representation of furnace program
- Checking the furnace functions

Open the **Furnace** window by clicking on  or via the menu item **Method Development** / **Furnace**.

Buttons in the window Furnace

Option	Description
Line	In this list field, select the analysis line for which the furnace parameters are displayed/varied.
[Check method parameters]	Transfer changes to the furnace parameters for the analysis line to the method.

9.3.1 Displaying the furnace program

The line-specific furnace program is displayed in the **Furnace** / **Furnace program** window. Select the line in the lower part of the window. The furnace program is created in the **Method** / **Furnace** window and can be edited here.

Open the **Furnace** / **Furnace program** window by clicking on  .

The parameters on display are:

Option	Description
Step	Step number in the furnace program
*	No function was assigned to this field so far.
Name	Name of furnace program step
Temp.	Target temperature in program step
Ramp	Heating rate/cooling rate in program step
Hold	Holding time of target temperature within program step
Time	Total duration of working step
Gas	Supply purge gas (**Purge**) and additional gas (**Add.**). Possible states **Stop**: No supply **Min**: Minimum feed rate (purge gas only) **Max**: Maximum supply rate
Inj.	Sample is injected into the furnace after this step.
E/P	Enrichment step (E = Enrichment) or thermal pretreatment step (P = Pretreatment) of the individual components

Use the **Check program** button to check the program for errors that make execution of the program impossible. If the program is correct, the indicator lamp next to the button lights up green. Otherwise, an error message indicating the incorrect step.

See also

Editing a furnace program [▶ 32]

9.3.2 Showing matrix modifiers, enrichment and pretreatment

In the **Furnace** / **Modif.Extras**, window you can view the following line-specific parameters for atomization in the graphite furnace:

- Use and volume of matrix modifiers
- Enrichment in the graphite tube through repeated pipetting and drying
- Thermal pretreatment of the sample

Click on  to open the **Furnace** / **Modif.Extras** window with the view of the matrix modifiers.

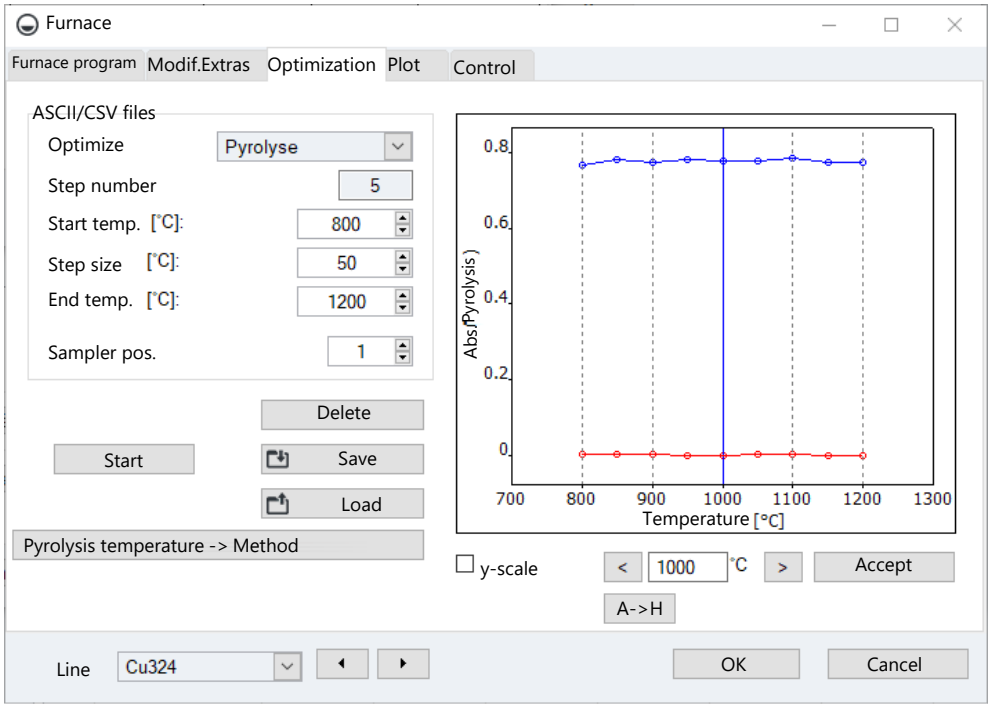
See also

Specifying matrix modifiers, enrichment, and pretreatment [▶ 35]

9.3.3 Optimizing the furnace program

In the window **Furnace** / **Optimization**, the optimum pyrolysis and atomization temperature for an element line is determined and set by carrying out a series of measurements with increasing step end temperatures. Once optimized, furnace parameter settings for atomization and pyrolysis can be saved and loaded to other methods.

Open the **Furnace** / **Optimization** window by clicking on  .



Parameters and control buttons

Option	Description
Optimize	Selects parameter for optimization: **Pyrolysis** or **Atomize**
Step number	Number of the selected step in the furnace program
Start temp.	The lowest end temperature of the furnace program step to be optimized within the measurement series.
Step size	The temperature of the step to be optimized is incremented by this amount for each measurement run.
End temp.	Highest final temperature of the step to be optimized within the measurement series **Note**: Available for selection are only such parameters which make sense for the particular furnace program.
Sampler pos.	The sample with which the optimization is carried out is located on this position of the autosampler.
Start / **Stop**	Automatically create a sequence for the optimization measurement Start/stop optimization
Delete	Delete determined values
Save	Save optimized furnace parameters
Load	Load saved furnace parameters
Pyrolysis temperature -> Method / **Atomization temperature** -> **Method**	Validates and transfers obtained values into currently selected furnace program.

Results display

The results of optimization can be displayed in a results window.

The graphical progression of the optimization is displayed on the right-hand side of the window. The curves of the autozero values and the absorbance are shown.

Option	Description
Red line	Background signal that depends on pyrolysis or atomization temperature

Option	Description
Blue line	Specific absorption depending on pyrolysis or atomization temperature
Vertical cursor	Selected optimum pyrolysis or atomization temperature
y-scaling	Scale the view to the background signal
A->H/H->A	Switch between display of signal area (A = Area) and signal height (H = Height)
< / >	Move the vertical cursors for the pyrolysis or atomization temperature to the left or right to set the desired optimum furnace temperature

Performing optimization

An autosampler is required to perform this series of measurements.

Program step	Optimization goal
Pyrolysis temperature	No specific absorption losses and minimal background signal
Atomization temperature	A constant specific absorbance

- Create and save a method with a furnace program for the analysis line.
- Click on  to open the **Furnace** / **Optimization** window.
- Enter the optimization parameters (see above).
- Prepare the sample on the autosampler.
- Start the optimization by clicking on **Start**.
  The optimization runs automatically.
  The measurement results are displayed in the main window and shown graphically in the **Furnace** / **Optimization** window.
- Display the sample single values by clicking on the measuring point in the graph or by double-clicking on the sample line in the main window.
- Move the vertical cursor to the optimum temperature using the < / > buttons or the arrow keys.
- Click on **Accept**.
  ✓ The optimized temperature is transferred to the furnace program.

Repeat this procedure for all other analytical lines included in the current method.

9.3.4 Displaying furnace program graphically and coating the graphite tube

The **Furnace** / **Plot** window contains the following functions:
- Graphical representation of furnace program
- Monitoring execution of current furnace program
- Coat graphite tube with iridium or gold for the hydrEA technique.

Graphical representation of furnace program

The furnace program is displayed as a graph in the temperature-time coordinate system.

Option	Description
Black line	Programmed temperature-versus-time graph
Red line	During a test of the processed part of the furnace program, a red line (realized temperature-time run) is superimposed on the black line.
Inj.	The injection step is marked with the flag **Inj.** above the diagram.
Green bar	The enrichment phase is indicated by a green horizontal bar.

Option	Description
Yellow-brown bar	Autozeroing (AZ*) is marked by a yellow-brown vertical bar.
Light pink bar	The integration step (measured value acquisition) is marked by a light pink vertical bar.

Testing furnace program in trial run

Execution of the current furnace program is checked in a test run, the process is displayed graphically. While this trial run is going on, temperature and time values will be displayed, but no sample will be injected.

- Start the test run by clicking on **Start**.
  The run is shown in the graph. The **Furnace program** window with the following values also appears:

Option	Description
Step	Furnace program step being performed
Temp.	Current furnace temperature
Time	Time elapsed since program start
Ramp	Current heating rate
Gas	Current gas flow

Graphite tube coating

The HydrEA technique requires a graphite tube coated with iridium or gold. Coating is controlled in the **Furnace** / **Plot** window.

If the **Graphite tube coating** checkbox is activated, the input parameters for this procedure are enabled.

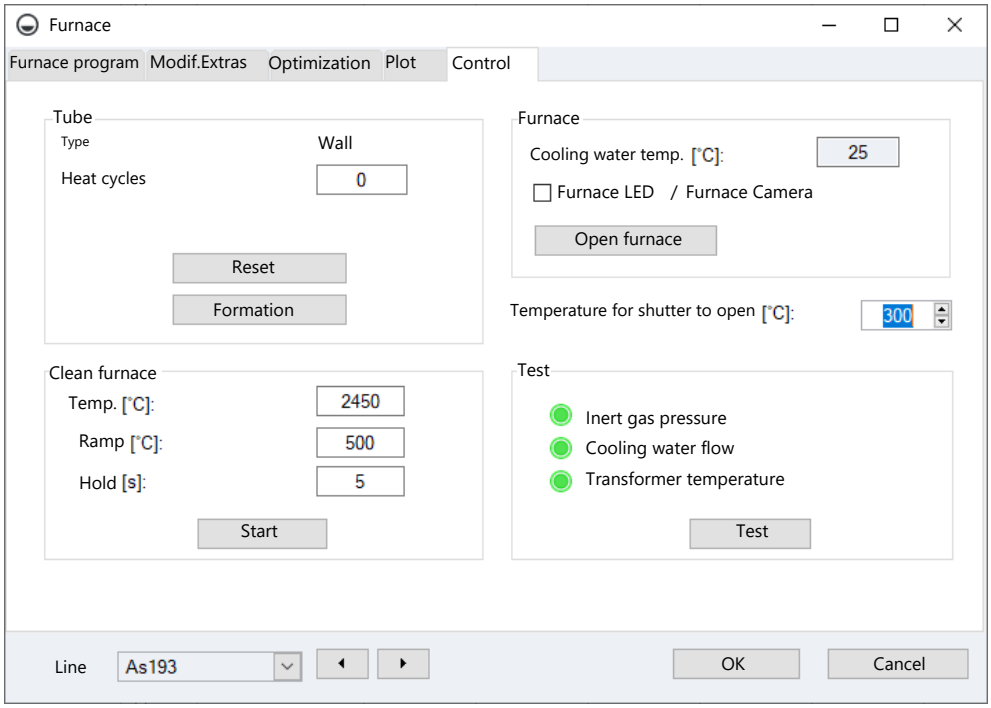
Option	Description
Cycles	Number of enrichment cycles for coating
Position	The sample tray position that contains solution for coating
Vol.	This volume of coating solution is pipetted into the graphite tube at each enrichment step.
Element	Selection of the coating material Use iridium (Ir) for hydride former analysis and gold (Au) for mercury analysis.
Start	Start coating

Note: A detailed description of the coating process can be found in the operating instructions for "HS 60 modular" and "HS 55 modular".

9.3.5 Further furnace functions

The **Furnace** / **Control** window contains the following functions:

- Information relating to the graphite tube
- Formatting the graphite tube
- Baking (cleaning) of graphite tube
- Opening / closing of graphite tube
- Indication of current cooling water temperature



Graphite tube data

The **Tube** area contains information about the graphite tube, which is entered when the tube is changed and then automatically updated.

Option	Description
Type	Tube type according to setting in the window **Quick Start**
Max. heating cycles	Number of heating cycles of this tube

Note: If you remove a graphite tube that is still usable, make a note of the data and enter the data when you reinsert it. The data can then be updated automatically. If you insert a new tube, reset the data by clicking on **Reset**.

Formatting the graphite tube

Formatting the graphite tube performs the following functions:

- Drive atmospheric oxygen out of the furnace and adjust the contact pressure of the moving furnace part
- Recalibrate tube temperature
- Format a newly inserted graphite tube
- Clean the furnace after breaks

Formatting must be performed in each case:

- After switching on the spectrometer
- After closing the open furnace

▶ Start the formatting by clicking on **Formation**.

✓ The **Format tube** window appears, which displays the currently measured furnace data. Nine temperature levels (300 – 1500 – 300 – 1500 – 300 – 1000 – 1600 – 2000 – 2400 °C) are run and the test temperatures in the tube are measured. After the last step, the determined data is stored for the tube temperature recalibration.

Cleaning the furnace

The tube is always baked out in a furnace program step after a measurement to remove analyte residues. You can also start the bake-out here. The bake-out is a one-step cleaning program while the tube is purged with maximum gas flow.

Option	Description
Temp.	Temperature of baking out (cleaning)

Option	Description
Ramp	Heating rate
Hold	The time for which baking lasts
Start	Start bake-out process The **Clean** window appears, which displays the currently measured furnace data.

Further furnace functions

Option	Description
Cooling water temp.	Current cooling water temperature
Furnace LED/Furnace Camera	Switch on furnace camera and LED A window with the image of the graphite tube appears, in which you can observe the sample injection and sample drying. As a default setting, the furnace camera is switched on all the time. The option for this is located in the window **Options** / **Analysis sequence**.
Open furnace / **Close furnace**	Open and close graphite furnace
Temperature for shutter to open	At this furnace temperature the furnace camera is switched off and the shutter of the spectrometer is opened. The high-energy radiation of the xenon lamp passes through the graphite tube and the measurement can begin.

Furnace test

In the Test group, you can check the furnace sensors. On successful completion of testing, the result will be reported by a green control lamp, on unsuccessful completion by a red control lamp. In the event of an error, a corresponding error message is output.

▶ Start the sensor test by clicking on Test.

See also

Options for analysis sequence [▶ 167]

9.4 Hydride system

The **Hydride system** window contains the following functions:

- Check the status of the hydride system
- Test system functions for errors
- Reinitialize hydride system
- Load system tubes with reagents before starting analysis
- Rinse the system, e.g. after the end of the analysis for cleaning

Open the **Hydride system** window by clicking on Hy or via the menu item **Method Development** / **Hydride**.

Initializing the hydride system

The hydride system is always initialized at the beginning of work with the AAS. Reinitialization may be necessary if the connection to the AAS has been interrupted.

▶ In the **Hydride system** window, click on **Initialize**.

✓ Communication between the autosampler, the AAS and the PC will be established.

Loading the hydride system

Loading with reagents is necessary before start of analysis, following a new installation or following cleaning of the hydride system.

- In the **Hydride system** window, click on **Load system**.
  - ✓ The tubes of the hydride system are loaded with reagents.

Flush hydride system

The hydride system can be flushed with acid or reductant to remove residues in the system. The associated parameters are specified in the **Method** / **Hydride** window.

- In the **Hydride system** window, click on **Clean system**.
  - ✓ The hydride system is flushed.

See also

Method / Hydride window [▶ 37]

9.4.1 Checking the functions of the hydride system

The **Hydride system** / **Control** window displays the status of the individual controllable modules of the hydride system.

Open the **Hydride system** / **Control** window by clicking on Hy.

Control of the pumps

This function switches the pumps on and off.

Option	Description
Components pump	The component pump transports the reagents and the waste of the hydride system.
Sample pump	The sample pump transports the liquid analysis sample.

Note: If neither of the two valves 3 or 4 is activated when one of the two pumps is switched on, valve 3 is automatically switched on to prevent backflow of the liquid. When the sample pump is active, the component pump is also activated to prevent a liquid blockage in the gas-liquid separator.

Control of the gas paths

In the **gas path** area, all paths of the argon gas flow that are relevant to the analysis process can be switched by means of the valves of the solenoid valve groups.

The **Gas -> valve 2 -> cell** option is used to switch a large gas flow directly to the cell for gas paths that do not go to the cell. This opens valve 2.

Valves in the gas flow

This function can be used to switch the valves.

Valve 1 switches the gas flow through the tip of the batch module on and off.

Valve 3 switches 6 L/h argon to the set path.

Valve 4 switches 25 L/h argon to the set path.

Checking the cell

Option	Description
Cell height	Adjust the cell height in the beam path
Heating on	Switch on the cell heating The function can be used for pre-heating the cell. The cell is heated to the temperature in the **Target** field. After switching the cell heater on and off, the temperature value is displayed in the **Actual** field.

Switching sample valves

In the **Sample valves** area, the solenoid valve pair (V6,V7) can be used to switch the sample path to either waste or the reactor.

Heating the gold collector

Only Hg/hydride systems with enrichment

In the **Collector** area, you can show and edit the gold collector settings.

Option	Description
off	Switch off the heating and cooling of the gold collector
Heating on	Switch on the heating of the gold collector
Cooling on	Switch on the fan of the gold collector The gold collector is cooled down.
Heat value	Parameters for the bake-out temperature of the gold collector The value is preset by the manufacturer and should only be changed if the thermal behavior of the gold collector heating has changed. A higher value corresponds to a higher cleaning out temperature. Click on **Set** to save a changed hydride system value.

Clean bubble sensor

Only for HS 60 and HS 60 modular

The bubble sensor gives a signal if liquid has entered the gas path after the gas-liquid separator. If this fault is reported during a hydride system fault test or during measurement by the bubble sensor then the gas path at the bubble sensor must be cleaned with an additional gas flow. The cleaning process is completed successfully if no bubbles are detected in the gas path for 30 s.

Option	Description
Bubble sensor	The indicator lamp is only active during cleaning of the bubble sensor. Red: Bubbles are detected in the gas path (liquid). Green: The gas path is free of bubbles.
Start	Start cleaning process.

9.4.2 Testing the hydride system for errors

The current status of the hydride system can be checked in the **Hydride system** / **Error test** window. Each analysis sequence is stopped as soon as one of the fault statuses listed here occurs and the relevant fault report is given on the screen.

Click on Hy to open the **Hydride system** / **Error test** window.

Connected hydride system

Option	Description
Type	Connected and initialized hydride system
Version	Version of the hydride system firmware
Line frequency	The measured line frequency 50 or 60 Hz is displayed. Deviations of 2 Hz up and down are tolerated, otherwise the error message "Line frequency" is output.

Fault test

You can start the fault test by clicking on **Test**. The results of the test are indicated by green (for successful test) and red (negative test result) indicator lamps. A negative test result can have the following causes:

Option	Description
Gas pressure	Argon gas pressure is not present.
+24 V	Operating voltage +24 V is not present.
Safety relay	Safety relay not switched on.

Option	Description
Transformer temperature	Transformer is too hot or sensor is defective.
Collector temperature	Gold collector is too hot or sensor is defective.
Gold collector heating time	Gold collector target temperature was not reached in the specified time.
Cell temperature	Cell is too hot or thermocouple is defective.
Cell heating time	Cell target temperature was not reached in the specified time.
Line frequency	Mains frequency is not 50 or 60 Hz.
Bubble sensor	Liquid is located in the gas path after the gas-liquid separator.
Cell temperature sensor	The temperature sensor in the cell is defective.

9.5 Autosampler parameters

9.5.1 Autosamplers for flame technique

The software supports the following autosamplers for the flame technique:
- AS-F and AS-FD
- AS 51s
- AS 52s

The autosampler is an optional accessory for the flame technique. The autosampler is identified during device initialization.

The **Autosampler** window contains the following functions:
- Display connected autosampler type
- Adjust the autosampler
- Additionally rinse / reinitialize the autosampler
- Perform a function test
- Display sample allocation
- Add reagent

You specify the parameters (allocation on the sample tray, dilution, mixing and rinsing steps) that are directly relevant for the analysis in the method, sequence and sample identification.

Open the **Autosampler** window by clicking on  or via the menu item **Method Development** / **Autosampler**.

Initializing the autosampler

The autosampler is always initialized at the beginning of work with the AAS in the **Quick Start**. Reinitialization may be necessary if the autosampler has lost its orientation, e.g. due to a mechanical impact.

▶ In the **Autosampler** window, click on **Initialize**.

✓ The connection between autosampler, AAS and PC is established by the initialization.

Washing the sample path

The sample path from the autosampler to the flame can be washed with the wash liquid of the autosampler. The cannula is immersed in the wash cup while the wash pump supplies fresh wash solution. With the SFS 6 injection module connected, the sample path is opened and thus the entire sample path is washed.

- In the **Autosampler** window, click on **Wash** or select the menu item **Routine** | **Wash**.
  - ✓ The sample path is washed.

NOTICE

Short circuit on the device due to incorrect connection of the autosampler

Switch off the AAS device before connecting the autosampler to the AAS device. Otherwise communication errors or destruction of the interface may occur.

9.5.1.1 Specifying autosampler for flame technique

The following settings are displayed or specified in the **Autosampler** / **Parameters** window:

- Autosampler type
- Washing parameters
- Setting options for controlled cleaning
- Function for washing the mixing cup (only autosampler with dilution function)

The **Wash** and **Controlled cleaning** parameters are taken from the current method. Changes in the **Autosampler** / **Parameters** window inversely update the entries in the method.

- Click on  to open the **Autosampler** / **Parameters** window.

Autosampler

Option	Description
Type	Display of the connected autosampler "-": No autosampler connected. **AS-F / AS 51s**: Autosampler without dilution function **AS-FD / AS 52s**: Autosampler with dilution function
Tray (AS-F / AS-FD)	"-": No tray attached. **139 Pos.**: Tray with 129 positions for 15 mL Sarstedt sample cups on the outer track and 10 positions for 30 mL Sarstedt cups on the inner track **54 Pos.**: Tray with 54 positions for 50 mL Sarstedt sample cups
Tray (AS 51s / AS 52s)	"-": No tray attached. **87 pos.**: Tray with 77 positions for 15 mL Sarstedt sample cups on the outer track and 10 positions for 30 mL Sarstedt cups on the inner track **49 pos.**: Tray with 49 positions for 30 mL Sarstedt sample cups on three tracks **30 Pos.**: Tray with 30 positions for 50 mL Sarstedt sample cups on three tracks
Version	Version number of the autosampler firmware

Wash

Option	Description
Wash mode	**off** Wash mode switched off. No washing performed automatically. **Between samples** Washing after each sample, but not within a statistical series.

Option	Description
Wash time Wash cup	Time in which wash agent is aspirated from the wash cup The wash agent is transported via the cannula through the nebulizer/ mixing chamber/burner system into the flame and the entire sample path is washed.
Mixing cup cycles	Number of rinse cycles for the mixing cup In a rinse cycle the mixing cup is filled with wash liquid / diluent and then emptied again.

Controlled cleaning

Option	Description
Controlled cleaning	Activate controlled cleaning if concentration is exceeded The cleaning progress is checked by repeated measurement.
Control limit (Abs)	The signal level must have returned to this value before the diluted samples or samples with lower concentrations are measured.

Special functions

The mixing cup is automatically washed during a running sequence. You can start the wash process of the mixing cup manually, e.g. to clean the cup after the end of the measurement.

Option	Description
Volume	Enter volume for cleaning.
Start	Start the wash cycle.

9.5.1.2 Technical parameters of the autosampler for the flame technique

In the **Autosampler** / **Techn. parameters** window, specify the following parameters:
- Immersion depth of the cannula in the various cups
- Working speed of the dosing unit
- Alignment of autosampler arm in relation to sample cups

Open the **Autosampler** / **Techn. parameters** window by clicking on  .

For the individual cup types the following actions are taken into account:

Cup	Action
Sample vials	Samples are taken up by a dosing unit or aspirated by a nebulizer (flame technique) or peristaltic pump (hydride technique)
Special cups	Take up or aspirate special samples
Mixing cup	Dispense analyte and diluent solution, and take up samples after dilution
Wash cup	Wash cannula and sample path
Reagent addition	Programmed addition of reagent to the sample

Elements of the actions table

Column	Description
Action	Available actions **Take up** Take up sample from cup for dispense into mixing cup or dispense into flame **Dispense** Dispense sample into the mixing cup

Column	Description
	Wash Take up wash solution
Type	Connected autosampler type
Location	This is the cup to which the action refers.
Depth	The depth to which the cannula submerges in units of 1 mm
Speed level	Working speed of the dosing unit Greater values cause the dosing unit to work faster, with smaller values it will work more slowly. Recommended values: Taking samples: Average speed levels Dispense into the mixing cup: One of the two highest levels, so that fast injection to ensure thorough mixing takes place. Besides, the complete mix up is supported by a fixed wait time before the take up from the mixing cup (or sample cup). The dilution solution is taken up at a fixed rate.

Table area

Use the controls in the **Table** area to change the parameters of the selected table row.

Option	Description
Speed	Speed of dosing unit
Depth	Immersion depth of the cannula / dosing tube The immersion depth is measured from the highest position of the sampler arm.
Depth at pos.	The special cup or the sample cup is checked at this position.
Set	Move the autosampler arm towards the cup. If the option is not activated, the immersion depth and speed are changed without the autosampler arm moving over a cup.

See also

Setting the immersion depth and dosing speed of the autosampler [▶ 136]

9.5.1.3 Setting the immersion depth and dosing speed of the autosampler

For the autosamplers for flame technique and graphite furnace technique, you can optimize the immersion depth of the cannula / dosing tube and the dosing speed of solutions in the various cups.

- Click on  to open the **Autosampler** / **Techn. parameters** window.
- Select a table row in the action table.
- When specifying sample or special cups in the **Depth at pos.** field, adjust the position on the sample tray.
- Only AS-GF and MPE 60/2: If dilution in sample cups is activated in the **Method** / **Sample transport** window, set the position of the mixing cups.
- Check the **Set** box to move the sample arm to the cup position.
- Observe the movement of the autosampler arm and change the **Speed** and **Depth** parameters until the desired result is obtained.

For information on setting the speed, refer to the description of the window **Autosampler** / **Techn. parameters**

See also

- Technical parameters of the autosampler for the graphite furnace technique [▶ 142]
- Technical parameters of the autosampler for the flame technique [▶ 135]

9.5.1.4 Functional test of the autosampler for flame technique

You can test the function of the connected autosampler in the **Autosampler** / **Function tests** window.

Open the **Autosampler** / **Function tests** window by clicking on  .

Tracker/Rotator

The autosampler arm is moved over different positions of the autosampler.

Option	Description
Cup no	Move to the sample cup selected in the list box
Wash position	Move to wash cup
Mixing position	Only autosampler with dilution function Move to mixing cup

Pipetter

Only for autosamplers with dilution function

These tests check the functions of the dilution unit (Fluidik module).

Option	Description
Speed	Dosing rate
Volume	Pipetting volume to be taken up
Take up	Take up the set volume at the set dosing rate.
Dispense	Dispense the volume at the dispense rate.
Valve to bottle	The valve switches the flow between the diluent bottle and the sample. In switching, you must hear the valve click.
Reset	Reset volume setting.

Dipping arm

The autosampler arm is lowered to the position selected under **Tracker/Rotator**.

- In the **Depth** field, set the depth in mm by which the autosampler arm is lowered.

Pumps

By activating and deactivating the checkboxes, you switch the pumps of the autosampler.

Option	Description
Wash pump	Pump for feeding the wash cup
Mix cup pump	Only autosampler with dilution function Pump for draining the mixing cup

Test programs

These tests are carried out with pre-configured, dry-running test programs. The cups approached in the test must be empty! When the test programs are finished, you are informed of the test success.

The selected test program is started by clicking on **Start**.

Option	Description
Test program 1	Driving to Position 1 and immersing in cup Rinsing of cannula Driving to Position 33 and immersing in cup Rinsing of cannula Driving to Position 42 and immersing in cup Rinsing of cannula
Test program 2	Execution of Test Program 1 Dispensing 5 mL diluent in mixing cup Rinsing of cannula Drains mixing cup Dispensing 5 mL diluent in mixing cup Rinsing of cannula Drains mixing cup
Test program 3 Only for AS-F and AS-FD	Immerse in every position

Error test

The autosampler is checked for sensor errors. If one of the error states listed here appears, every measurement will be aborted (on the screen a corresponding error message will be displayed). Start the error test with **Test**. If the test was successful, the indicator will light green; if the test fails, it will light red.

If a test fails, this may have the following causes:

Error	Description
Wash bottle level	Only AS 51s / AS 52s Fill level in the bottle for wash solution too low
Diluent bottle level	Only AS 52s Fill level in the bottle for diluent too low
Tracker/Rotator	Swivel drive of sampler arm and rotary drive of tray are defective.
Tray ident.	Sample tray not detected.
Pipetter (drive)	Dosing unit error
Pipetter (volume)	The volume taken up by the pipettor was too large.

Adjust sampler

Click on **Adjust sampler** to open the window for readjusting the autosampler.

See also

Adjusting the autosampler [▶ 138]

9.5.1.5 Adjusting the autosampler

The autosamplers are supplied factory-adjusted. An adjustment must be carried out in exceptional cases (e.g. following inappropriate transport), if the sampler arm no longer immerses centrally in the cups. The readjustment is computer-controlled in the **Adjust sampler** window.

The **Adjust sampler** window contains the following options and buttons.

Alignment position

The autosampler arm can be adjusted to the following positions:

Option	Description
Mixing positions	Only autosampler with dilution function Mixing cup
Tray	Position 1 on the sample tray
Wash position	Wash cup

Alignment

Customized options are provided for adjusting the positions.

Option	Description
Depth	This field is used to lower the cannula into or out of the respective cup. This allows a better assessment of the position relative to the center of the cup. The immersion depth parameter is only optimizable for the wash position.
Dipping arm	Click on the buttons to swivel the position of the autosampler arm Alternatively, use the left/right arrow keys on the keyboard to move the arm.
Sampler tray	Click on the buttons to rotate the sample tray. Alternatively, move the tray with the up/down arrow keys on the keyboard.
Steps	
Save	Save new parameters for the selected position

Wash pump

Only autosamplers with newer firmware version

Here you can set the rate at which the pump delivers solution into the wash cup.

- Select the rate (1 – 24) in the **Level** list.
- Accept the setting by clicking on **Save**.
  - ✓ The setting is stored permanently.

Adjusting the autosampler

- Place a sample cup on position 1 of the sample tray.
- Click on  to open the **Autosampler** / **Function tests** window. Then click on **Adjust sampler**.
- Select a position for adjustment.
- Adjust the immersion depth so that the position to the cup can be easily evaluated.
- Readjust the position of the autosampler arm using the buttons.
- Additionally with **Tray**: Readjust the position of the sample tray using the buttons.
- Accept the new parameters of the position by clicking on **Save** in the firmware of the autosampler.
- Repeat the previous steps for the positions that have not yet been adjusted.
  - ✓ The new positions are permanently stored in the autosampler firmware.

9.5.1.6 Position overview of the sampler for flame technique

The **Autosampler** / **Positions** window displays the sample tray positions used in the current sequence.

Click on  to open the **Autosampler** / **Positions** window.

You can select the **all positions** or **only special positions** modes for the display.

Note: To display this window, at least one line must be loaded in the current method.

9.5.1.7 Supply of reagents for sample

In the **Autosampler** / **Add reagent** window, a reagent can be automatically pipetted to the samples using the autosampler. The reagent must be kept ready in a sample cup on the sample tray. The **Add reagent** tab is only displayed if a method and an associated sequence are activated.

- Load the sample tray with samples according to the sequence. Place the reagent on an empty tray position.
- Click on  to open the **Autosampler** / **Add reagent** window.
- Click on **Pos. from sequence**.
  The sample positions are transferred from the sequence to the sample table of the window.
- Enter a name for the reagent in the **Name** field and the tray position in the **Position** field.
- Activate the **Consider factor** option if the addition of the reagent is to be taken into account for the dilution factor of the sample.
- For samples to which the reagent is to be added, enter the sample volume and the added reagent volume in the sample table.
- Select the samples in the sample table by clicking with the mouse. Several items can be selected by pressing and holding the Shift key or the Alt key.
- Start the addition of reagent by clicking on **Start add.**.
  ✓ The reagent is added. All processed samples are marked with "*".

9.5.2 Autosamplers for graphite furnace technique

The software supports the following autosamplers for the graphite furnace technique:
- AS-GF: Autosampler without dilution function
- MPE 60: Autosampler with dilution function
- MPE 60/1: Autosampler without dilution function

The autosampler is mandatory for the graphite furnace technique. The connected autosampler is detected during device initialization.

You specify the parameters (allocation on the sample tray, dilution, mixing and rinsing steps) that are directly relevant for the analysis in the method, sequence and sample identification.

Open the **Autosampler** window by clicking on  or via the menu item **Method Development** / **Autosampler**.

The **Autosampler** window contains the following functions:
- Display connected autosampler type

- Adjust the autosampler
- Additionally rinse / reinitialize the autosampler
- Perform a function test
- Display sample allocation
- Add reagent

You specify the parameters (allocation on the sample tray, dilution, mixing and rinsing steps) that are directly relevant for the analysis in the method, sequence and sample identification.

Open the **Autosampler** window by clicking on  or via the menu item **Method Development** / **Autosampler**.

Initializing the autosampler

The autosampler is always initialized at the beginning of work with the AAS in the **Quick Start**. Reinitialization may be necessary if the autosampler has lost its orientation, e.g. due to a mechanical impact.

▶ In the **Autosampler** window, click on **Initialize**.

✓ The connection between autosampler, AAS and PC is established by the initialization.

Wash sample tube

Wash liquid is pumped through the sample tube via the dosing unit of the autosampler and dispensed into the wash cup.

▶ In the **Autosampler** window, click on **Wash** or select the menu item **Routine** | Wash.

✓ The sample tube is washed.

NOTICE

Short circuit on the device due to incorrect connection of the autosampler

Switch off the AAS device before connecting the autosampler to the AAS device. Otherwise communication errors or destruction of the interface may occur.

9.5.2.1 Specifying the connected autosampler for graphite furnace technique

The following settings are displayed or specified in the **Autosampler** / **Parameters** window:

- Autosampler type
- Washing parameters
- Setting options for controlled cleaning
- Function for washing the mixing cup (only autosampler with dilution function)

The **Wash** and **Controlled cleaning** parameters are taken from the current method. Changes in the **Autosampler** / **Parameters** window inversely update the entries in the method.

▶ Click on  to open the **Autosampler** / **Parameters** window.

Autosampler

Option	Description
Type	Display of the connected autosampler "-": No autosampler connected **AS-GF / MPE 60**: Autosamplers for graphite furnace technique
Tray	"-": No tray attached

Option	Description
	89 Pos.: For MPE Tray with 77 sample cups (V = 2 mL), 4 special sample cups (V = 5 mL) and 8 special sample cups (V = 2 mL) **108 Pos.**: For AS-GF Tray with 100 sample cups (with V = 1.5 mL) and 8 central cups for diluents, special samples, standards, modifiers etc. (with V = 5 mL)
Version	Version number of the autosampler firmware

Wash

Option	Description
Wash mode	**off** Wash mode switched off. No washing performed automatically. **Between samples** Washing after each sample, but not within a statistical series **Between runs** Washing after each measurement, including within a statistical series **Between components** Washing after transfer of each component (modifier, standard, sample, etc.) into the graphite tube
Wash cycles Wash cup	Number of wash cycles per wash, 1 to 5

Controlled cleaning

Option	Description
Controlled cleaning	Activate controlled cleaning if concentration is exceeded The cleaning progress is checked by repeated measurement.
Control limit (Abs)	The signal level must have returned to this value before the diluted samples or samples with lower concentrations are measured.

Washing MPE 60 mixing cup

On the MPE 60 autosampler with dilution function, the mixing cup can be washed.

Option	Description
Wash mix cup	Wash mixing cup separately outside the measurement.
Volume	Volume of wash solution
Mixing cup cycles	Number of wash cycles for the mixing cup
Start	Wash the mixing cup

9.5.2.2 Technical parameters of the autosampler for the graphite furnace technique

In the **Autosampler** / **Techn. parameters** window, specify the following parameters:

- Immersion depth of the cannula in the various cups
- Working speed of the dosing unit
- Alignment of autosampler arm in relation to sample cups
- Automatic depth adjustment for volume decrease during the analysis
- Alignment of the autosampler to the graphite furnace

Click on  to open the **Autosampler** / **Techn. parameters** window.

For the individual cup types the following actions are taken into account:

Option	Description
Sample vials	Take up samples through dosing unit
Special cups	Take up special samples
Mixing cup	Dispense analyte and diluent solution, and take up samples after dilution
Graphite tube	Inject samples or special samples into the graphite tube

Elements of the actions table

Column	Description
Action	Available action options: **Take up** Take up sample from the sample cup, special cup or mixing cup **Dispense** Dispense sample into the mixing cup **Inject sample** / **Dispense special** Inject sample or special sample into the graphite tube.
Type	Connected autosampler type
Location	This is the cup to which the action refers.
Speed level	Working speed of the dosing unit Greater values cause the dosing unit to work faster, with smaller values it will work more slowly. Recommended values: Taking samples: 3 Dispense into the mixing cup: 9 Injection into the graphite tube: 1 The diluent and the separating air segment are taken up at a fixed rate.

Table area

Use the controls in the **Table** area to change the parameters of the selected table row.

Option	Description
Speed	Speed of dosing unit
Depth	Immersion depth of the cannula / dosing tube The immersion depth is measured from the highest position of the sampler arm.
Depth at pos.	The special cup or the sample cup is checked at this position.
Set	Move the autosampler arm towards the cup. If the option is not activated, the immersion depth and speed are changed without the autosampler arm moving over a cup.

Automat. depth correction

With automatic depth adjustment, the immersion depth of the dosing tube in sample cups and special cups is automatically adjusted to the new volume after sampling. This ensures that the dosing tube is optimally immersed according to the fill level in the cups and reduces the risk of contamination of the sample.

Option	Description
Automat. depth correction	Automatically adjust the immersion depth of the dosing tube to the fill level in the cups
Sample cups	Opens the **Sampler positions, volumes and depths** window for setting deviating cup geometries and volumes for individual cups. The settings are taken into account during automatic depth adjustment

Additional functions

Option	Description
empty mixing cups	Only MPE 60/2 and AS-GF The button is active if sample cups have been defined as mixing cups in the sample transport window. Clicking on the button releases these positions for reuse.
Open furnace / Close furnace	Open and close furnace to change graphite tube
Align sampler to furnace	Start software-assisted alignment of the autosampler to the graphite furnace

See also

- Setting the immersion depth and dosing speed of the autosampler [▶ 136]
- Automatic depth adjustment of autosamplers for graphite furnace technique [▶ 144]
- Aligning the autosampler to the graphite furnace [▶ 145]

9.5.2.3 Automatic depth adjustment of autosamplers for graphite furnace technique

The automatic adjustment of the immersion depth of the dosing tube into the sample and special cups prevents unwanted contamination of the dosing tube. To draw in a sample volume, the dosing tube will dip into a sample cup just as much as necessary to accomplish this. As total volume removal increases, the immersion depth will automatically be corrected.

The immersion depths for sample cups or special cups set in the **Autosampler** / **Techn. parameters** window initially apply to all cups on the sample tray.

Fill volumes or cup sizes at variance with standard cups can be separately specified and duly considered for automatic depth correction.

- Click on  to open the **Autosampler** / **Techn. parameters** window.
- Activate the **Automat. depth correction** option and click on **Sample cups**. The**Sampler positions, volumes and depths** window appears.
- Make separate settings for each sample cup or special cup.
- Exit the window with **OK**.

  ✓ All settings are saved and taken into account at the next sequence start.

With regard to individual special cups or sample cups, the following parameters can be specified:

Option	Description
Position	Adjust the cup position on the sample tray Settings must be made individually for each cup that is intended to be modified.
Volume	Displays the sample volume already taken from the cup If the cup is not full, you can enter the missing sample volume. The value is updated by the program after each sampling.
Depth	Displays additional depth corresponding to the sample volume already taken. This value is recalculated after each sample take-in sequence. The total immersion depth is the sum of the specified immer-

Option	Description
	sion depth (**Autosampler** / **Techn. parameters** window) and the additional depth displayed here. This value is used as input for calculation of the depth, based on the amount of withdrawn volume.
Diameter	Displays the cup diameter If the cup diameter differs from the value shown, select the **Diameter** checkbox and enter the value in this field.
Delete volumes	Reset the volume values for all special cups or sample cups to 0.
Reset	Set volumes and depths for all cups to 0, reset diameters to the values last saved with **OK**

Maximum immersion depth (auto adjustment)

A maximum allowed immersion depth can be specified in order to prevent the dosing tube from hitting the cup bottom and getting twisted.

Option	Description
Sample cup	The maximum immersion depth settings apply to sample cups and special cups.
Depth	Maximum immersion depth in the sample cup or special cup
Position	This sample tray position is used to test the immersion depth for the selected cup type.
Set	The dosing tube dips into the cup according to the depth set under **Depth**. The immersion depth can be checked visually. **Important**: If the **Set** checkbox is activated, the dosing tube immediately dips to the specified depth. Make sure that the autosampler path is not blocked.
Save	Save the changed immersion depth for the cup type.

See also

Technical parameters of the autosampler for the graphite furnace technique [▶ 142]

9.5.2.4 Aligning the autosampler to the graphite furnace

The fine alignment of the AS-GF with the furnace is software-supported. The autosampler is aligned in such a way that the dosing tube can optimally dispense the samples in the graphite tube without touching the dosing insert. The injection depth for the sample is set in the same process.

- Click on  to open the **Autosampler** / **Techn. parameters** window.
- Click on **Align sampler to furnace**.
  - ✓ The autosampler alignment instructions start. Follow the further instructions on the screen.

9.5.2.5 Functional test of the autosampler for graphite furnace technique

You can test the function of the connected autosampler in the **Autosampler** / **Function tests** window.

Open the **Autosampler** / **Function tests** window by clicking on  .

Tracker/Rotator

The autosampler arm is moved over different positions of the autosampler.

Option	Description
Cup no	Move to the sample cup selected in the list box
Wash position	Move to wash cup
Mixing position	Only autosampler with dilution function Move to mixing cup
Tube position	Start up graphite furnace

Pipetter

This test checks the dosing unit.

Option	Description
Speed	Dosing rate
Volume	Pipetting volume to be taken up
Take up	Take up the set volume at the set dosing rate.
Dispense	Dispense the volume at the dispense rate.
Valve to bottle	The valve switches the flow between the diluent bottle and the sample. In switching, you must hear the valve click.
Reset	Reset volume setting.

Dipping arm

The autosampler arm is lowered to the position selected under **Tracker/Rotator**.

- In the **Depth** field, set the depth in mm by which the autosampler arm is lowered.

Test programs

These tests are carried out with pre-configured, dry-running test programs. The cups approached in the test must be empty! When the test programs are finished, you are informed of the test success.

The selected test program is started by clicking on **Start**.

Program	Description
Test program 1	■ Aspirates volume from position 1 ■ Aspirates volume from position 41 ■ Discharges volume into graphite tube ■ Washes dosing tube two times
Test program 2	Only autosampler with dilution function ■ Aspirates diluent solution from waste bottle ■ Aspirates volume from position 10 ■ Discharges volume into mixing cup ■ Aspirates volume from mixing cup ■ Discharges volume into graphite tube ■ Purging the dosing tube ■ Drains mixing cup ■ Washes and drains mixing cup
Test program 3	Immerse in every position

Error test

The autosampler is checked for sensor errors. If one of the error states listed here appears, every measurement will be aborted (on the screen a corresponding error message will be displayed). Start the error test with **Test**. If the test was successful, the indicator will light green; if the test fails, it will light red.

If a test fails, this may have the following causes:

Error	Description
Wash bottle level	Only MPE 60 Fill level in the bottle for wash solution too low
Diluent bottle level	Only MPE 60 Fill level in the bottle for diluent too low
Tracker/Rotator	Swivel drive of sampler arm and rotary drive of tray are defective.
Tray ident.	Sample tray not detected.
Pipetter (drive)	Dosing unit error
Pipetter (volume)	The volume taken up by the pipettor was too large.

Adjust sampler

Click on **Adjust sampler** to open the window for readjusting the autosampler.

See also

Adjusting the autosampler [▶ 138]

9.5.2.6 Position overview of the autosampler for graphite furnace technique

The **Autosampler** / **Positions** window displays the sample tray positions used in the current sequence.

Click on  to open the **Autosampler** / **Positions** window.

You can select the **all positions** or **only special positions** modes for the display.

Note: To display this window, at least one line must be loaded in the current method.

9.5.3 Solids autosampler

The SSA 600 solids sampler is used in automated solids analysis. The **Solid sampler** window contains the following functions:

- Functional test
- Alignment to the graphite furnace

The solids sampler can be operated with or without liquid dosing, therefore the function test and adjustment is based on the autosampler specified in the method.

Open the **Solid sampler** window by clicking on  or via the menu item **Method Development** / **Autosampler**.

Transporting the sample platforms back

You can have all sample platforms that are on different positions of the autosampler or in the graphite furnace transported back to the sample trays.

- In the **Autosampler** window, click on **Reset**.
  - ✓ The platforms are transported back to their places on the sample trays.

Initializing the autosampler

The autosampler is always initialized at the beginning of work with the AAS in the **Quick Start**. Reinitialization may be necessary if the autosampler has lost its orientation, e.g. due to a mechanical impact or due to pressing the stop button on the autosampler.

- In the **Autosampler** window, click on **Initialize**.
  - ✓ The connection between autosampler, AAS and PC is established by the initialization.

Aligning the gripper to the graphite furnace

The gripper of the autosampler must be aligned to the furnace using the software. To do this, you need the adjustment aid included with the autosampler.

- In the **Autosampler** window, click on **Align** and follow the instructions on the screen.
  - ✓ When the adjustment routine is complete, the autosampler is aligned with the furnace.

A detailed description of the adjustment procedure can be found in the "SSA 600 Solids Sampler" operating instructions.

NOTICE

Short circuit on the device due to incorrect connection of the autosampler

Switch off the AAS device before connecting the autosampler to the AAS device. Otherwise communication errors or destruction of the interface may occur.

9.5.3.1 Function test of solid sampler

You can test the function of the connected autosampler in the **Autosampler** / **Function tests** window.

Open the **Autosampler** / **Function tests** window by clicking on  .

The following options are available for the functional test:

Option	Description
Status/Buttons	Display the autosampler status and the button pressed on the autosampler since the last query in the respective color (green, orange, red) Press **Update** to query the status again or to update the button display.
Move to position	Select a position in the **Pos.** list and move to it No platform is taken up or dispensed.
Rotate tray	Rotate the sample tray to the selected position
Transport	Transport a platform from a starting position (**from**) to a target position (**to**) If **Take-up platform** is activated, the gripper picks up a platform. If **Put-down platform** is activated, the gripper places the platform at the target location.
Gripper	Open and close gripper Lower the cannula
Balance	Determine the weight of a platform located on the tray at the set position (**Pos**). **Weighing with tare** Before weighing the platform, the scale is tared. #1 indicates the tare weight. #2 contains the weight of the platform (with dosed sample, if applicable). **Internal calibration** During this calibration, the internal calibration curve of the scale is determined again. To do this, first reset the scale, determine the zero

Option	Description
	point and then weigh an internal weight. The values obtained for zero-point and internal weight will provide the input for determination of the scales calibration graph.
Loop	The autosampler transports two platforms (positions 1 and 2) back and forth between the sample tray, the scale and the furnace. The number of transports can be entered in the **Cycles** field.

9.5.3.2 Adjusting the solids autosampler

The **Solid sampler** / **Alignment** window contains the following functions:

- Check and adjust the movement to individual positions
- Align the autosampler to the graphite furnace
- Autosampler with dosing unit: Automatic depth adjustment for the take up of matrix modifiers and liquid special samples
- Test liquid dosing

Click on  to open the **Solid sampler** / **Alignment** window.

The following options are available in this window:

Option	Description
Alignment position	Selection of the position on the autosampler
Buttons in the group **Adjust position**	Align the gripper to the set position
Open gripper/Close gripper	Open and close gripper with software control, e.g. for changing the gripper tips

Only autosamplers with liquid dosing:

Option	Description
Lower cannula	Lower the cannula
group **Automat. depth correction**	Automatic depth adjustment for immersion in the sample cups
Wash	Wash the dosing tube with the preset number of wash cycles confirmed by clicking on  .
Test liquid dosing	Check liquid dosing
Change dispenser syringe	Move the piston of the dosing syringe downwards for the changeover

Monitoring & aligning individual positions

- ▸ Select the position in the **Alignment position** list.
- ▸ Click on **Move to** in the **Adjust position** group.
  The autosampler moves to the selected position.
- ▸ Place a platform at this position and check the position of the platform.
- ▸ Correct the position with the buttons in the **Adjust position** group.
- ▸ Save the changed settings by clicking on **Save**.

Aligning the gripper to the graphite furnace

The gripper of the autosampler must be aligned to the furnace using the software. To do this, you need the adjustment aid included with the autosampler.

- ▸ In the **Autosampler** window, click on **Align** and follow the instructions on the screen.
  - ✓ When the adjustment routine is complete, the autosampler is aligned with the furnace.

A detailed description of the adjustment procedure can be found in the "SSA 600 Solids Sampler" operating instructions.

Washing the system

Only autosamplers with liquid dosing:

When cleaning the system diluent is taken from the supply bottle and pumped through the entire path via the dosing device to the dosing tube and dispensed into the wash cup.

- Enter the number of repetitions in the **Wash cycles** input field.
- Save the entry by clicking on .
- Start the wash process by clicking on **Wash**.

Automatic depth correction for dosing unit

In general, the depth adjustment of the solids sampler is automatic, i.e. the immersion depth is readjusted as more sample is drawn from the cups of the dosing unit. Starting volumes other than those which were set via Method can be corrected in this window. The settings are made in the same way as for the autosampler for the graphite furnace technique.

See also

Automatic depth adjustment of autosamplers for graphite furnace technique [▶ 144]

10 Data management

This section provides information on the following topics:
- Print functions
- Management of methods, sequences and sample IDs
- Management of device-specific files
- Definition of units for concentrations and contents
- Management of frequently used stock solutions and QC samples

10.1 Information on print functions

The software has a large number of output formats for data output. In addition to output to the printer, the data can be exported to Excel, PDF, HTML, XML or text format or saved as bitmap or scalable graphics.

Report templates are used for the output of analysis results or the contents of windows. A set of report templates is installed by default. If required these sheets can be adapted individually with the report designer "Report-/Print module List & Label"

10.1.1 Printing results data

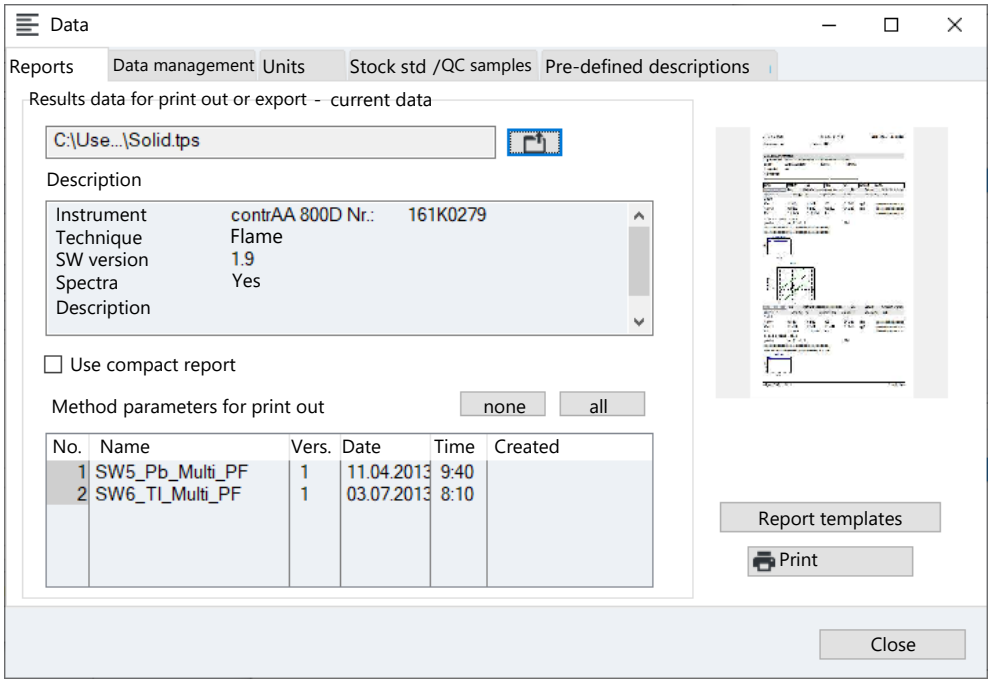
The software offers different possibilities to print results data:
- Print the complete record. The complete record of an analysis contains the method parameters, the calibration and analysis results with individual sample values (statistic runs). A report may be printed of the current results in the main window and the saved data.
- Print current results. In this printout only the data of the main window are printed. Here you can choose between a complete and a compact printout.
- Print selected data from the **Overview** tab. For this printout you can select the analysis lines and results in a dialog window.

Print complete record

The complete record of an analysis contains the method parameters, the calibration and analysis results with individual sample values (statistic runs). The complete records can be printed of the results in the main window or the saved files.

▶ Click on  to open the **Data** / **Reports** window.
Alternatively, open the window with the menu items **Extras** | **Data** or **File** | **Print** | **Report**.

✓ The name of the current file, file information (description list), and all method versions that were used to generate the current results file are displayed.



- To print a saved file, click and select the desired file in the standard **Open** window.
- In the table, select all method versions you want to print out by clicking with the mouse.
  Click the mouse and hold down the Shift or Ctrl key to select more than one method version. Click on **all** to select all versions. Click on **none** to remove all selections.
- Click on **Print** to open the **Aspect CS Report** window.
- Select the output format in the **Output to** list. Click **Options** and set specific parameters for the output format.
- Select the **Save settings permanently** checkbox if you want the selected output medium to be the default setting for this print template.
- Click on **Start** to start the printout.
  ✓ The output is sent to the selected medium.

Note:
Use the **Preview** setting for the printout. By clicking on **Start** the pages to be printed are first displayed in the print preview. This allows you to check that all desired data or whether unnecessary data are being output before they are sent to the printer.

Print current results

The results displayed in the main window can be printed.

- In the main window, select the results tab you want to print.
- Select the menu item **File** | **Print** | **Active Window**.
  The**Results report format** window appears.
- Select the size of the printout.
  complete output: Results with the signal graphs
  compact output: Results in a compact overview
- Proceed as described above for "Printing the complete report".

Note: If you activate the **Always use this results report type** checkbox in the **Results report format** window, this window will no longer appear the next time you print the results and the last results report type will be used automatically. You can reset this setting in the **Options** / **View** window.

Print selected data

- Select the **Overview** tab in the main window.
- In the bottom section of this tab, click on or select the menu item **File** | **Print** | **Active Window**.
- The **Print** / **Overview** window appears.
- Select all desired lines and parameters for the printout by clicking with the mouse and confirm the selection with **OK**.
  The **ASpect CS Report** window appears.
- Proceed as described above for "Printing the complete report".

See also

View options [▶ 164]

10.1.2 Print further analysis parameters and settings

The following parameters and settings of the analysis can be printed:

- Method
- Sequence
- Result data and results overview
- Sample ID
- QC (Quality Control charts)
- Calibration
- Autosampler positions

The printing of the parameters occurs from the respective window.

- Activate/open the window on the workspace of the software.
- Click on in the window.
  Alternatively select the menu command **File** | **Print** | **Active Window**.
  - ✓ The **ASpect CS** Report window opens.
- Select the output format in the **Output to** list. Click Options and set further parameters for the output format.
- Click on **Start** to start the printout.

10.1.3 Adapting report templates

Use report design mode

The report templates installed by default can be individually adapted. For a better overview report views can be edited with real values.

- Select the menu item **File** | **Report design mode**.
- Open the window whose report template you want to change.
- Select the menu item **File** | **Print** | **Active Window**.
  - ✓ The report designer opens.
- Make the changes and save the report template.
  - ✓ The template has been changed and must now be linked to the corresponding print contents (see "Managing report templates" below).

Short introduction to the report designer

The individual components of the report template are called Objects. For example, a table can consist of one object each for the header, the list values and a graph.

These objects again contain the information to be printed and carry the associated layout properties such as fonts, alignment, breaks, colors etc.

The report designer makes various types of objects available, e.g. text objects, graphs, barcodes. These can be freely placed in the working area and the size can be changed. Depending on type an object can present different information or have different characteristics.

The desired objects are as a rule pulled onto the working area with the mouse and then provided with the relevant contents and layout characteristics. Alternatively you can pull a variable from the variables list onto the working area by "Drag & Drop". If there is still no object at the target position, one is automatically created and the variable is assigned to the object.

In order to process an existing object, it must first of all be selected. For this click on the object with the left mouse button. You will recognize a selected object by its highlighted frame. If you create a new object it is automatically selected and can be directly changed in terms of size and position. A dialog window is started via a double-click, in which further settings can be changed.

Further information on the operation and functions of the report designer can be found in the manual "designer_deu.pdf" / "designer_eng.pdf" on the installation CD for the software.

The Report templates window

The **Report templates** window is where you edit templates and assign them to the windows of the software. Several sheets can be assigned to one window by using a file mask, from which the desired report is selected at the start of printing. The names of the format templates offered must be chosen in such a way that they can be entered with wildcards.

- Click on  to open the **Data** / **Reports** window.
- Click on **Report templates** to open the window of the same name.

For the following windows a report template must be available:

Name	Description
Results	Content of the **Result** tab in the main window
Compact results	
Results (Overview)	
Calibration	**Calibration** window: Calibration of the analysis
Method	**Method** window: Method parameters
Method/Results	Full report
Sample ID	**Sample ID** / **Sample Information** window: Sample information data
Sampler pos.	**Autosampler** / **Positions** window: Assignment of the autosampler
QC chart	**QC**: Quality control chart data
QC sample information	**Autosampler** / **QC sample information** window: Information data of the QC samples
SSA600 table	Content of the **Solid** tab in the main window
Sequence	**Sequence** window: Sequence order

Change assignment

You must assign a new/edited report template to the corresponding print function again.

- In the list, select the window whose report template you want to change.
- Click **Modify** to open the dialog box for assigning the files.
- Assign only one report template: Activate the **Use report template file (*.lst)** option, click on  and select the template file.

- Offer several templates at the same time when printing: Activate the option Allow file selection and enter the mask name in the input field using wildcards.
- Confirm the settings with **OK**.
  - ✓ The new report template is displayed in the **Report templates** window.

Editing a report template

You can select a report template here and edit it in the report designer.

- Select the report template in the list by clicking with the mouse.
- Use **Edit** to open the report designer window.
  - ✓ You can edit the report template. Detailed information about the report designer can be found in the file "Designer.pdf" on the installation CD.

Restoring default settings

You can restore the settings according to the program installation.

- Click on **Default settings**.

10.2 Management for all file types

The following data is generated in the software:

- Methods
- Sequences
- Results files
- Line/wavelength file
- Correction models
- Correction spectra
- Report templates
- Worksheets

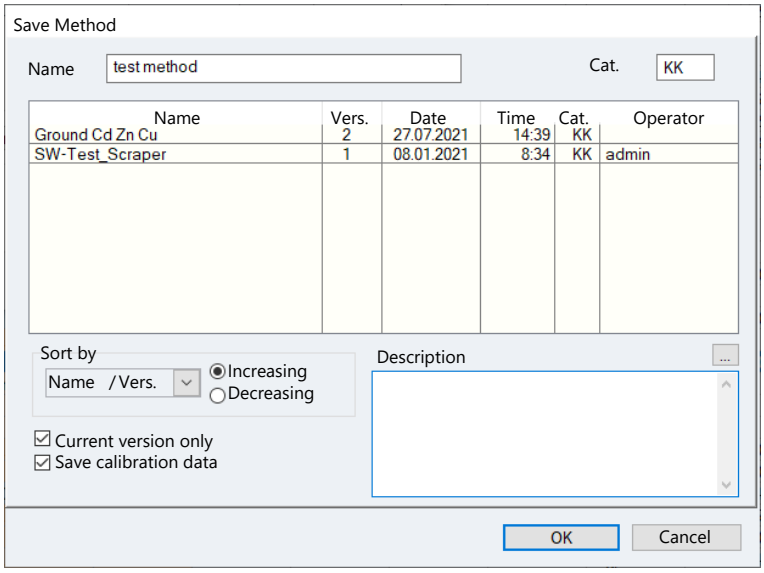
The above data is organized in the **Data /Data management** window. The window appears after you click on or select the menu item **Extras** | **Data**.

10.2.1 Managing methods and sequences

Methods and sequences are stored separately in a database. The method database is saved as "method.tps". The database containing the sequences is called "sequ.tps". In the text of this section, methods and sequences will hereafter be referred to as "data records".

Elements in the database window

When saving, opening, deleting, importing and exporting methods and sequences, database windows are opened, that have identical elements.



Option/display	Description
Name	Entry or display of the name of the selected method or sequence.
Cat.	Additional property for searching the method/sequence in the database A maximum of three digits can be entered as the category name. You can limit the display of the list by entering the category name in the **Cat.** field. If you want to display the records of all categories, clear the entry in the **Cat.** field.
List of records	Stored records with name, version, date, time, category and operator
Sort by	Sort the list according to various properties Sorting can be done in ascending or descending order, depending on the option selected.
Description	Enter or display additional notes, e.g. on the use of the records. You can create predefined notes in the **Data** / **Pre-defined descriptions** window.
Current version only	If several versions of a method/sequence with the same name have been created, only the method/sequence with the highest version number is displayed.

In the software, methods/sequences with the same names are not overwritten, but another version is created and the version number is increased by 1.

The databases also provide functions for importing, exporting or deleting individual methods or sequences from the respective databases.

Note
Hold down the Ctrl or Shift key while selecting with the mouse to select multiple records in the database window.

Opening the data management

- Click on  to open the **Data** / **Data management** window.
- Select the record type you want to edit in the **Type** list. Method or sequence.

Exporting data records

Using the export function, you can make records available to other devices/computers. You may export several data records to a common file. Export files get the following extensions: Method data records - ".met", sequence data records - ".seq".

- Click on **Export spectrum data** to open the database window.
- Select the records by clicking with the mouse and then click **Export spectrum data**.

- In the standard **Save as** window, enter a file name and click **Save**.
  The database window with the exported files is displayed.
- Exit the database window with **Close**.

Importing data records

Using the import function, you can load data records from other devices/computers into your database. An import file can contain several records from which you select the records you want to load.

- Click **Import** to open the **Select file to import** window.
- Select the file to import and click **Open**.
  This will bring up the database window with the presentation of name, date of creation and category of the data records contained in the file. In the title bar of the window, the name of the import file is displayed.
- In the database window, select the records you want to import and click **Import**.
  The records are imported into the database. If a method/sequence with the same name already exists, a new version of the record is created. In the database window, the current versions of the available data records appear.
- Exit the database window with **Close**.
  - ✓ The imported records can now be used in the software.

Deleting data records

Using the delete function, you can permanently delete data records from the database.

- Click on **Delete** to open the database window.
- Select the records you want to delete.
- Click on **Delete**.
  - ✓ The database window is updated, displaying only the remaining data records. For data records of the same name, the version number is reduced by 1.

Deleting records via the File menu

Alternatively, you can open the database window for deleting records using the menu item **File** | **Delete** | **Method** or **File** | **Delete** | **Sequence**. Then, proceed as described above.

10.2.2 Managing results data

Results data are stored in a database during the measurement. A new database file is created each time a sequence is started, but you can also append measurements to an existing file that already exists. Results data is saved with the extension TPS.

In addition, a spectrum file with the same name as the TPS file and the extension SPK is generated with the measurements. This file contains the measured spectra and is needed to display and evaluate the spectra in the **Spectra** window. All other information required for analysis and evaluation is stored in the TPS file. If measurements are appended to an existing TPS file, the spectra are also added to the corresponding SPK file. When managing in the **Data** window, the TPS file is imported, copied or deleted at the same time as the SPK file.

- Click on  to open the **Data** / **Data management** window.
- Select the **Results** option from the **Type** list.

Importing results data

You can import results data into the software. During this process, the data is placed in the results folder of the active atomization technique within the file structure of the software.

- In the **Quick Start** window, select the atomization technique for which data is to be imported.

- In the **Data** / **Data** window, click on **Import**.
  The**Select results files** window appears.
- Select the TPS files by clicking with the mouse and then click **Open**.
- Select the subfolder where you want to save the results and click on **OK**.
  - ✓ The TPS files and associated SPK files (if any) are copied to the results folder of the active atomization technique.

Exporting results data

Use this command to copy one or more results files to another folder.

- In the **Data** / **Data** window, click on **Export**.
  The **Export** window appears with the overview of existing TPS files. The files are listed with name, size and time of the last change.
- Select the TPS files by clicking with the mouse.
- Use **Export** to open the **Find folder** window.
- Select the destination folder and confirm by clicking on **OK**.
  - ✓ The TPS files and the SPK files are copied to the destination folder.

Deleting results files

You can permanently delete results data.

- In the **Data** / **Data** window, click on **Delete**.
  The **Export** window appears with the overview of existing results databases.
- Select the TPS files by clicking with the mouse.
- Click on **Delete** and confirm the subsequent query to delete files by clicking on **OK**.
  - ✓ The data are permanently deleted.

Searching for results of individual samples

You can search for individual samples with known sample names in the databases.

- In the **Data** / **Data** window, click on **[Search Sample]**.
  Alternatively, select the menu item **Extras** | **Search Sample**.
  This **Search Sample** window appears.
- Enter the sample name in the **Sample type** field.
  If the entered string is part of the name, select the **Substring search** checkbox.
- Limit the time of the measurement by activating the **Date** checkbox.
- Click on **Start**.
  All results which contain samples with the sample name entered are displayed in the table.
- To open one of the displayed results files, select the file in the list and click on **Open**.
  - ✓ The results are displayed in the main window.

10.2.3 Exporting line/wavelength files

The line/wavelength file with the analysis lines and the saved main peaks is device-specific. It is stored on the computer used to control the analyzer. To use the line/wavelength file on another computer, follow these steps:

- Click on  to open the **Data** / **Data management** window.
- In the **Type** list, select the **Lines/wavelength file** option and click on **Export**.
- Select the folder where you want to save the file and click **OK**.
  - ✓ The file is saved in the selected folder with the name "lines.dat".

10.2.4 Managing correction models

Correction models are used for background correction of analyte spectrum overlays by matrix components. They can be transferred from one device to another. Correction model files have the extension MOD.

- Click on  to open the **Data** / **Data management** window.
- Select the **Correction models** option from the **Type** list.

Importing correction models

Use this command to import correction models into the software.

- Click on **Import**.
- Select the correction model MOD and click on **Open**.
  The **Import** / **Correction model** window appears.
- Click on **Import**.
  - ✓ The correction model is transferred to the database of the software.

Exporting correction models

With this command you export the correction model for use on another computer.

- Click on **Export spectrum data**.
- In the **Export** window, select the **Correction model** with the mouse. Multiple selection is possible.
- Click on **Export**.
- In the **Save as** window, enter the name and save path and click **Save**.
  - ✓ The file with the correction model is saved.

Deleting correction models

With this command you delete correction models no longer required.

NOTICE

Deleting correction models can make methods unusable

Note that no check takes place whether the correction model is used in a method.

- Click on **Delete**.
- Select the model in the **Correction models** window.
- Click on **Delete**.
  - ✓ The correction model is deleted from the database.

10.2.5 Deleting correction spectra

Correction spectra no longer required can be deleted from the database.

- Click on  to open the **Data** / **Data management** window.
- In the **Type** list, select the **Correction spectra** option and click on **Delete**.
- In the **Correction spectra** database window, select the spectrum and click **Delete**.
  - ✓ A check takes place whether the spectrum is used in a correction model. If this is not the case, the correction spectrum is deleted.

10.2.6 Importing report templates

Templates for print reports that were created externally must be imported into the software via data management.

- Click on  to open the **Data** / **Data management** window.
- In the **Type** list, select the **Report templates** option and click on **[Import]**.
- In the **Open** window, select the report file LST and click on **Open**.
  - ✓ The report template is imported into the software. Now assign the report template to the print content in the **Data** / **Reports** window.

See also

Adapting report templates [▶ 153]

10.2.7 Managing worksheets

You manage worksheets in the **Data** / **Data management** window. You can import or export worksheets into or from the software. Optionally, you can specify the stored methods and sequences. You can delete worksheets that you do not need. Worksheets have the extension WST.

- Click on  to open the **Data** / **Data management** window.
- Select the **Worksheet** option from the **Type** list.

Importing a worksheet

- Click on **Import**.
- In the **Import Worksheet** window, click on **Import**. Activate the **including sequence and method(s)** option to import methods and sequence.
- In the **Import Worksheet** window, select the worksheet and click on **Open**.
  - ✓ The worksheet is imported.

Exporting a worksheet

- Click on **Export**.
- In the **Export Worksheet** window, select the worksheet by clicking with the mouse. Activate the **including sequence and method(s)** option to export methods and sequence.
- Click on **Export**.
- In the **Save as** window, enter a folder and a name for the export file and click **Save**.
  - ✓ The worksheet is exported.

Deleting a worksheet

- Click on **Delete**.
- In the **Delete** window, select the worksheet and click on **Delete**.
  - ✓ The worksheet is deleted.

10.3 Managing units

In the **Data** / **Units** window, you can manage the units available throughout the program. 3 preferred versions (for solutions: mg/L, µg/L, ng/L; for solid samples: mg/kg, µg/kg, ng/kg) are available. These units cannot be changed by the operator. Units deviating from these can be freely defined.

- Click on  to open the **Data** / **Units** window.

The table contains the overview of the available units.

Table column	Description
Unit	Name of the unit (max. 10 characters)
Comment	Remarks on the unit (max. 20 characters)
Factor	Factor 1 corresponds to 1 µg/L or µg/kg, factor 1000 corresponds to 1 ng/L or ng/kg The factor must be entered for units you have entered yourself.
Type	**solid**: Unit related to solid sample **liquid**: Unit related to liquid sample (solution)

Use the buttons to manage your own entries.

Button	Description
Append	Insert new row at the end of the list
Insert	Insert row above a selected row in the list
Delete	Only delete custom units. The preferred units cannot be deleted.
Save	Save changes and entries

10.4 Managing databases for stocks and QC samples

The databases with the frequently used stock standards and QC samples are managed in the **Data** / **Stock std**/ **QC samples** window. You can add, delete or edit entries in the database. The stock standards and QC samples are available in method development.

- Click on  to open the **Data** / **Stock std** / **QC samples** window.
- Select the options **Stock standard** or **QC samples**.
- Enter or edit the parameters of a stock standard in the table:

Column	Description
Name	Name of the standard/QC sample Max. 20 characters
Unit	Unit of the standard/QC sample
Elements and concentrations	The element concentration is entered in the format "element symbol concentration" in the selected unit, e.g. Fe 0.5; Cu 10; Co 0.005. Alternatively, click on **Concentration** to open the window with the same name and assign the concentration to each element there.

Use the buttons to manage the entries:

Button	Description
Append	Insert new row at the end of the list
Insert	Insert row above a selected row in the list
Delete	Delete the selected row
Save	Save changes and entries
Concentration	Open input window for element and concentration of the selected row

10.5 Creating predefined notes

User-defined notes can be defined for the following operations:
- Saving a method
- Saving a sequence
- Starting reprocessing
- Starting a measurement

The user-defined notes can be inserted by clicking on ••• next to the **Remarks** field in the corresponding windows.

Frequently used notes are already stored in the software. Notes can be created, edited or deleted.

- Click on  to open the **Data** / **Pre-defined descriptions** window.
- Select the process in the **Select category** list.
- Click **Edit template** to open the list of notes.
- Create a new note by clicking on **New**.
  Enter the new note in the **Enter pre-defined descriptions** window.
  Name field: The note can be selected under this name.
  Text field: Enter the actual note.
- You can edit a note by clicking on **Modify** or remove it from the selection list by clicking on **Delete**.

10.6 Using the Windows clipboard

Copying results to the clipboard

The application lets you copy the results of selected samples directly to the Windows clipboard thus making them accessible to other Windows applications. The commands for this can be found in the **Edit** menu.

Edit	
Copy visible Columns only	Copies the visible sample results of the current table.
Copy all Columns	Copies the sample results of all tables.
Column Titles	If activated (check mark), the copy action includes the column headers.

- Select the samples in the table of the results list.
  Holding the ctrl or shift key depressed, choose the samples by mouse clicks on the respective row.
  Select all sample rows with the menu item **Edit** | **Select All**.
- If the title row is also to be copied, activate the menu item **Edit** | **Column Titles**.
- Select the corresponding menu item to copy the results to the clipboard.
  ✓ The results can now be pasted into the application, e.g. a spreadsheet program.

Copying graphics as screenshots

Graph windows and graphs of calibration curves, absorbance signals or emission signals can be copied to the clipboard as a screenshot.

- Right-click on the graph.
  A submenu with two copy commands opens.

- Select the copy command to copy the desired object: copy only the graph or the entire displayed window.
  - ✓ The selected object is copied onto the clipboard and is available for other Windows applications.

11 Options – Customizing ASpect CS

The following settings are configured in the **Options** window, and are valid for the entire operation of the software:

- View options
- Save paths of files
- Parameters for data export
- Generally applicable settings for the analysis sequence

The settings are retained after exiting and restarting the software.

Open the **Options** window with the menu item **Extras** | **Options**.

Resetting settings

The **Default settings** button resets all options and saved window positions to default values.

11.1 View options

In the **Options** / **View** window, you can define the functions visible on the workspace.

Open the **Options** / **View** window with the menu item **Extras** | **Options**.

Elements in the window Options / View

Option	Description
Show toolbar	Display the toolbar with the buttons for the measurement routine.
Show iconbar	Display toolbar with large icons for quick access and select toolbar position. The position of the toolbar can also be changed by dragging it with the mouse. The setting is not saved until the next program start.
Hide event windows	Do not display the event windows (e.g. delay time). Instead of this, the messages appear in the status bar of the main window.
Calib. table column by column	Rotate the calibration table for defining the standards. The individual calibration standards are arranged in columns and the selected analysis lines in rows.
Hide results windows automatically	Result windows are hidden when sub-windows (e.g. Method window) are opened to avoid overlaps. After closing the sub-windows the result windows are displayed again.
Show lamp operating lifetime (spectrometer)	The operating time of the XBO lamp is displayed in the Spectrometer window (only for lamp power supplies from version 4). When the program is started, a message is displayed if the guaranteed lamp operating time of 1000 hours has been exceeded.
Display note on recommended flame type	Flame technique: When checking the method parameters, the system checks whether the flame type recommended in the cookbook is used for the analysis of an element. A message appears if the flame type is different.
Display tooltips	Small help texts (tooltips) are displayed above buttons and column titles in tables.
Net signal and **Background**	Select signal colors for the graph view. Click on ••• to open the color selection window.
Scientific Mode	Activate spectrum display. If this option is deactivated, the functions for displaying and editing spectrum data are not accessible.
Allow screensaver	Turn on Windows screen saver during input pauses.

Option	Description
Ask for results report type (compact or complete) when printing	When printing results windows via the menu item **File** | **Print** | **Active Window**, you can choose between a complete or a compact report. Clicking this button resets the **Always use this results report type** selection so that the report type can be selected again.

11.2 Storage paths

During the installation the storage paths for data are defined. They are displayed in the **Options** / **Folder** window and can partly be edited here.

Open the **Options** / **Folder** window with the menu item **Extras** | **Options**.

Functions in the Options / Folder window

Folder	Description
Program	Installation path of the executable program files
Work directory	Directory for operator data The working directory contains further subfolders. It is defined during installation or by the optional user administration.
Temporary data	Directory for temporary application files.
Export/Import	Default path for opening and saving sample information files This path can be changed. Click ••• to select the new folder. A different path can also be selected when opening and saving the sample information files.
Sample Information	Default path for export and import of method and sequence data and export of results data as CSV files This path can be changed. Click ••• to select the new folder. During export and import a different path can also be selected.
Results	Directory for results data This default directory can contain further subfolders for saving results. These folders are available for saving results files at the start of measurements.
Application data	Directory for internal program data

The **Add** button creates new subfolders for saving results below the results folder. Besides, it is possible to delete and rename empty folders here.

11.3 Options for ASCII/CSV export

In the **Options** / **ASCII/CSV export** window, you can define the parameters for the ASCII export of results data. The parameters apply to both the automatic continuous data export and the manual data export.

Open the **Options** / **ASCII/CSV export** window with the menu item **Extras** | **Options**.

Functions in the Options / ASCII/CSV export window

Option	Description
Decimal separator	Defines the separator for decimal numbers.
List separator	Defines the character separating the individual elements of a list.
Results export	**all** Export the entire results table.

Option	Description
	only selected fields Custom results export. Click on ••• and use the mouse to select all fields/columns you want to export in the **Field selection** window.

E-mail notification

The **E-mail notification** button opens the configuration window for the e-mail interface. This automatically sends e-mails at the end of the analysis run or when the analysis run is aborted due to errors.

Option	Description
Server (SMTP)	Name or address of the SMTP server
Port	The port number used for SMTP (usually port 465 or 587).
E-Mail address	Your complete e-mail address
Account name	User name for logging on to the SMTP server
Password	Password for logging on to the SMTP server. The password is stored in encrypted form.
Recipients adresses	Up to three e-mail addresses can be entered.
Activate e-mail notification	If activated, e-mails are always sent to the entered e-mail recipients after the end of the analysis run or only if errors have occurred. In the event of a premature abort due to errors, the notification indicates the error that caused the abort.
Send test mail	A test e-mail is sent to the e-mail recipients entered.

11.4 Options for continuous ASCII export

In the **Options** / **Continuous ASCII export** window, you can activate the automatic export of results data during the analysis run. The export file is updated respectively after the output of a new row in the process and results window. The result data will be appended to already existing files.

Further export options are defined in the **Options** / **ASCII/CSV export** window.

Open the **Options** / **ASCII/CSV export** window with the menu item **Extras** | **Options**.

Export of results data

The **Continuous ASCII export of results data** checkbox activates the export function. The data is stored in the default path for export/import (**Options** / Folder window).

You can select the following file names:

Option	Description
Method name.csv	The file name corresponds to the name of the method. The data is stored in the default path for export/import (**Options** / Folder window).
Results file name.csv	The file name corresponds to the name of the results file. The data is stored in the default path for export/import (**Options** / Folder window).
other	You may freely define file name and save path. The data is written to this file continuously until a new name is assigned or another naming option is selected. Click on the ••• icon and enter the destination folder and file name in the **Save as** window.

Option	Description
Create separate file for each sample (result row number and sample name is appended to file-name)	The file name is appended with the row number of the results list and the sample name. Characters that are not allowed are replaced by underscores (e.g. Test method-001 QC 1 mg_L.csv).

Spectral export

For the spectrum export, activate the **Continuous export of spectra (CSV)** option and select a storage path.

The spectra are additionally exported as CSV files to the specific export path. The file name is generated based on the schema "ListRow-SampleName-LineName-RepeatMeasurement", e.g. 0007-Sample-Al309-02.csv.

11.5 Options for analysis sequence

In the **Options** / **Analysis sequence** window, you define generally valid settings for the analysis procedure.

Open the **Options** / **Analysis sequence** window with the menu item **Extras** | **Options**.

Aborting a sequence after the following errors

The analysis is monitored for the following errors and can be canceled if these errors occur:

Option	Description
Offset of optical system	Stops if the wavelength configuration (Ne correction) is faulty.
Invalid calibration function	Stops if the calibration function could not be calculated.

Additional error checking

Option	Description
Monotony of calibration points	The calibration points will be tested for monotony. The monotony test serves to determine if higher standard concentrations also lead to higher measured values.

Display windows

During the analysis process, display windows with signal curves and further information on the measurement can be shown.

Option	Description
Signal Plot	Time-dependent measurement signal curve
Spectrum Plot	Recorded spectral range
Bar graph	Bar graph of the measured absorbance or emission values
Scaling of max. signal value	Set the maximum of the measured value axis for the displays of the signal curve. Alternatively, this setting can also be made using the **View** | **Scale (Abs)** menu function.
Report window	Status information on the atomizer used
Sample conc. in calibration curve	Current calibration curve and recalibration curve

Option	Description
	After the measurement of the sample, the calculation of the uncorrected concentration from absorbance/emission data is illustrated by red auxiliary lines. If addition calibration is used, the converted calibration curve will be displayed.
Furnace Camera	Picture of the furnace camera with the graphite tube image This allows you to directly watch as a sample droplet is deposited and drying. When the temperature for the shutter opening is reached, the furnace camera is switched off.

Miscellaneous

Option	Description
Always save spectra	The spectrum data is always saved during the measurement regardless of the method parameters (Method / Output window).
Attach date/time to the results filename	The current date and PC/time are automatically appended to the name of the result file when the measurement is started.
Continuous export also during reprocessing	After reprocessing the results are automatically exported.
Do not update timestamp when reprocessing	After reprocessing the results, the original measurement times are retained.
Take-up components during cooling phase	While the graphite tube is cooling down, the autosampler is used to take the next sample. This option may be used to accelerate a measuring sequence.
Beep after end of cooling phase	A beep will sound as soon as the graphite tube has completely cooled down.
Stop after transformer overheating	Enabled: Measuring program is stopped in case of overheating of the transformer for graphite furnace technique and is not continued again. Disabled: The program is interrupted if the transformer overheats. Resumes the interrupted program after the transformer has cooled down.
Readjust wavelength before each measurement	The wavelength is reset before each individual measurement. This improves repeatability (default: enabled).
Formation required after opening furnace	At the start of a measuring sequence, a message is displayed indicating that formatting has not taken place after opening the furnace or switching on the device.
Update straylight data for lines below	At sequence start, the stray light level for lines below the selected wavelength (nm) is updated once a day. You can also record the stray light values manually at the next measurement start. To do this, click the **[Reset values]** button.
Clean mixing chamber when flame is extinguished	When the flame is extinguished, the mixing chamber is washed.
Activate tube and drying detection (after restart)	The furnace camera detects the type of tube and the completion of the drying phase. Activating this option requires the software to be restarted.

11.6 Options for optics purging

contrAA 800 only

In the **Options** / **Optics purging** window, you define parameters for purging the spectrometer of the contrAA 800. Optics purging protects the spectrometer from contamination. Purging with argon also improves the limits of detection in the short-wave UV range.

Open the **Options** / **Optics purging** window with the menu item **Extras** | **Options**.

Option	Description
Optics purging	off: No optics purging. Air: Purging with air Argon: Purging with argon
Argon stabilisation time	The spectrometer is purged with argon. This time is required until the air in the spectrometer has been displaced by argon and stable optical conditions have been established after starting the argon purge.
Argon drive out time	The spectrometer is purged with air. This time is needed to expel the argon from the spectrometer.
Activate optics purging at software startup	Optics purging is always started when switching on the device.

When optics purging is switched on, a message appears in the toolbar of the main window indicating the optics purge and the time remaining until the purge has stabilized. If a measurement routine (sequence) is started during the current stabilization time, a message appears indicating that the purge is still running.

11.7 Calibration and blank correction options

Calibration

In this group you configure basic settings for the calibration. All checkboxes are disabled as default.

Option	Description
Show R instead of R^2(adj.)	If enabled, the correlation coefficient is displayed. By default the corrected (adjusted) coefficient of determination is provided.
Show prediction instead of confidence interval	If enabled the prognosis band for the calibration is displayed. The confidence band is provided as default.
auto compares with quadratic instead of rational function	"auto" indicates the automatic selection of the calibration function. If enabled the quadratic function is used for the comparison. The default setting is the broken ratio function.
Compute slope for mean conc instead of 0	If enabled the slope of the calibration graph is calculated for the mean concentration of the calibration range. As default the slop is calculated for 0 concentration.

NOTICE

All options mentioned above must be enabled for compatibility of the calculation of the quadratic calibration function in accordance with DIN 38402 and ISO 8466-2.

Blank correction

For blank correction you can choose between two different calculation methods: Conc.1-based or conc.2-based.

In the conc.2-based calculation, the original concentration of the blank ($Conc2_{BV}$) is first calculated based on the sample IDs of the blank. $Conc2_{BV}$ is taken into account when determining the conc.2 of the sample.

In the conc.1-based calculation, the blank concentration ($Conc1_{Blank}$) determined directly from the sample is used to calculate the sample concentration. This method can be used if the sample ID data (e.g. dilutions) do not strongly influence the concentration of the blank solutions and therefore no sample ID data is entered for the blanks.

Calculation example for liquid original sample with predilution:

- Conc.1-based: $Conc2_{Sample} = (Conc1_{Sample} - Conc1_{Blank}) * DF_{Sample}$
- Conc.2-based: $Conc2_{Sample} = (Conc1_{Sample} * DF_{Sample}) - Conc2_{Blank}$

$Conc1_{Sample}$	Concentration of the sample without taking into account the information in the sample ID
$Conc2_{Sample}$	Original concentration of the sample
$Conc1_{Blank}$	Concentration of the blank without taking into account the information in the sample ID
$Conc2_{Blank}$	Original blank
DF_{Sample}	Dilution factor of the sample

The default setting for blank correction is the conc.2-based method. If you want to revert to the shorter conc.1-based method without taking into account the sample ID of the blank value, activate the **Blank correction based on Conc1** option.

Limits of detection/quantitation

You can edit the factors and number of repeat measurements for the limits of detection/quantitation. The calculated limits of detection/quantitation are displayed in the **Calibration** window. If the settings are to be applied to existing results, the results must be reprocessed. The factors and number of repeat measurement are output in the **Calibration** window and in the printouts of the calibration and results/blank measurements.

To edit the limits of detection/quantitation settings, click on **LOD** / **LOQ**. The following default settings are provided:

Parameter	Value
Factor LOD	3
Factor LOQ	9
Replicates	11

12 Optional FDA 21 CFR Part 11 Compliance module

The optional FDA 21 CFR Part 11 Compliance module for ASpect CS includes the following functions in accordance with the FDA Requirements for Electronic Records and Electronic Signatures (21 CFR Part 11):

- User management
- Electronic signatures
- Audit trail
- AJ File Protection to protect files against intentional and unintentional data tampering

The user management provides for one administrator level and four user levels. The following functions are accessible to a user with administrator rights:

- Flexible system configuration (password and login policies, audit trail, signatures, data directories)
- Creation of users in user levels with graduated user rights
- Assignment of passwords
- Assignment of a separate working directory for methods, sequences and results for the user
- View and export the generated audit trail (event report)

If user management is installed and configured, the **System** menu item in ASpect CS is activated, through which the functions of user management can be accessed.

Any change in user data will be permanently saved in an encoded database on exiting the relevant window.

Note: In order to meet safety requirements, Microsoft Windows must be used as the operating system with adequate configuration options. This applies to file access rights and other setting actions of a kind that should be performed by an authorized system administrator.

12.1 User management

12.1.1 Hierarchy and access to functions

The user management provides for one administrator level and four user levels.

The hierarchy structure for user levels is as follows:

Administrator > level 1> level 2 > level 3 > level 4.

The following functions are assigned to the individual user levels

Administrator level

The user has full access rights to ASpect PQ and to any function of user management.

Level 1

Level 1 users have unlimited access to all Aspect PQ functions, but are denied access to user management.

Level 2

Same as level 1 users, except:

- Deletion of methods (M1 ID code)
- Deletion of sequences (P1 ID code)
- Deletion of QC rule tabs (Q1 ID code)
- Deletion of results files (R1 ID code)

Level 3

Same as level 2 users, except:

- Saving of methods (creating methods in a method data base) (M2 ID code)

- Saving of sequences (creating sequences in a sequence data base) (P2 ID code)
- Accept peak offsets (W1 code)

Level 4

Same as level 3 users, except:

- Changes in method parameters (E1 ID code)

Users of this category can only load previously created methods and sequences and perform measurements.

Function	ID code*	Admin.	Level 1	Level 2	Level 3	Level 4
Working with user management		+	-	-	-	-
Delete methods	M1	+	+	-	-	-
Delete sequences	P1	+	+	-	-	-
Delete QC rule tabs	Q1	+	+	-	-	-
Delete results files	R1	+	+	-	-	-
Save methods	M2	+	+	+	-	-
Save sequences	P2	+	+	+	-	-
Change peak offsets	W1	+	+	+	-	-
Change report templates	L1	+	+	-	-	-
Make changes in methods	E1	+	+	+	+	-
Load methods and sequences		+	+	+	+	+
Perform measurement		+	+	+	+	+

*ID code is used in operating advice.

12.1.2 User management – Display and settings

User management setups can be made by a user with administrator rights as part of initial installation of the user management package or at any time thereafter.

An account is created for each user. An account contains a given user profile. Where a user account is not required any longer, it can be disabled or inhibited. User accounts cannot be deleted.

▶ Select the menu item **System** | **User management** or start user management via the entry in the Windows start menu.

▶ Log in with an administrator profile.

✓ The**User Management** window appears.

User Management window

The window contains a list with the registered user names and the corresponding full names. The right-hand side of the window displays the details of the selected user's profile.

Indicator and control elements

Option	Description
User ID	Login name of user
Full name	Full name of user
User level	Administrator, level 1 to level 4
E-signature	**Yes**: User is authorized to electronically sign result data. **No**: User has no authorization for electronic signature.

Option	Description
Status	Active: User name allowed for use (green circle). Disabled: User name is disabled and cannot be used (red circle).
Passwd. protect.	Active: User login requires a password (key). Inactive: User login allowed without a password (key crossed out)
Valid until:	**Indefinitely**: Password never expires. **Date/ days**: User must change his/her password on expiry of specified term.

Buttons

Button	Description
New ...	Create new user The **Add user data** window appears.
Modify ...	Edit user data for selected table row The **Modify user data** window for a selected user appears. The window can also be opened by double-clicking on the user.
Preferences	Change the user management configuration
Audit trail	Open event report
?	Open help
Exit	Exit the application

12.1.3 Configure general settings of the user management

In the **Preferences** window, you can configure the user management in general with the following options:

- Password policies
- Login and audit trail
- Signature meanings
- Data directories used

The settings apply to newly created user accounts and should therefore be made after installation, before user accounts are created.

▶ In the **ASpect CS** / **User Management** window, click on **Preferences**.
The**Preferences** window appears.

▶ On the left, select the option group you want to change.

▶ Carry out the configuration.
Click **Default settings** to restore the default settings for the selected option group.
The settings of the other groups remain unaffected.

▶ Click **OK** to apply the settings.

Log-on

Settings for login and password policies

Option	Description
Number of login attempts:	Shows the number of invalid login attempts (max. 10). If this is exceeded, **ASpect CS** terminates after a waiting period and must be restarted for another login. An entry (warning) is added to the audit trail file.
Disable account after failed login attempts	The user is blocked after exceeding the number of login attempts.
Minium user name length:	Only passwords consisting of letters and numeric characters can be assigned.

Option	Description
	Maximum number of characters: 10
Enforce login with password	A password must be assigned to newly created user names.
Password and user ID must be different	Only passwords which contain both letters and figures can be issued. This policy equally applies to changes in password.
Password and user ID must be different	Only passwords which are different from the respective user name will be accepted. This policy equally applies to changes in password.
"User must change password at next login" is active	By default, new users must change their password the first time they log in.
Password expires in	After the time limit has expired, the user is prompted to change the password when logging in. The password is then extended by a term as set in Policies. This value is then acknowledged as a template that can be modified for other single users (max. 999 days).
Minium password length:	Minimum number of characters for newly created passwords 3 to 10

Folders

The ASpect working directory and the directory for the audit trail file can be specified.

Option	Description
ASpect working directory	Working directory of **ASpect CS** The working directory contains the method and sequence databases and the results files. The working directory was defined during the installation of **ASpect CS** and can be changed here.
Audit trail	Path of the audit trail file The path can be changed.
User database	Path of the user database This path can only be changed using the installation program.
AJ File Protection	Additional protection is provided by the optional AJ File Protection software. This protects files against intentional and unintentional data tampering, e.g. deletion or modification of data. If AJ File Protection is installed, the button is active and indicates the protection status by a marker. Green – file protection is active; Red – file protection driver is not active. After clicking the button, a window appears with a list of protected directories.

Audit trail

In this action group, you specify the activation of the audit trail, the use of methods, and the basic validity period of calibrations.

Option	Description
Inactive (no entries)	No entries are added to the audit trail file.
Active	Entries are added to the audit trail file.
Allow measuring only with saved methods	If activated, a measurement can only be started if a method has been loaded and this method has not been changed since the last time the method was saved.
Calibration validity period [h:mm]:	If activated, the validity period of the calibration can be specified. For user level 3 and 4, the calibration must be updated before starting the measurement. A message is displayed for other levels.

Signatures

The list shows the signature meanings and the corresponding user level that can be selected when signing.

Button	Description
Add	Add new signature meaning After clicking the button, the **Edit list of signature meanings** window appears in which you an select a new signature meaning and the valid user level.
Modify	Edit selected signature meaning
Delete	Delete selected signature meaning

12.1.4 Creating a new user account

Only users with administrator access rights can create a new user account. A new user is configured with corresponding rights in the **Add user data** window.

Options in the Add user data window

Option	Description
User ID	The user logs in with this name. Not case sensitive. The minimum length depends on the general configurations of the user management.
Full name	Full name of the user This name is used as part of the electronic signature. Maximum number of characters: 32
Description	Field for notes The entry is optional.
User level	Selection of the user level with the corresponding rights
Password ...	Set password Passwords are case sensitive. If the password dialog is acknowledged without a password entry, the password protection will be canceled. The minimum length and other password policies are specified in the general configurations of the user management. Max. password length: 20 characters
Padlock symbol	Password protection is active.
Open padlock symbol	The user does not use a password.
Password never expires	Password will remain valid for unlimited time if this box is active. If it was disabled, the given password will expire within a preset term. The specified value is sourced from password policies. A user may also extend his/her password in advance.
User-specific working directory	A separate working directory is set for the user according to the following schema: \ASpect-Working directory\User name. The directory structure is created when the user logs on for the first time.
Use e-signature	The user is allowed to sign measurement results electronically. The signatures of their user level and lower user levels are available.
View audit trail	The user can open the event report.
Disable user ID	Disable the user account The user name can be temporarily disabled. Disabling a user account, as opposed to removing it, prevents the user name from being reassigned for newly created users.
User must change password at next login	The next time the user logs on, they will be prompted to change the password.

Specifying user data

- In the **User Management** window, click on **New ...**.
  The**Add user data** window appears.
- Configure the settings in the fields and options and confirm by clicking on **OK**.
  ✓ The new user account appears in the **ASpect CS User Management** window.

See also

- Configure general settings of the user management [▶ 173]
- Hierarchy and access to functions [▶ 171]

12.1.5 Changing an existing user account

You can change the properties of a user account.

- In the **User Management** window, select the user account and click on **Modify ...**.
  The **Modify user data** window with the account settings appears.
- Configure the settings and click on **OK**.
  ✓ The changes are applied and take effect the next time the user logs on.

See also

- Creating a new user account [▶ 175]

12.1.6 Changing a password

Depending on the specification in the user account, the user must change the assigned password at regular intervals.

- In **ASpect CS**, select the menu item **System** | **Change password**.
  The**Change password** window appears.
- Enter the old password and the new password twice and confirm by clicking on **OK**.
  ✓ If the entry is correct, the **Password is changed!** message appears.

12.2 Viewing, printing and exporting the audit trail

The audit trail file records system events as well as all warning and error messages. To view the audit trail, permissions must be granted in the user account.

You can open the audit trail via the menu item **System** | **Audit Trail** or in the user management by clicking on **Audit Trail**.

The following functions are available for the audit trail:
- Display
- Refresh
- Export as CSV file (only if the audit trail was called from the user management window)

The following parameters are documented in an audit trail file:

Table column	Description
Type	Display the event type The following event types are recorded in the audit trail and identified by symbols: Info, Warning, Error, Login and Logout

Table column	Description
Date/Time	Date and time of the entry (PC clock) The [+] and [-] buttons in the table header of both columns are used to sort the entries by ascending and descending time or date.
Time zone	Indicates the time zone to which the time of an entry is referenced (Windows system control)
Name	Name of the event, details see field **Description**
Category	Category of the event The category "USRMGMNT" identifies all entries which originate from the user management. All other categories are entered by **ASpect CS**.
User	Designates the user in login state at the moment of an entry.
Description	More detailed information about the cause of the selected entry

Updating an audit trail

Click **Refresh** to refresh the audit trail entry list. This may be necessary if further entries were added to a previously created audit trail display.

Exporting the audit trail

You can export the audit trail entries to a CSV file if you have administrator rights. The export function is only available if the audit trail has been opened in the user management.

- Click on **Export** to open the **Save as** window.
- Enter a path and the name and confirm by clicking on **OK**.
  - ✓ The audit trail file is exported.

Filtering the audit trail

You can filter the audit trail by specific labels, categories, or users, and narrow down the time period of the entries.

- Click on **Filter** and specify the search filter in the Filter audit trail window.
- Click **Reset filter** to clear the restrictions imposed by the filter.

Printing the audit trail

You can print the audit trail. If you have filtered the entries, only the filtered entries are printed.

- Start the printout of the current audit trail view by clicking on **Print**.
  The print window opens.
- Select the output format in the **Direct to** list.
- Start the printout by clicking on **Start**.
  - ✓ The audit trail is output in the selected output format.

12.3 Electronic signatures

Results data can be signed electronically in ASpect CS. A signature will close work on a particular file so changes in this file made at a later point in time will cause an invalid signature state. Signature meanings are created in the general settings of the user management. A signing user must have the appropriate permissions in their user account.

A signing procedure will encode a given file and assign to this file a signed state and the data of the signing user. In addition, an encrypted signature file is created with the same name as the results file, but with the file extension ".sig". It contains the check sums of the related results file, including those of (if included) a spectrum file.

A file may be signed by more than one user.

12.3.1 Signing measured results

Measurement results files can be provided with an electronic signature in the **Sign off** window after the measurement or after the file is loaded at a later time by users with the appropriate rights.

Options in the Sign off window

Option	Description
User ID	Login name of the current user The user name can be changed. This makes signing by other users possible.
Password	Password of the user
Meaning	Signature meaning The list of signature meanings is defined by the administrator of the user management.
Comment	For optional comment (max. 256 characters)
Sign off	Sign document with the settings made above

Signing results

- Display measurement results for signing in the main window of the software.
- Select the menu item **System** | **Sign off results**.
- Enter user name and password.
- Select signature meaning.
- Click on **Sign off**.
  - ✓ You will be asked whether the signature should be granted or the process should be canceled. Successful granting of a signature will be confirmed.

See also

Configure general settings of the user management [▶ 173]

12.3.2 Displaying signatures

When previewing or printing signed results data, a **Signatures** section is appended to the end of the report. This contains all electronic signatures of the corresponding file:

Option	Description
Issued by	Full name and login name of the user who signed the file
Signed on	Date/time of signature granting
Status	The signature state may take on one of the following meanings: **Valid** Signature and results data are complete and correct. The calculated checksums of the files show no differences to the checksums stored in the signature file at the time of the signature. **Invalid (missing or invalid signature file)** The signature file associated with the record was not found or is corrupt. **Invalid (TPS data)** The results file was changed after signing. Comparison between newly calculated check sums and previously saved check sums reveals variances.

Option	Description
	Invalid (SPK data) The file with the raw spectra data was changed after signing. Comparison between newly calculated check sums and previously saved check sums reveals variances.
Meaning	The meaning of signatures
Comment	Optional comment in the signature

12.4 AJ File Protection

The optional AJ File Protection software protects files against intentional and unintentional data tampering, 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, the AJ File Protection software guarantees complete data privacy for method creation, data acquisition and evaluation, and archiving.

13 Annex

13.1 Overview of markings used in the display of values

Comment	Meaning	Values	Edition
> KAL	The mean value is larger than the working range of the calibration curve.	Mean values	Process and results window
< KAL	The mean value is smaller than the working range of the calibration curve.	Mean values	Process and results window
< LOD	The value is smaller than the limit of detection.	Mean values	Process and results window
< LOQ	Sample value is less than the limit of quantitation and greater than the limit of detection	Mean values	Process and results window
RSD !	Sample mean or standard mean is outside the range of the specified relative standard deviation	Mean values	Process and results window
RR!	Sample mean or standard mean is outside the range of the specified relative range	Mean values	Process and results window
Factor!	Limit of recalibration factor for the calibration curve was exceeded	Calibration curve	Process and results window
R^2(adj.) or R	Coefficient of determination of the regression R^2(adj.) or R (depending on the selection in the Options / Calibration window) of the calibration curve falls below the specified value	Calibration curve	Process and results window Calibration curve window
MAN	Sample single value or standard single value was manually excluded from the calculation of the sample means	Single values	Sample single values window
KOR	Sample single value or standard single value was automatically excluded from the calculation of the sample means by Grubbs outlier test	Single values	Sample single values window

13.2 Description of the algorithms used for spectral background correction

The spectral background correction is performed separately for each individual spectrum. A time-resolved absorbance signal is obtained with a number of absorbance values that depends on the measurement time. A single absorbance value is calculated for each evaluation pixel (**Method** / **Evaluation** window, **Eval.Pixels** column) and summed over the number of evaluation pixels. Depending on the AAS technique, a height, area or mean value is calculated from the absorbance signal.

13.2.1 "without reference" background correction

Calculation of the reference value

The reference value is formed by averaging the statically set pixels of the measuring range. If no static pixels are set, then averaging is done over all pixels in the range, ignoring a range of +/-10 pixels around the measurement pixel. A separately recorded reference spectrum is not required.

Calculation of the absorbance spectra

$Abscorr=lg(I_0/I_{peak})$

I_0	Mean of the pixels within the gap, except measuring pixel +/- 10 pixels
I_{peak}	Measuring pixel

Limits

Flame and other molecular structures that would be detected in a separate reference spectrum are not compensated. Due to uneven CCD illumination, the absorbance spectrum may show a falling or rising baseline.

This correction corresponds to the broadband D2 correction of the lines AAS.

13.2.2 "with reference" background correction

Calculation of the reference value

The individual absorbance spectra are calculated from the individual spectra of the sample and the mean normalized reference spectrum. The mean normalized reference spectrum is obtained by dividing (normalizing) the areas (sums) of the individual reference spectra by the area of the mean reference spectrum. The normalized individual spectra are then averaged again.

Calculation of the absorbance spectra

Due to the fluctuation of the light source and the atomizer, the obtained absorbance spectra have more or less strongly inclined and curved baselines with different offset values. In a further step, therefore, a baseline is adjusted for each individual spectrum. To do this, support points (BGC points) are set, through which a polynomial is applied. The fitting polynomial is at most a second degree polynomial. The degree is determined by the number and the distribution of the support points, whereby support points that are less than 10 pixels apart are combined into a group.

The fitted baseline is subtracted from the absorbance spectra. The absorbance value can then be determined directly.

The BGC points can be set either statically or dynamically (automatically).

Statically: The BGC points are set manually or from a list in the range center pixel+/-0.5 x measuring range.

Dynamically: The BGC points are found by an algorithm.

- Target: Identify pixels that are not significantly different from the baseline noise. To do this, the gradients of the pixel under consideration to the +/-3 neighboring pixels are calculated and tested for gradient changes.
- The BGC points of the individual spectra are combined. If a particular BGC pixel is found with a defined frequency, then that pixel is taken as the BGC point for the mean spectrum.
- Constraints: If all BGC points are on one side of the measurement pixel, an error is issued. If the connection is one-sided, the extrapolation of the polynomial can lead to large errors. The search algorithm detects a gradient only when the absorbance difference between four adjacent pixels exceeds a certain amount (>2E-4/pixel).
- The range measuring pixel +/- 10 pixels is excluded from the search.

Limits

With overlapping structures over the entire range of the spectral gap, the algorithm has fundamental problems, since then no area is dominated by baseline noise. In this case, the frequency is adjusted dynamically, i.e. the decision criterion is gradually relaxed. If this does not result in a sufficient number of BGC points, then static pixels are set, which are stored as default in the line table.

13.2.3 "IBC" and "IBC-m" background correction

The **IBC** background correction (IBC= Iterative Baseline Correction) is based on an iterative filtering of the intensity spectra. Background structures wider than the analyte peak are eliminated. The algorithm is suitable for complex spectral backgrounds.

IBC-m is a special iterative filter algorithm for the determination of broadband molecular structures.

13.2.4 Spectrum subtraction (correction of permanent structures)

Intended use

Multivariate correction of flame structures and other interferences present in reference and sample spectra at different intensities.

Assumptions

- The sum spectrum is the weighted sum of the spectra of the pure substances and the noise.
- Other wavelength ranges (e.g. additional analyte bands that are not present in the correction spectrum) are not present or are masked out.
- No wavelength shifts, or very small wavelength shifts between sample spectrum and correction spectrum, as these lead to artifacts.

The flame structure spectrum is calculated from the reference spectrum according to $Abs_{corr}=lg(I_0/_{I0\text{-}Offset})$; further molecular corrections require spectra of the pure substances.

The basis for the calculation is the multivariate classical calibration:

$y=X*b+e$

m – number of wavelengths/pixel

n – number of pure substance spectra

y – sum spectrum (mx1)

X – matrix of pure substance spectra (mxn)

b – coefficient vector

$b(estimated)=X+y$ where $X+=(X'*X)^{-1} X'*y$ (pseudoinverse)

The product of the pure substance spectrum and the coefficient can then be subtracted from the sample spectrum:

$y_N= x_N-\Sigma(b_ix_i)$, where i = 1... except N (index of the spectrum of interest)

See also

Creating a correction model for spectral corrections [▶ 94]

13.3 Storage location of ASpect CS files

The folders used to store files differ depending on the installation options and the version of Windows you are using. The following summary shows the folders used by default. The folders used by the current installation are displayed in the Options / Folders window.

Working directory and subfolders

Drive:>User>Public>Documents>Analytik Jena>ASpect CS

Type	Folder	Files
Results	C:\User\Public\Documents\Analytik Jena\ASpect CS\<Technique>\Results	*.tps – results list *.spk – spectrum data
Method, sequence and correction spectrum data	C:\User\Public\Documents\Analytik Jena\ASpect CS\<Technique>\meth	*.tps
Optimization results (e.g. optimization of the furnace program)	C:\User\Public\Documents\Analytik Jena\ASpect CS\<Technique>\opt	*.tps
Default parameters	C:\User\Public\Documents\Analytik Jena\ASpect CS\<Technique>\tables	*.dat
Sample ID files, unit files and exported files (*.csv)	C:\User\Public\Documents\Analytik Jena\ASpect CS\user	*.tps; *.csv
Report templates	C:\User\Public\Documents\Analytik Jena\ASpect CS\user\Reports	*.lst – template *.jpg – preview file
Options and adjustment values	C:\User\Public\Documents\Analytik Jena\ASpect CS	*.cfg; *.ini

Application data (and subfolders)

Drive:>ProgramData>Analytik Jena>AspectCS

Type	Folder	Files
Line lists	C:\ProgramData\Analytik Jena\ASpectCS\<Technique>\tables	Lines.dat
Device data and predefined comments	C:\ProgramData\Analytik Jena\ASpectCS	*.dat: *.tps
User management data and audit trail data	C:\ProgramData\Analytik Jena\ASpectCS\UserMgmt	Usrlrv.tps – user database Eventlog*.tps – audit trail

Program

Drive:>ProgramData>Analytik Jena>ASpect CS or

Drive:>Program Files (x86)>Analytik Jena>ASpectCS

Type	Folder	Files
Devices and system configuration	C:\Program Files (x86)\ASpectCS	ASpectCS.ini

Technique: FL – Flame, EA – Graphite furnace, EAS – Solid graphite furnace, HS – Hydride, HF – HydrEA

Before a complete restore (applications and data), the ASpect CS installation must also be executed.

Information on the display of folders and file name extensions

Some folders may be hidden folders. It is also possible that the display of file name extensions is switched off. In Windows Explorer, select **View** to show hidden files, folders, and extensions.