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Operating Manual

ASpect PQ
Software für ICP-OES

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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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1 ASpect PQ software

ASpect PQ is the control and analysis software for the following ICP-OES devices:

- PlasmaQuant PQ 9000
- PlasmaQuant 9100
- PlasmaQuant 9200

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

In addition to the software description, this manual contains information on the maintenance and care of the ICP-OES device. Many of the maintenance instructions are enriched with animations and videos.

Described software version

This document is based on the version ASpect PQ 1.4.

Intended use

ASpect PQ software 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 PQ.

ASpect PQ and the device to be controlled by it may only be operated by appropriately qualified and instructed personnel. The user must be familiar with the information given herein and in the user's manual of the device.

1.1 Data protection information

This software uses sample names and allows optional information about the sample (notes). The sample name serves as an identifier for the test results of a specific sample. Particularly in clinical settings, the sample name could be used to assign test results to the natural person on whom the tests were performed. Personal data should be minimized as much as possible to ensure that no one can derive personal information from the sample name or the optional notes. Direct identifiers such as names, social security numbers, national identification numbers, dates of birth or other personal attributes should not be used. It is the responsibility of the data controllers in the laboratories to comply with applicable data protection laws and obligations.

Analytik Jena may request that files containing measurement results, including sample names or notes, be shared as part of service-related activities such as customer support, troubleshooting and complaint investigation.

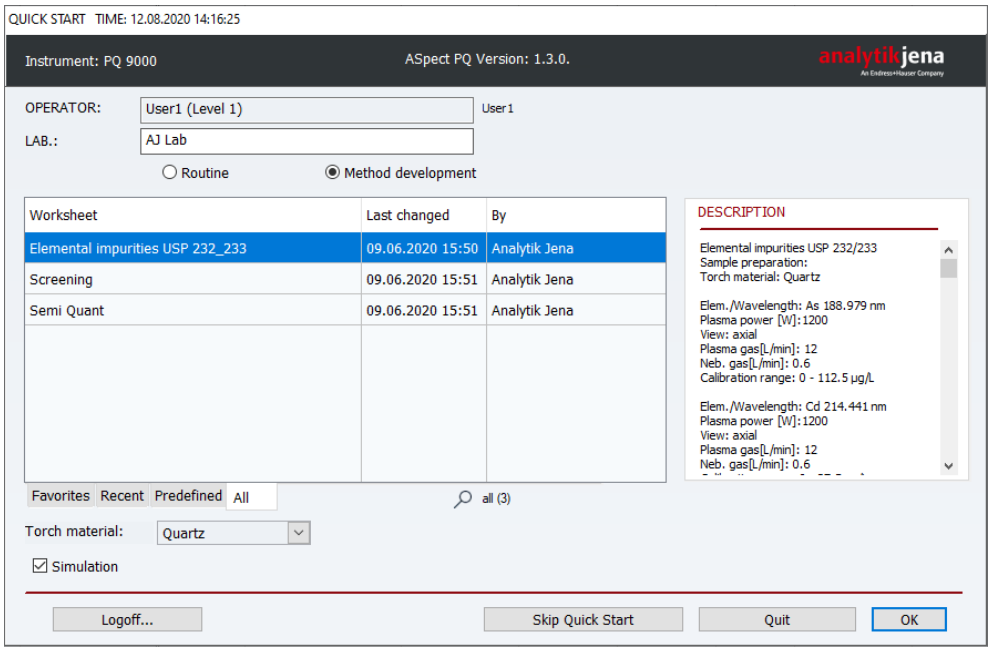
1.2 Starting ASpect PQ

- ▸ Switch on the device and the autosampler.
- ▸ Click on the ASpect PQ icon on the Windows desktop.
  - ✓ ASpect PQ is started.
- ▸ If the user management option has been installed, you will be prompted to enter a user name and password. The ASpect PQ program will only be accessible after successful entry of this data.

After the software starts, the Quick Start opens. Here you have the option of selecting worksheets with preset methods and sequences to quickly start a measurement or switching directly to the ASpect PQ interface.

1.2.1 Quick Start window

After the software has been started and a user logged in (only if user management is installed), the**Quick Start** window appears. From here you can load a worksheet or switch to ASpect PQ without any further settings. You can also open the **Quick Start** window in ASpect PQ with the menu command **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 a user name manually.
Lab.	You can enter up to 30 characters. The name entered last is saved and issued as information on result reports.
Routine	Start program for routine operation. In routine operation, only methods that are enabled for routine operation are displayed. If the optional "21 CFR Part 11 Compliance ASpect PQ" module is installed, the **Routine** option is preset. There is no choice between **Routine** and **Method development**.
Method development	Start the full program. All configurations in method development have been released.
Torch material	Select the torch material used (quartz or ceramic) to adjust the sensitivity of the optical plasma sensor.
Simulation	For training and demonstration purposes, it is possible to operate ASpect PQ without a connected analyzer. When enabled, all device functions (including data acquisition and analysis) are run in simulation mode.
Skip Quick Start	Switch to the ASpect PQ interface without selecting a worksheet.

Option / button	Description
Configuring ports: AX/ SDX	Only when the Teledyne Cetac SDXHPLD dilution system is connected to the ASX-560 autosampler. After clicking on the button, the USB ports used by the autosampler and dilution system are automatically configured. If the optional "21 CFR Part 11 Compliance ASpect PQ" module (User Management) is installed, this function can only be performed by a user with administrator rights.
Quit	Close the **Quick Start** window and exit ASpect PQ.
OK	After selecting a worksheet, switch to the ASpect PQ interface.

Worksheet table

The worksheet table displays the currently available worksheets. The 4 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 during the installation of ASpect PQ
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 several elements, all worksheets that contain at least one of the elements in the stored method (OR logic) are displayed. This search includes both methods directly linked to a worksheet and methods loaded within a linked sequence.

1.2.2 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 the accessories on the analyzer and then switch on the accessories and the device.
- Start the software.
  - ✓ The **Quick Start** window appears.
- Enter the required information in the **Operator** and **Lab.** fields.
- Under **Torch material**, select quartz glass or ceramic.
- Select the required worksheet in the worksheet table.
- Click on **OK**.
  - ✓ The ASpect PQ interface 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.

1.2.3 Starting without a worksheet

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

- Install the accessories on the analyzer and then switch on the accessories and the device.
- Start the software.
  - ✓ The **Quick Start** window appears.
- Enter the required information in the **Operator** and **Lab.** fields.
- Under **Torch material**, select quartz glass or ceramic.
- Click on **Skip Quick Start**.
  - ✓ The ASpect PQ interface 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** in a method (method development). Load a method.
- 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 is 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. This data is 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 start of the measurement the result data is 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.

1.2.4 Opening a second instance of ASpect PQ

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 **File** | **Start Offline Program Instance** menu item.

1.2.5 Locking ASpect PQ

The application can be locked for operation whilst measurements continue to be performed when it is locked. In combination with the optionally available user management a password confirmation is required to unlock the screen.

- Select the **Extras** | **Lock** menu item.
- To unlock the application click on the padlock icon on the screen.

1.3 Exiting ASpect PQ

- Extinguish the plasma.
- Quit the program by selecting the **File** | **Quit** menu item.
- If, at this time, method, sequence or sample information data files are open that have not been saved yet, you will be informed accordingly. Click on **Yes** if you want to save the files.
- The ICP-OES device still requires time for system cooling after the plasma has been switched off. If the target temperature has not yet been reached, a progress window will appear with a message about safely switching off the device.
  Do not switch off the ICP-OES device until you have exited ASpect PQ.

NOTICE

If you exit ASpect PQ while the plasma is burning, the plasma will be automatically extinguished after a query!

See also

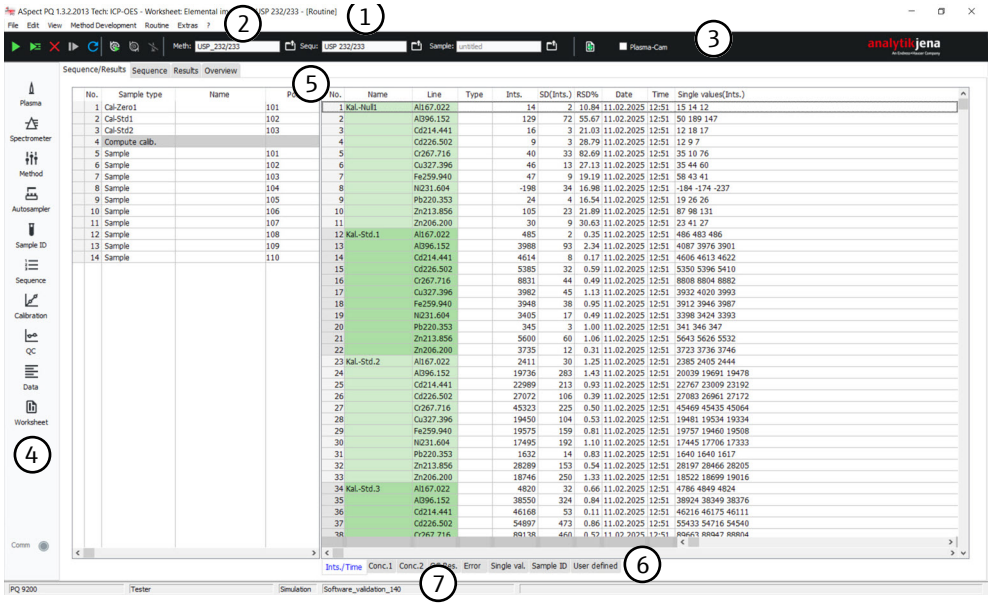
Switching on the spectrometer and igniting the plasma [▶ 64]

1.4 General information on operation

1.4.1 The workspace

After starting the ASpect PQ program, the **Quick Start** window is first opened. From here, you can access the workspace.

Main components of the workspace



No.	Description
1	In the **title bar** you will find information about the software version, the connected device, the technology and (if loaded) the worksheet.
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 on the button behind the fields to load the data record. You will also find the button for creating a new worksheet here.
4	This **icon bar** 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.
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 database.

See also

- Displaying results and analysis progress in the main window [▶ 73]
- Quick Start window [▶ 8]

1.4.2 The Help function

Help on using ASpect PQ is available via the **?** | **Help topics** menu item. While working with ASpect PQ windows, you can activate context-sensitive help by pressing the **F1** function key.

The program displays tooltips (brief information) for toolbar and icon bar buttons, other icon buttons and for column titles in the **Method**, **Sequence** and **Sample ID** windows when you hover the mouse pointer over them.

1.4.3 Overview of the menu bar, toolbar and icon bar

Functions in the menu bar

The menu bar is located at the top of the ASpect PQ interface and is used to initiate all software operations. 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 depending on whether other windows are 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** window ■ 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
View	■ Open and close windows showing graphs and information during the analysis sequence, e.g., signal curves ■ Select the scale of the signal axis for graphs
Method Development	■ Open windows required for method development ■ Record overview spectrum
Routine	■ Start, pause and cancel measurement ■ Reprocess results ■ Delete calibration ■ Extinguish plasma ■ Wash system
System	Available if the optional "21 CFR Part 11 Compliance ASpect PQ" module is installed ■ Configure user management ■ Changing a password ■ View audit trail ■ Sign results
Extras	■ Open **Data** and **Options** windows ■ Open line list ■ Search for samples ■ Print current screen display ■ Check and perform maintenance (recirculating chiller) ■ Lock workstation
?	■ View help and version information

Toolbar

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

Tools	Description
	Start measurement routine
	Measure selected rows in the sequence

Tools	Description
	Pause running measurement routine
	Continue paused sequence measurement
	Reprocess results
	Start/stop the pump at the ICP-OES device
	Speed up the pump (flush sample path)
	Extinguish plasma (quick shutdown)
	Open file Saved methods, sequences or sample IDs can be loaded into the program and used for the current analysis.
	Create new worksheet
Plasma-Cam	Activate plasma camera The software continuously displays the camera image with a recording of the plasma. Possible irregularities, such as the formation of a ring plasma during the ignition process, are quickly detected. The camera image can be cropped using the **Settings** | **Crop camera image** menu command in the camera window.

Icon bar

The icon bar provides quick access to the key functions of the ASpect PQ program. Clicking on the icon 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.

Icon	Description
	Check atomization: ■ Igniting/extinguishing the plasma ■ Setting the gas flows ■ Check the pump for the sample conveyance to the nebulizer ■ Adjustment of the transfer optics ■ Optimization of plasma power and nebulizer gas
	Check spectrometer functions: ■ Device data ■ Test of wavelength corrections ■ Start a measurement on a test wavelength ■ Start a continuous measurement for device optimizations
	Open method window
	Specify autosampler
	Open sample information data window
	Open sequence window
	Open window with calibration

Icon	Description
	Open window with quality control data
	Open the data management
	Manage worksheets, open saved worksheets

1.4.4 Frequently used control elements

Various button, mouse and keyboard functions are used in Aspect PQ, which always have the same or very similar meanings.

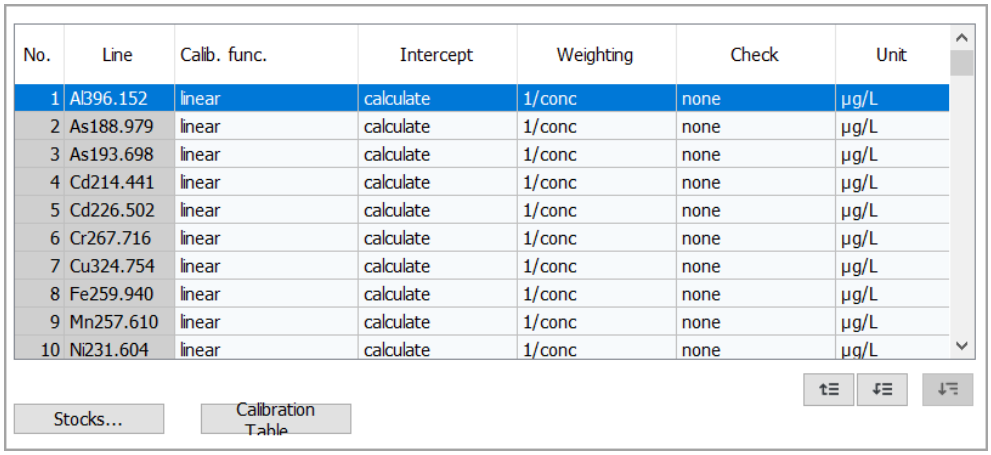
These control elements are described here in general. Specific information is given, where necessary, in the description of the respective windows.

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 table row, click on the corresponding row in the first table column highlighted in gray. You can then move the selection bar using the arrow buttons on the keyboard.

- To change the column width, move the mouse pointer over the boundary line between two columns until a double arrow appears. Press the left mouse button and adjust the column width.

The following additional functions are available in input fields:

- F2 activates the edit mode. In this mode, the arrow keys on the keyboard are used for editing character by character. Pressing **F2** again reactivates the standard mode where the cursor keys are used to navigate between the cells.
- Text can be copied to the Windows clipboard and pasted again using the **Edit | Copy** and **Edit | Insert** menu or the Ctrl+C and Ctrl+V key combinations.

Buttons accessible in tables

Button	Function
Append	Appends a new table row to the end of the list.
Insert	Inserts a new table row before the selected line.
Delete	Deletes the selected table row.
	Shifts up the selected table row 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.
	Shifts down the selected table row by one position.
	Transfers the value of the selected cell to all following table rows of the same sample type (sample, standards, QC, etc.). With the **inc.** checkbox enabled (inc. means increment), this value will be incremented automatically, e.g., Sample001, Sample002 ...

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:

Icon	Function
	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 returns 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

Icon	Function
F1	Open the context-sensitive help
F2	Edit table cells
F5	Start printing a screen image
F6	Measure the selected row of the sequence (menu item **Routine | Run Selected Sequence Row...**)

Icon	Function
F7	Display additional graphical windows (e.g., signal curve)
F8	Close additional graphical windows
F10	Switch between the menu bar of the workspace and results window for operation via keyboard
F11	Continue a previously halted measurement (menu item **Routine** | **Continue**)
F12	Start or stop the measurement process (menu items **Routine** | **Start Sequence...** and **Routine** | **Stop**)

Using the printer

If you have already set up a Windows default printer, this printer will be used in ASpect PQ.

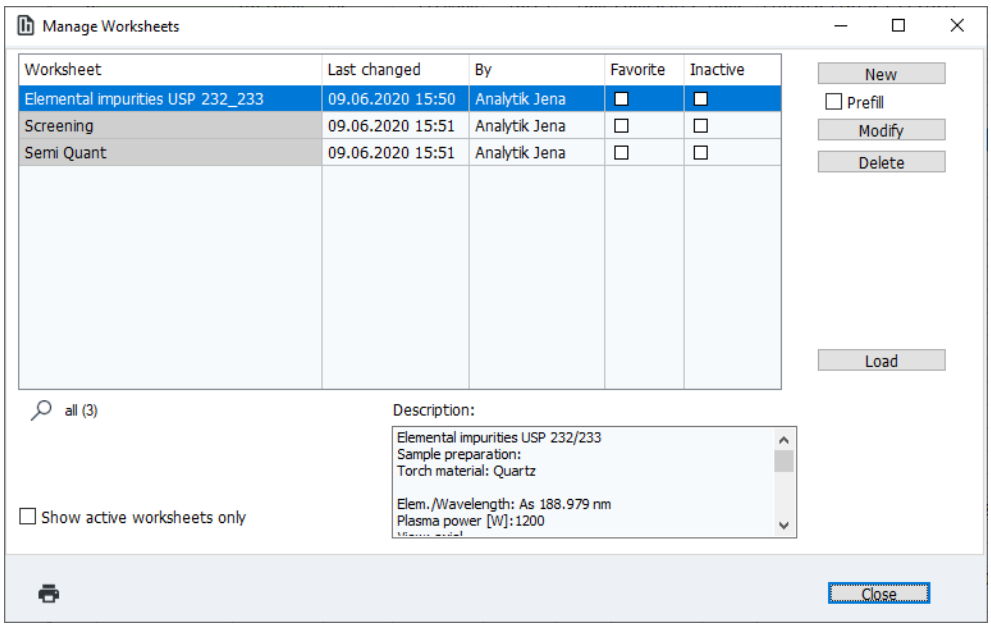
2 Worksheets

A worksheet is a folder that summarizes a method and a sequence. In addition, settings for a sample ID file and for results data can be stored 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



Buttons / options	Description
New	Create new worksheet
Prefill	An already loaded sequence and method are transferred to the worksheet.
Modify	Edit selected worksheet
Delete	Delete selected worksheet
Load	Load selected worksheet for a measurement
Show active worksheets only	Hide all worksheets in the table that are marked **Inactive**.
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	If activated, displays the worksheet on the **Favorites** tab in the **Quick Start** window.
Inactive	If activated, this worksheet will not be shown in the Quick Start.

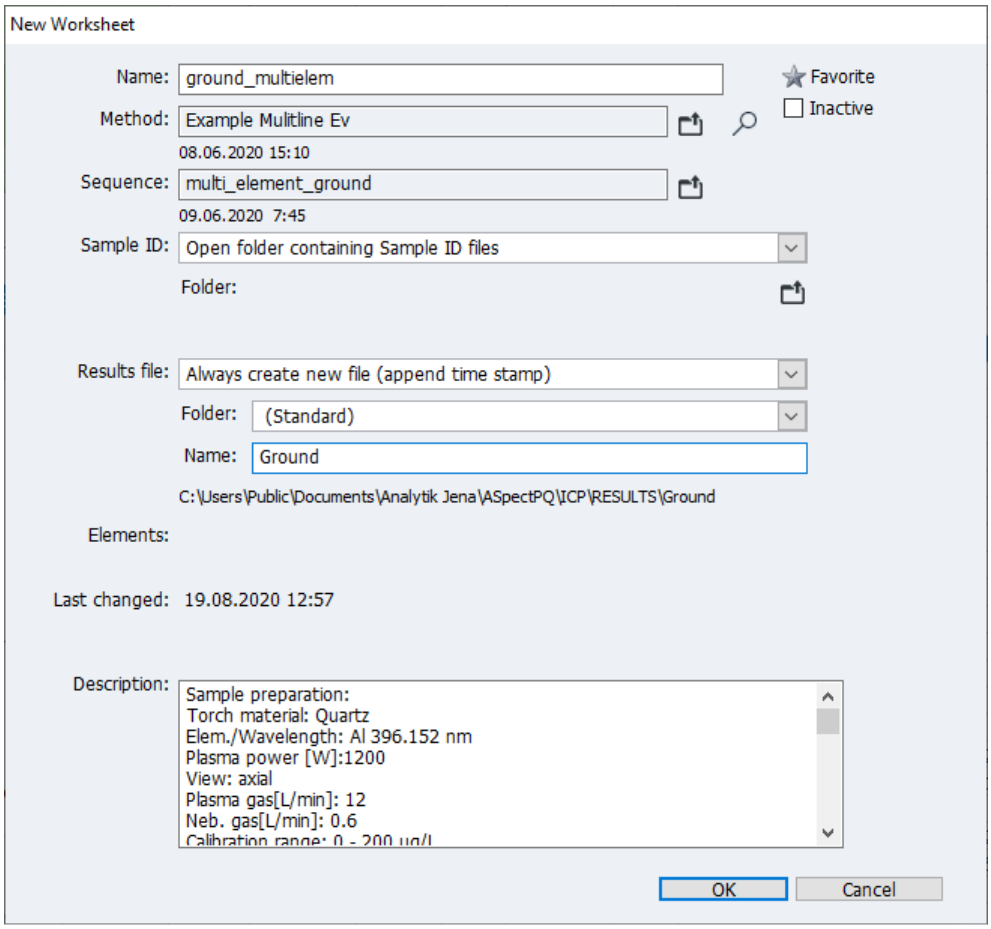
Table column	Description
	However, a worksheet marked as inactive can be loaded from the **Manage Worksheets** window.

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

Field/option	Description
Name	Enter the name of the worksheet
Method	Method stored in the worksheet Click to open the database window and select the method.
Sequence	Sequence stored in the worksheet Click to open the database window and select the sequence.
Sample ID	Optionally, you can define 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, a folder is opened in which the sample ID file is available. Click on and select the folder.

Field/option	Description
	Load Sample ID file: When the worksheet is loaded, a sample ID file is automatically loaded. Click on and select the file. You can also define a file mask using the "*" and "?" wildcards.
Results file	Optionally, you can define settings for saving the results: **(none)** Measurement starts with the Start window, in which the name of the results file and the storage location are assigned. **Always create new file (append time stamp)** Results files of a sequence 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 the sequence is started for the first time. Each subsequent time the sequence is started, 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 the 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, this worksheet will not be shown in the Quick Start. A worksheet marked as inactive can be loaded from the **Manage Worksheets** window.

Specifying a worksheet

- To create a new worksheet, click on in the icon bar to open the **Manage Worksheets** window and click on **New**.
  Alternatively, you can click in 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, you can enter specifications for saving the results file and the use of a sample ID file and edit the description (see below).
- Exit 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 [▶ 67]

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 the changes in the same way as when creating a new worksheet.

2.3 Loading a worksheet

You can select a worksheet in the **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 with a mouse click and click on **Load**.
  - ✓ The worksheet is loaded and the 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.

NOTICE

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.

2.4 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.

3 Methods

Methods store the parameters required for an analysis.

- Selection of analysis lines
- Parameters for line analysis
- Plasma and spectrometer 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. Sequences define the order in which samples and actions are to be processed within the measurement routine. Saved methods can 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 you have not loaded a method after starting ASpect PQ, the window displays will contain the default settings or be empty.

3.1 Creating, saving and loading methods

Methods are saved in a database. If you change an existing method and save the changed method under the same name, the software creates a new version of the method. The existing method can therefore not be overwritten or be unintentionally deleted in this way.

Further functions for exporting, importing or deleting methods can be found in the **Data** | **Data management** window.

See also

Managing methods and sequences [▶ 123]

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 **File** | **Create new Method** menu item.
If you have not yet activated a method, you can alternatively click on .

▶ Enable one of the three options in the **New method** window:

- **Based on default parameters**: Open the **Method** window only with default settings for calibration and statistics.
- **Based on current parameters**: Open the **Method** window with the currently set method parameters.
- **Based on saved method**: Select a method in the **Load method** database window.

▶ Confirm your selection with **OK**.

✓ The **Method** window with the selected default settings appears.

▶ Specify the method on the various tabs and make the necessary optimizations.

▶ Enable the set 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.

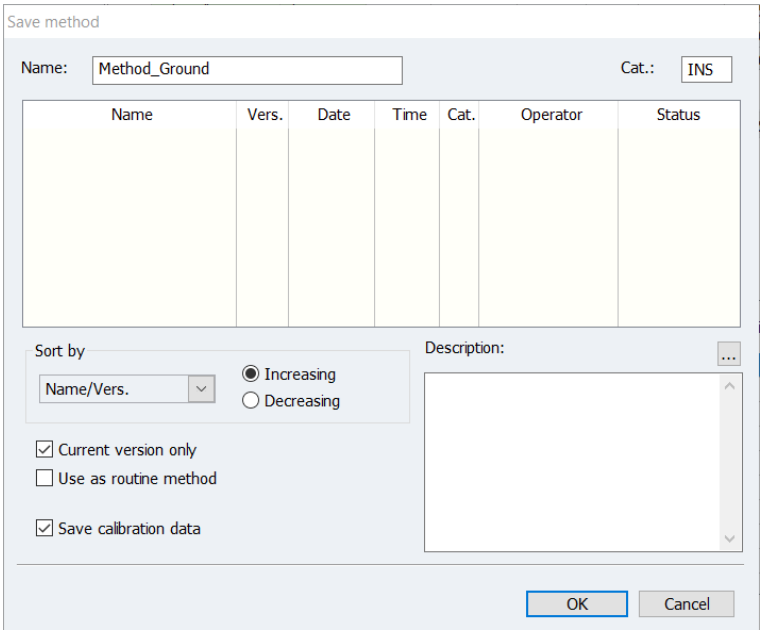
See also

Specifying method parameters [▶ 25]

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 worksheets. Methods are saved in the database in the **Save method** window. You can enter additional data to categorize the method and make it 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. If the FDA 21 CFR Part 11 Compliance module is installed, you can use selected categories to mark a method as approved. You define the categories for approved methods in the user management settings.
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 will be displayed for methods with the same name.
Use as routine method	If enabled, the method is available in the **Routine** program mode. The program mode is selected in the **Quick Start** window. If the optional "21 CFR Part 11 Compliance ASpect PQ" module is installed, this option is not available for selection.
Predefined methods	Save any available calibration curves with the method The calibration curves can be used for further analyses.

Option	Description
Description	Optionally enter further explanations for the method Click on ... to open a list of predefined comments. You manage these comments in the **Data** | **Default descriptions** window.

Saving a method

- In the **Method** window, click on **Save** or select the **File** | **Save** | **Method** menu item.
  - ✓ The **Save method** window appears.
- Enter the name of the method and select further parameters.
  - ✓ 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.

NOTICE

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

See also

- Configure general settings of the user management [▶ 148]
- Quick Start window [▶ 8]
- Managing methods and sequences [▶ 123]

3.1.3 Loading a method

You can load saved methods and start a measurement routine 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 **File** | **Load method** menu item.
  - In the **Method** window, click on **Open**.
- Choose the desired method from the list.
- In the **Cat.** field, you can limit the displayed methods by selecting a category. If you want to see all methods, delete the entry in the **Cat.** field.
- Enable the **Current version only** checkbox if only the method with the latest version is to be shown for methods with the same name.
- Exit the **Method** window with **OK**.
  - ✓ You have loaded the desired method. The method is displayed in the toolbar under **Meth**.

Loading from a results file

The method can be extracted from a results file displayed in the main window.

- Right click on any sample.
- In the context menu, select the **Load method from results** item.
- After a query whether current method parameters should be overwritten the method can be displayed 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 window Method

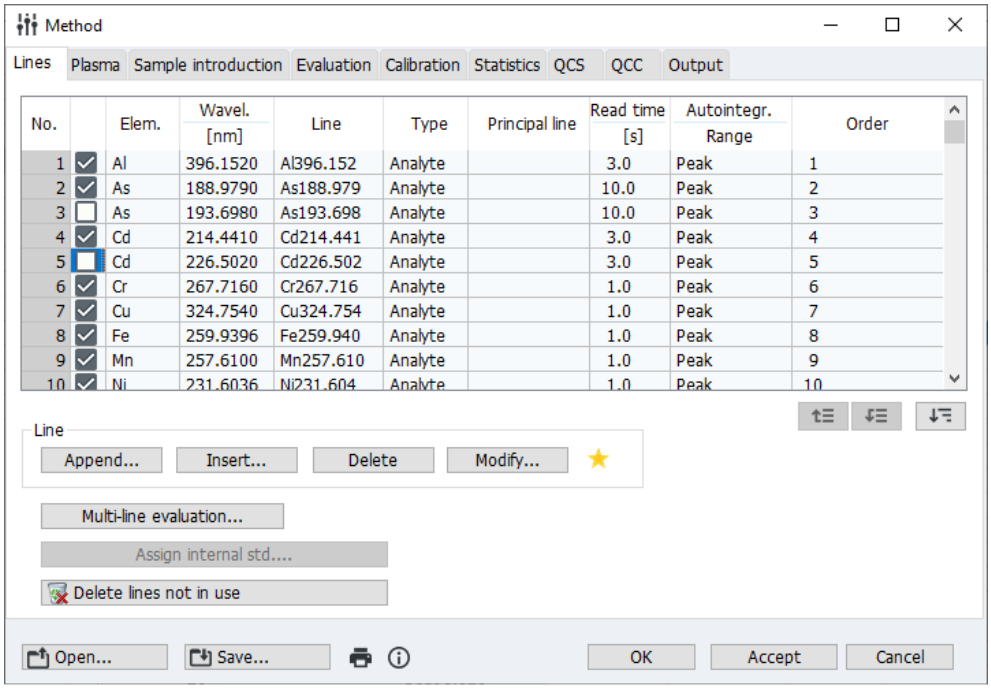
The bottom part of the window contains buttons that are available at all times.

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

3.2.1 Specifying analysis lines (Method | Lines window)

In the **Method** | **Lines** window, select the analysis lines for the measurement.

Method | Lines window



Line table parameters

Table column	Description
No.	Sequence of selected lines in the table
/	Only available in **Method Development** mode (not with "21 CFR Part 11 Compliance ASpect PQ" module) The marking eases method development, where several lines of an element are measured at the beginning and then the appropriate line is selected. If an element line is activated with a checkmark, this line is used and mea-

Table column	Description
	sured for the analysis. Deactivated lines are excluded in the following analysis and are not measured. Deactivated lines are not yet explicitly deleted from the line table.
Elem.	Element icon of the element to be analyzed
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. The name can be edited freely and must be unique.
Type	Selection between **Analyte** (line to be analyzed) and **Int.std.** (internal reference line)
Principal line	Selection and display of the analysis line with which the current line is measured simultaneously (simultaneous measurement) The measuring time can be shortened by measuring lines that are close together with one spectrometer setting. Click on **Multi-line evaluation** to display the possible combinations.
Read time	Total measuring time for an analysis line
Autointegr. Range	The integration time is automatically chosen for optimum exposure of the CCD detector and to avoid over-exposure With over-exposure the charge absorbed by a pixel spills over to adjacent pixels and causes measuring errors (blooming effect). To determine the integration time the area under consideration must be selected: **Spectrum** The integration time is optimized for the highest peak within the spectral range of the line. This is the default option and leads to a safe result. **Peak** The integration time is optimized for the analysis peak. When selecting this option the dynamic range of the CCD detector is used optimally for the analysis. It must, however, be ensued that no higher peak is present in the immediate vicinity of the analysis pixel. In this case the measuring result could be distorted by the blooming effect. **etector** The integration time is adapted to the highest peak on the detector. In this option no area of the detector is over-exposed; it may be possible that the pixels of the analysis peak are not optimally exposed.
Order	Analysis order The measuring order can be freely defined. **Note:** After highlighting a number the numbers are assigned to the subsequent lines in ascending order after clicking on . You can arrange selected lines (element lines) in the desired measuring order in the table with and ; enter "1" under Order in the first row and assign the measuring order to all other analysis lines in ascending order with .

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 and checkboxes

Button	Description
Multi-line evaluation	Find combinations of analysis lines that can be measured together with one spectrometer setting These analysis lines can be measured simultaneously.
Assign internal std.	Combine and correct analysis lines with an internal standard
Delete lines not in use	Only available in **Method Development** program mode (not with "21 CFR Part 11 Compliance ASpect PQ" module) Delete all disabled lines from the method list. **Note:** Methods can only be saved and used as routine methods if all lines in the line table are being used.
Optimized measuring order	Automatically sort analysis lines by wavelength and measurement conditions to shorten the total measuring time If the checkbox is enabled, manual sorting of the analysis lines is no longer possible. **Note:** The measuring time depends on the number and sorting of the analysis lines and the measurement conditions. Therefore, selecting similar parameters for plasma and transfer optics for many analysis lines can also shorten the measuring time.

See also

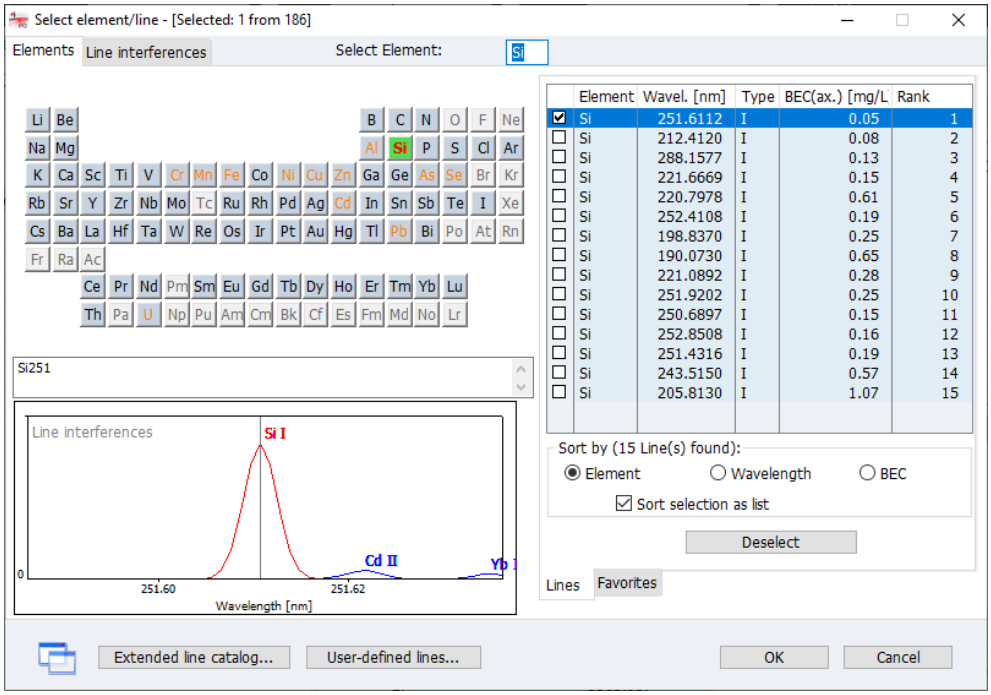
- Measuring lines simultaneously [▶ 29]
- Frequently used control elements [▶ 15]
- Defining internal standards [▶ 31]

3.2.1.1 Inserting analysis lines into the line table

The analysis lines are selected in the **Select element/line** window.

Elements in the Select element/line window

The **Elements** tab contains the periodic table with all elements analyzable with the ICP-OES technology (dark gray buttons and black element symbols). "Grayed out" elements are not available. The **Line interferences** tab shows the known possible interferences for a selected line with relative sensitivities.



The **Favorites** spreadsheet contains a preselection of lines with the recommended applications (key words). When selecting these lines, optimized method parameters are simultaneously transferred to the method. You can also add your own lines to these favorites.

The **Lines** spreadsheet contains all selectable lines with the following information:

Table column	Description
Element	Element
Wavel.	Analysis wavelength in nm
Type	Atomization type display: I: Atom line II: Ion line
BEC	Typical BEC value of the analyte line The BEC value (background equivalent concentration) is the concentration of the analyte producing an intensity equivalent to the background. A lower value corresponds to a higher sensitivity. The BEC values were determined under the following conditions: axial monitoring, output 1200 W, plasma gas flow 12 L/min, auxiliary gas flow 0.5 L/min, nebulizer gas flow 0.6 L/min.
Rank	Ranking of the recommendation of the analysis line The recommendation of an analysis line depends both on the sensitivity and on the possible interference from adjacent lines of other elements. The further forward a line is in the ranking, the better the chances of achieving good results with the analysis line.

Using the **Element, Wavelength** or **BEC** options you can sort the line table in ascending order by chemical symbol, wavelength or BEC.

If the **Sort selection as list** option is enabled, the lines are inserted into the line table of the method in the sorting order of the list (**Sort by**). If the option is disabled, the lines are inserted in the order they are selected.

Selecting lines

- In the **Method** | **Lines** window, click on **Append** or **Insert**.
  - ✓ The **Select element/line** window appears.
- If you click on one of the dark gray element symbols in the periodic table, only the lines of the selected element are displayed in the **Lines** and **Favorites** tables.
  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.
- In the **Favorites** spreadsheet select the lines for your application or enable the checkboxes of the desired lines in the **Lines** table.
- Change to the **Line interferences** tab and check the selected lines for known interferences.
- Continue until you have selected the lines for each analyte. Exit the window with **OK**.
  - ✓ The selected lines are transferred to the **Method** | **Lines** window.

Note:
When working through the methods, select several lines for each analyte.

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.

- In the **Select element/line** | **Elements** window, click on **Extended line catalog**.
- Select the desired 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 lines table** to transfer the selection to the line list.

NOTICE

The lines added from the extended line catalog can no longer 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.

- In the **Select element/line** window, click on **User-defined lines**.
- In the **Edit lines** window, enter the data for the **Element** and the **Wavelength** and select the **Type** in the list box.
- Transfer the entries to your own line list with **Add**.
- Click on **Close** to transfer your own lines to the line list.

Own lines can be edited or removed again from the line list.

- To edit a line in your own list, select the line by mouse click in the list of the **Edit lines** window.
  Enter the new line data and then click on **Modify**.
- You can remove a selected entry in the list by clicking on **Delete**.

See also

Defining your own line favorites [▶ 31]

3.2.1.2 Measuring lines simultaneously

Lines that are recorded together with one spectrometer setting can be measured simultaneously to shorten the analysis time. With the **Multi-line evaluation** function you can find these lines in the current method and combine them for analysis.

- 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.

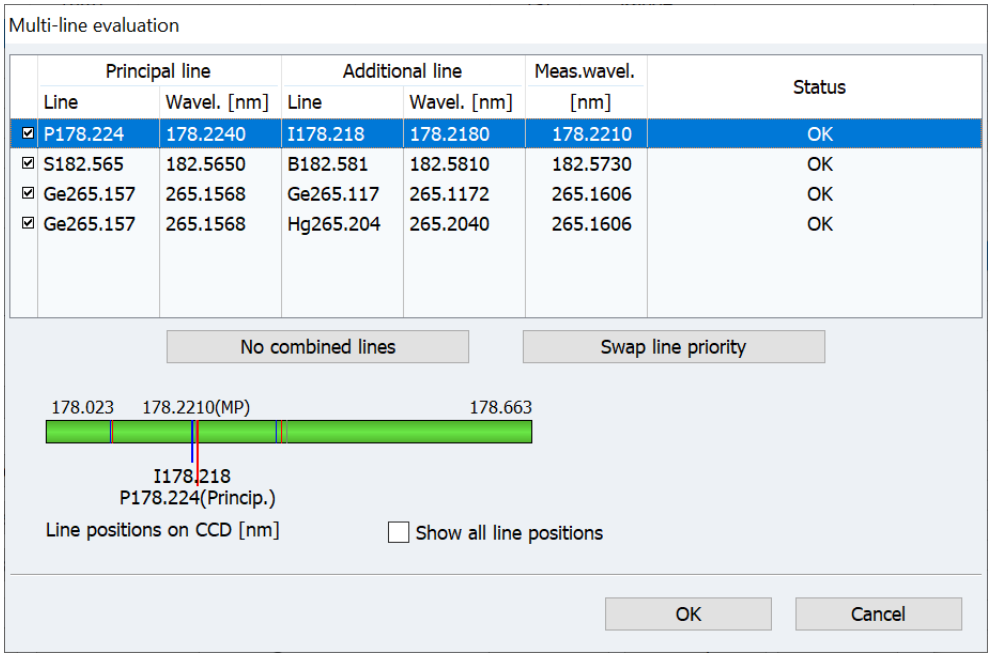


Table columns / button	Content
Checkbox	If enabled the respective line combination is measured simultaneously in the method.
Principal line	The measurement parameters of the **Principal line** are used to measure the line combination. **Line** Line name of the principal line **Wavel.** Wavelength in 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)
Status	Comments
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 plasma parameters from the principal line. With **Swap line priority** this assignment can be reversed.

3.2.1.3 Defining your own line favorites

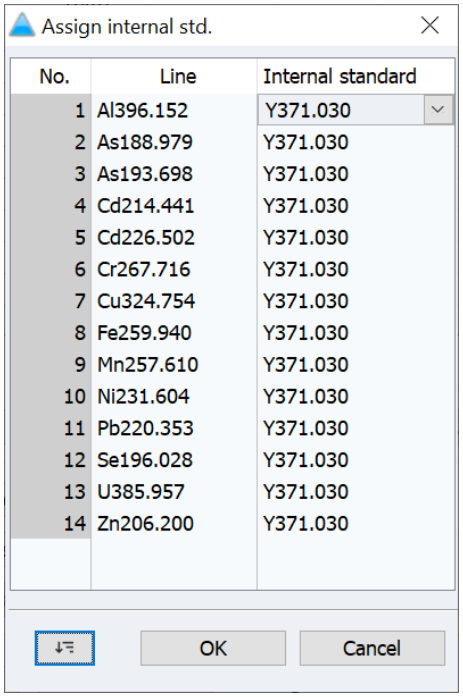
You can add favorite analysis lines to a favorite list with notes on the preferred application. The information on the analysis lines is saved with all line-relevant method parameters in this entry. The favorite list is available during each selection of element lines.

- Mark the line in the table of the **Method** | **Lines** window and click on ☆.
- In the **Add to favorites** window edit the line name.
- In the **Comment** field you can enter additional notes for the line.
- In the **Tags** list select one or several applications.
  You can supplement the key word list with your own entries. Predefines key words are highlighted in blue.
  ✓ The line is available in the **Select element/line** window.

3.2.1.4 Defining internal standards

Internal standards are mainly used to correct non-spectral interference caused, e.g., by sample transport faults. You define the internal standards in the line table of the **Method** | **Lines** window.

- Insert the analysis line that you want to use as an internal standard into the line table and in the **Type** table column select the **Int.std.** option**.**
- Click on **Assign internal std.**.
  The **Assign internal std.** window appears.
- In the table, assign the internal standard or standards to the desired analysis lines. To do this, click on the corresponding line in the **Internal standard** column and select the internal standard from the list.
- Click on ↓ to transfer the settings for an analysis line to all subsequent lines in the table.
- Click on **OK** to apply the settings to the method.



3.2.2 Configuring parameters for plasma and transfer optics (Method | Plasma window)

In the **Method** | **Plasma** window make the following settings:

- Gas flows for the plasma in the torch
- Selection of the monitoring direction of the plasma and its adjustment

Elements in the Method | Plasma window

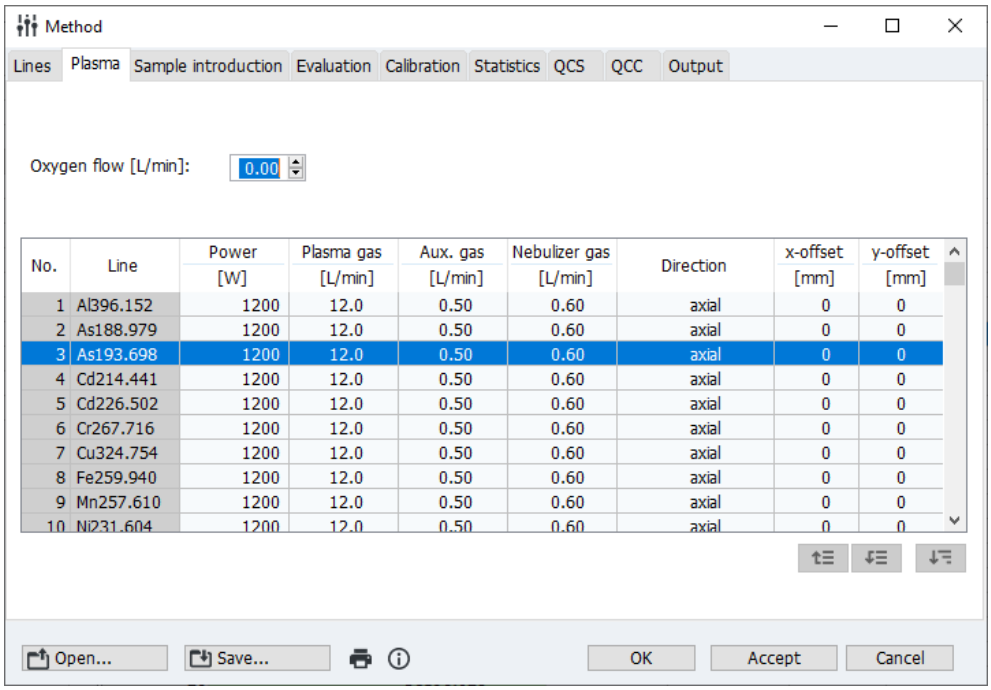


Table column	Description
No.	Sequence of selected lines in the table
Line	Name of the analysis line
Power	Effective plasma power in watts Increasing the plasma power improves the stability of the plasma, e.g., with organic solvents or samples with a high salt content as measuring solution. At the same time a higher plasma power also requires a higher plasma gas flow to prevent melting or damage of the torch.
Plasma gas	Plasma gas flow in L/min The plasma gas flows between the outer and inner quartz tube of the torch. It is put into the plasma state by the induction of the coil and simultaneously cools the outer tube of the torch. A higher plasma gas flow can improve the lifetime of the torch.
Aux. gas	Auxiliary gas flow in L/min The auxiliary gas flows between the inner quartz tube and the injector. It supports the development of the measuring channel and pushes the plasma away from the injector tip. A higher auxiliary gas flow is required, e.g., for measuring solutions with organic solvents or higher salt concentrations.
Nebulizer gas	Nebulizer gas flow in L/min The nebulizer gas is introduced at the nebulizer. It nebulizes the sample and moves it through the spray chamber and injector into the plasma.
Direction	Monitoring direction of the plasma With the transfer option the emission radiation from the plasma can be coupled to the spectrometer from two directions. Dependent on the analyte line the optimum monitoring direction can be selected.

Table column	Description
	radial The plasma is monitored from the side at a specific height above the upper coil edge. **axial** Monitoring is from the top along the longitudinal axis of the plasma. Both monitoring directions can also be weakened. This avoids an overflow of the detector for high intensities and increases the analytical range.
x-offset and **y-offset**	Correction of the transfer optics in mm By shifting the optics along the measuring channel (for radial observation) and out of the center of the measuring channel (for radial and axial observation), areas of varying hotness can be scanned and the optimum emulsion temperature of the analysis line can be determined. The optimum for a line can be determined automatically in the **Plasma** window.

NOTICE

During the first phase of method development (selection of suitable lines) the preset plasma parameters are sufficient. These parameters can be changed after defining the analysis lines, the necessary background corrections and the determination of the linearity range to further optimize the method parameters.

Using oxygen

For special applications, e.g., organic matrices, oxygen can be used as an additional gas.

- Set the gas flow in the **Oxygen flow** field.

See also

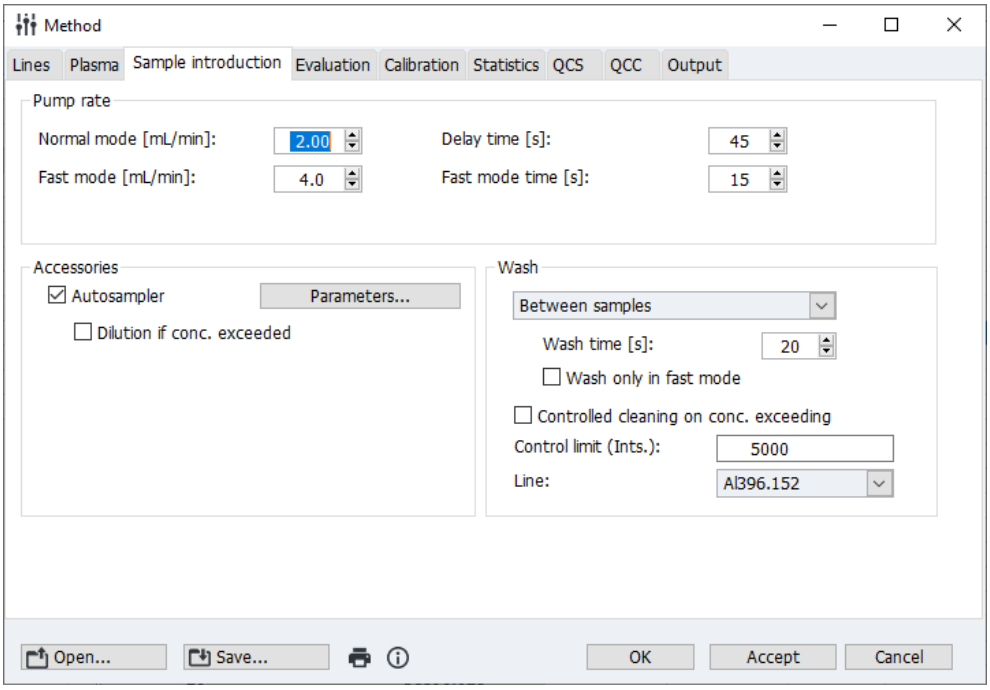
- Adjustment and optimization of plasma [▶ 107]

3.2.3 Configurations for sample introduction (Method | Sample delivery window)

In the **Method** | **Sample delivery** window you make the following settings for the analyzer:

- Pump rate of the pump at the analyzer
- Use of the autosampler
- Purging option

Method | Sample delivery window



Pump times on the ICP-OES device

Option	Description
Normal mode	Normal pump speed at which the sample is transported during analysis This speed should ensure optimal nebulization of the sample and should be based on the recommended pumping rate of the nebulizer used.
Fast mode	Increased speed at which washing (with washing solution) can be performed during the measuring pauses and at which the sample can be transported up to the nebulizer Activating this speed optimizes the transport time. However, this speed must not be used during the measuring time, because the homogeneous nebulization of the sample will then no longer be ensured.
Delay time	Time from the start of sample aspiration up to the actual measuring start This time is required to wash the entire sample path up to and including the torch with the sample and ensure stable atomization. **Note:** The delay time also includes the time entered in the **Fast mode time** field.
Fast mode time	Time with which the sample is transported with a high pump rate during the passing of the delay time

NOTICE

In the **Method** | **Sample delivery** window set the pump rates of the tube pump of the ICP-OES device. The pump rate at the autosampler for the transport of the washing solution can be regulated with the rotary knob above the pump at the autosampler or at the Cetac samplers in the **Autosampler** | **Techn. parameters** window.

Using the autosampler

If an autosampler is used for the analysis, enable the **Autosampler** option. Via **Parameters** you get to the autosampler settings.

Washing and controlled cleaning

During the completion of a sequence you can set the washing steps after each sample measurement. The washing solution is then taken from the wash cup of the autosampler during automatic measurement. During manual measurement a prompt is shown to provide the washing solution.

If the concentration of the sample exceeds the measuring range of the calibration curve by more than 10 %, the sample path and the torch can be washed to remove contamination from the previous measurement. During washing, the intensity is measured to check the cleaning result and washing continues until the control limit is reached. The automatic cleaning control is recommended after the measurement of highly concentrated samples.

Option	Description
Wash	**off** Wash mode switched off. No washing performed automatically. **Between samples** Washing after each sample, but not within a statistical series
Wash time	During this time, the sample path up to the torch is washed.
Wash only in fast mode	The wash step only takes place with the fast mode time. If the option is disabled, washing is initially carried out in fast mode for the entered fast mode time (**Fast mode time**) and in normal mode for the rest of the wash time.
Controlled cleaning	If enabled, controlled cleaning takes place automatically if the concentration is exceeded
Control limit (Ints.)	Value of the signal level that must be reached during washing before the next solution is measured
Line	Element line that is used as a control line

3.2.4 Evaluating peaks (Method | Evaluation window)

In the **Method** | **Evaluation** window you define the parameters for peak evaluation.

NOTICE

In method development you determine the optimum settings for the background correction of the respective analysis line in the **Edit spectra** | **Evaluation** window and then transfer it to the method.

Method | Evaluation window

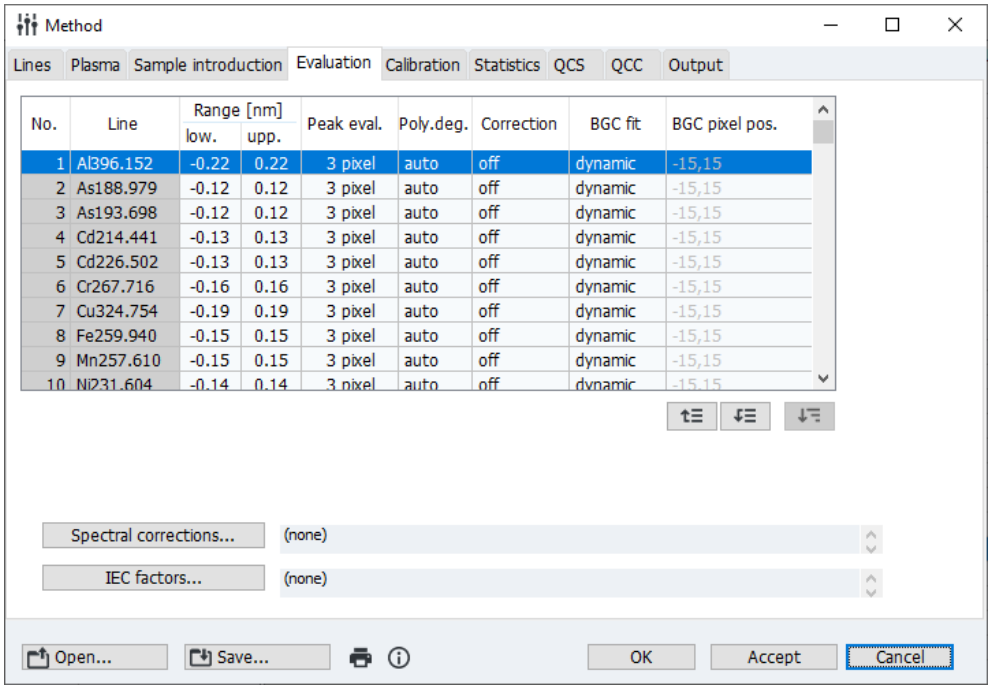


Table column	Description
No.	Sequence of selected lines in the table
Line	Name of the analysis line
Range	**low.** Lower limit of the wavelength range for spectral analysis relative to the measuring wavelength **upp.** Upper limit of the wavelength range relative to the measuring wavelength
Poly.deg.	Selection of the polynomial degree of the regression graph for static background correction Polynomial degrees of 0, 1st, 2nd and 3rd order are available for selection or an automatic search for the polynomial degree (**auto** option).
Peak evaluation	Selection of the peak evaluation **Pixels** Number of pixels used to analyze the intensity and ultimately for generating the measuring values. The intensities of the evaluation pixels are totaled. In this manner analysis inaccuracies can be reduced by fluctuations in the peak position. 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 Sample entry: 50,120-130 forms the total across the measuring values of the pixels 50 and 120 to 130
Correction	Algorithm for spectral correction (see below). **off** Apply no spectral correction **LSM** Spectral correction with Least Squares Model **IEC** Spectral correction with Inter Element Correction

Table column	Description
BGC fit	Adjust pixels for background correction **off** Do not apply background correction **dynamic** 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 pixel pos.** column.
BGC pixel pos.	Position of the pixels relative to the measuring pixel for static adaptation of the background correction Enter the pixel numbers for the background correction.

Buttons

Buttons	Description
Spectral corrections	Specify a model for spectral correction for analysis line
IEC factors	Specify an interelement correction for analysis line

See also

Evaluating the peak and determining the background correction – Edit spectra | Processing window [▷ 84]

3.2.4.1 Spectral corrections with Least Squares Model

With spectral corrections structured background emissions can be removed by way of calculations that were caused by the overlap of analysis lines with lines of the matrix elements. A precondition is that for the respective analysis line the possible interference spectra have been combined in a correction model.

- In the **Method** | **Evaluation** window click on **Spectral corrections** and configure the suitable correction model separately for each line.
  - ✓ Lines to which a correction model has been assigned are identified in the **Correction** column with **LSM**.

See also

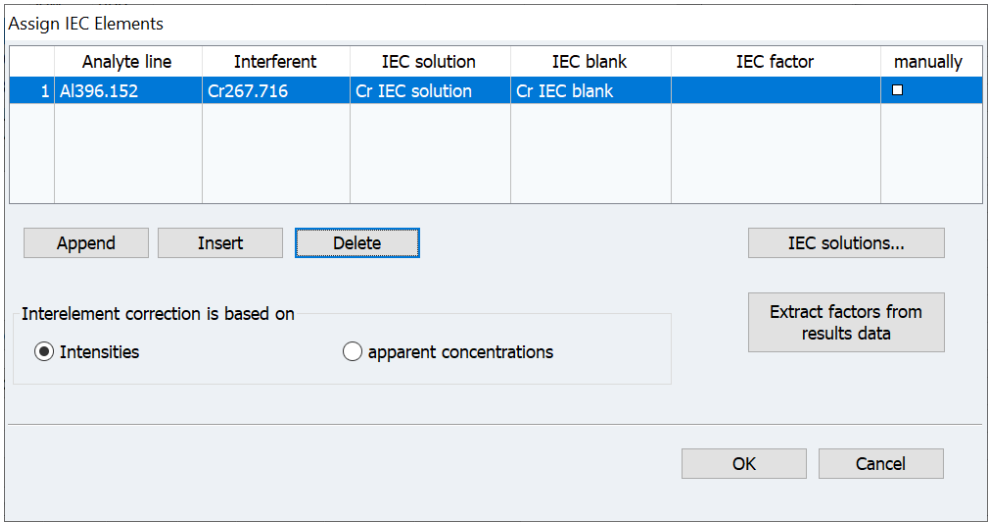
Removing spectral interference – Edit spectra | Spectral corrections window [▷ 86]

3.2.4.2 Interelement correction

With the interelement correction it is possible to correct direct line overlaps. A condition is an additional, interference-free wavelength of the interferent.

With a single element solution (IEC solution) the ratio of the two lines of the interferent (overlapped analysis line and interference-free line) is determined. The quotient (IEC factor) is used during subsequent sample measurements to subtract the apparent intensity or concentration of the interferent from the analyte line.

Elements in the Assign IEC Elements window



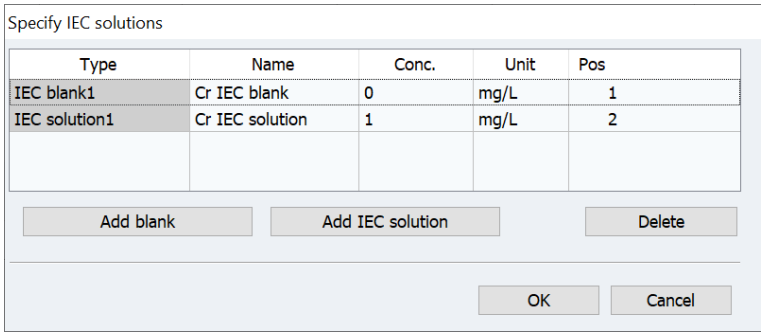
Control element	Explanation
IEC solutions	Input of name, concentration, unit and sampler position of the IEC element solutions and blank values used for the interelement correction
Append	Append a new row at the end of a list
Insert	Inserts a new row at the selected list position
Delete	Delete the selected row
Interelement correction is based on	**Intensities** Correction takes place by subtracting the intensities **Concentration** Correction takes place by subtracting the apparent concentrations
Extract factors from results data	Extract calculated IEC factors from a loaded result file

Table contents

Table column	Description
Specify IEC solutions	Name of the analysis line with interference
Interferent	Name of the interference line
IEC solution	Name of the single element solution containing the interferent. IEC solutions are specified via the **IEC solutions** button.
IEC blank	Name of the blanc value solution subtracted from the intensity or concentration of the interferent. Blank value solutions are specified via the **IEC solutions** button.
IEC factor	IEC correction factor Calculated factors are highlighted in gray.
manually	If enabled, an IEC factor can be entered manually. No measuring solutions are required.

Assign interelement correction

- In the **Method | Evaluation** window, click on **IEC factors.**
  - ✓ The **Assign IEC Elements** window appears.
- First specify the IEC solutions. You need a blank value and an IEC solution (single element solution) for each interferent.
  - – Click on **IEC solutions**.



- In the table in the **Analyte line** window, add a blank value and an IEC solution for each interferent by clicking on **Add blank** and **Add IEC solution**.
- In the corresponding table cells enter a name for each solution.
- For the IEC solutions enter the concentration of the interferent in the IEC solution into the **Concentration** column.
- Confirm the entries with **OK**.

▶ Back in the **Assign IEC Elements** window select the interfered line of the analyte in the **Specify IEC solutions** table column.

▶ In the **Interferent** column select the interference-free line of the interferent.

▶ In the **IEC solution** and **IEC blank** columns configure the corresponding single element solution and blank value solution.

▶ Select the type of Interelement correction either based on **Intensities** or **apparent concentrations**.

▶ Confirm the entries with **OK**.

✓ Lines which have an interelement correction assigned are identified in the line table of the **Method | Evaluation** window in the **Correction** column with **IEC**.

The measurement of the IEC solutions must be carried out in the sequence following the measurement of the calibration standards or calculation of the calibration.

Entering factors manually

Instead of determining the factors for the interelement correction by measuring the single element solution, known factors can be entered directly into the table.

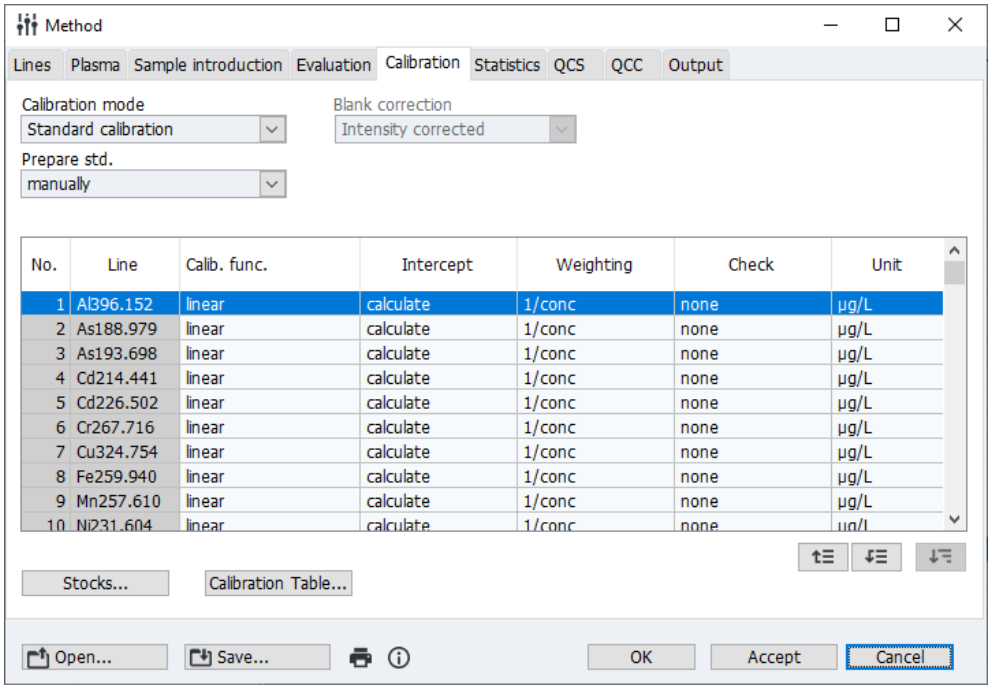
▶ After entering the **Specify IEC solutions** and **Interferent** enable the **manually** checkbox.

▶ In the **IEC factor** column enter the already calculated factor.

3.2.5 Entering calibration parameters (Method | Calibration window)

In the **Method | Calibration** window you define the type of calibration and blank value correction. Generally, multiple element standards are used for calibration, which you can enter as stock standards.

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. No further entries are required on the **Calibration** tab. The sequence list should, logically, only consist of samples.
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 quantities of a known sample are added to the unknown sample and the resulting substance 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.

Standard preparation

Option	Description
manually	The calibration standard solutions are prepared manually.
by diluter system	Only when using the Cetac SDXHPLD autosampler with automatic dilution function The standards are prepared by diluting a stock in the vortexer (mixing vessel) of the autosampler.

Blank correction

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

Correction	Description
Intensity 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.

Correction	Description
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.

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** | **Calibration** 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. **calculate** The zero value is included in the calculation like any other calibration point.
Weighting	**none** Consider all calibration points equally. **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**

Table column	Description
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.

See also

Options for analysis sequence [▶ 136]

3.2.5.1 Specifying stock standards

If you use the stock standards, you can enter the respective dilution factors for the individual standards instead of the concentrations. To this end you must specify the stock standards before completing the calibration table, and it is possible to use several stock standards with different elements and concentrations.

- In the **Method | Calibration** window, click on **Stocks**.
  - ✓ The **Stock standards** window opens.
- Click on **New** or **Insert** to add a new line to the stock list.
  Max. number of stock standards: 20
- For the **From stock database** option select the stock name in the list. The stock database is managed in the **Data | Stock std/QC samples** window.
- Select the **Enter manually** option if you do not use a stock from the database.
- Back in the **Stock standards** window enter the data of the stock directly into the table:

Table column	Description
Name	Name of the standard

Table column	Description
Elements and concentrations	Elements and corresponding standard concentrations With **Concentrations** you can open a list for entering the concentrations. Alternatively enter the values in the following input format directly into the row in the format *Element symbol-space-Concentration*, e.g., nickel with a concentration of 0.5 mg/L: Ni 0.5 Further elements and their concentrations are simply added separated by a semicolon. An example of the input format is given under the stock list.
Unit	Concentration unit of the elements in the standard.

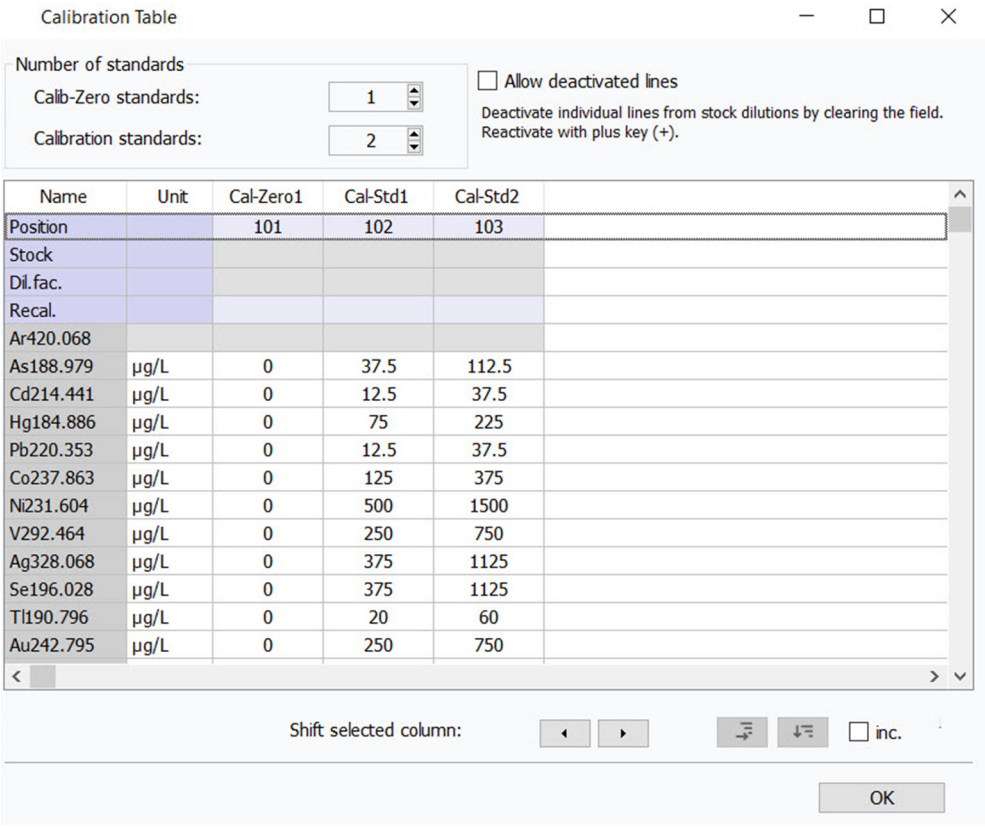
See also

Managing databases for stocks and QC samples [▶ 130]

3.2.5.2 Entering the calibration table

Enter the standard data in the calibration table.

Calibration Table window



- In the **Method** | **Calibration** window, click on **Calibration Table**.
- First enter the number of standards into the input fields. Dependent on the calibration method chosen, various standards must be selected.

For the standard method the number of calibration standards (**Calibration standards**) and calibration zero standards (**Calib-Zero standards**) must be entered. Several zero standards can be entered, e.g., if the elements to be 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.

For **Method of additions** and **Method of additions calib.** the number of **Addition standards** must be entered in each case.

- For the preparation of standards by a connected dilution system, you must select the stock standard used in the **Stock** row and the dilution factor in the **Dil.fac.** row for each calibration standard.
  The following dilution factors can be selected: 1, 2, 5, 10, 15, 20, 25, 50, 75, 100, 200, 250, 500, 1000, 1500, 2000, 2500, 5000. The number of dilution factors is limited according to the range settings in the **Autosampler | Dilution** window. For the dilution factors 1 ... 100 the dilution is carried out in one step, for higher values in two steps.
  - ✓ After the stock standard and dilution factor have been selected, the software automatically calculates the concentration for each calibration standard and each analysis line.
- Standard concentrations that are not to be measured can be manually deleted from the table after activating the **Flexible selection** checkbox.
  To reactivate deleted entries, enter a plus sign (+) in the relevant fields and confirm with the Enter key or by moving to the next cell with the mouse.
- If you prepare the calibration standards manually, you can also have the software calculate the concentrations of the calibration standards by selecting a stock standard and entering a dilution factor.
  Alternatively, enter the concentration for each analysis line for each standard in the table.
- For manually prepared standards, you can define the position of the standards in the autosampler in the **Pos** line.
  If the autosampler is not used, the entries in this line are not considered.
  For autosamplers with dilution function, the position of the stock is taken from the stock database.
  The assignment of the autosampler positions can be entered or changed in the sequence.
- For recalibrations specified as sequence actions or as a sequence of QC actions, at least one calibration zero standard and one calibration standard or at least two calibration standards must be selected in the **Recal.** line. If more than two recalibration standards are selected for a line, the lowest and the highest recalibration standard is used.

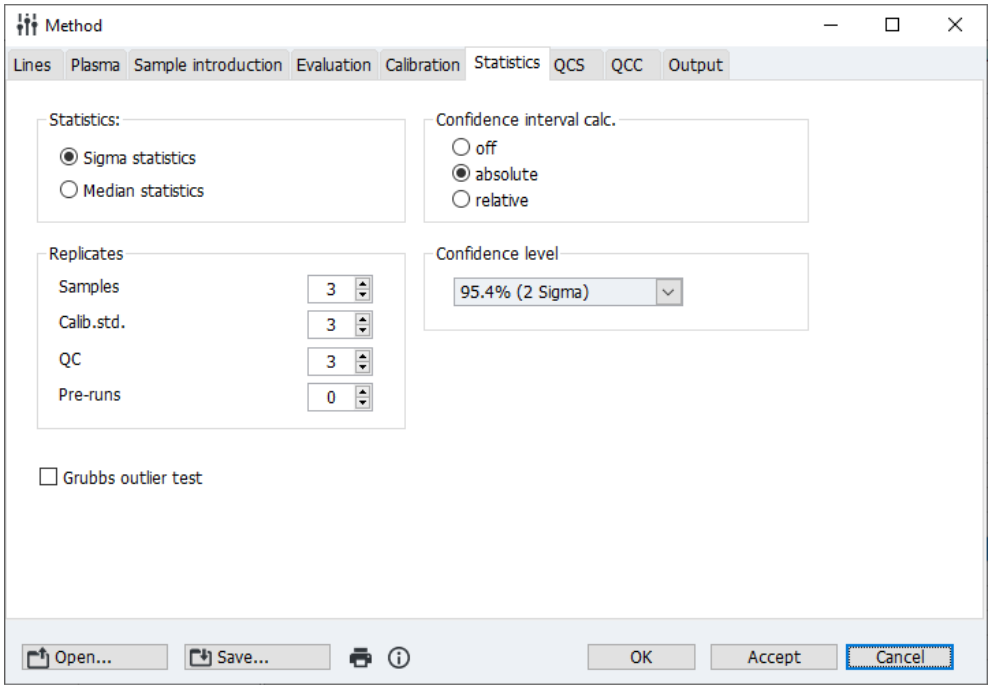
See also

- Specifying stock standards [▶ 42]
- Dilution function [▶ 114]

3.2.6 Specifying statistical analyses (Method | Statistics window)

In the **Method | Statistics** window, select the statistical methods to be applied to the calibration and sample measurement. The settings are independent of the selected calibration method and remain unchanged with each change of method.

Method | Statistics window



Statistics type

Option	Description
Sigma statistics	Calculate mean value and standard deviation Error statistics according to the arithmetic mean: The sample is measured several times after the blind cycles. Based on the measurement results, the arithmetic mean, the standard deviation and the relative standard deviation are calculated.
Median statistics	Calculates 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 displayed median is: ■ 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.

Number of replicate measurements

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	Number of repeats of blank measurements Blank measurements are sample measurements preceding the statistics series and disregarded for the calculation of the measurement result.

Grubbs outlier test

For mean value statistics with at least 3 repeat measurements per sample

Status	Description
Disabled	Includes all values of the statistics series for the calculation of the mean value.
Enabled	Outliers are eliminated and are not used in the calculation of the statistics. The average values determined in this manner are marked with "!" in the output table.

Confidence interval calc.

The calculation of the confidence interval is based on the chosen statistical certainty (see below). In the calculation of the confidence interval, the errors in sample measurement and particularly the calibration errors are included, so that a value will be presented even if the statistics function has been deactivated.

Setting	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** (selectable between 68.3 ... 99.9%) is used to calculate the confidence interval of the samples and the prognosis ranges of the calibration curves.

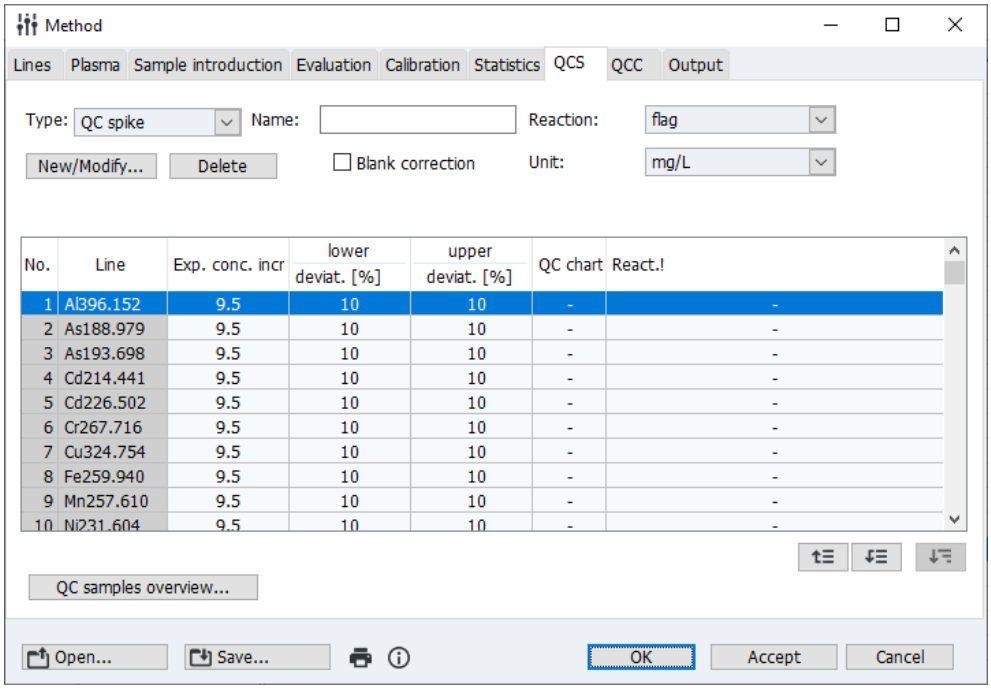
See also

Specifying quality control (Method | QCS window) [▶ 46]

3.2.7 Specifying quality control (Method | QCS window)

In the **Method | QCS** window, you can specify the quality control (QC) samples. During the sequence, control measurements with samples are then inserted at predetermined points, which should provide known measurement 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 can be automatically documented on quality control (QC) charts. The system of QC charts is used for quality monitoring over a long period of time. The QC charts are saved with the method and continued with each measurement with the method.



Elements in the Method | QCS window

Elements	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	Deletes the displayed QC sample
Blank correction	Optionally, a blank value correction can be activated for all QC samples, except QC standards and QC blank values
Unit	List box for selecting the corresponding concentration unit.
QC samples overview	Opens a list with the 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 **Method** | **QCS** window. **enter manually** Enter the concentrations of the QC sample directly into the 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 With this option, 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 the measurement the concentration difference (Conc1 of sample and QC stock sample) is compared to the expected concentration increase specified here (Exp. conc. increase) and the recovery rate calculated.

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 saved when the control sample first appears in the analysis sequence. 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. Both portions are separately subjected to all steps of sample preparation. They are placed separately on the autosampler tray as QC Trend and QC Matrix. The difference between the determined concentrations is evaluated.

Procedure if error limits are exceeded

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

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

Option	Description
	QC sample or the last (re)calibration will be re-measured. If the QC sample is again outside the permissible error limits, the measurement program will be stopped. **next method** The current measurement program is canceled and the measurement program of the next method is started if the sequence includes another method. **Stop** The current measuring program is aborted.
QC spike	**flag** **recal. + continue** **cal. + continue** **next method** **Stop**
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.

Option	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 stock volume and the concentration of the stock solution.
Exp. ints.	For **QC blank** Expected intensity in QC blank value
lower lim.	Lower range of error limit in percent.
upper lim.	Upper range of error limit in percent.
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	For **QC std.** Unit of the expected concentration

Entering parameters of QC samples

- Click on **New/Modify** to create a new parameter set for a QC sample type or to edit the selected sample type.
  - ✓ The **Add/modify QC sample type** window opens.
- Select the sample type in the **Type** list.

- Only QC samples: If you define multiple QC samples, assign a consecutive number in the 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.

  ✓ The QC samples are defined in the method.

See also

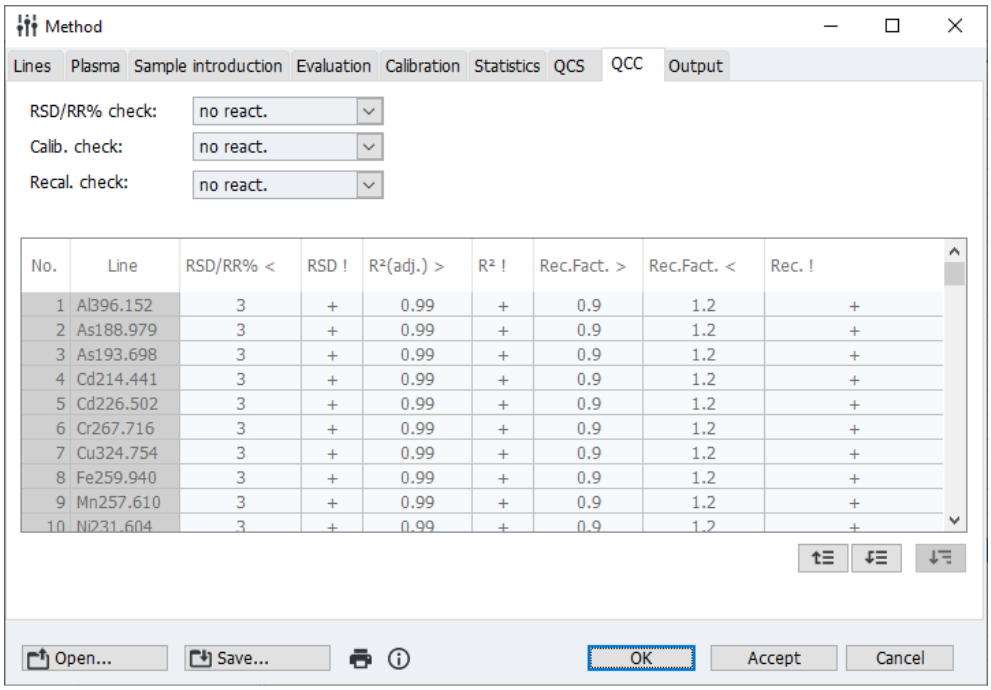
Managing databases for stocks and QC samples [▶ 130]

3.2.8 Specifying quality control (Method | QCC window)

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

- Relative standard deviation (mean value 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.



Types of quality control

Control type	Description
RSD/RR% check	Control of the relative standard deviation or relative range
Calib. check	Control of the coefficient of determination of the calibration
Recal. check	Control of recalibration factor

Reactions if error limits are exceeded

Reaction	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

Reaction	Description
repeat + continue	Only with **RSD/RR% check** Repeats the measurement of the respective sample if the serial precision limit was exceeded before the next sample is measured
cal. + continue	Only **Calib. check** and **Recal. check** Runs a new calibration if the error limits for the calibration or the recalibration factor were exceeded. Afterwards, measurement is continued with the next sample
next method	Only **Calib. check** and **Recal. check** If error limits are exceeded, the current measuring program is aborted and the measuring program of the next element line in the method is started. This option can only be selected if more than one element line has been specified in the method.
Stop	Only **Calib. check** and **Recal. check** Stops the measurement of the currently running method, if the error limits were exceeded.

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. If one or more of the controlled lines exceed the error limits, the reaction chosen above will be triggered.

Quality control	Parameter / meaning
RSD/RR% check	**RSD/RR% <** The system will respond with the defined procedure if the relative standard deviations or the relative ranges are larger than or equal to the specified value. **RSD !** For lines marked with "+", the RSD% or RR% will be checked.
Calib. check	**R^2(adj.)** The coefficient of determination of the regression R^2(adj.) must be larger than or equal to the specified value. Otherwise, the system will respond as selected. **R^2 !** For lines marked with "+", **R^2(adj.)** will be checked.
Recal. check	**Rec.Fact. >** Upper limit of recalibration factor **Rec.Fact. <** Lower limit of recalibration factor The selected response will be released, if the calibration factors are outside these specified limits. **Rec. !** For lines marked with "+", the recalibration factor will be checked.

See also

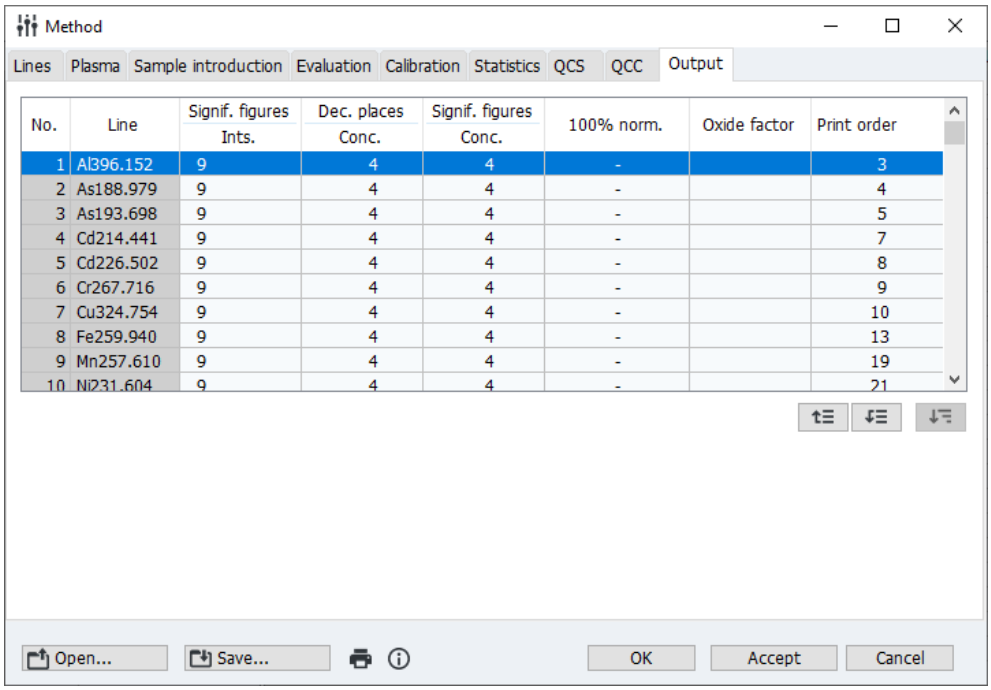
Specifying statistical analyses (Method | Statistics window) [▶ 44]

3.2.9 Specifying output formats for results (Method | Output window)

In the **Method** | **Output** window, you specify the number of decimal places with which results are presented on the screen and on the printouts, additional output types, and the order of lines for an analysis of several elements on the printout.

In the table below, define the number of decimal places for the display and printout of intensity and concentration values, and the order in which the analysis lines shall appear on the printout.

Elements in the Method | Output window



Elements	Description
Signif. figures Ints.	Number of significant figures of intensity values
Dec. places Conc.	Number of decimal places of concentration values
Signif. figures Conc.	Number of significant figures of concentration values
100% norm.	The output concentration **Conc. 2** is converted to the percentage value in relation to the total concentration. The total concentration is the sum of the concentrations of the lines marked with "+".
Oxide factor	If an oxide is selected, the output concentration **Conc. 2** is converted to the concentration/content of the oxide. The oxide factor is displayed in parentheses, e.g., Ti is converted to TiO_2 by multiplication with 1.6681.
Print order	Order in which the lines are displayed in the report

4 Sequences

The sequence defines the order in which samples and actions are to be processed within the measuring routine. Some sample describing data such as sample name and position on the sample rack 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 on the type of calibration, statistical analyses, quality control, etc.

4.1 Creating, saving and opening sequences

Like methods, sequences are saved to a 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 [▶ 123]

4.1.1 Creating a new sequence

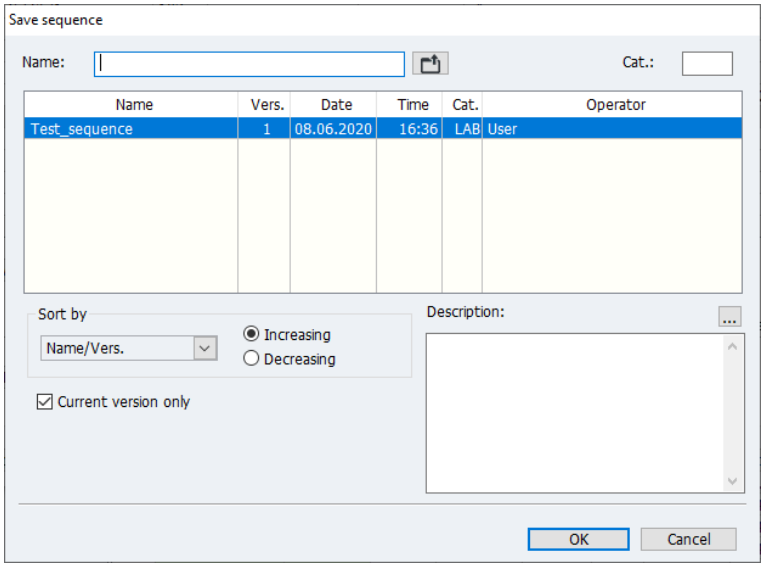
First create or load a method. You can specify a new sequence of sample measurements and actions based on this method.

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

4.1.2 Saving a sequence

After entering the measurements and actions, save the sequence to the database in the **Save sequence** window. This allows you to reuse the sequence for later measurements. When saving the sequence, you can add additional data to categorize the sequence and make it easier to find.

Elements in the Save sequence window



Option	Description
Name	Sequence name
Cat.	Category (three characters) for further identification and sorting the sequences 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 will be displayed for sequences with the same name.
Description	Optionally enter further explanations for the sequence Click on ... to open the list of predefined comments. You manage these comments in the **Data** | **Default descriptions** window.

Saving a sequence

- In the **Sequence** window, click on **Save** or select the **File** | **Save** | **Sequence** menu item.
- In the **Save sequence** window, enter the name for the sequence and select further parameters.
- Confirm the settings with **OK**.
  - ✓ On doing so, the sequence will be saved to the database. If you choose an existing sequence name, the existing method will not be overwritten, but a new version created in the database.

See also

Creating predefined comments [▶ 131]

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 icon next to the **Sequ** field.
  - Select the **File** | **Open Sequence** menu item.

– In the **Sequence** window, click on **Open**.

- Optionally, you can limit the display of the sequences by selecting a category in the **Cat.** field. If you want to see the sequences from all categories, delete the entry in the **Cat.** field.
- Enable the **Current version only** checkbox if you want to see only the sequence with the highest version number for sequences with the same name.
- Select the sequence in the table 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 during the analysis.

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

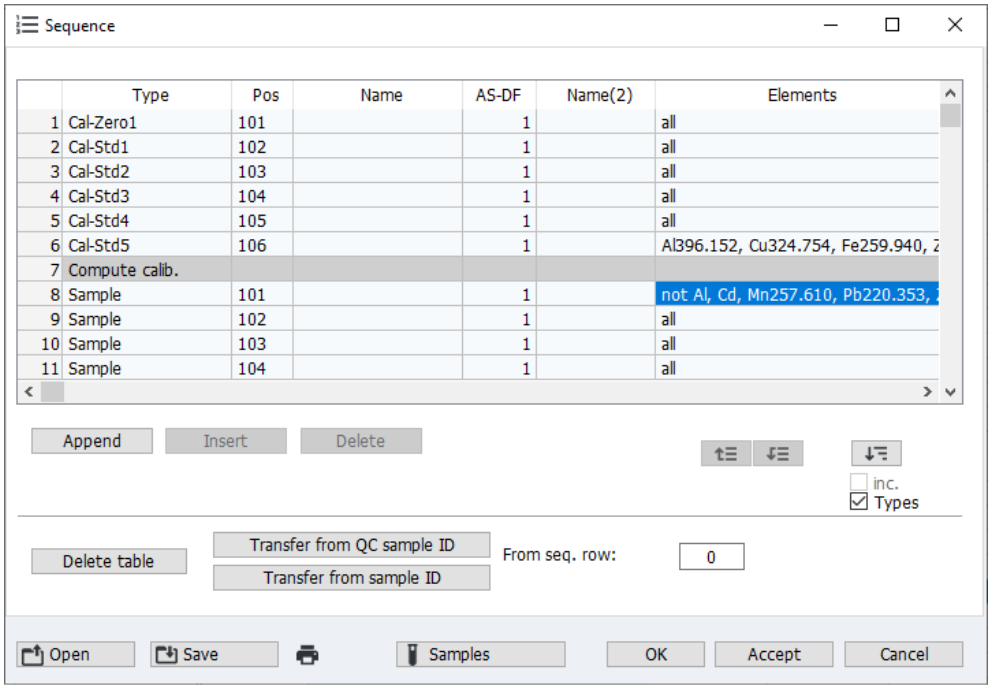


Table of sample and action sequences

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

Table column	Explanation
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 and QC samples the names can be transferred from the sample information file.
Name (2)	Additional name for sample identification (optional)
Elements	Select the elements to be analyzed in a sample or for which special actions are performed. ■ **none** Current selection is deleted.

Table column	Explanation
	■ **all** All elements defined in the method will be determined (default). ■ Element symbol Only the specified elements will be determined, e.g., "Cu, Pb". ■ Element line (symbol + wavelength) Only the specified element lines will be determined, e.g., "Mn 257.610, Ca 315.887". ■ **not Element symbol** or **not element line** The specified elements or element lines are not determined, e.g., "not Cu, Pb", "not Mn 257.610, Ca 315.887"

Buttons

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

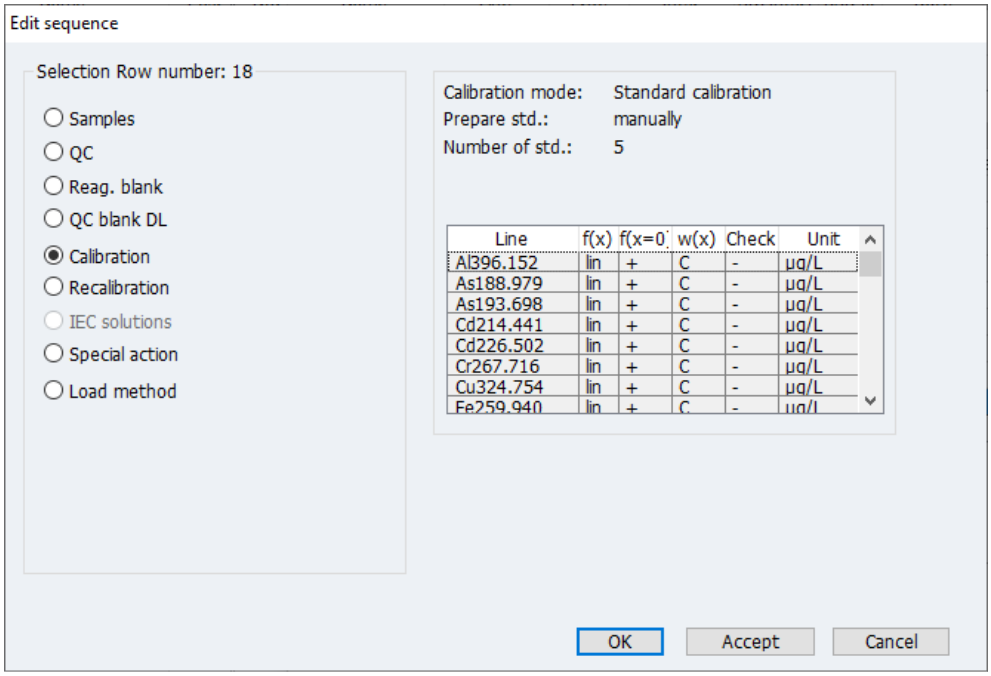
Button	Explanation
Append	Add new row at the end of the list and open the **Edit sequence** window
Insert	Inserts a new row above the selected list position
Delete	Delete selected rows
Delete table	Delete entire sequence list
Transfer from QC sample ID	Transfer information about names of QC samples and their position in the autosampler from the **Samples** | **QC sample information** window The information from the QC sample ID table is entered in the sequence table. The first row with new sample identification is defined in the **From seq. row** field.
Transfer from sample ID	Transfer information about sample names, the position in the autosampler and the elements to be analyzed from the **Samples** window The information from the sample ID table is entered in the sequence table. The first row with new sample identification is defined in the **Samples** field.
Samples	Open **Sample ID** window

See also

- Frequently used control elements [▶ 15]
- Selecting elements/lines for a sample analysis/action [▶ 59]

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 method settings.

Sample/Action	Description
Samples	Measure the number of samples specified under **Number**.
QC samples	Measure a QC sample and evaluate it as specified in the method In the list select a QC sample specified in the method. The parameters of the QC sample are displayed in the opposite field.
Reag. blank	Measure the blank value analytes
QC blank DL	Measure a blank to determine the limits of detection and quantitation according to the blank method
Calibration	Measure the calibration samples and calculate the calibration according to the specification in the method
Recalibration	Measure the calibration sample intended for recalibration and calculate a recalibration
Sample-addition	For the calibration process Method of additions calib. Add this sample and determine the calibration curve and sample concentration
Blank-addition	For the calibration process Method of additions calib. and the blank correction Concentration corrected Add this blank sample and determine the blank
IEC solutions	Only for peak corrections with IEC Measure the IEC solutions
Special action	These actions do not directly affect the measurement of the samples (see below).
Load method	Load a saved method, e.g., to start another analysis within the sequence With ... open the database window with the saved methods. Select one of the two saved methods.

Special actions

Action	Description
Extinguish plasma	Extinguish plasma
Dark current meas.	Perform additional dark current measurement With this measurement of the dark current the signal is determined with the shutter closed. The dark current measurement is always performed automatically, even if it was not inserted into the sequence.
Waiting time	Wait for the time (in minutes) entered in the field and then continue the analysis When using an autosampler, the cannula remains in the wash position and further washing solution is aspirated.
Pause	Stop the analysis The sequence can then be continued by clicking on or using the **Routine** | **Continue** menu item.
Beep	Allow the PC to generate a signal tone, e.g., in order to indicate the end of the calibration
Repeat / **While**	Define a loop (repetition) in the sequence. The part of the sequence enclosed by the starting point **Repeat** and the end point **While** is repeated until the cancellation criterion has been met. As a cancellation criterion a number of loop cycles or a time in minutes can be specified. For an online measurement (as part of remote maintenance) the **autom.** option must be enabled. This prevents the prompt for sample metering during the manual mode.
Show calib. plots	Display the calibration curve during the running sequence until the waiting time (in minutes) has elapsed. After the waiting time has elapsed or after clicking on **OK** the software continues the measurement. If you activate the **Show calib. plots** action without entering a waiting time, the software will not continue the measurement until you confirm the calibration with **OK**. If you click on the **Stop** button in the **Calibration** window, the software will close the window and interrupt the analysis sequence, regardless of the set waiting time.
Clean system	Wash the sample path up to the torch with wash solution with normal pump speed Enter the wash time in the input field.

Specifying a sequence

- Open the **Sequence** window by clicking on .
- Click on **Append**.
  - ✓ The **Edit sequence** window appears.
- Activate the required actions one after the other and transfer them to the sequence table using **Accept**.
- Confirm the last action with **OK**.
  - ✓ You return to the **Sequence** window. The sequence table now contains all actions in the order of selection.
- As the default for the elements to be analyzed the **all** option has been selected in the sequence table for each sample/action. By clicking on the **Elements** table cell of the relevant sample/action, you can change this setting in the window.

- When using the autosampler:
  Specify the position **Pos** of the samples in the autosampler. The positions of calibration and QC samples are automatically taken from the method. However you can change the positions here, the positions set in the sequence always have priority.

It is best to enter the data of the samples to be analyzed in the **Sample ID** window and then transfer them to the sequence list.

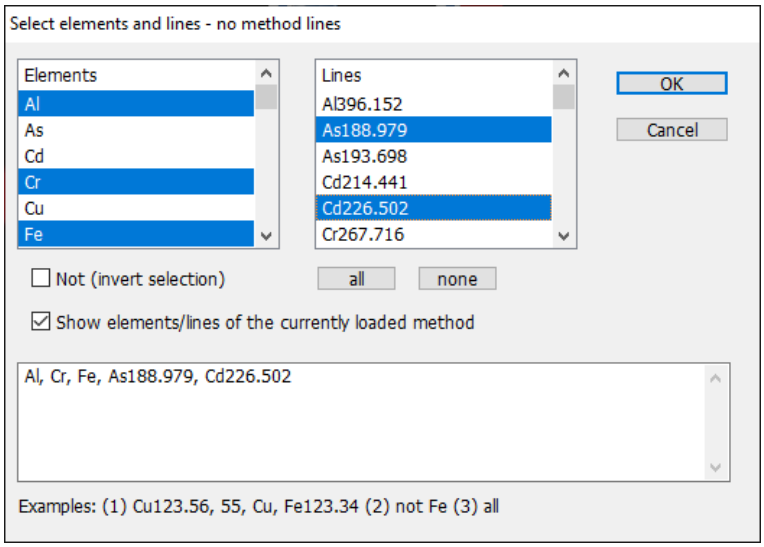
4.4 Selecting elements/lines for a sample analysis/action

In the sequence all elements for the analysis of samples or the execution of actions have been enabled by default. If you want to exclude elements for the analysis of a sample or an action, proceed as follows:

- In the **Sequence** window, click on the table cell of the corresponding sample or action. The **Select elements and lines** window appears.
  Enable the **Show elements/lines of the currently loaded method** checkbox.
  - ✓ In the **Elements** list all elements/lines set in the method are highlighted in blue.
- To fully exclude an element, remove the selection by clicking on the corresponding element. To enable the element, click on the element again.
- If several lines have been set for an element in the method and you only want to use selected lines, select the desired line with a mouse click in the **Line** list.
- With the **all** and **none** buttons you either enable all elements or exclude all elements for the analysis/action.
- Using the **Not (invert selection)** option all selected elements/lines are excluded from the analysis/action. Only the unselected elements/lines will be analyzed. The list of elements/lines is preceded by "**not**".

In the output field all selected elements/lines are listed. The elements/lines can be edited directly in the table cell after returning to the sequence window.

Select elements and lines window



5 Sample information data (sample ID)

The sample information data (sample IDs) includes the specific data for the current analysis samples and QC samples, such as sample name, position on the autosampler, initial 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.

The **Sample ID** window is opened by clicking on in the icon bar.

5.1 Creating, saving and opening sample information data

Creating a new sample ID set

- In the icon bar, click on or select the **Method Development** | **Sample ID** or **File** | **New Sample Information File** menu items.
  - ✓ The **Sample ID** window appears.
- Specify the data for samples and QC samples.
- Click on **Transfer to sequence** to transfer the data record to a sequence.
  - ✓ The samples 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** or select the **File** | **Save** | **Sample information** menu item.
- Save the data record in the **Save as** default window.
  - ✓ The sample ID is saved in CSV format. You can load the data for further analysis or edit it in a spreadsheet program.

Open sample information data

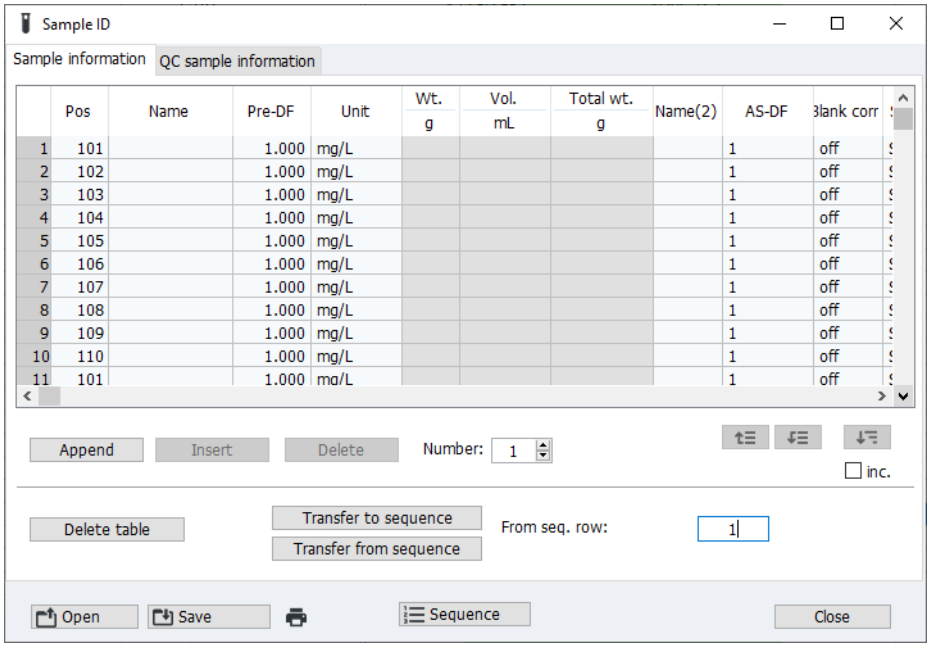
- You can open a sample ID using one of the following alternatives:
  - In the toolbar, click on the icon next to the **Samples** field.
  - Select the **File** | **Open Sample Information File** menu item.
  - In the **Sample ID** window, click on **Open**.
- In the **Open** default window, select the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

See also

Specifying sample information [▶ 62]

5.2 Sample ID | Sample information window

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



Tab Sample information

The **Sample information** tab contains a list of the samples and their characteristics.

Table column	Description
Pos	Position of sample on autosampler
Name	Sample name This entry is optional. Maximum number of characters: 20
Pre-DF	For unit type **liquid** and **solid** The pre-dilution factor of the sample designates the factor by which the original sample was diluted before being placed on the autosampler or supplied to the plasma, if no autosampler is used. The factor is required for the calculation of the concentration of the original sample (**Conc. 2**).
Unit	Concentration unit of sample.
Wt.	Initial weight in grams (only for the unit type **solid**) The mass of the original sample which was dissolved in sample preparation. The initial weight is necessary to calculate the concentration of the original sample (**Conc.2**).
Vol.	Total volume or filling volume in mL (only for the unit type **solid**)
Total wt.	Total initial weight of the sample and solvent in grams (only for the unit type **liquid grav.**, e.g., for oils).
Name (2)	Additional sample name. This entry is optional. Maximum number of characters: 20
AS-DF	Dilution factor of the autosampler.
Blank corr.	Blank value correction (only for sample type **Sample**) **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. You select the blank correction procedure in the **Options** | **Calibration** window.
Sample type	Selection between **Sample** and **Blank**

Table column	Description
Elements	Elements or lines to be analyzed in the sample After clicking on the table cell the **Select elements and lines** window opens in which these settings are made.

Buttons

Buttons	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 marked row.
Number	Input field for the entry of the number of rows to be inserted.
Delete table	Deletes the complete table of sample information.
Transfer to sequence	Transfer sample names, positions in the autosampler and elements to be analyzed to the sequence list. The first row of the sequence list from which the sample data should be transferred must be defined in the **From seq. row** input field.
Transfer from sequence	Transfer sample names, positions in the autosampler and elements to be analyzed from the sequence list to the sample ID table. The first row of the sequence list from which the sample data should be transferred must be defined in the **From seq. row** input field.

QC sample information tab

Analog to the **Sample information** tab, this tab contains the QC samples. In addition, the **Type** column contains information about the QC type. The **Unit** column is omitted because the unit is defined in the method. The blank correction is defined in the method for QC samples and cannot be selected here.

Button

Button	Description
Transfer to sequence	Transfer QC sample names and positions on the autosampler to the sequence list

See also

- Options for analysis sequence [▶ 136]
- Selecting elements/lines for a sample analysis/action [▶ 59]
- Specifying units of measurements [▶ 130]

5.3 Specifying sample information

If you require further data on samples or QC samples for the analysis, such as the initial weight or the pre-dilution factor, you must specify the data in the **Sample ID** window. Sample names and positions in the autosampler specified here can be transferred to the sequence.

- Open the **Sample ID** | **Sample information** window by clicking on  .
- Then enter the number of samples to be analyzed in the **Number** field. Then click on **Append** to insert the rows into the table.
- In the table, enter the required information for every sample.

- If the entries in a column are identical, you can use  to copy the entry of the selected cell to all subsequent cells in the column. If you enable the **inc.** checkbox (inc. means increment), the value is increased by 1 each time the information is transferred to the next cell. In this way, you can easily, e.g., assign successive places on the tray of the autosampler or number a sample name consecutively.
- You can copy text from input fields to the clipboard and paste it again. To do this, use the Ctrl+C and Ctrl+V key combinations or right-click on the table cell and use the context menu commands.
- When all information has been entered, in the **From seq. row** field, enter the row in the sequence from which you want the sample information to be transferred to the sequence. Transfer the information by clicking on **Transfer to sequence**.
- Specify the QC sample information in the same way in the **Sample ID** | **QC sample information** window. Click on **Transfer to sequence** to transfer the QC sample information to the sequence.

  ✓ The sample information will 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

Measurement routines (analysis processes based on a sequence) are started with the icons in the toolbar or via the **Routine** menu.

Icon	Menu item	Function
	**Routine | Run sequence**	Starts a measurement routine
	**Routine | Run Selected Sequence Row...**	Runs 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**	Stops a measurement routine
	**Routine | Continue**	Continues a stopped measurement routine

6.2 Switching on the spectrometer and igniting the plasma

CAUTION

Risk of poisoning due to ozone and nitrous gases

- Switch on exhaust unit prior to igniting the plasma.
- Leave the exhaust unit switched on during operation.

To ensure safe plasma operation, the device monitors the following conditions using safety circuits.

- The plasma compartment door is closed.
- The plasma torch is in working position.
- Sufficient cooling is supplied.
- Exhaust air extraction is active.
- Argon supply is ensured.

Do not ignite the plasma unless all conditions are met. If one of the safety circuits reports a fault during operation, the device extinguishes the plasma.

Igniting the plasma

- ▶ Switch on the PC using the power switch and start the operating system.
- ▶ Switch on the ICP-OES device using the power switch.
- ▶ Open the argon supply. Set the preliminary pressure to 500 to 700 kPa (5 to 7 bar).
- ▶ Switch on the exhaust unit.
- ▶ Switch on the recirculating chiller using the power switch.
- ▶ Open the plasma compartment door. Check if the torch is in starting position. The injector tip must be situated approx. 1 to 2 mm below the bottom edge of the induction coil.

- Inspect the cone of the window for axial observation for contamination and wear. Use the supplied hook wrench to check that the cone is tight.
  NOTICE! If the cone is loose, it will not be cooled sufficiently and will corrode.
- Close the plasma compartment door.
- For PlasmaQuant 9200 Elite: Switch on the optional sampling compartment lighting.
- Check the tube hoses. Replace tubes that are no longer flexible or show signs of heavy abrasion.
- Clamp each of the tube hoses between the stoppers in the pump on the ICP-OES device.
- Place the clamping brackets over the tubes and fasten the guides with the clamping levers. Make sure that the clamping levers snap into place!
  NOTICE! Note the pump direction. This pump rotates anti-clockwise.
- Ensure that sufficient wash solution is in the bottle for the analysis.
  NOTICE! The wash solution should have the same acid content as the samples and standards. Use a 2 % nitric acid solution unless specified differently.
- Check the filling level of the waste bottle and empty the bottle if there is not enough reservoir available for analysis.
- For manual operation without an autosampler, immerse the sample aspiration tube in the wash solution. No air must follow during the plasma ignition process.
- Start the ASpect PQ program.
- In the **Quick Start** window, make the following settings:
  - Select the **Routine** or **Method development** option.
  - If using the HF kit, under **Torch material** select the **Ceramic** option to adjust the sensitivity of the optical plasma sensor.
  - Optionally: In the **Worksheet** area, select the worksheets prepared for the Quick Start, e.g., for the analysis of elemental impurities in pharmaceutical products according to USP 232/233. The worksheets contain method settings and prepared sequences.
- If you start the software with a worksheet, complete the Quick Start in the **Quick Start** window with **OK**.
- If you start the software without a worksheet, click on **Skip Quick Start** to go to the ASpect PQ interface.
- If the system has been out of service for an extended period or the nebulizer chamber was dismantled, purge the nebulizer chamber and the torch using nebulizer gas to expel any air from the system. Click on  to open the **Plasma** | **Control** window and click on **Purge spray chamber**.
- Ignite the plasma. In the **Plasma** | **Control** window, click on the **Ignite plasma** button.
  - ✓ This is followed by an initial phase in which the torch is purged with argon and the safety circuits of the ICP-OES device are checked. If everything is OK, the plasma is ignited.
- Observe whether the plasma has formed correctly. The plasma must be conical, extend beyond the induction coil, and taper towards the top.
- If a ring plasma forms, the plasma is only forming within the induction coil, or a crackling noise will be heard. In this case, press the red plasma off button on the device.
- Before the next ignition attempt, check that the sample tube is immersed in the wash solution and that the gas supply and recirculating chiller are working properly.

✓ The spectrometer is only cooled after successful ignition and stable plasma formation. After 1 to 2 min the ignition routine is complete and the tube pump starts. The emission spectrometer is ready to measure.

- Only now make further settings on the analysis system and start the measurement routine.

See also

Starting ASpect PQ [▸ 7]

6.3 Extinguishing the plasma and switching off the spectrometer

- After the end of the analysis, pump the wash solution through the system for approx. 3 min followed by water for 1 min. Then let the device run dry. If you need to replace the tubes, there will be no acid left in them!
- Extinguish the plasma in the ASpect PQ program by clicking on in the toolbar. Alternatively, use to open the **Plasma** window and click on **Extinguish plasma**.
- Exit the ASpect PQ program with **File** | **Quit**.
- Confirm the query to turn off the purge gas for the detector with **Yes** if you want to turn off the purge gas.
  If you are only interrupting work for a short time (up to 30 min) or are working in the UV range, do not turn off the purge gas. This saves you the waiting time during the ignition process until the detector is sufficiently purged. Leave the device switched on during the measurement break.
- Wait for the message to appear that the device and the cooling can be switched off.
- Switch off the ICP-OES device and, if applicable, the autosampler using the power switches.
- During daily measuring operations, you can alternatively switch off the ICP-OES device using the standby switch on the front of the device. The device is still connected to the power supply. The gas supply is switched off in standby mode.
- Release the pump tubes on the ICP-OES device. Loosen the pressure levers so that the clamping brackets no longer press on the tubes and pull the tube stoppers on one side of the pump out of the lock.
- If using the autosampler, release the pump tube in the same way.
- After switching off the devices, close the gas supply.
- Switch off the recirculating chiller using the power switch.
- Switch off the exhaust unit.
- Shut down Windows and switch off the PC.

✓ The analyzer is now switched off.

NOTICE

Wait for the ICP-OES device to cool down before switching it off!
After extinguishing the plasma, wait at least 30 s before switching the device off using the power switch.

6.4 Starting a measurement routine

In preparation for a measurement, create a method and a sequence or use one of the prepared worksheets.

If necessary, prepare a sample ID containing additional sample information such as dilutions.

Prepare the device for measurement:

- Switch on the PC, the device and accessories and ignite the plasma.

Prepare the samples for measurement, e.g., on the autosampler tray.

Start measurement

- Switch on the PC.
- Switch on the emission spectrometer and accessories. Ignite the plasma.
- Load a method:
  - In the toolbar, click on the folder icon next to the **Meth** field. Select the method in the **Open Method** window.
- Create a new sequence or load an existing sequence:
  - Perform a calibration at the beginning of the sequence.
  - When loading the sequence, make sure that the calibration matches the method. The analysis lines of the calibration standards must match the analysis lines that you selected in the method on the **Calibration** tab.
  - After calibration, measure a QC sample to verify the correctness of the calibration.
- If necessary, create a sample ID table with additional information about the samples.
- Start the measurement routine by clicking on  or using the **Routine** | **Run sequence** menu item.
- In the **Start** window, select a file name for the results file.
  You can save the result in a new file or append it to an existing file. Overwriting an existing file is not possible.
  - ✓ After selecting the file name, the measurement routine starts according to the settings in method and sequence. When using the autosampler, the measurement runs automatically.
- For manual sample introduction without an autosampler, follow the sample preparation instructions on the screen.

See also

Options for analysis sequence [▷ 136]

6.5 Displaying and saving the results during the analysis run

Display during the analysis sequence

During the measurement routine, the results are displayed in real time in the main window. Additional windows with the current result can also be displayed.

- **Spectrum Plot**: View of the analysis line
- **Signal plot**: Measurement signal curve
- **Bar graph**: Measured values in a bar graph
- **Report window**: Plasma report
- **Sample conc. in calibration curve**: Sample valuesin the calibration curve

You select these display windows in the **Options** | **Analysis sequence** window. The display windows can be shown or hidden during the analysis.

- Use the **View** | **Open Results Windows** menu command or the F7 function key to open the windows.
- Use the **View** | **Close Results Windows** menu command or the F8 function key to hide the windows.
- With the windows can also be opened during the analysis.

In the sequence list of the main window, the measurement progress is logged. The rows with the successive actions are marked by the following symbols in the table column:

Icon	Meaning
-	Not measured/executed yet.
O	Just being measured.
+	Already measured/executed.

Buttons in the icon bar

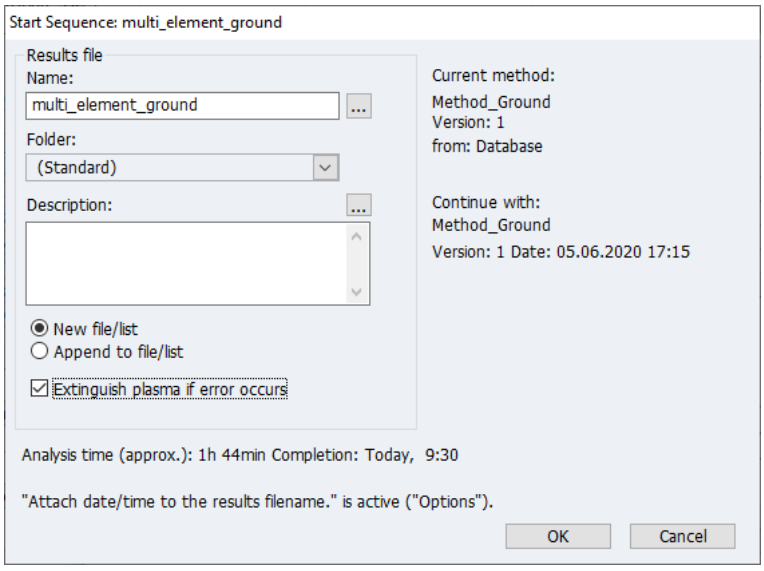
The following buttons are displayed in the icon bar during the measurement:

Button	Description
	Open and close display windows
	Display sequence window A method can only be read, it cannot be changed.
	Display sequence window The sequence can be expanded during the ongoing analysis. The sequence window contains the **Samples** button, which opens the **Sample ID** window for adding sample data.

Saving result data during the analysis sequence

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 saved optionally to a new database or added 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 related **Start** window opens with the following options for the results file:



Option	
Name	Enter the file name for the result database **New file/list** If enabled, 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 on ... to open a selection window from whose list you can select an existing results file.
Folder	Choose the storage path for the results file In the **Options** | **Analysis sequence** window, if the **Attach date/time to the results filename** option is enabled, this information is automatically appended to the results name. A message about the enabling of this option appears in this window.
Description	Here, you may enter an additional comment that is saved along with the analysis results You can click on ... to select user-defined descriptions.
Extinguish plasma if error occurs	The plasma is extinguished if the measurement is canceled with an error message

The file contains the measurement and evaluation results as well as the sample ID information. In addition the method parameters are saved in the result database.

The result database is saved with the extensions ".tps" (method parameters, intensities and concentrations) and ".spk" (raw spectral data).

6.6 Interrupting and continuing the analysis sequence

An analysis sequence can be interrupted and then continued again.

- With the **Routine** | **Stop** menu item or the analysis sequence is stopped immediately.
- With **Routine** | **Continue** or an interrupted routine is continued.
  - ✓ The **Continue sequence** window opens in which the action status before the interruption is displayed.
  - ✓ If the method is changed, enable 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.The measurement can be continued as follows:

Option	Description
Continue	Continue with current sample, current line and current statistical run
First statistical run	Continue with current sample, current line and the first statistical run
First element	Continue with current sample, first line and the first statistical run
From table row ->	Continue with the table row displayed in the text box

6.7 Repeating actions of the sequence

Single actions in a sequence can be repeated.

- In the main window, on the **Sequence** or **Sequence/Results** tab, select the row or rows with the action to be repeated.
  You can make multiple selections by clicking on the relevant rows while holding down the Ctrl or Shift key.
- Start the measurement routine by clicking on  or using the **Routine** | **Run Selected Sequence Row...** menu item.
- In the **Start** window, select a file name to which the result of the repeat measurement should be saved.
  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.
  ✓ Next the repetition of the selected action will start.

NOTICE

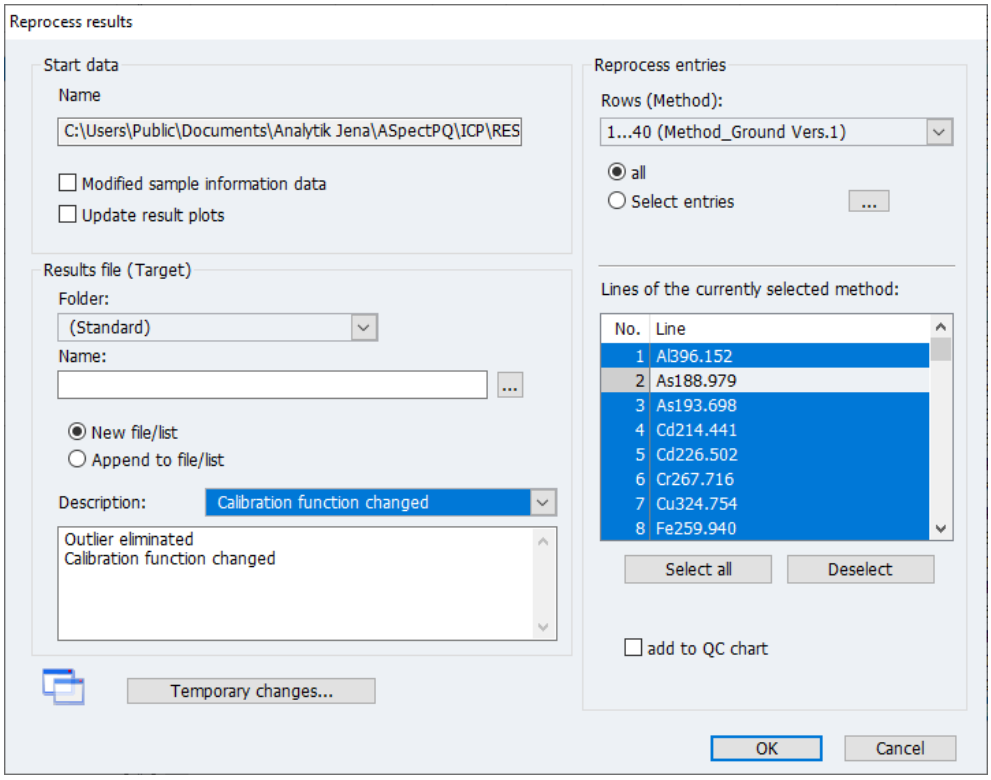
If changes have been made to the method in the meantime, the changed method will be used when repeating a sequence or single lines and saved as a new version with the results.

6.8 Reprocessing analysis results

The reprocessing of analysis results is used for changes in the analysis conditions, e.g., change of the calibration function or method, to take effect in the analysis. A change of sample information data, e.g., sample name, dilution factors, also requires a reprocessing to take account of it in the output of the analysis results.

The reprocessed data can optionally be appended to the current results file or saved to a new file. Manipulation of the original data is ruled out. If in a results file the reprocessing is repeated several times with different parameters, each reprocessing refers back to the original data of the results file.

NOTICE! With every reprocessing a new method version is saved.



Input options in the Reprocess results window

Option/field	Description
Start data	Selection of the start data **Name** Display of the name of the results file whose data is reprocessed. **Modified sample information data** To be enabled if data in the sample information file, e.g., the dilution factor, has been changed. If the option is not enabled, changes in the sample information file will not be taken into account when reprocessing the results. **Update result plots** The result windows, e.g., **Display spectra**, are updated as for the measurement. **Note:** This slows down the reprocessing.
Results file Target	Select the location for saving the reprocessed results data. **New file/list** Save results data in a new file For the results file select the storage location for the calculated data under **Folder** and **Name**. **Append to file/list** The reprocessed data is appended to the existing results file.
Description	This additional note is saved with the reprocessed analysis results. The entry is required if the optional 21 CFR Part 11 compliance module is installed. User-defined descriptions can be selected from the list.
Reprocess entries	Select the rows for reprocessing. **all** Reprocess all entries in the results list.

Option/field	Description
	Select entries Only reprocess selected sequence rows. Click on ... and in the **Select entries** window select all sequence rows to be reprocessed. **Lines of the currently selected method** In the list select all lines to be reprocessed. **Select all** selects all lines. **Deselect** removes all selections in the line list.
Temporary changes	Save temporary changes for reprocessing (wavelength offsets, deletion markers) (file extension ".rep"). The data is subsequently loaded automatically with the corresponding results file (of the same name).
add to QC chart	When active, QC sample type results are entered into QC charts during reprocessing.

Performing reprocessing

- Changes are made in the method parameters or in the **Sample ID** window.
- Click on or select the **Routine** | **Reprocess** menu item.
  The **Reprocess results** window opens.
- Specify the start data (name, modified sample information data, updated results plot), the storage location and the name of the target file.
  Note: If you are recalculating because of changes in the sample information, enable the **Modified sample information data** option. Otherwise, these changes will not be considered.
- Select the rows/lines for reprocessing.
- Start reprocessing with **OK**. If no target file has been specified, the query "Reprocess data without saving to a permanent file?" appears.

Replacing a calibration standard

An existing calibration standard can be replaced by one that has been measured at a later time. To do this, proceed as follows:

- In the main window, on the **Sequence** or **Sequence/Results** tab, select the row of the calibration standard to be replaced.
- Start the measurement of the sequence row with a click on .
- In the **Start** window define that the result is to be appended to the already existing file.
  Next, the measurement of the calibration standard starts.
- Open the **Reprocess results** window by clicking on .
- Enable the **Select entries** option and open the window of the same name by clicking on ....
- Select the last measured standard and use the arrow keys to move it to the position of the standard to be replaced.
- Select all rows to be reprocessed. Deactivate the old standard that should no longer be included in the calculation.
- Click on **OK** to return to the **Reprocess results** window and specify the start data, the storage location and the name of the target file.
- Start reprocessing with **OK**.
  ✓ The data is reprocessed for the selected rows.

Replacing individual lines of a calibration standard

Alternatively, you can replace the standard as follows:

- In the main window, on the **Sequence** or **Sequence/Results** tab, select the row of the calibration standard to be replaced.
- Start the measurement of the sequence row with a click on .
- In the **Start** window define that the result is to be appended to the already existing file.
  Next, the measurement of the calibration standard starts.
- In the results list, right click on the standard (line) you want to replace. In the context menu, select the **Sample single values** item.
- In the **Sample single values** window enable the **Replace with entry number** checkbox and enter the row number of the standard to be replaced into the input field.
- Start reprocessing as described above.
  ✓ The data is reprocessed for the selected rows.

See also

- Creating predefined comments [▶ 131]
- Specifying quality control (Method | QCS window) [▶ 46]

6.9 Evaluating measurements parallel to running analyses (offline mode)

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.

- Start ASpect PQ in the second program instance using the **File** | **Start Offline Program Instance** menu item.
- Open the results file of the currently running measurement using the **File** | **Open Results** menu item.
  The results measured so far are loaded into the results window.
- Additional results from the current measurement are loaded by clicking on in the toolbar or using the **View** | **Update results list** menu item.
  ✓ The results display is updated. The results can be edited further.

NOTICE! In reprocessing, the recalculated results are saved to a new database. It is not possible to access the original results file.

6.10 Displaying results and analysis progress in the main window

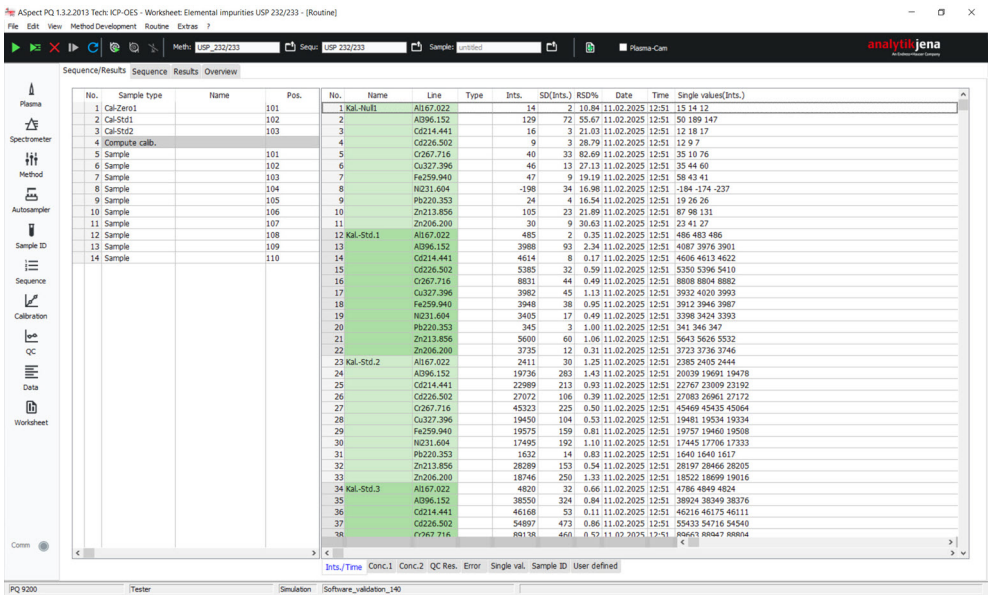
The measurement results and the sequence are extensively displayed in the main window in the background of the workplace. The presentation on different tabs in the main window provides a good overview of measurement results and statistical analyses.

The following tabs are selectable:

- **Sequence/Results** (content of the **Sequence** and **Results** tabs on one tab)
- **Sequence** (display of the current sequence)
- **Results** (display of the measurement results)
- **Overview** (summary of the measurement results)

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

Main window of ASpect PQ with results



6.10.1 Sequence/Results tab

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

See also

- Sequence tab [▶ 74]
- Results tab [▶ 74]

6.10.2 Sequence tab

On the **Sequence** tab, the active sequence is listed.

On this tab, you can follow the progress of the running analysis. The various samples and special functions are marked in the first column of the table as follows:

Icon	Meaning
-	Not measured/executed yet.
O	Just being measured.
+	Already measured/executed.

NOTICE! After the measurement, you can remeasure a selected sample.

To this end, you must have marked the sample row in the sequence. Then, click on on the toolbar.

6.10.3 Results tab

The **Results** tab contains all measurement results and statistical evaluations. The values are split up in further tables for a clear presentation. 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.

Table Ints./Time

The table contains the intensities and the statistical analyses according to the method settings (**Method** | **QCC** window).

Column	Description
No.	Number in analysis sequence
Name	Name of the sample, standard or QC sample/standard
Line	Element line
Type	Internal standard or analyte
Ints.	Mean value of the measured individual intensities of the sample
SD(**Ints.**)	Standard deviation (mean value statistics)
RSD%	Relative standard deviation (mean value statistics)
Date/**Time**	Time of the measurement
Single values (**Ints.**)	Individual values of the intensity measurements

Conc.1 table

The **Conc.1** table shows the analyzed concentration of the sample as supplied to the ICP-OES device. The unit used is the calibration unit set in the method.

Column	Description
No.	Number in analysis sequence
Name	Name of the sample, standard or QC sample/standard
Line	Element line
Type	Internal standard or analyte
Unit	Concentration unit
Conc.1	Analyte concentration in the sample / analyte concentration in the standard
SD1	Standard deviation of Conc.**1** (mean value statistics)
RSD%	Relative standard deviation of Conc.**1** (mean value statistics)
R	Range of Conc.**1** (median statistics)
R%	Relative range of Conc.**1** (median statistics)
Cf	Confidence interval
DF	Pre-dilution factor of the sample Factor by which the original sample was diluted before being placed on the autosampler or supplied to the plasma, if no autosampler is used.
Rem.	Remarks when determining values
Ints.	Mean value of the measured individual intensities of the repeat measurements
SD(Ints.)	Standard deviation of the intensity (mean value statistics)
Date/**Time**	Measuring time
Single values (Ints.)	Individual values of the intensities of the repeat measurements

Conc.2 table

The **Conc.2** table shows the concentrations of the original sample. In calculating conc. 2, the sample information data is considered:

- Pre-dilution
- Initial weight for solids and solution volume
- Conversion factors for other units

Column	Description
No.	Number in analysis sequence
Name	Name of the sample, standard or QC sample/standard
Line	Element line
Type	Internal standard or analyte
Unit	Concentration unit
Conc.	Concentration of original sample taking sample information data into account
SD2	Standard deviation of the Conc.**2** (mean value statistics)
RSD%	Relative standard deviation of the Conc.**2** (mean value statistics)
Cf	Confidence interval of Conc.**2**
100% norm.	Conc.**2** normalized to the percentage of the total concentration
Ints.	Mean value from the determined individual intensities
SD(Ints.)	Standard deviation of the intensity (mean value statistics)
R(Ints.)	Range of the intensity (median statistics)
Date / **Time**	Measuring time
Single values (Ints.)	Individual values of the intensity measurements

QC Res. table

The **QC Res.** table shows the results of the QC samples:

- Target value and actual value of the concentration
- Recovery rates (all types except blank value)
- Reactions to any deviations (all types except blank value).

Column	Description
No.	Number in analysis sequence
Name	Name of the sample, standard or QC sample/standard
Line	Element line
Type	Internal standard or analyte
QC (for calibration functions)	**R^2(adj.)** or **R** **Slope** **BEC** Background equivalent concentration
QC(for QC samples, not for QC blank)	**Conc.1** 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 blank measurements **LOD** Detection limit **LOQ** Limit of quantitation
Rem.	Comments on QC events (e.g., >cal.)
Ints.	Mean value of the measured individual intensities
SD	Standard deviation of the intensity (mean value statistics)

Column	Description
Date / **Time**	Measuring time
Single values (Ints.)	Individual values of the intensity measurements

Error table

If errors occur during the measurements, the corresponding measurements are marked in red in all tables. In the **Error** table, the respective measuring error including error number is documented in writing.

Single values table

The **Single values** table contains the measured individual values of the intensity and the corresponding background intensity.

Sample ID table

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

Column	Description
No.	Number in analysis sequence
Name	Name of the sample, standard or QC sample/standard
Line	Element line
Pos	Position of sample on autosampler
Pre-DF	Pre-dilution factor Factor by which the original sample was diluted before being placed on the autosampler or supplied to the spectrometer, if no autosampler is used. The factor is required for the calculation of the concentration of the original sample.
Wt.	Initial weight in gram The mass of the original sample which was dissolved in sample preparation (in g). The mass is necessary to calculate the concentration of the original sample (**Conc.2**).
Vol.	Volume of solvent used to dilute the initial weight (in mL). This value is required for the calculation of the concentration of the original sample (**Conc.2**).
Total wt.	Total weighed portion, includes sample and diluent (only for the unit type **liquid**, **liquid grav.**)
Name(2)	Additional sample name from the sample information table
AS-DF	Dilution factor of the autosampler.
Blank corr.	Blank correction **off** No blank value correction took place. **on** For the calculation of the concentration of the original sample, the blank measured last in the sequence will be subtracted.

User defined table

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

- Click on the **Select columns** button in the bottom right corner of the table.
- In the **Select columns** window select the desired parameters by clicking with the mouse.
- To change the order in the display, select the parameter whose position you want to change and move it with the keys and in the list.

- 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 moving the table column with the mouse button held down to the desired width.

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

- Options for analysis sequence [▶ 136]
- Overview of markings used in the display of values [▶ 156]
- Sample information data (sample ID) [▶ 60]

6.10.4 Overview tab

The results of the analysis are summarized on the **Overview** tab. You may choose among various presentation options:

Value	Description
Conc.1	Concentration 1
Conc.(RSD%)	Concentration 1 (relative standard deviation)
Conc.2	Concentration 2
Conc.2(RSD%)	Concentration 2 (relative standard deviation)
Ints.	Intensity
Ints.(RSD%)	Intensity (relative standard deviation)
Ints.(SD)	Intensity (standard deviation)
LOD	Detection limit
LOQ	Limit of quantitation
Recovery(Nominal val.)	Recovery rate (setpoint)
R^2/ Recal. factor	Coefficient of determination / recalibration factor
100% norm.	Conc. 2 normalized to the percentage of the total concentration

By activation of the respective checkboxes, the following sample types can be displayed:
- Sample
- QC sample
- Cal-Std
- Other

Use 🖶 to open the **Print Overview** window from where you can start the printout of the data displayed in the current overview.

See also

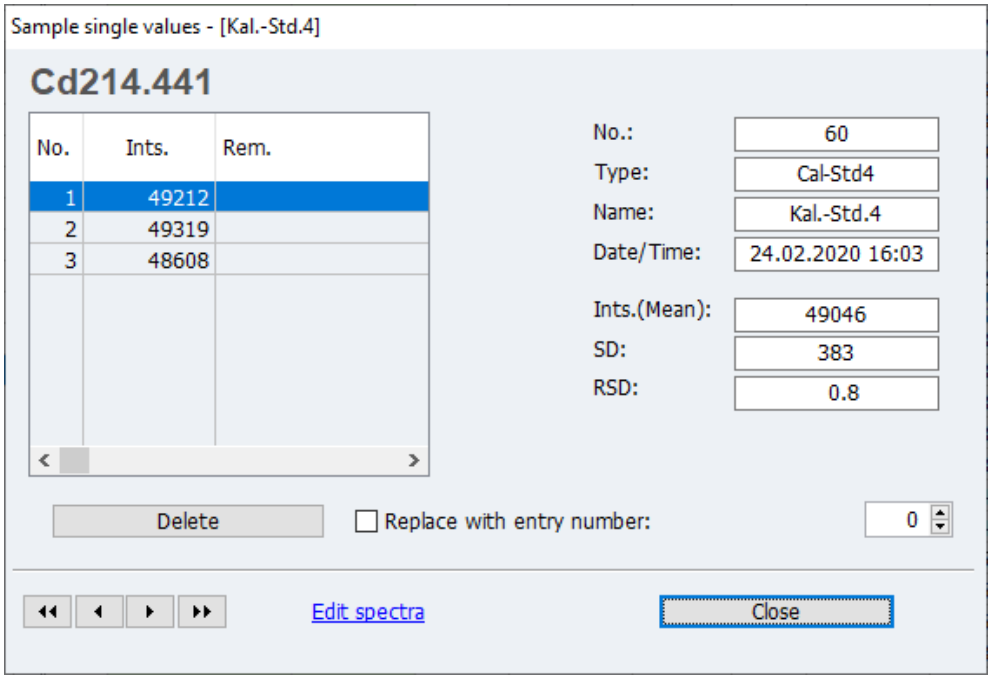
- Print functions in ASpect PQ [▶ 117]

6.11 Displaying and editing sample single values

You can display the single values of a sample and exclude single values from the calculation of the sample concentration.

- Right-click on the row in the results table and select the **Sample single values** item from the context menu.
  Alternatively, select the sample row and select the **View** | **Sample single values** menu command.

Autosampler adjustment window Sample single values



Single value display (table)

The sample single values are shown in the table.

Table column	Description
No.	Number of single value within the sample measurement
Ints.	Intensity of the single value
Conc.1	Concentration of the analyte in the analyzed sample.
Rem.	**none** The single value is included in the calculation of the sample mean. **#MAN** The value was manually excluded from the calculation of the sample value. **#KOR** The value was automatically excluded from the calculation of the sample value due to the Grubbs outlier test.

Sample data

Field	Description
No.	Number of measurement in the result table
Type	sample type (sample, standard or QC sample type)
Name	Sample name
Date / Time	Date and time of the measurement selected in the table
Ints.(Mean)	Intensity averaged for 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) This parameter is displayed independently of the statistical method chosen for the measurement (mean/median).

Additional buttons and options in the Sample single values window

Option / buttons	Description
Delete / **Reactiv.**	Remove the sample single value from the mean value calculation or reactivate it for the calculation
Edit spectra	Display wavelength-dependent line spectra
Replace with entry number	Only for calibration standards The current sample is to be replaced by the sample at position **Enr.** in the results table during reprocessing
	Switch between the lines of individual samples and from one sample to the next in the results table

Excluding sample single values

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

- To this end, mark the single value to be excluded in the table.
- Click on **Delete** to exclude the value from the calculation of the sample average for result reprocessing.
- Click on **Reactiv.** to include the selected single value in the calculation again.

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

See also

Displaying and editing intensity spectra [▶ 80]

6.12 Displaying and editing intensity spectra

The display of intensity spectra in the **Edit spectra** window is used for the following tasks:

- Calculate the main peak of an analysis line and save it in the line file
- Calculate the background correction with consideration of the sample matrix and transfer it to the method
- Create spectral corrections
- Identify lines adjacent to the analysis line

The intensity spectra can be displayed and edited for each measurement in the results window.

- Open the **Edit spectra** window by double-clicking on the corresponding sample row in the results table.
  Alternatively, right-click on the row in the results table and click on **Edit spectra** in the context menu. You can also select a sample row and select the **View** | **Edit spectra** menu command.

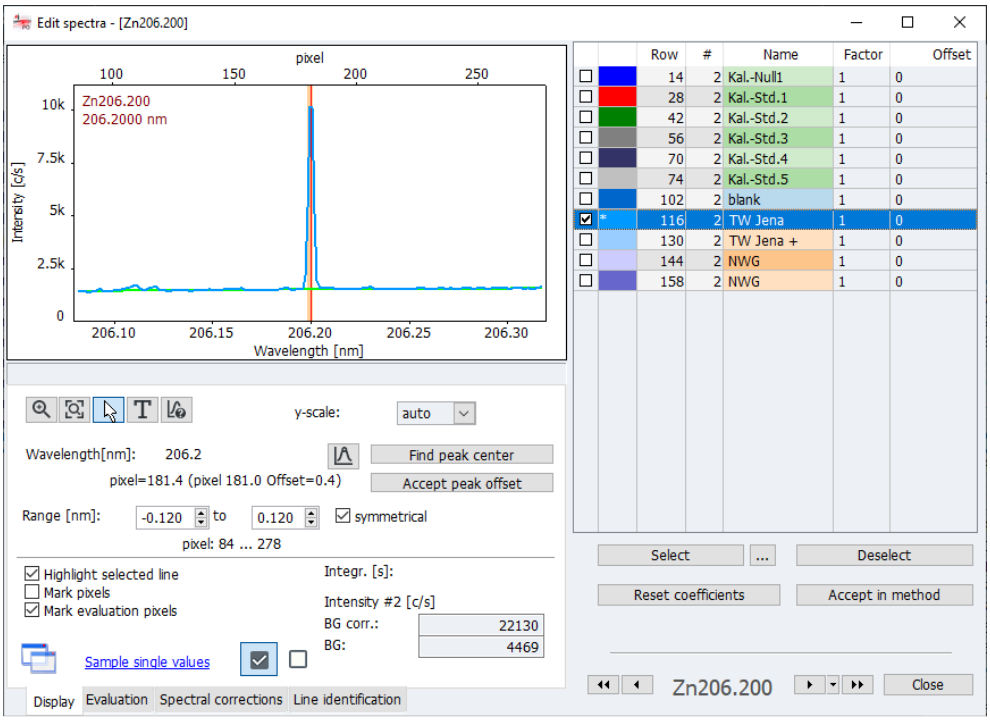
In the **Edit spectra** window, all measured samples with all single values are listed for one analysis line at a time. It is possible to change between the individual analysis lines.

The left side of the **Edit spectra** window contains the graph of the intensity spectrum of the selected sample or samples and four tabs for the analysis and editing of the spectrum. On the right side the sample single values to be displayed are selected from the overview.

6.12.1 Displaying spectra – Edit spectra / Display window

The **Edit spectra** | **Display** window displays an overview of the sample spectra. You can determine the position of a peak and transfer the found parameters to the line/wavelength file and the method.

Edit spectra | Display window



Selecting spectra / sample list

The sample list on the right side lists all sample single values of the analysis line.

- Enable the checkboxes of the single values you want to display in the graph.
  The spectra of the sample single values are shown as overlayed. The color of the field at the front in the table is assigned to the individual spectra.
- The single sample selected with the mouse (blue bar in the table) is highlighted in bold in the graph if the **Highlight selected line** option in the bottom left corner of the window has been enabled.
- You can filter the display of the samples/repeat measurements in the sample list and the selection for the graphical display of spectra (enable the checkbox in the sample list) using the buttons below the table:
  - Next to **Select** click on ...
  - In the **Selection** window make the following settings:

Option	Description
all	Select all rows of the result list in the main window for the graphical display (enable the checkbox for the graphical display).
from/to	Only select the spectra in the result list between set rows from/to.
Replicate	Select sample single values of a sample: **all** Select all sample single values of a sample. Reference number, e.g., "2." Only select the selected single value of a sample
show selected replicate(s) only	If enabled only the entries for the selected repeat measurement are displayed in the sample list.

Option	Description
	If disabled, all individual spectra are displayed and the entries of the main window selected above (all or from/to) are loaded.

- By clicking on **Select** you can display and select the spectra with the parameters set above.
- Use **Deselect** to disable all checkboxes for the display of the single values.

Entry of factor and offset

- For every spectrum you can enter a factor and/or an offset in the sample table. A spectrum manipulated in this manner is spread out/compressed and moved along the x-axis.
- By clicking on **Reset coefficients** the factor and offset are reset again and the spectrum is displayed in its original state.

Display of the line spectra

The selected spectra are displayed on the left. The intensity in counts/second is plotted against the wavelength in nanometers. At the top margin of the graph the pixel allocation is shown. The spectrometer is adjusted to map the main peak to the measuring pixel, e.g., 180. The main peak offset must be corrected for each analysis line, see below.

The buttons for the spectral view have the following functions:

Option / button	Description
	Enable graphic zoom. After clicking select the spectral section to be enlarged with the left mouse button held down.
	After zooming restore the original coordinates.
	Enable the selection mode in signal or spectral plots. The measuring points are selected with the left mouse button. The values of the selected measuring point are displayed in the output field below the buttons.
	Enable text mode. With the left mouse button pressed it is possible to select an area for a window for adding text to a graph. Double-clicking on existing text opens the window where you can edit or delete the text. Existing text can be moved using the Ctrl key and the right mouse button.
	Enable line identification mode. By clicking or dragging with the mouse element lines at the selected wavelength position are searched for in a line database. The found line is displayed below the graph.
y-scale	Select the scaling of the graph: **auto.** Autoscaling: The spectrum is displayed with optimum ordinate expansion. **Value** Manual scaling. The upper ordinate limit must be selected in the list.
Wavelength	Display the wavelength of the analysis line.
	Set the main peak manually.
Find peak center	Automatically search for the peak and correct the offset.
Accept peak offset	Save the peak offset in the line library. The offset will be used from this time onwards for each measurement of this element line.
Range (nm)	Select the wavelength range below and above the analysis line. This wavelength range is available for spectral analysis, e.g., background correction.

Option / button	Description
	If the **symmetrical** checkbox has been enabled, the wavelength range below and above the wavelength is identical. The corresponding pixel range is displayed below the input fields. Transfer the settings for the wavelength range of the selected line to the current measuring method by clicking on **Accept in method**. This range is used for dynamic background adjustment (or automatic background correction) for calculation. The data is also changed in the method window on the **Evaluation** tab.
Highlight selected line	The single spectrum selected in the right overview is highlighted with a bold line in the graph.
Mark pixels	Pixels are identified with a circle in the graph.
Mark evaluation pixels	The central analysis pixel at the main peak is highlighted with a red line. If several pixels are used for the analysis, their range is highlighted in light red.
Intensity	**BG corr.** Background-corrected intensity **BG** Intensity of the background
Sample single values	Link to the **Sample single values** window
	If the icon has been highlighted in this manner, the line is used in the method. You can select suitable lines in this manner during method development in the **Edit spectra** window.
	Do not use line in the method.

Automatically setting the main peak

During method development you need to correct device-related peak offsets and offsets caused by line interference, e.g., duplicates.

- Click on **Find peak center**. The automatic determination of the main peak is well suited for determining most peaks.
  Alternatively, click on  and select the main peak manually in the spectrum.
- Optionally you can recalculate the results to evaluate the new peak offset.
  Change to the results window and start reprocessing by clicking on  .
- Save the peak offset found with **Accept peak offset** to the line/wavelength file of the device.
  - ✓ The data is now available for every subsequent analysis of the analysis line.

See also

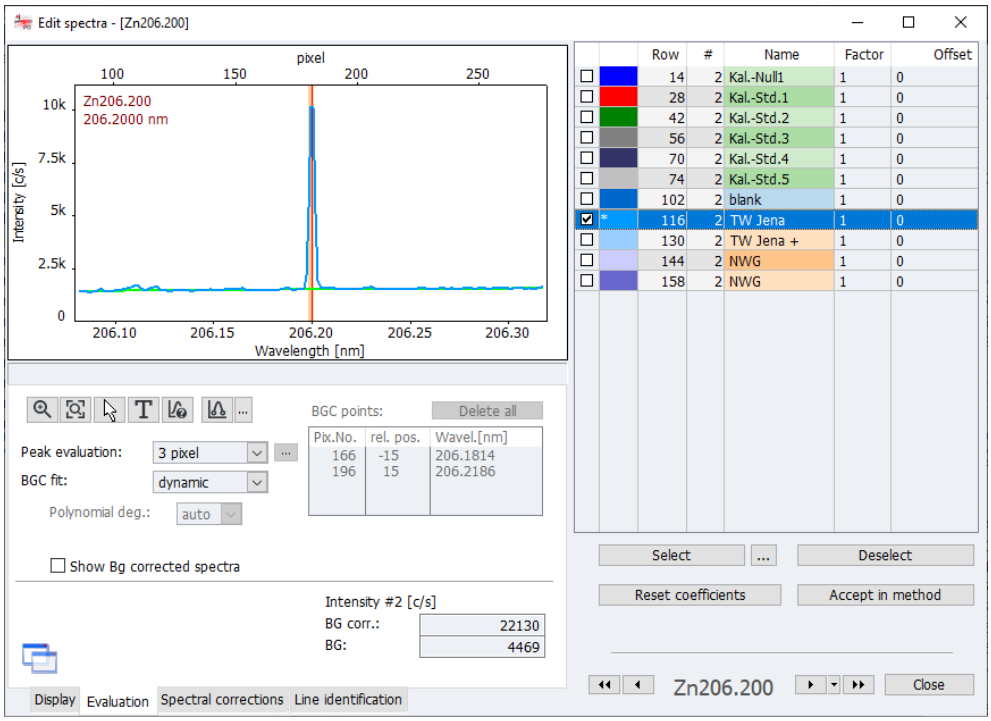
- Specifying analysis lines (Method | Lines window) [▶ 25]
- Reprocessing analysis results [▶ 70]
- Finding lines – Edit spectra | Line identification window [▶ 88]

6.12.2 Evaluating the peak and determining the background correction – Edit spectra | Processing window

Continuous background emissions causing intensity fluctuations across a wide spectral range around an analysis line can be compensated using background correction. Pixels (background corrections points) are selected on both sides of the analysis line, a regression is calculated through the points and the regression graph used for background correction.

In the static method for selecting the background correction points the points are set manually and the polynomial degree of the regression graph determined independently. In the dynamic method the regression graph is automatically calculated using the ABC algorithm (ABD = automatic baseline correction).

A discontinuous background interference, e.g., due to line overlap with a matrix element, can be minimized with the aid of correction spectra.



Element overview for peak analysis and background correction

The buttons for the spectral view, some value outputs and the selection of sample single values have been described in the section on the **Edit spectra** | **Display** window.

Option/ button	Description
Peak evaluation	Set the number of pixels for the peak evaluation. **1** The measuring signal is only determined at the pixel at which the main peak is located. Value **> 1** Number of pixels across which the measuring signal is determined. The individual signals of the pixels are totaled. The result is therefore greater than the maximum peak. The pixel with the main peak is located in the center of the range. **Height** The peak height is used for evaluation.

Option/ button	Description
	User defined The evaluation range is defined by the user. This is the preferred option for the evaluation of duplicates. After clicking on ... enable all pixels in the list that are used for the evaluation.
BGC fit	Select the type of background correction: **dynamic** The background correction is automatically calculated using a mathematical algorithm. No other settings are required for this option. **static** The background correction points are set manually via mouse click in the spectrum. For the correction function the polynomial degree must additionally be selected.
	For static adaptation set or delete the background correction points A cross is shown when moving the mouse over the spectral graph. Clicking on ... opens the function list: **Set background correction points** Set the correction points to the desired wavelength on the spectrum with a mouse click. If you move over a range with the mouse button held down, you select the entire range. **Delete background correction points** Clicking on an already selected point deletes the respective background correction point. Ranges can be deleted by dragging the mouse. **Delete all background correction points** Delete all selected points
BGC points Delete all	Delete all manually set background correction points
Table	Displays the manually set background correction points
Polynomial deg.	Select the polynomial degree for the regression of the background correction graph With the **auto** option the regression is selected automatically.
Show Bg corrected spectra	Show background-corrected spectra The adapted background (green line) is subtracted from the sample spectrum. The background then corresponds to the zero line.

Transferring data to the method

Transfer the settings for the peak evaluation and for background correction for the selected line to the current measurement method by clicking on **Accept in method**. The data is also changed in the method window on the **Processing** tab.

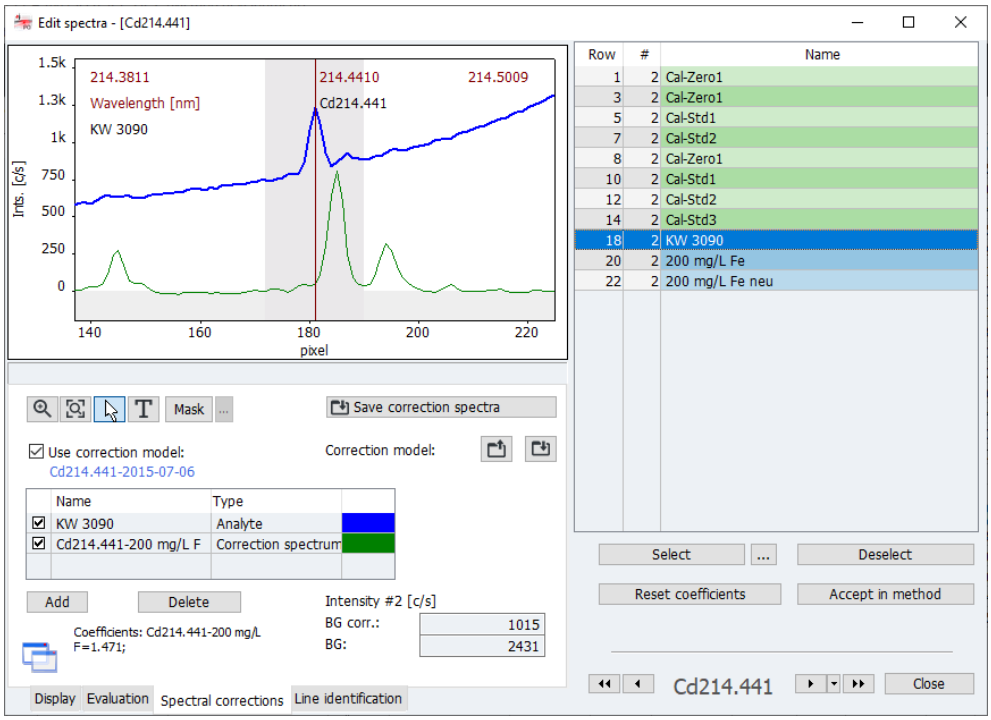
See also

- Removing spectral interference – Edit spectra | Spectral corrections window [▶ 86]
- Displaying spectra – Edit spectra / Display window [▶ 81]

6.12.3 Removing spectral interference – Edit spectra | Spectral corrections window

During the routine it is attempted to select lines for the analysis that are without interference and/or feature an easily corrected background. If this is not possible, correction spectra can be used to eliminate the discontinuous interference, e.g. caused by line overlaps 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.

The functions for saving the individual correction spectra and combining the correction model are available in the **Edit spectra** | **Spectral corrections** window.



Option/button	Description
Save correction spectra	Save spectra of the pure components of a matrix as correction spectra
Use correction model	If enabled the correction model is applied to the analyte
Correction model	Save the current correction model Load an existing correction model

The line table lists the analyte and the correction spectra used in the model. By enabling the checkboxes the individual spectra are displayed in the diagram. With **Add** further spectra are added to the correction model. With **Delete** the spectrum selected with the mouse is deleted from the model.

NOTICE! All correction spectra in the line table are used for the calculation in the model, irrespective of whether the checkbox for their display has been enabled or not. If a correction spectrum is to be excluded, it must be deleted.

6.12.3.1 Creating a correction model for spectral corrections

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.
- Measure the analyte in the matrix and load the spectrum in the **Edit spectra** window (double-click on the sample row in the main window).
- In the **Edit spectra** | **Line identification** window identify the possible interference lines.

Step 2: Measuring and saving correction spectra

- Add to the sequence the measurement of the interfering matrix components that cause spectral overlap and measure these components in single element solutions.
  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.
- Load a spectrum of a matrix component to the **Edit spectra** | **Spectral corrections** window**.**
- Click on **Save correction spectra**.
  ✓ The database window for saving the correction spectra opens.
- Issue a name and finish the process with **Save**.
- Save the spectra of the other matrix components in the same manner.

Step 3: Creating a correction model

- Load the spectrum of the analyte in the matrix again.
- Enable the **Use correction model** checkbox.
- Click on **Add** to open the selection of the already saved correction spectra.
- Select a correction spectrum in the list and click on **Load**.
- Add all correction spectra in this manner.
- Check in the spectral view whether the resulting sample spectrum is not free of overlaps.
- Using the **Mask** button you can mask ranges with the mouse button held down that are not to be included in the calculation of the correction model.
  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 on  and issue a name for the model. Finish the process with **Save**.

Step 4: Transferring analysis line with correction model to the method

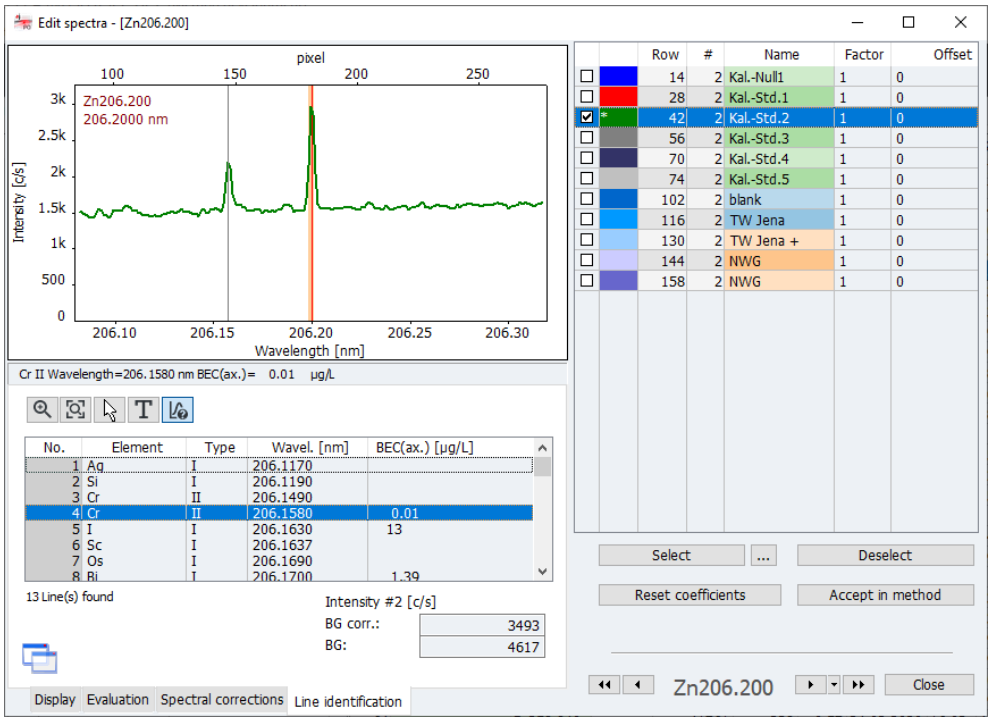
- Transfer the parameters of the analysis line with the correction model to the current method with **Accept in method**.
  ✓ In the **Method** | **Evaluation** window the analysis line is identified in the **Correction** column with **LSM** (Least Square Model).

After saving the method the future measurements will be performed with this method with the created correction model. Already completed measurements can be reprocessed with the new method version making it unnecessary to repeat the measurement.

The spectral correction models and correction spectra are saved with the results data. If the results data are transferred to a different computer on which the correction models have not been saved, the models are imported after a query.

6.12.3.2 Finding lines – Edit spectra | Line identification window

In the **Edit spectra** | **Line identification** window you can identify lines in the measured spectra based on the line database.

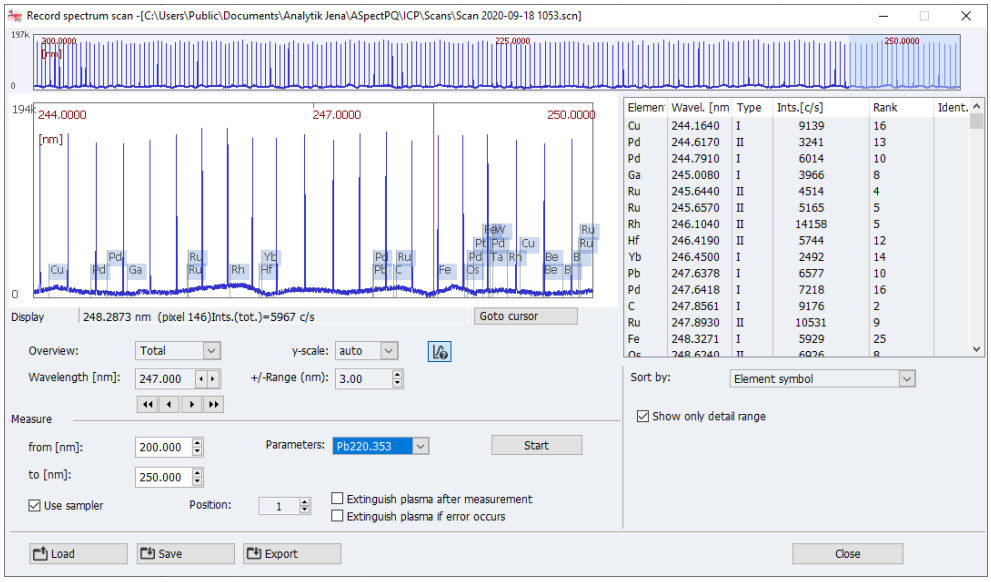


In the table below the spectrum all lines identified in the spectral section are displayed.

- Enable the button .
- Click on the peaks of interest in the spectrum.
  The nearest line is displayed below the spectrum and highlighted in the table.
- Inversely, you can also select a line in the table which is then displayed in the spectrum.

6.13 Recording an overview spectrum

With the **Method Development** | **Overview Scan** menu item you can record an overview spectrum in a specified wavelength range.



- Select the **Method Development** | **Overview Scan** menu item.
- In the **Measure** area enter the desired wavelength range (**from/to**).
- If you have activated a method, you can select the parameters of a line of the method for the spectrum scan. If no method is loaded, preset parameters are used.
- Prepare the sample. If you want to work with an autosampler, activate the **Use sampler** option and select the position of the sample on the autosampler.
- Start the scan by clicking on **Start**.
  When the scan is finished, the overview spectrum is displayed in the upper part of the window.
- If you click on a section in the overview spectrum, a detail area with the selected line is displayed in the graphic. You set the width of the detail area in the **+/-Range**.
- The lines found are displayed in the table on the right side. You can limit the display to the spectral range shown with the **Show only detail range** option.

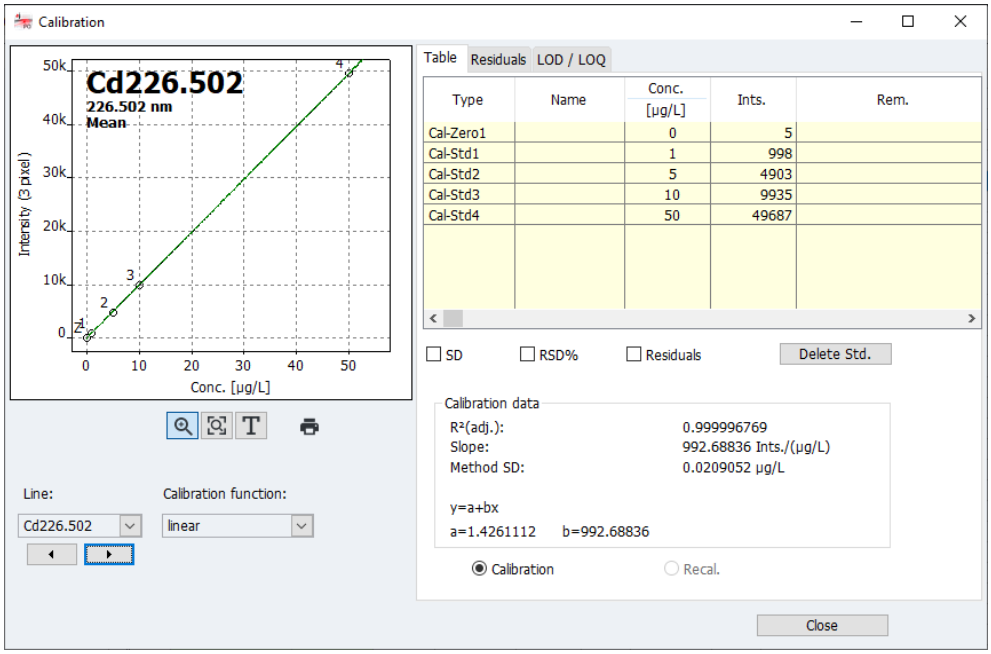
7 Calibration

The calibration is carried out during the measurement according to the options selected in the sequence. The calibration curves and functions can be displayed and edited after the measurement.

- Open the **Calibration** window by clicking on in the icon bar.
  Alternatively, double-click on one of the **Compute calib.** sequence rows or select the **Method Development** | **Calibration** menu item.

Calibration window

The **Calibration** window shows the calibration curve calculated taking into account the graph parameters.



The window contains for each of the analysis lines defined in the sequence:

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

Selecting a line

In the **Line** list box select the analysis line for the calibration view. Use the arrow keys below the list to change between the displays of the individual lines.

Selecting a calibration function

In the **Calibration function** list select between the possible regression calculations of the calibration curve:

Calibration option	Description
linear	Linear progression of the calibration function $y = a + bx$
nonlin. ratio.	Non-linear progression of the calibration function described by a rational function $y = \frac{a + bx}{1 + cx}$

Calibration option	Description
nonlin. quadr.	Non-linear progression of the calibration function described by a quadratic function $y = a + bx + cx^2$
automatically	For the calibration a linear and non-linear function each are calculated. This is followed by a Mandel test in which the sums of the squared residues are compared. 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** | **Calibration** window. As default setting the broken ratio function has been provided.

See also

General settings for calibration and blank correction [▶ 137]

7.1 Graphic presentation of 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 statistical certainty is selected in the **Method** | **Statistics** window. In the **Options** | **Calibration** window you can choose between displaying the prognosis or confidence band.

Enlarge the calibration curve

After clicking on a graphical area can be enlarged with the mouse button held down. reverses the enlargement again.

Insert remark

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

- Click on .

- With the left mouse button held down drag the frame for the text field onto the graph.
- In the open input window select the font by clicking on **Font**.
- Enter the text and click on **OK**.
  - ✓ The text is displayed on the graph.

Printing the calibration curve

The calibration curve and the calibration data are output to the printer after clicking on .

See also

- General settings for calibration and blank correction [▶ 137]
- Specifying statistical analyses (Method | Statistics window) [▶ 44]
- Print analysis results [▶ 117]

7.2 Displaying calibration results

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

See also

- General settings for calibration and blank correction [▶ 137]

7.2.1 Calibration – Table tab

In the **Calibration** window the value pairs of the standards (calculated concentration / measured value) are displayed on the **Table** tab.

If the standards were measured multiple times and a statistical analysis option set in the method, you can additionally output the standard deviation (SD) and the relative standard deviation (RSD%) or the range (R) and the relative range (R%) by enabling 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.**.

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

Under the measured value table the calibration data are displayed provided they can be meaningfully calculated:

Parameters	Meaning
R^2(adj.)	Coefficient of determination
Slope	Slope of calibration curve
Method SD	Method standard deviation
BEC	The BEC value (background equivalent concentration) is the concentration of the analyte producing an intensity equivalent to the background. A lower value corresponds to a higher sensitivity.

7.2.2 Calibration – Residuals tab

In the **Calibration** window the deviations of the calibration points from the calculated calibration curve and the limits of the prediction band are displayed on the graph on the **Residuals** tab.

7.2.3 Calibration – LOD/ LOQ tab

In the **Calibration** window the limits of detection the limits of quantitation of the ICP-OES device are displayed on the **LOD/ LOQ** tab. These limits are calculated based on the current calibration results. In this area, values of the blank method and the calibration curve method will only be displayed if the device has been calibrated already.

Parameters	Meaning
Limit of detection	The weight (concentration) of the element to be analyzed that can be detected with a defined statistical certainty.
Limit of quantification	The minimum weight (concentration) of the element to be analyzed that can be determined with a defined confidence level.
SD Blank (DL)	Only for blank value method Measured standard deviation of the blank (IDL sample)

With **calculate** start the calculation of the limits of detection and quantitation.

Calibration curve method

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

- 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 curve 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 included in the sequence.

For the blank method the following calculation rule is used:

- 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 quantitation:

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

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

See also

Specifying measurements and actions in a sequence [▶ 56]

7.2.4 Calibration – LOD/ LOQ tab

In the **Calibration** window the limits of detection the limits of quantitation of the ICP-OES device are displayed on the **LOD**/ **LOQ** tab. These limits are calculated based on the current calibration results. In this area, values of the blank method and the calibration curve method will only be displayed if the device has been calibrated already.

Parameters	Meaning
Limit of detection	The weight (concentration) of the element to be analyzed that can be detected with a defined statistical certainty.
Limit of quantification	The minimum weight (concentration) of the element to be analyzed that can be determined with a defined confidence level.
SD Blank (DL)	Only for blank value method Measured standard deviation of the blank (IDL sample)

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- 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 curve method can be considered useful only if the calibration was run in the lower concentration range.

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For the blank method the following calculation rule is used:

- 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 quantitation:

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

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

See also

Specifying measurements and actions in a sequence [▶ 56]

7.3 Editing the calibration curve

You can edit an existing calibration curve in the **Calibration** window as follows:

- Changing the used calibration function
- Enabling/disabling standards
- Replacing a measured standard

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

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

The modified calibration parameters will be applied to the results when you reprocess the results. To do this, select the **Routine** | **Reprocess results** menu item or click on  in the toolbar.

A standard can also be measured again and the results be reprocessed.

See also

Reprocessing analysis results [▶ 70]

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 defined for a method and included in the sequence.

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 are defined in the **Method | QCS** window and in the sequence the integration of the QC sample.

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 in the icon bar or select the **Method Development | QC** menu item.

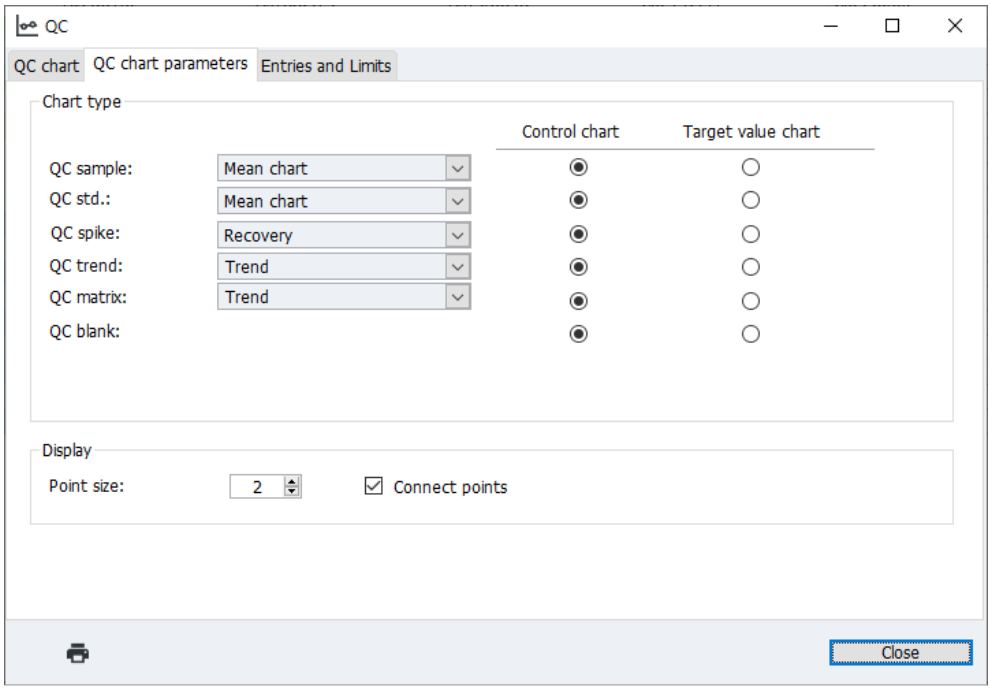
See also

- Specifying quality control (Method | QCS window) [▶ 46]
- Specifying measurements and actions in a sequence [▶ 56]

8.1 Parameters of QC charts

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

QC | QC chart parameters window



QC sample types and evaluations

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.)** – Not for target value chart
	Recovery
QC spike	**Recovery**
QC trend	**Trend**
QC matrix	**Ranges** – Not for target value chart
	Precisions – Not for target value chart
QC blank	No selection provided. The intensity of the blank is displayed.

For the **Control chart** chart type (process control chart), the target parameters and the control (K) 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** chart type, the target values and exclusion limits are determined from the expected values and limits of the quality control samples.

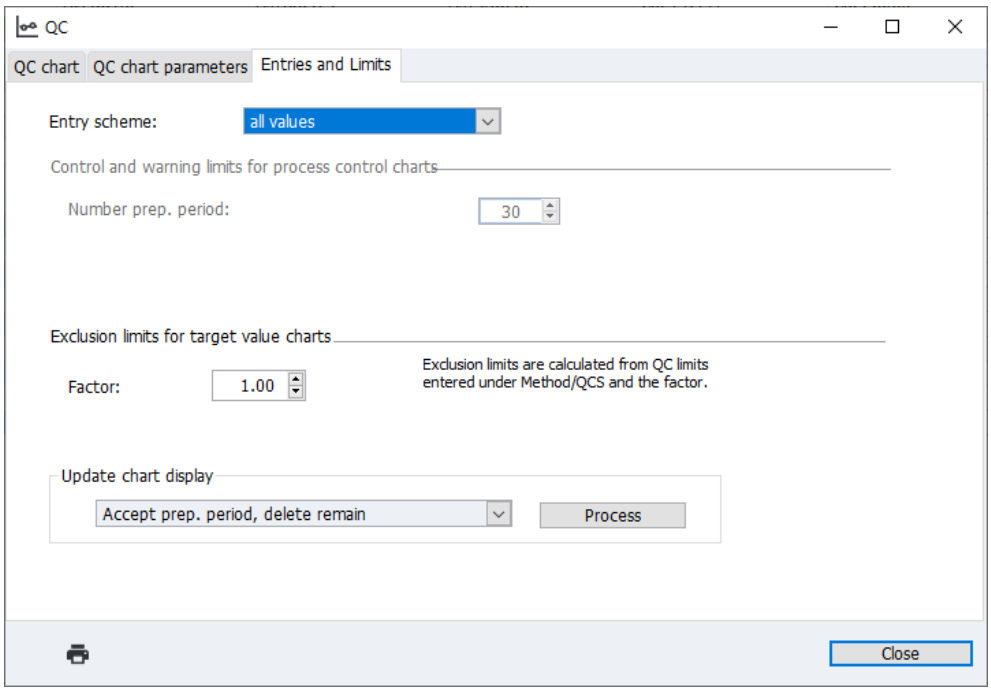
Display

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	Connects the points on the graph with each other by a line.

8.2 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 laboratory with regard to the frequency of the entries.



Option	Description
Entry scheme	**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. **Note** A "day" corresponds to one day according to the PC clock, i.e., 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	**Control chart** only: The preparation period is a number of QC chart entries that are used for the calculation of control (C) and error (E) 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.
Exclusion limits for target value charts	**Target value chart** only: The exclusion limits are calculated from the limits specified for the quality control samples multiplied by the **Factor** (default is 1).

Renewing charts

Define the procedure for (almost) full charts. To this end select one of the options from the list:

Option	Description
Accept prep. period, delete remain	**Control chart** only: Accepts the preparation period of the old chart for application to the new chart and deletes remaining values.
Last values -> new prep. period	**Control chart** only: 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. **Control chart** only: New measured values will first fill the preparation period.

By clicking on **Process** you replace the QC charts in accordance with the option selected above.

8.3 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.

Options/views

Options/views	Description
Control sample	Here, choose the QC sample type to be displayed.
Line	Here, choose the element line to be displayed.
Displayed values	Number of displayed values and the date of the first and the last value displayed.

Options/views	Description
Saved values	Total number of entries on the current QC chart and the date of the first and the last value.
x(min) / **x(max)**	Select the start entry and number of entries to be displayed on the graph.
y-scale	**Entries** Maximum of y-axis is scaled according to the highest value. **Control limits** Maximum of y-axis is scaled to the range of the control limits or exclusion limits.
	Prints the QC graph inclusive of alphanumerical data and measured values.

Graph area

Color/marking	Meaning
Yellow field	Control chart only: Preparation period
Light gray horizontal line	Control chart only: Mean value calculated from preparation period Target value chart only: Target value
Red horizontal lines	Control chart only: Upper and lower control limit (C) calculated from preparation period (3 Sigma) Target value chart only: Upper and lower exclusion limits (EU, EL) depending on the limits of the QC sample
Green horizontal lines	Control chart only: Calculated warning limits (W; 2 Sigma).
Small circles	Measuring points (black: active entry; gray: inactive entry)

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
Value	Measured value (converted according to the presentation type of the QC chart)
Date / **Time**	Measuring time
Operator	user logged in at the time of 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

9 Controlling and monitoring spectrometer and accessories

9.1 Spectrometer

The **Spectrometer** window serves to test the spectrometer functions and set the spectrometer parameters.

The following data can be adjusted or viewed and the following actions performed:
- Device data
- Display of the readout parameters of the detector
- Start measurements for device optimization

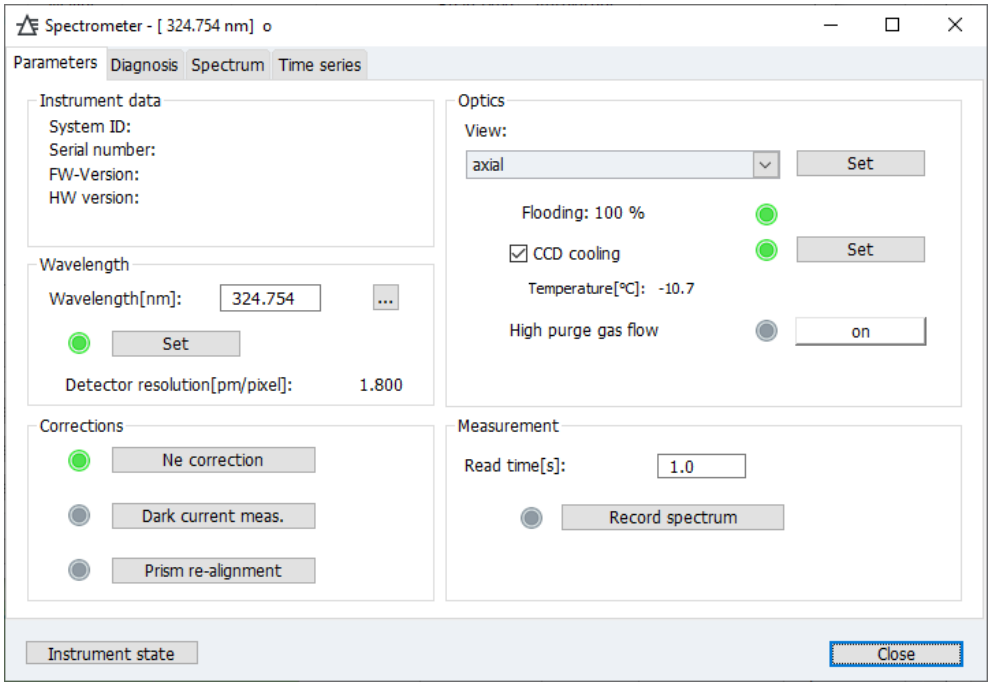
Open the **Spectrometer** window by clicking on or using the **Method Development** | **Spectrometer** menu item.

Click on **Instrument state** to display a graph for the output of the messages from the safety sensors. In case of problems with the plasma, you can view the error messages of the sensors here.

9.1.1 Configuring spectrometer parameters and testing functions

The **Spectrometer** | **Parameters** window contains the following functions:
- Check basic device functions
- Start automatic corrections to the optical system
- Start a test measurement at a selected wavelength

Elements in the Spectrometer | Parameters window



Parameters	Description
Instrument data	In the **Instrument data** group various service and version numbers are displayed that are required for the device service.
Wavelength	In the **Wavelength** field the selected wavelength is displayed. A wavelength can be adjusted after clicking on ... in the **Select element/line** window.

Parameters	Description
	Clicking on **Set** moves the spectrometer to the selected wavelength.
Ne correction	Perform a wavelength calibration of the detector
Dark current meas.	Correct the dark signal
Prism re-alignment	Optimize the mapping of the dispersion order on the detector by prism adjustment (adjustment for energy maximum).
View	Select the monitoring direction of the plasma in the list box (**axial** – from above, **radial** – from the side)
CCD cooling	If the checkbox is enabled, the cooling of the CCD detector can be started with **Set**. If the checkbox is disabled, the cooling is stopped. The CCD cooling is started automatically with the ignition of the plasma. Manual control is only necessary in exceptional cases, e.g., after an error message during automatic. In the **Operating temperature** field the current temperature of the CCD detector is displayed.
High purge gas flow	Purge the spectrometer with increased argon flow
Measurement	To start a measurement at the selected wavelength the total measurement period must be entered under **Measurement**. Click on **Record spectrum** to start the measurement. For the measurement the main settings for the plasma are used. The sample must be supplied manually. The autosampler is not used.

Measuring spectral peak at a selected analysis line

Start a test measurement at a selected analysis line in the **Spectrometer | Parameters** window.

- Ignite the plasma.
- In the **Wavelength** area use ••• to open the **Select element/line** window and set the desired line.
  Alternatively, enter the value directly into the **Wavelength** input field.
- Move the spectrometer with **Set** to the desired wavelength.
  When the setting is completed successfully, the marker next to the setting turns green.
- Start a dark current measurement with **Dark current meas.**.
- For the following measurement select the view direction **axial** or **radial.**
- Set the **Read time**.
- Provide the sample and immerse the intake tube in the sample.
- Wait for the time period to achieve stable nebulization of the sample. Start the measurement with **Record spectrum**.
  - ✓ The measurement takes place and the measurement results are displayed in the **Edit spectra** window.

See also

- Inserting analysis lines into the line table [▶ 27]
- Displaying and editing intensity spectra [▶ 80]

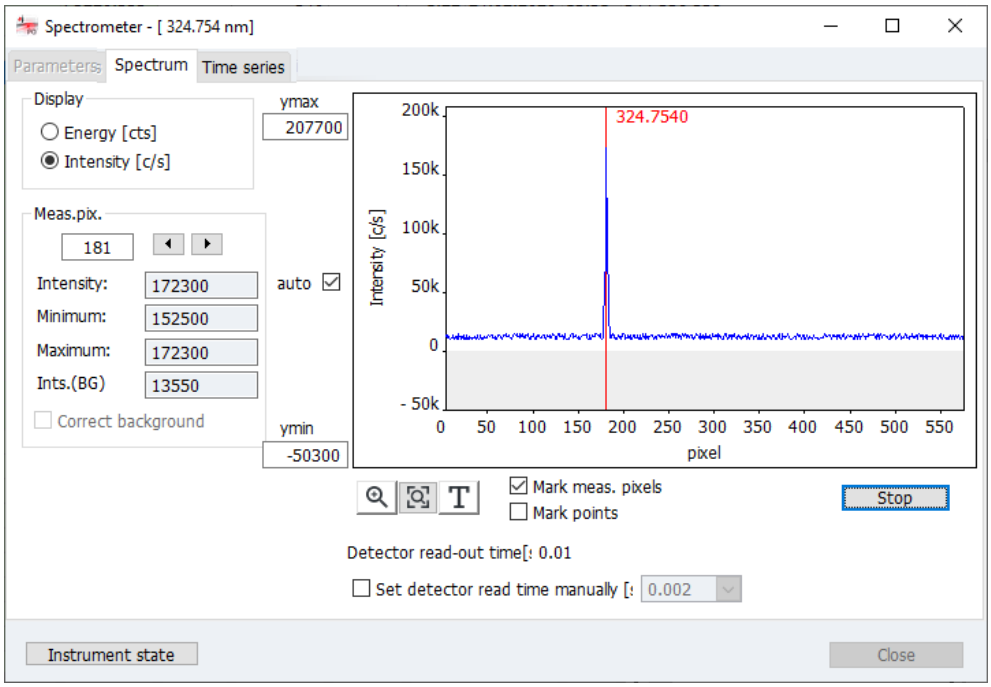
9.1.2 Diagnosis of device parameters

Service-relevant parameters are displayed in the **Spectrometer** | **Diagnosis** window.

9.1.3 Performing continuous peak measurements

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

Graphical display and digital analysis



Option	Description
Display	Options for displaying the spectrum. **Energy** Display of the energy spectrum, measuring unit: cts (counts) To obtain measurement results with as little noise as possible, the integration times for the detector are chosen for the energy maximum to be at approx. 30000 cts. **Intensity** Presentation of the energy per time unit, measuring unit: cts/s (counts per second) Based on the intensity different peaks can be compared irrespective of the integration time.
Meas.pix.	Selection of the pixel whose value is continuously displayed in the **Energy** or **Intensity** fields The **Maximum** and **Minimum** fields display the corresponding results of the continuous measurement.
Mark meas. pixels	Mark the set measuring pixel in the graph with a vertical red line
Mark points	Mark the measuring values for each pixel in the graph with a point
Set detector read time manually	Select the read-out time for the CCD detector from the list box Longer read-out times result in higher energy values. The default for the read-out time of the CCD detector is 0.01 s.

Option	Description
Graph scaling	Enter values for the start and end points of the ordinates directly into the input fields at the axes. Alternatively, after enabling zoom mode select the range to be displayed by holding down the left mouse button. Reverse scaling by enabling the **auto** option or clicking on .

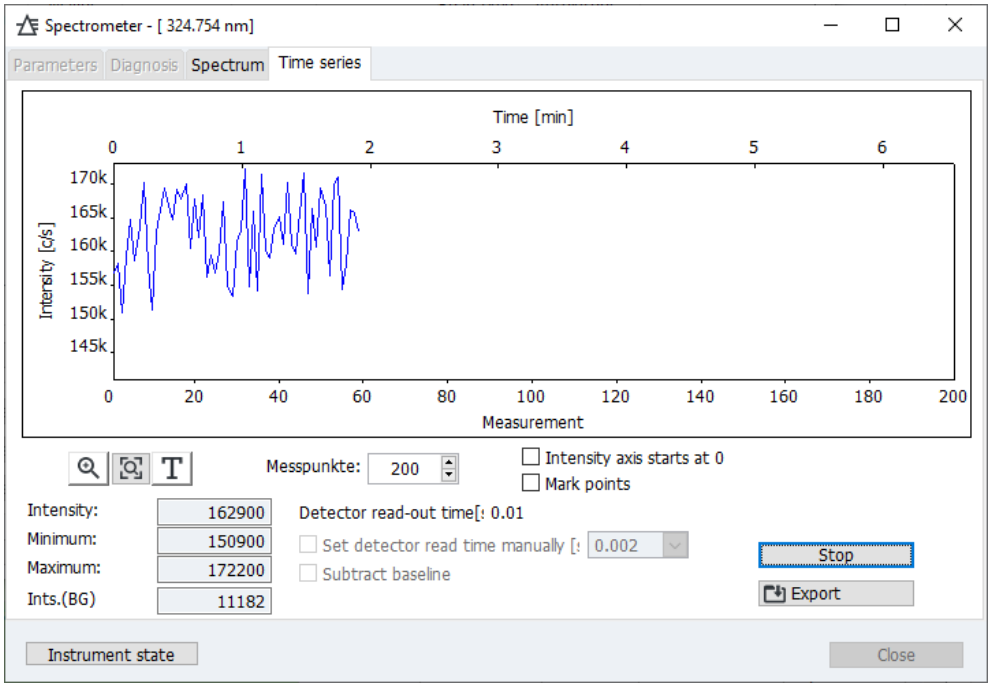
Starting a peak measurement

- In the **Spectrometer** | **Parameters** window set the wavelength and the view direction.
- Change to the **Spectrum** tab.
- Start continuous measurement by clicking on **Start**.

The measuring values are recorded with the set parameters and repeated continuously until **Stop** is pressed.

9.1.4 Recording signal progression

In the **Spectrometer** | **Time series** window record the signal progression of the intensity for the wavelength currently set in the spectrometer across a selected number of measuring points.



In addition to the graphical display the digital values of the current intensity, the maximum and minimum intensity values reached and the intensity of the background are output.

You can set the following parameters for recording the signal progression:

Option	Description
Scaling	After enabling zoom mode select the range to be displayed by holding down the left mouse button Reverse scaling by clicking on
Intensity axis starts at 0	Do not set the scaling of the y-axis automatically, but let it start at "0"

Option	Description
Messpunkte	Select the number of measuring points from the list
Mark points	Mark the measuring points in the graph with a point
Set detector read time manually	Select the read-out time for the CCD detector from the list box
Subtract baseline	Show background-corrected intensity values

9.2 Plasma

The **Plasma** window contains the following functions:

- Ignite plasma/extinguish plasma
- Control of the HF generator
- Setting the gas flows
- Control of the analyzer pump
- Adjustment of the transfer optics
- Automatic optimization of nebulizer gas flow and plasma power

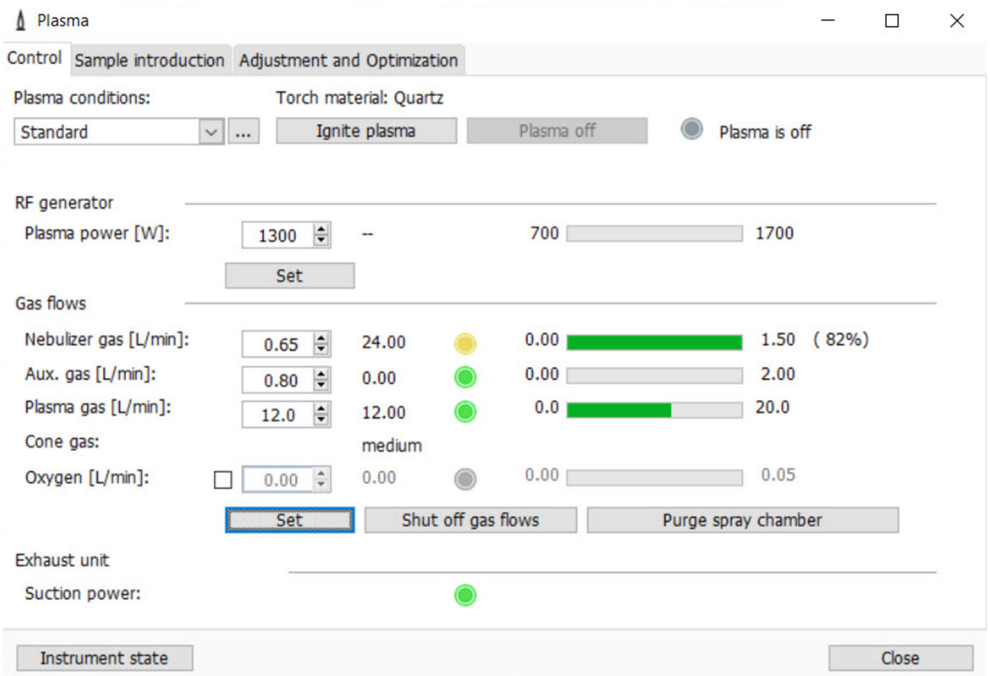
▶ Open the **Plasma** window by clicking on in the icon bar or select the **Method Development** | **Plasma** menu item.

With **Instrument state** a graph is displayed for the output of the messages from the safety sensors of the ICP-OES device. In case of problems with the plasma, you can view the error messages of the sensors here.

9.2.1 Igniting the plasma and setting up the plasma conditions

In the **Plasma** | **Control** window you ignite/extinguish the plasma and adjust the gas flows in the device.

Functions in the Plasma | Control window



Option	Description
Plasma conditions	Select the plasma conditions (plasma power and gas flows).

Option	Description
Ignite plasma/Extinguish plasma	Ignite the plasma and extinguish it when the ICP-OES device is ready.
RF generator	Set the effective plasma power. The plasma power defines the plasma temperature. The generator current is controlled via the firmware to achieve the effective plasma power.
Gas flows	Switch on and adjust the gas flows. **Plasma gas** The plasma gas flows along the outer tube and is used to generate the plasma. **Nebulizer gas** The nebulizer gas nebulizes the sample and transports the sample aerosol into the plasma. It is connected to the nebulizer. The percentage value in the nebulizer gas row indicates how permeable/clean the nebulizer is (see below). **Aux. gas** The auxiliary gas pushes the plasma away from the injector and flows between the inner tube and the injector. **Cone gas** The cone gas removes the "cold" plasma tail to eliminate interference due to recombination in the plasma in the axial direction of observation. At the same time the cone gas supports the cooling of the cone. **Oxygen** Oxygen can be added to the nebulizer gas as an additional gas for selected applications. The oxygen flow must be activated with the checkbox in front of the gas setting before it can be changed.
Shut off gas flows	Close all gas valves.
Purge spray chamber	The nebulizer gas is activated for 1 minute to purge air from the spray chamber. This facilitates the ignition of the plasma after interrupted operations. A countdown is displayed during this time.
Suction power	A safety circuit checks that the power of the connected extraction is sufficient for the operation of the ICP-OES device. If this is the case the indicator lamp is illuminated in green.

With the **Set** buttons you configure the modified parameters (plasma power and gas flows) at the ICP-OES device.

Evaluating the nebulizer function

The nebulizer must be cleaned if sample particles or high concentrations of salt in the samples have clogged it up. An indicator that the nebulizer has clogged up is increased nebulizer gas pressure.

Compare the current percentage (pressure) of the **Nebulizer gas** parameter with the value achieved after installation of the new or cleaned nebulizer.

Clean the nebulizer as described in the operating instructions of the ICP-OES device if the percentage has increased significantly (by more than half the original value), at the latest however if 75 % is reached.

Selecting the plasma conditions

The **Plasma conditions** list contains saved plasma parameters for different sample matrices and, if a method has been loaded, the line-specific parameters of the method.

By clicking on ... a context menu opens with functions for managing the parameters selected in the list:

Function	Description
Save current plasma parameters	Save configured plasma conditions (plasma power and gas flows) and add them to the list
Delete entry	Delete the selected entry The **Standard**, **Kerosine** and **Hydride technique** defaults cannot be deleted.
Set plasma conditions	Configure the plasma parameters of the selected entry at the ICP-OES device
Copy to method line	Available if a method line has been selected in the list Transfers the plasma conditions to the method parameters of the selected line.
Copy to all method lines	Available if a method line has been selected in the list Transfers the plasma conditions to the method parameters of all lines.
Set as method defaults	Save the current plasma conditions as default values for newly inserted method lines (does not apply to line favorites)

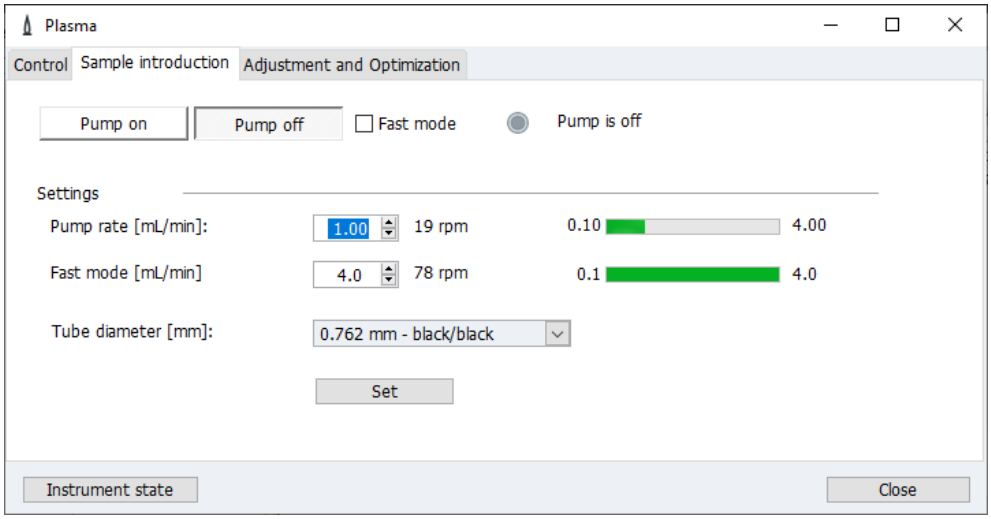
See also

Switching on the spectrometer and igniting the plasma [▶ 64]

9.2.2 Checking the sample introduction and the pump

In the **Plasma** | **Sample introduction** window check the function of the tube pump at the ICP-OES device.

Functions in the Plasma | Sample introduction window



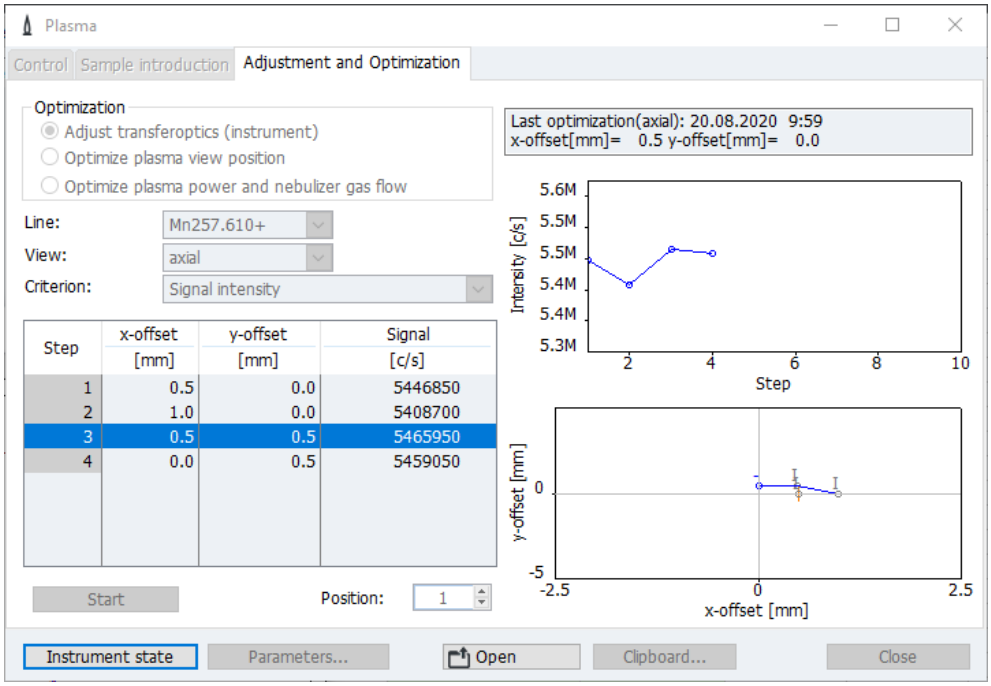
Function / parameters	Description
Pump on/ **Pump off**	Switch the pump on and off. In the original state after activation of the ICP-OES device the pump is switched on.
Fast mode	Move the pump manually into fast mode The function can be used to manually purge the sample introduction system. After successful purging the checkbox must be disabled to move the pump back to sample transport.
Pump is running/ **Pump is off**	Pump status The current pump speed is displayed with the unit RPM (rotations per minute).

Function / parameters	Description
Pump rate	Set the pump rate for the sample transport during the measurement
Fast mode	Set the pump rate for fast mode With the fast mode the transport time during a change of sample or the transport time of the purging solution to the nebulizer is optimized.
Tube diameter	Select the tube type used The transported sample volume (pump rate) is calculated from the information of pump speed and tube diameter. The tubes have been coded with colored stoppers. Select the stopper combination of the tube used from the list.
Set	Apply the settings

9.2.3 Adjustment and optimization of plasma

In the **Plasma | Adjustment and Optimization** window make the following adjustments:

- Alignment of the transfer optics with the optical axes of the spectrometer
- Calculation of the offset values of the transfer optics for an analysis line from the method
- Optimization of plasma power and nebulizer gas flow



Two different methods are available for adjustments and optimization and can be selected by clicking on **Parameters**:

Method	Description
Grid search	The range is scanned based on a grid. From the number of measuring points the one with the highest intensity is determined. The adjustment is exact but takes a long time due to the determination of a large number of measuring points.

Method	Description
Simplex optimization	The energy maximum is determined iteratively. From a start measuring point the measuring point with the highest value in the vicinity is determined. Starting from this measuring point, the measuring point with the highest energy is determined again. The process continues until the energy maximum has been found. This method is faster than the grid search but less certain. In the various hot zones of the plasma several energy maxima may occur and thus an incorrect energy maximum be found if the start point was unfavorable. For the simplex method a **Stopping criterion** must be defined as a percentage value. If 3 consecutive values do not differ by more than this percentage value, the adjustment is ended. If **Start with optimized values** is enabled, the optimized parameters of the last adjustment/optimization are used as start-up values for the current optimization.

For the adjustment of the transfer optics (device) the signal intensity is used as a criterion.

The criterion for optimization is configured automatically dependent on the wavelength of the analysis line, but can be modified manually:

Criterion	Wavelength range of the analysis lines
Signal intensity	< 200 nm
Signal/background	200 to 350 nm
Signal/square root of background	> 350 nm

Adjusting the transfer optics on optical axes (plasma centers)

The adjustment of the transfer optics on optical axes takes place using a Mn solution. Prepare Mn solution for the adjustments with the following concentration:

Monitoring direction	Mn solution
axial	1 mg/L
radial	10 mg/L

- Enable the **Adjust transferoptics (instrument)** option.
  - ✓ The Mn analysis line is automatically set in the **Line** list.
- Select the adjustment method under **Parameters** (see above).
- Select the monitoring direction:

Option	Description
axial	Monitoring from above
radial	Monitoring from the side
attenuated axial	Monitoring of the attenuated energy from above
attenuated radial	Monitoring of the attenuated energy from the side
closed	Monitoring with the shutter closed (for service purposes)

- Immerse the intake tube into the sample. When using an autosampler, set the position on the sample rack.
- Click on **Start**.

✓ The adjustment of the transfer optics runs automatically. At the end of the adjustment the new data are displayed.

▶ Accept the new adjustment values by clicking on **OK**.

Optimizing the monitoring position for an analysis line of the active method

The plasma has zones of different heat. During this optimization the monitoring point in the plasma is detected where the analyte has the greatest signal intensity. The values are saved in the method as **Offset**.

▶ In the **Line** list select the analysis line from the method.

▶ Enable the **Optimize plasma view position** option.
The information about the monitoring direction is automatically transferred from the method and the criterion is set for the optimization (see above).

▶ After clicking on **Parameters** select the adjustment method (see above).

▶ Immerse the intake tube into the sample. When using an autosampler, set the position on the sample rack.

▶ Click on **Start**.

✓ The adjustment of the monitoring position runs automatically. At the end the optimized offset values are displayed.

▶ Transfer the new offset values to the method by clicking on **OK**.

Optimizing the plasma conditions for a sample

After having defined the monitoring position of the analytes in a sample you can optimize the plasma conditions (plasma power and nebulizer gas flow).

▶ Enable the **Optimize plasma power and nebulizer gas flow** option.

▶ In the **Line** list select the analysis line from the method.

✓ The information about the existing plasma conditions is automatically transferred from the method and the criterion is set for the optimization (see above).

▶ Select the adjustment method under **Set** (see above).

▶ Immerse the intake tube into the sample. When using an autosampler, set the position on the sample rack.

▶ Click on **Start**.

✓ The optimization of the plasma power and nebulizer gas flow runs automatically. At the end the optimized values are displayed.

▶ Transfer the new values to the method by clicking on **OK**

9.3 Autosampler

The autosampler is an optional accessory. The autosampler is detected during the initialization in the **Quick Start** window after starting the ASpect PQ program.

The **Autosampler** window contains the following functions:

- Show connected autosampler type
- Configuring the autosampler
- Adjust the autosampler
- Rinse sample paths additionally
- Reinitialize the autosampler
- Perform a self-test

The parameters directly relevant to the analysis (charging on the sample racks and wash steps) are to be specified in the method, the sequence and the sample identification data (sample ID).

Open the **Autosampler** window by clicking on in the toolbar or using the **Method Development** | **Autosampler** menu item.

Initializing the autosampler

The autosampler is generally initialized when the mains switch is activated. Re-initialization may be necessary if the autosampler has lost its orientation, e.g., due to mechanical impact. This re-establishes the connection between the autosampler, ICP-OES device and PC.

- By clicking on **Initialize** you can re-initialize the autosampler if necessary without re-starting the ASpect PQ program.

Detecting the autosampler

If the autosampler was only switched on after starting ASpect PQ, the use of the autosampler must be registered in the program.

- To do this, click on **Detect** and then on **Initialize**.

Note: When using the Cetac ASX-560 with dilution system, the **Detect** button is hidden.

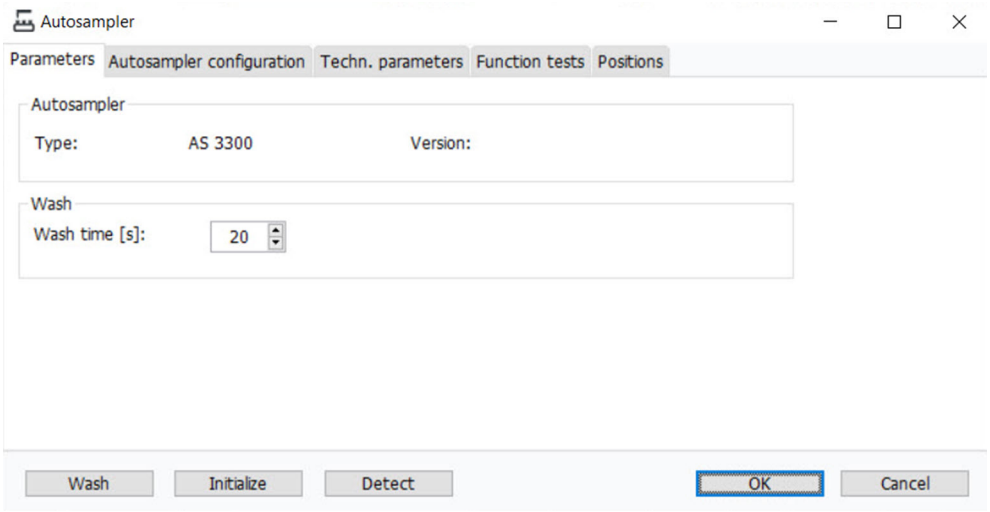
Flushing the sample paths

- In the **Autosampler** | **Parameters** window set the **Wash time**.
  The default for the wash time is transferred from the current method.
- Click on **Wash**.
  Alternatively, select the **Routine** | **Wash** menu item.
  - ✓ The sample paths (tubes-nebulizer-spray chamber-torch) are washed for the specified wash time with the pump in fast mode.

9.3.1 Displaying the connected autosampler

In the **Autosampler** | **Parameters** window the following parameters are displayed or configured:

- Autosampler type
- Washing parameters



Autosampler type

The **Autosampler** | **Parameters** window displays the autosampler type detected during initialization and the autosampler firmware version.

Washing parameters

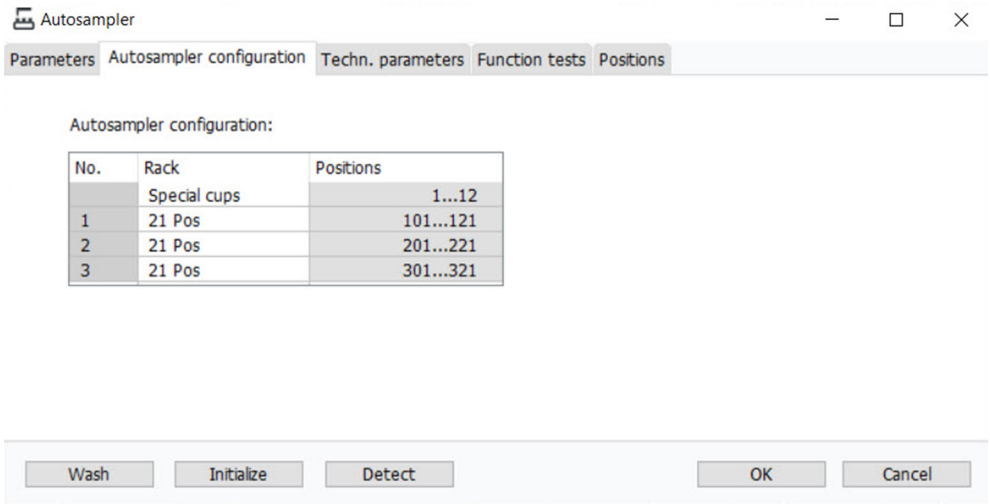
The system wash time of the sample path from the sample cup through to the torch is transferred from the current method. Conversely, changes in the **Autosampler** | **Parameters** window do not affect the entries in the method. During system washing using the autosampler the wash solution is taken from the wash cup of the autosampler.

See also

Configurations for sample introduction (Method | Sample delivery window) [▶ 33]

9.3.2 Configuring the autosampler rack

In the **Autosampler** | **Autosampler configuration** window configure the sample racks used on the autosampler.

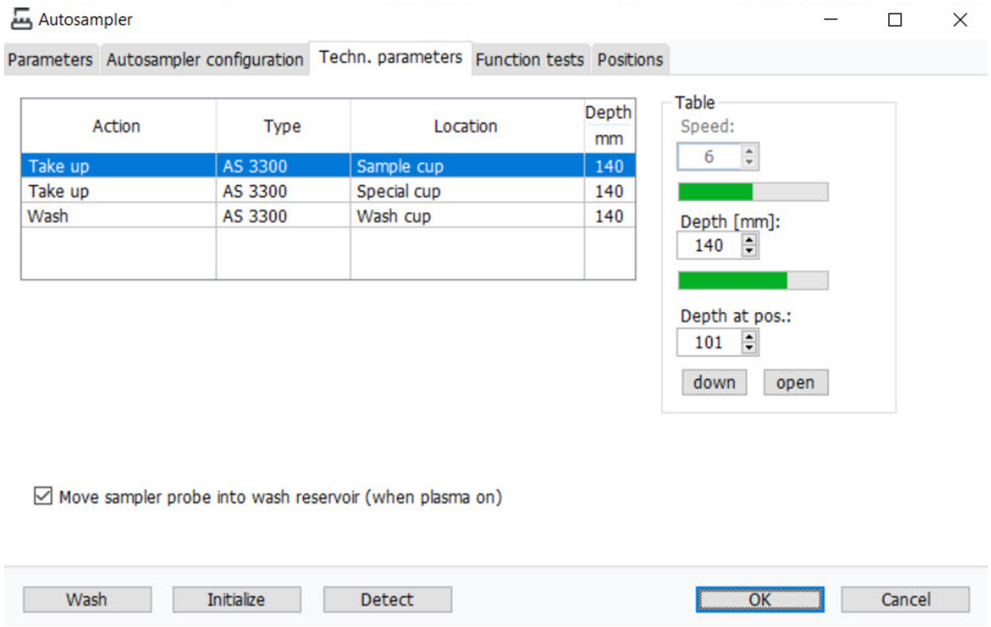


Depending on the autosampler used, different sample racks and racks with special samples can be positioned.

Select the sample racks in the table. For the variable sample racks, three-digit numbers are provided as position numbers. The first digit indicates the position of the sample rack on the autosampler, and the other two indicate the position on the sample rack. For example, the number 113 indicates position 13 on sample rack 1. The variable sample rack 1 is located on the autosampler in front of the wash cup, followed by sample racks 2 and 3.

9.3.3 Technical parameters of the autosampler

In the **Autosampler** | **Techn. parameters** window specify the immersion depth of the cannula into the various cups.



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

Cup	Action
Sample cups	Aspire samples through tube pump.
Special cups	Aspire special samples through tube pump.
Wash cup	Flush cannula and intake path.

Elements of the actions table

Option	Description
Action	Available action options: **Take up** Take up sample from the cup for transport to the torch. **Wash** Take up wash solution.
Type	Connected autosampler type
Location	Cup to which a given action refers
Depth	The depth to which the cannula submerges in mm

Table subarea

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

Option	Description
Depth	Set immersion depth of the cannula The immersion depth is measured from the highest position of the autosampler arm.
Depth at pos.	Position of special or sample cup at which the immersion depth is measured.
Set	If activated, the autosampler arm moves over the cup for which the positioning has to be adjusted. With sample and special cups, this is the position selected under **Depth at pos.** If not activated, the immersion depth and speed are changed without the autosampler arm moving above the cup.

Additional options

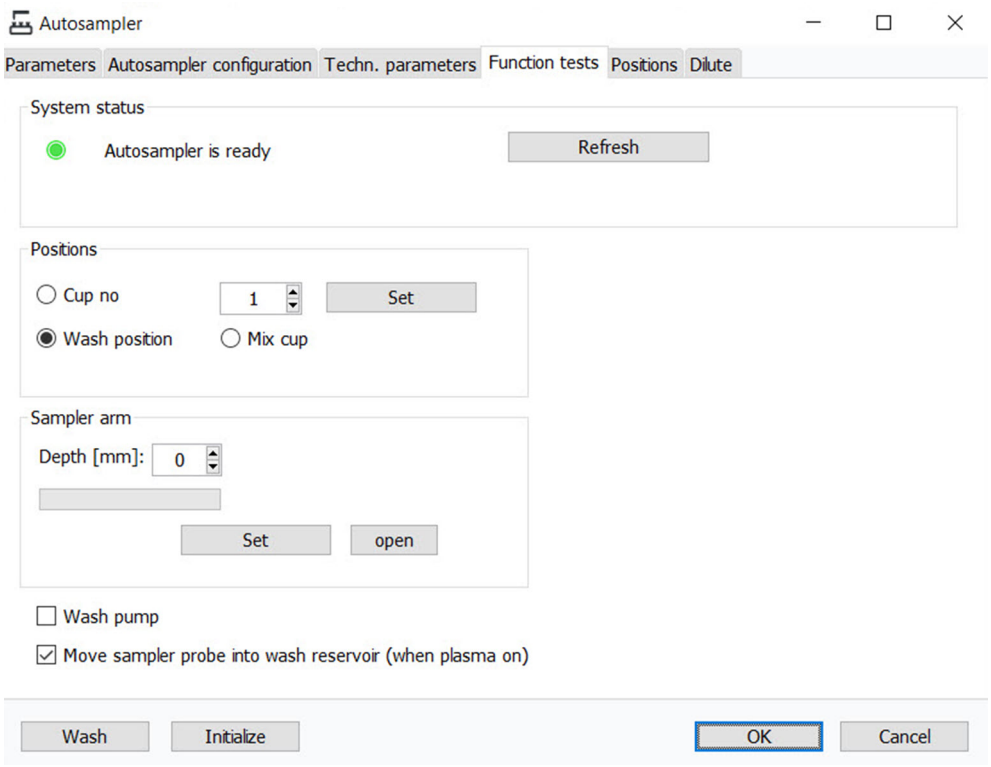
If the **Move sampler probe into wash reservoir (when plasma on)** option is enabled, the cannula is automatically immersed into the wash reservoir after the window is closed.

ASX-560 only: Set the speed of the wash pump (levels: 0...99). Use **Set** to permanently store this value in the autosampler.

9.3.4 Testing the autosampler functions

In the **Autosampler | Function tests** window you can check whether the autosampler is ready for use.

Autosampler | Function tests window



The following functions of the autosampler are tested:

Function	Description
System status	Check for operational readiness. With **Update** operational readiness is checked again.
Positions	After clicking on **Set** the autosampler moves to a selected position. **Cup no** The autosampler moves to the position selected in the list. **Wash position** The autosampler moves to the wash cup.
Sampler arm	Lower the autosampler arm to the **Depth** set in the list box.
Wash pump	Switch the wash pump on and off.

Move autosampler canula into wash reservoir

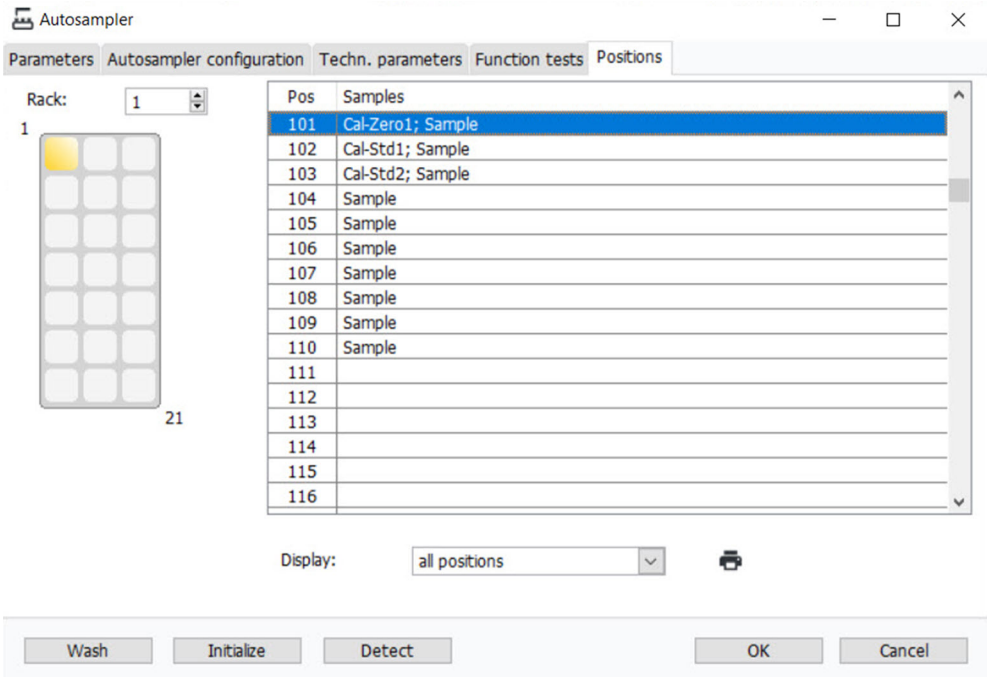
If the **Move sampler probe into wash reservoir (when plasma on)** checkbox is enabled, the cannula is immersed into the wash reservoir after the **Autosampler** window is closed.

9.3.5 Displaying the sample positions on the autosampler

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

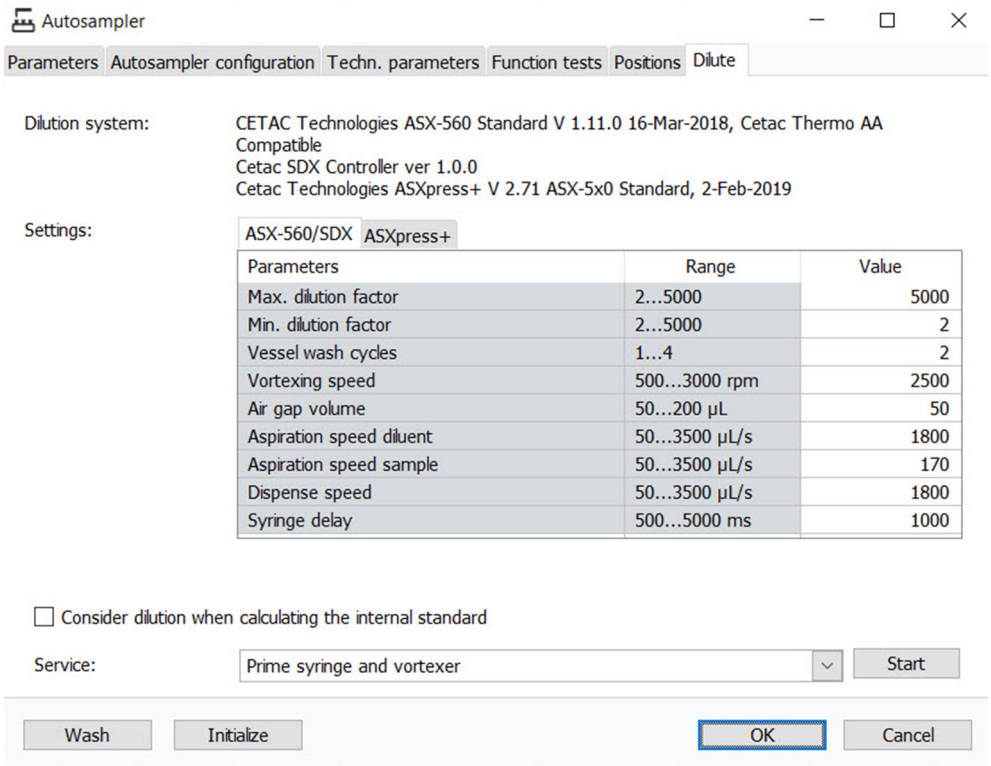
For the display it is possible to choose between the options **all positions**, **only sample positions** and **only special positions**.

A diagram of the sample rack with the currently selected sample position is shown next to the table. The sample position can be selected both in the diagram and in the table.



9.3.6 Dilution function

The parameters for sample dilution when using the Cetac ASX 560 autosampler with the Cetac SDX_{HPLD} are displayed in the **Autosampler** / **Dilute** window.



Configuration

The parameters in the **Settings** section are preset settings that provide good results for sample dilution. You can vary the parameters within the setting ranges during a method optimization.

Consider dilution when calculating the internal standard

If you enable this checkbox, the software will take the dilution into account when calculating the internal standard.

- If you add the internal standard to the original sample, the internal standard in the sample will also be diluted. Enable this checkbox to take the dilution into account in the calculation.
- If you also add the internal standard to the diluent or add it to the sample solution via the internal standard kit, the internal standard will not be diluted. In this case, do not enable this checkbox.
- Even if you use argon as the internal standard, do not enable this checkbox.

Service

In the **Service** list you can select service functions on the SDX_{HPLD} and execute them with **Start**:

Option	Function
Prime syringe and vortexer	Dilution fluid is pumped through the system with the syringe pump and dispensed into the vortexer. This removes air bubbles from the system and conditions the vortexer.
Move syringe to removal position	If the syringe pump needs to be removed for maintenance, the syringe plunger must first be moved into the correct position using this function.
Re-home ASXpress+ after disassembling for cleaning	Only if the ASXpress+ is installed: Initialize the ASXpress+ after installation or maintenance.

9.4 Recirculating chiller

In the cooling circuit a valve is switched in the ICP-OES device to open and close the circuit. The replacement of the cooling water is therefore supported by a wizard.

NOTICE

Observe the notes on the maintenance of the recirculating chiller and the preparation of the cooling water in the operating instructions for the ICP-OES device.

- Select the **Extras** | **Maintenance** menu item.
- In the **Maintenance** window, start the coolant change by clicking on **Change**.
- Follow the instructions of the wizard.

10 Data management

This section contains information about
- Print options
- Method and sequence management
- Management of results data
- Definition of units for concentrations and contents
- Management of data for frequently used stock solutions and QC samples

10.1 Print functions in ASpect PQ

For the output of data ASpect PQ has a large number of output formats available. 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.

For the output of analysis results and the content of windows (e.g., the **Method** or **Sequence** windows) report templates are used. 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 Print analysis results

ASpect PQ offers a variety of options for printing results data:
- Print the complete record. The complete record of an analysis contains the method parameters, the calibration and analysis results with single 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 is 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

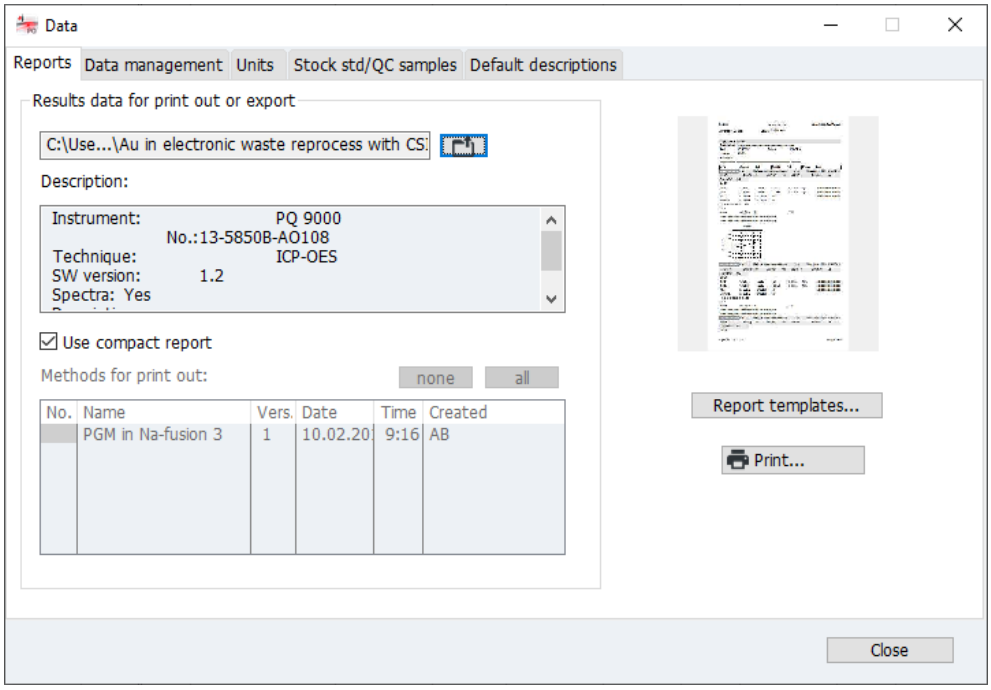
The complete record of an analysis contains the method parameters, the calibration and analysis results with single sample values (statistic runs). The complete records can be printed of the results in the main window or the saved files.

▶ Open the **Data** | **Reports** window using the  icon.

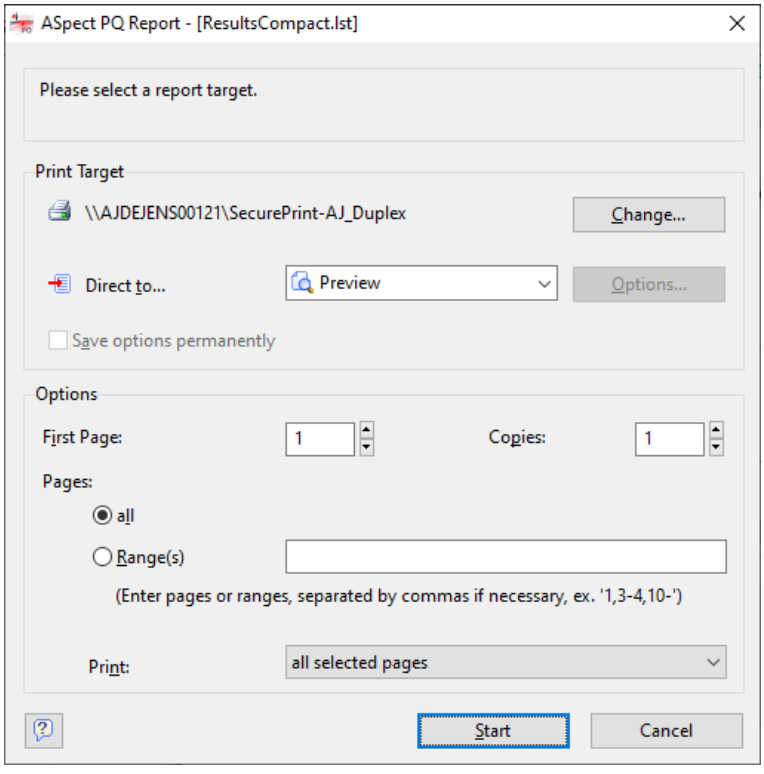
▶ Alternatively, open the window using the **Extras** | **Data** or **File** | **Print** | **Report** menu items.

The name of the current file, file information (**Description** list), and all method versions used for creating the current results file are displayed.

Data | Reports window with selection of the results data for printing



- If you want to print a saved file, use to open the **Open** default window and select the desired file.
- If you want to print the shortened compact report, enable the **Use compact report** option.
- Select all method versions to be printed in the table.
  With the shift or Ctrl key held down click on the method versions you want to select.
  Use the **all** button to select all versions and the **(none)** button to remove all selections.
- Click on **Print** to open the **ASpect PQ Report** window with the selection of output formats.



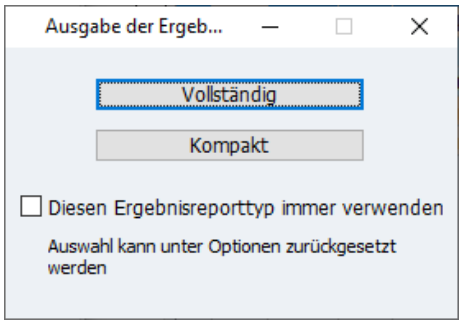
- If necessary change the output format in the **Direct to** list and set special parameters of the output format with **Options**.
- Start the printout with **Start**.

NOTICE! Use the **Direct to** | **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 is being output before it is sent to the printer.

Print current results

The results displayed in the main window can be printed:

- Activate the Results tab in the main window, the content of which you wish to print.
- Start the printout using the **File** | **Print** | **Active Window** menu item.
  - ✓ The **Results report format** window appears.

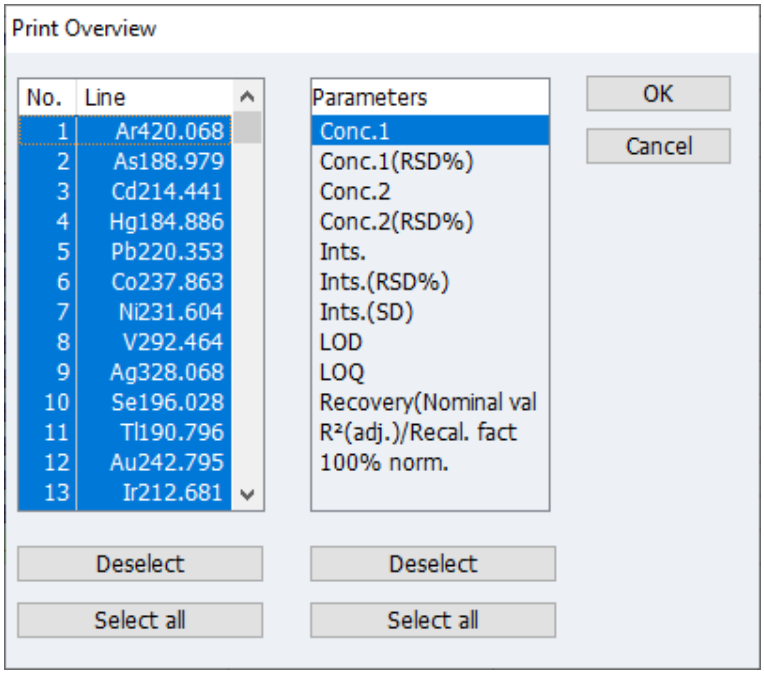


- Click on **Complete** if you want to print the results with the signal diagrams. Select **compact** for printing the results in a compact overview.
- Continue as described above for "Print complete record".

NOTICE! If you enable the **Always use this results report type** checkbox in the **Results report format** window and then click on **Complete** or **compact**, this window no longer opens for the next result printout; the last results report type is automatically used. You can reset this setting in the **Options** | **View** window.

Print selected data

- Change to the **Overview** tab in the main window.
- Click on in the bottom area of this tab or select the **File** | **Print** | **Active Window** menu item.
  The **Print Overview** window appears.



- Select all desired lines and parameters for printing and confirm your selection with **OK**.
  The **ASpect PQ Report** window appears.
- Continue as described above for "Print complete record".

See also

View options [▶ 133]

10.1.2 Print further analysis parameters and settings

The following parameters and settings of the analysis can be printed from the respective window:

- Method
- Sequence
- Results data on the **Overview** tab in the main window
- Sample ID
- QC (Quality Control charts)
- Calibration
- Autosampler positions

- On the Aspect PQ workspace enable the window whose content you want to print.
- Start printing the parameters with a click on in the window.
- Alternatively, open the **File** | **Print** | **Active Window** menu command.
  ✓ The **ASpect PQ Report** window appears.
- If necessary, change the output format in the **Direct to** list and set special parameters of the output format with **Options**.
- Start the printout with **Start**.

10.1.3 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.

- Activate the **File** | **Report design mode** menu item.
- Open the window whose report template you want to change.
- If present, click on there. Otherwise, select the **File** | **Print** | **Active Window** menu item.
- Confirm the query about editing the report template with **Yes**. The report designer opens.
- Make the desired changes and save the changed report template.
- Link the report template to the corresponding print contents (see "Change assignment" 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.

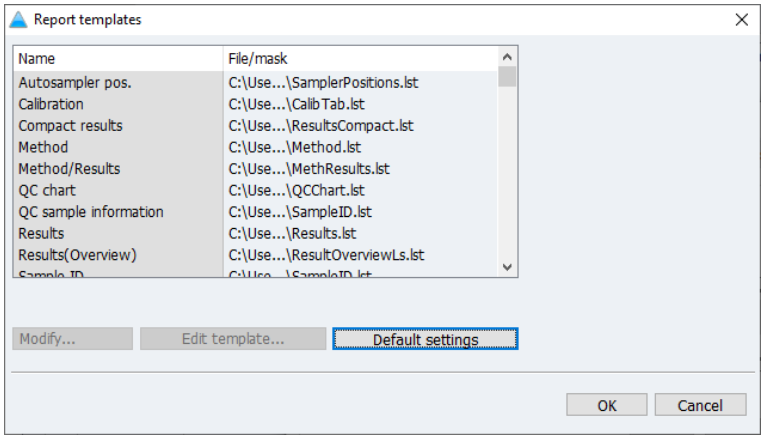
In order to process an existing object, it must first of all be selected. For this click on the object with the left mouse button. You will recognize a selected object by its highlighted frame. If you create a new object it is automatically selected and can be directly changed in terms of size and position. 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

In the **Report templates** window the templates are edited and assigned to the ASpect PQ windows. 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.

- Use the icon to open the **Data** | **Reports** window.
- Click on **Report templates**.



For the following windows a report template must be available:

Name	Description
Results	Content of the **Results** tab in the main window
Compact results	Compact overview of the results
Results (Overview)	Content of the **Overview** tab in the main window
Calibration	Analysis calibration: Window **Calibration**
Method	Method parameters: Window **Method**
Method/Results	Full report
Autosampler pos.	Autosampler assignment: Window **Autosampler** | **Positions**
Sample ID	Sample information data: **Sample ID** | **Sample Information**
QC chart	Data of the QC charts: Window **QC**
QC sample information	Information data of the QC samples: Window **Sample ID** | **QC sample information**
Sequence	Sequence: Window **Sequence**

Change assignment

- In the **Report templates** window select the window whose report template is to be changed.
- With **Modify** open the dialog window to assign the files.
- If only one report template is to be assigned, enable the **Use report template file (*.lst)** option and then select the desired file by clicking on .
- If several templates are to be offered simultaneously at the start of printing, enable the **Allow file selection (mask, e.g. c:\Reports\Results*** option. Enter the mask name while using wildcards in the input field.
- Confirm the settings with **OK**.

Editing a report template

- In the **Report templates** window select the window whose report template is to be edited.
- Click on **Edit template** to open the **Report designer** window.

Restore default settings

You can restore the settings according to the program installation.

- Click on **Default settings**.

10.2 Data management for all data types in ASpect PQ

The following data is generated in ASpect PQ:

- Methods
- Sequences
- Results files
- Line/wavelength file
- Correction models
- Correction spectra
- Report templates
- Line favorites
- Worksheets

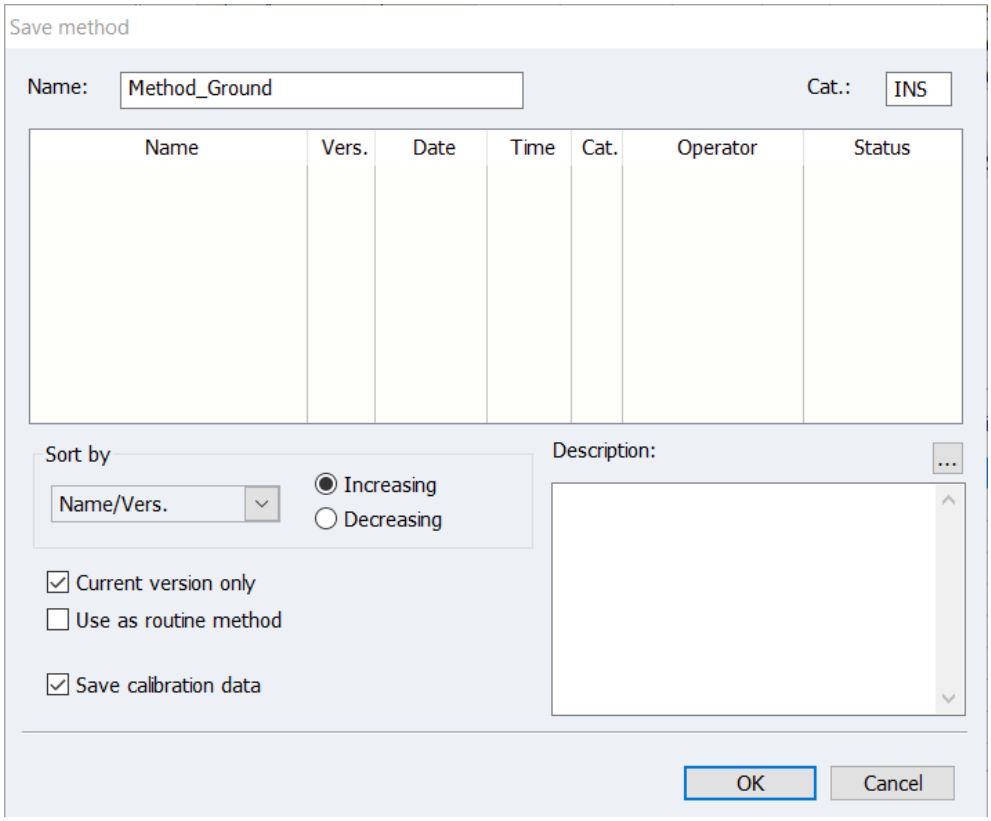
The above data types are organized in the **Data** | **Data management** window. The window appears after clicking on or after selecting the **Extras** | **Data** menu command.

10.2.1 Managing methods and sequences

Methods, sequences and correction models are saved 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

Option/display	Description
	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 data records of all categories, clear the entry in the **Cat.** field.
List of records	Display of the stored methods/sequences 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 comments in the **Data** | **Default descriptions** window.
Current version only	If multiple versions of a data record with the same name exist, only the data record with the highest version number is displayed.
Predefined methods	Save any available calibration curves with the method The calibration curves can be used for further analyses.

In the software, data records with the same name 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
To select multiple data records in the database window, hold down the Ctrl or Shift key during selection with the mouse.

Open the data management

- Open the **Data** | **Data management** window by clicking on .
- In the **Type** list select the data record type to be edited: **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 are given the following extensions: method data records ".met", sequence data records ".seq".

- Open the database window with **Export**.
- Select the data records and click on **Export**.
- In the **Save as** default window enter a file name and confirm it with **Save**.
  - ✓ The database window with the exported files is displayed.
- Click on **Close** to close the database window.

Importing data records

Using the import function, you can load data records from other devices/computers into your database. An imported file can contain multiple data records from which you can select those to be loaded.

- Use **Import** to open the **Select the method file for import** or **Select the sequence file for import')** window with the default functions for opening files.
- Choose the file to be imported.
  - ✓ 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 data records to be imported and click on **Import**. The data records are imported into the database. If a data record with the same name already exists, a new version of the data record is created. In the database window, the current versions of the available data records appear.
- Exit the database window with **Close** and return to the **Data** window.

Deleting data records

Using the delete function, you can permanently delete data records from the database.

- Open the database window with **Delete**.
- Select the data records to be deleted.
- 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 **Delete method** or **Delete sequence** database windows with the **File** | **Delete** | **Method** or **File** | **Delete** | **Sequence** menu command.
- Then, proceed as described above.

10.2.2 Managing results files

Results data is saved to the database during the measurement. A database containing results data may be copied or deleted.

- Open the **Data** | **Data management** window using the **Extras** | **Data** menu item or by clicking on .
- In the **Type** list select the **Results** option.

Importing results data

You can import results data into the software. During this process, the data is placed in the results folder within the file structure of the software.

- Click on **Import**.
  - ✓ The **Select results files** window appears.
- Select the TPS files and click on **Open**.
- Select a subfolder for the results memory and click on **OK**.
  - ✓ The TPS files and associated SPK files (if any) are copied to the selected results folder.

Exporting results data

Use this command to export one or more databases as well as existing spectrum files to another folder.

- Click on **Export**.
  The **Export** window appears with an overview of available results databases.
- Select the results databases to be copied by mouse click. You can select multiple databases by holding down the Ctrl or Shift key.
- Click on **Export** to open the **Find folder** window.
- Select the target folder and click on **OK**.
  - ✓ The TPS files and the SPK files are copied to the destination folder.

Deleting results files

You can permanently delete results data.

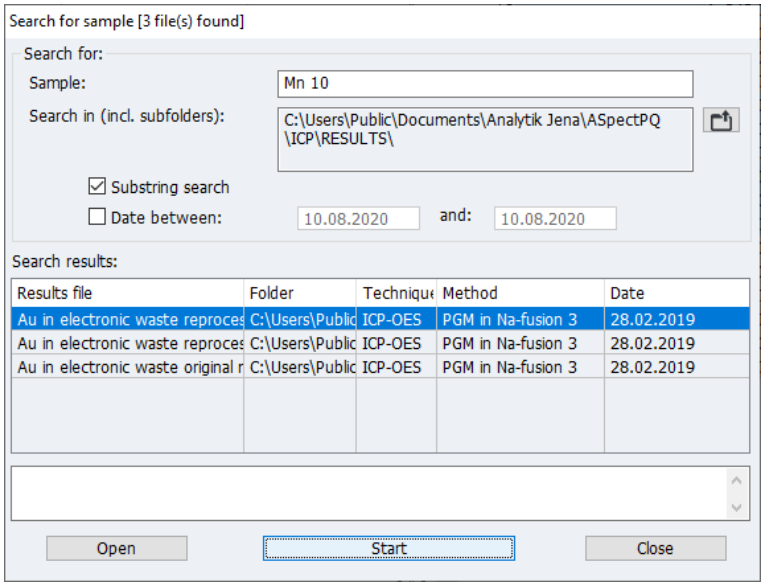
- Click on **Delete**.
- In the **Delete results files** window select the results database to be deleted by mouse click.

- Click on **Delete** and confirm the delete query with **OK**.
  - ✓ The data is 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 management** window, click on **Search for sample**. Alternatively, select the **Extras** | **Search Sample** menu item.



- In the **Sample** input field enter the sample name.
- To search for samples where the entered string is part of the name, enable the **Substring search** checkbox.
- Limit the time of the measurement by enabling the **Date between** checkbox.
- Start the search with **Start**.
  - ✓ All results which contain samples with the sample name entered are displayed in the table.
- To open one of the displayed results databases, select this database 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 has been saved to the computer controlling the ICP-OES device. To use the line/wavelength file on another computer, follow these steps:

- Open the **Data** | **Data management** window using the **Extras** | **Data management** menu command or by clicking on the icon.
- In the **Type** list, select the **Lines/wavelength file** option and click on **Export**.
- Select a folder to save the file and click on **OK**.
  - ✓ The file with the name "lines.dat" is saved in the selected folder.

10.2.4 Managing correction models

Correction models are used for spectral corrections. They can be transferred from one device to another. Correction model files have the extension MOD.

- Open the **Data** | **Data management** window using the **Extras** | **Data management** menu command or by clicking on the icon.
- In the **Type** list select the **Correction models** option.

Importing correction models

With this command you import correction models to ASpect PQ.

- Click on **Import**.
- Select the correction model file to be imported and click on **Open**.
  The **Import Correction model** database window appears.
- Click on **Import**.
  ✓ The correction model is transferred to the database.

Exporting correction models

With this command you export the correction model for use on another computer.

- Click on **Export**.
- In the **Export Correction model** database window select the desired model. Multiple selection is possible.
- Click on **Export**.
- In the **Save as** window enter the name and storage path and click on **Save**.
  ✓ The file with the correction model is saved.

Deleting correction models

With this command you delete correction models no longer required.

- Click on **Delete**.
- In the **Correction models** database window select the desired model.
- Click on **Delete**.
  ✓ The correction model is deleted from the database.

NOTICE

Deleting correction models can make methods unusable

Note that no check takes place whether the correction model is used in a method.

See also

Removing spectral interference – Edit spectra | Spectral corrections window [▸ 86]

10.2.5 Deleting correction spectra

Correction spectra no longer required can be deleted from the database.

- Open the **Data** | **Data management** window by clicking on the icon.
- In the **Type** list, select the **Correction spectra** option and click on **Delete**.
- In the **Correction spectra** database window select the spectrum to be deleted and click on **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

Print report templates created externally must be imported to ASpect PQ via the data management:

- Open the **Data** | **Data management** window by clicking on .
- In the **Type** list, select the **Report templates** option and click on **Import**.
- In the **Open** window select the file and click on **Open**.
  Report files have the extension ".lst".
  ✓ The report template is imported to ASpect PQ. Now assign the report template to the print content.

See also

Report templates [▶ 121]

10.2.7 Managing line favorites

Line favorites can be defined the **Method** window. They contain the analysis line used for a specific application and the line-dependent method parameters. Line favorite files have the extension ".fav".

- Open the **Data** | **Data management** window by clicking on .
- In the **Type** list select the **Favorites** option.

Importing line favorites

With this command you import a favorite record into ASpect PQ.

- Click on **Import**.
- In the **Favorites details** database window click on **Import**.
- Select the line favorite file to be imported and click on **Open**.
  ✓ After a query the favorite record is added to your line favorites.

Exporting line favorites

- Click on **Export**.
- In the **Favorites details** database window select the desired data record. Multiple selection is possible.
- Click on **Export**.
- In the **Targetfile (new or existing file)')** window enter the name and storage path and click on **Save**.
  An already existing file can also be used as the target file. In this case the data record will be integrated there.
  ✓ The file with the record of line favorites is saved.

Deleting line favorites

With this command you delete line favorites no longer required.

- Click on **Delete**.
- In the **Favorites details** database window select the data record.
- Click on **Delete**.
  ✓ The selected record is deleted from the database.

See also

Defining your own line favorites [▶ 31]

10.2.8 Importing, exporting and deleting worksheets

You can import, export and delete worksheets in the **Data** | **Data management** window. Optionally, you can specify the stored methods and sequences during the export. Worksheets have the extension WST.

- Open the **Data** | **Data management** window using the **Extras** | **Data management** menu command or by clicking on the icon.
- In the **Type** list select the **Worksheet** option.

Exporting a worksheet

- Click on **Export**.
- In the **Export Worksheet** window select the relevant worksheet. To export the methods and sequences contained in the worksheet, enable the **including sequence and method(s)** option.
- Click on **Export** and enter a folder and a name for the export file.
- Confirm the entries with **Save**.
  - ✓ The worksheet is exported with the extension WST.

Importing a worksheet

- Click on **Import**.
- In the **Import Worksheet** window select the worksheet and click on **Import.** To also import the methods and sequences contained in the worksheet, enable the **including sequence and method(s)** option.
- In the default window select the worksheet and click on **Open**.
  - ✓ The worksheet is imported.

Deleting worksheets

- Click **Delete**.
- In the **Delete** window select the worksheet and click on **Delete**.

10.3 Saving results in ASCII/CSV format

Measurement and analysis results can both be saved automatically and manually in ASCII/CSV format. For both export formats, the parameters for the decimal separator and the column separator are defined in the **Options** | **ASCII/CSV export** window.

Automatic continuous data export

With automatic continuous data export option enabled, every entry in the results table is instantly exported to the defined ASCII file. You specify the name of this ASCII file in the **Options** | **Continuous ASCII export** window.

Manual data export

If you intend to export data manually, you can select the rows of the results table to be exported.

- Select the samples in the results table.
  Hold down the Ctrl or Shift key and select the samples by clicking on the sample row.
  Select all sample rows using the **Edit** | **Select All** menu command.
- Use the **Edit** | **Save Selection** menu item to open the **Save as** default window.
  Alternatively, you can right-click on the selected lines and select a corresponding menu item from the context menu.
- Enter the file name and confirm it with **OK**.
  The data is saved in a format that can be read by spreadsheet programs with the extension ".csv".

See also

- Export options [▶ 135]
- Options for continuous ASCII export [▶ 135]

10.4 Specifying units of measurements

You can define the units of measurement available throughout the program in the **Data** | **Units** window.

- Open the **Data** | **Units** window by clicking on the icon.

3 preferred versions (for solutions: mg/L, µg/L, ng/L, mg/kg(liq); for solid samples: mg/kg, µg/kg, ng/kg, m-%) are available. These units cannot be changed by the operator. Units deviating from these can be freely defined. For freely defined units it is necessary to enter the conversion factor under Factor :

Option	Description
Unit	Name of the unit (max. 10 characters)
Comment	Comments 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
Type	**solid** Unit related to solid sample **liquid** Unit related to liquid sample (solution) **liquid grav.** Unit related to liquid sample to be weighed, e.g., oil

Use the buttons to manage your own entries.

Button	Description
Append	Append new row to the end of the list
Insert	Insert new line above the current row selection
Delete	Only user-defined units, preferred units cannot be deleted
Save	Save changes and entries

10.5 Managing databases for stocks and QC samples

The databases with 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 these databases. The stock standards and QC samples are available in method development.

- Open the **Data** | **Stock std/QC samples** window by clicking on the icon.
- Select the **Stock standard** oder **QC samples** option.
- Enter or edit the parameters of the standards in the table:

Table column	Meaning
Name	Here, enter the name of the standard (max. 20 characters).
Unit	Select the name of the unit (max. 10 characters) for the standard.

Table column	Meaning
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, use **Concentrations** to open the **Concentration entry** input field where you can assign the concentration to each element.

Use the buttons to manage the entries:

Button	Function
Append	Appends a new row to the end of the list.
Insert	Inserts a row in the list above the currently selected row.
Delete	Delete the marked row.
Save	Save the lists of the stock standards/QC samples.
Concentrations	Opens the input window for the entry of the element(s) and concentration(s) of the selected standard.

10.6 Creating predefined comments

User-defined comments can be defined for the following operations:
- Saving a method
- Saving a sequence
- Starting reprocessing
- Start measurement

The user-defined comments can be inserted by clicking on ... next to the **Description** field in the corresponding windows.

Create comment

- Open the **Data** | **Default descriptions** window by clicking on the icon.
- Select the process from the **Select category** list.
- Click **Edit template** to open the list of comments.
- Create a new comment by clicking on **New**. Under **Name** enter a description under which the comment can be selected. In the **Text** field, enter the actual comment.
- A comment can be edited via **Modify** or removed from the selection list via **Delete**.

10.7 Using the Windows clipboard

Copying results data 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 corresponding commands can be found in the **Edit** menu:

Edit... menu	Description
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 (checkmark), the copy action includes the column headers.

- Select the samples from the desired table of the results list.

- Hold down the Ctrl or Shift key and select the samples by clicking on the sample row.
- Select all sample rows using the **Edit | Copy all Columns** menu command.

▶ If necessary, activate the **Edit | Column Titles** menu command to have the column header included in the copy action.

▶ Activate the desired menu command to copy the results to the Windows clipboard.

Copying graphics as screenshots

You may also copy graphic windows and graphs of calibration curves, intensity signals or emission signals as screenshots to the Windows clipboard.

▶ Click on the right mouse button on the graph. A context menu 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 Customizing ASpect PQ

In the **Options** window, you can make the following settings which apply to all operations in ASpect PQ:

- View options
- Save paths of files
- Parameters for data export
- Generally applicable settings for the analysis sequence, for calibration and blank correction

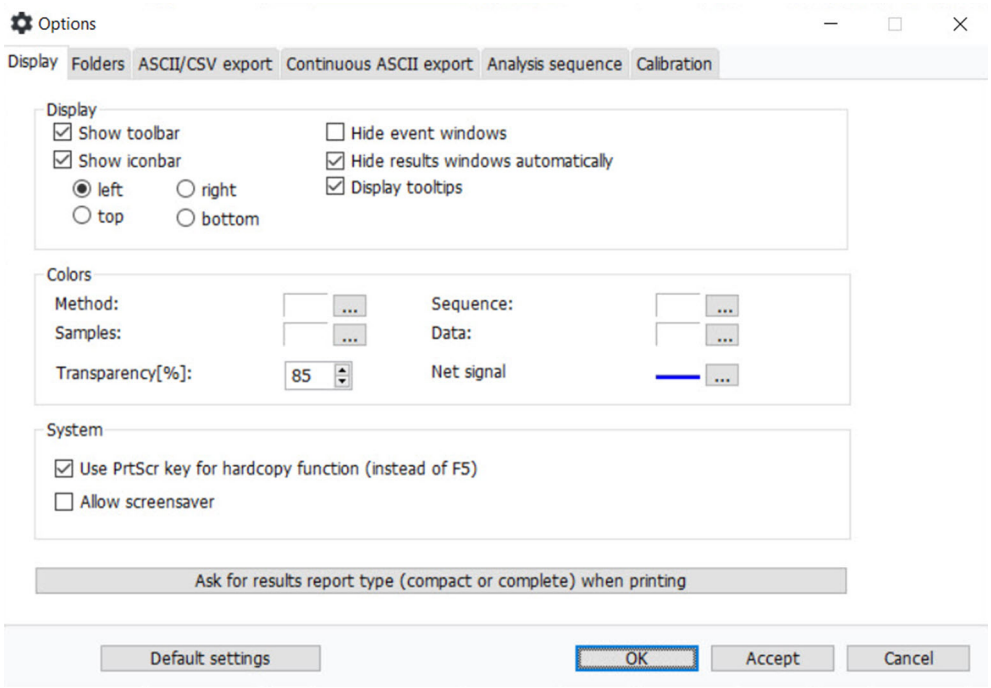
The settings made remain active after exiting and restarting ASpect PQ. The **Default settings** button resets all options to default values.

Open the **Options** window using the **Extras** | **Options** menu item.

11.1 View options

In the **Options** | **Display** window, you can define the functions visible on the workspace.
Screenshot

Options | Display window



Option	Description
Show toolbar	Display the toolbar with the buttons for the measurement routine
Show iconbar	Display the icon bar with the large buttons for fast access and select the icon bar position The position of the icon bar can also be changed by dragging it with the mouse, but the setting is not saved until the next program start.
Hide event windows	Hide the event window (e.g., **Delay time**) The messages are instead shown in the status bar of the main window.
Hide results windows automatically	Results windows are hidden if sub-windows (e.g., **Method** window) are opened. After closing the sub-windows the results windows are displayed again.

Option	Description
Display tooltips	Displays brief help texts (tool tips) with mouse-over on all icon buttons and for the column headers in the **Method**, **Sequence** and **Sample ID** windows.
Colors	The ... button opens the color selection dialog. There, you may choose predefined or newly defined colors as list background.
Use PrtScr key for hardcopy function (instead of F5)	By default, the printout of the screenshot is started with F5. In this case, the **Print** key on the keyboard is used for the Windows clipboard function. If this checkbox is enabled, the **Print** button starts the printout of the screenshot. This option only becomes active after restarting ASpect PQ.
Allow screensaver	If enabled, the Windows screensaver activates during input pauses.
Ask for results report type (compact or complete) when printing	When printing results windows via the **File** | **Print** | **Active Window** menu item it is possible to 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. These paths are displayed in the **Options** | **Folder** window and can be partially edited here.

Folder	Description
Program	Installation path of the executable program files
Work directory	Directory for user data The work folder contains further subfolders. It is defined during installation or by the optional user management.
Temporary data	Directory for temporary application files.
Sample Information	Default path for opening and saving sample information files This path may be changed. Click ... to select the new folder. When opening and saving the sample information data a deviating path can be selected.
Export/Import	Default path for exporting and importing method and sequence data and exporting results data as CSV files This path may be changed. Click ... to select the new folder. During export and import a different path can also be selected.
Results	Folder for results files This default folder may contain additional subfolders for result storage. These folders are available for saving results files at the start of measurements.
Application data	Directory for data in which ASpect PQ stores necessary data

11.3 Export options

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.

Configuration

Option	Description
Decimal separator	Defines the separator for decimal numbers
List separator	Defines the character separating the individual elements of a list

For exporting the results lists select the **Decimal separator** and the **List separator.**

In the **Results fields for export** field, you may define which columns of the result table are exported to the ASCII file. The **all** option exports all columns of the results list (with all sub tabs). The **only selected fields** option opens a list in which the columns to be exported can be selected.

See also

Saving results in ASCII/CSV format [▶ 129]

11.4 Options for continuous ASCII export

In the **Options** | **Continuous ASCII export** window the automatic export of results data during the analysis sequence is enabled. 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.

Export of results data

The **Continuous ASCII export of results data** checkbox activates the export function. Next an option for the file name must be selected:

Option	Description
Method name.csv	The file name corresponds to the name of the method. The file name extension is ".csv". The file is saved to the default export/import path (**Options** | **Folder** window).
Results file name.csv	The file name corresponds to the name of the results file. The file name extension is ".csv". The file is saved to the default export/import path (**Options** | **Folder** window).
other	You may freely define file name and save path. The **...** button opens the **Save as** default window to issue a storage path and a file name. The data will be continuously written to this file until a new name is given or another naming option is selected.
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. Impermissible characters are replaced by underscores (e.g., Testmethod-001 QC 1 mg_L.csv).

Spectral export

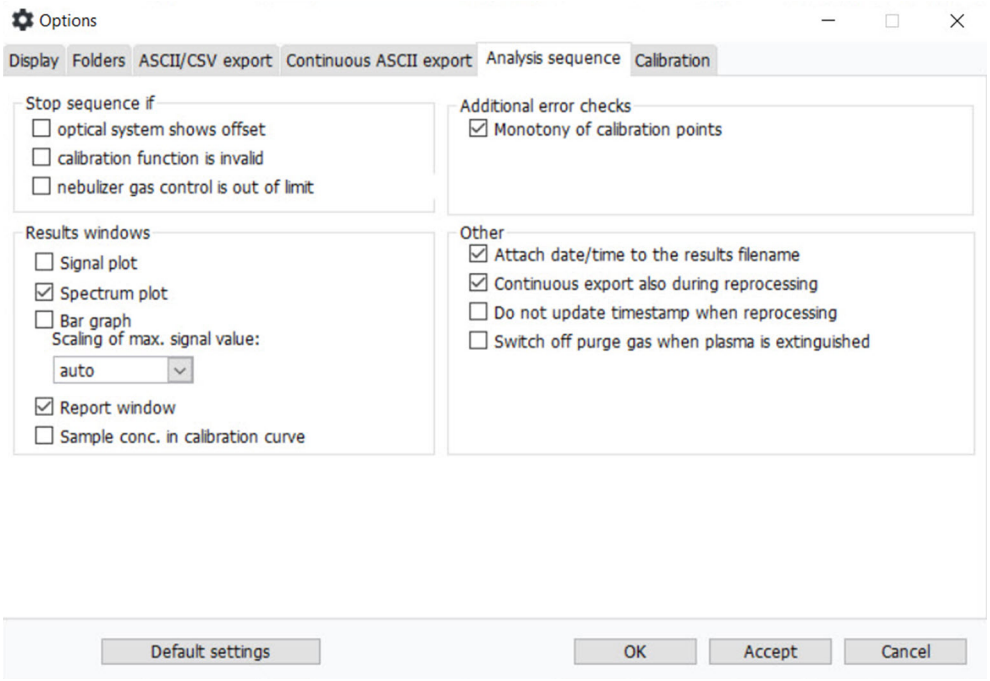
For the spectrum export, enable the **Continuous export of spectra (CSV)** option and select a storage path.

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-AI309-02.csv.

11.5 Options for analysis sequence

In the **Options** | **Analysis sequence** window you can define general options for the analysis sequence. Screenshot

Options | Analysis sequence window



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
optical system shows offset	Stops if the wavelength configuration (Ne correction) is faulty
calibration function is invalid	Stops if the calibration function could not be calculated
nebulizer gas control is out of limit	Stops when the nebulizer control value is exceeded During calibration, the nebulizer flow control value is determined. If the control value changes during subsequent analysis, this is an indication that particles are clogging the nebulizer.

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.

Results displays

Option	Description
Signal Plot	A window is displayed during the analysis sequence showing a graph of the measured signal as a function of time.
Spectrum Plot	A window is displayed during the analysis sequence showing a graph of the recorded spectral range.
Bar graph	Displays measured intensities as a bar graph
Scaling of max. signal value	Defines the maximum of the measurement value axis for the presentation of the signal curve **auto**: Automatic axis scaling. Alternatively, this setting can also be made using the **View** | **Scaling** menu function.
Report window	A window is displayed during the analysis sequence showing status information about the plasma.
Sample conc. in calibration curve	Displays the **Sample conc. in calibration curve** window with the current calibration curve and, if already measured, the recalibration curve. After the measurement of the sample, the calculation of the uncorrected concentration from the emission is highlighted by red auxiliary lines. If addition calibration is used, the converted calibration curve will be displayed.

Miscellaneous

Option	Description
Attach date/time to the results filename	Current PC/time at the start of measurement is automatically appended to the name of the result file.
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.
Switch off purge gas when plasma is extinguished	To save gas the purging gas is switched off if the plasma is extinguished.

See also

- Calibration [▶ 90]
- Entering calibration parameters (Method | Calibration window) [▶ 39]

11.6 General settings for calibration and blank correction

In the **Options** | **Analysis sequence** window you can make basic settings for the calibration and select a blank correction procedure.

Calibration

In this group you configure basic settings for the calibration. All checkboxes are disabled as default.

Option	Description
Correlation coefficient	Select the ratio for the calibration curve's goodness of fit **R**: Correlation coefficient **R^2 !**: Coefficient of determination **R^2(adj.)**: Adjusted coefficient of determination

Option	Description
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 rational function.
Compute slope for mean concentration instead of 0	If enabled the slope of the calibration curve 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) does 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 pre-dilution:

- 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, enable the **Blank correction based on Conc1** option.

Limits of detection (LOD) and limits of quantitation (LOQ)

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 used 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 factors and measurement repetitions, click on **LOD and BG**. The following default settings are provided:

Parameters	Value
Factor LOD	3
FactorLOQ	9
Replicates	11

12 Setting up data exchange with an external job management system

You can export measurement results in ASCII/CSV format from ASpect PQ to a laboratory information management system (LIMS) or another external program via a data interface.

In addition, you can import sample information data (sample ID) in ASCII/CSV format from external programs such as LIMS or Microsoft Office applications.

12.1 Exporting measurement results

You can export measurement results both automatically and manually in ASCII/CSV text formats for further processing in other applications such as a LIMS.

Defining export options

- Open the **Options** window using the **Extras** | **Options** menu item.
- On the **Folder** tab under **Export/Import** define the storage path for exporting results data.
- On the **ASCII/CSV export** tab define the separators:
  - **Decimal separator**: Select the separator for decimal numbers.
  - **List separator**: Select the character that separates the elements of a list.
- Define the fields for the results export:
  - **all**: Export all columns of the results list, with all sub tabs.
  - **only selected fields**: Click on ... to open a list where you can select the columns to be exported.
- Accept the export settings by clicking on the **Accept** button.
  - ✓ You have defined the export options. The settings apply to automatic and manual export.

Configuring automatic export

Configure the automatic export of results data during the analysis sequence. The software updates the export file immediately after the output of a new row in the process and results window. The software appends the new data to the existing export file.

- In the **Options** window go to the **Continuous ASCII export** tab.
- Enable the **Continuous ASCII export of results data** checkbox.
- Define the file name for the export file:
  - **Method name.csv**: The file name corresponds to the name of the method, with the file extension ".csv".
  - **Results file name.csv**: The file name corresponds to the name of the results file, with the file extension ".csv".
  - **other**: Click on the ... button to open the **Save as** default window. Issue a storage path and file name.
  - ✓ The software will continuously write the data to the file until you give a new name or select another file naming option.
- Enable the **Create separate file for each sample (result row number and sample name is appended to filename)** checkbox if you want to create a file for each sample.

✓ The software adds the row number of the results list and the sample name to the file name. Impermissible characters are replaced by underscores (e.g., Test-method-001 QC 1 mg_L.csv).

- Enable the **Continuous export of spectra (CSV)** checkbox if you also want to automatically export spectra. Under **Export path** select the storage path.
- Accept the export settings by clicking on the **Accept** button.
- Change to the **Analysis sequence** tab.
- Enable the **Continuous export also during reprocessing** checkbox if you want to automatically export results even after reprocessing.
- Close the window by clicking on **OK**.

  ✓ You have configured automatic data export.

Exporting results manually

Alternatively, you can export measurement results manually.

- Change to the **Results** tab in the main window.
- Select the samples in the results list.
  Hold down the Ctrl or Shift key and select the data to be exported by clicking on the respective sample row.
  Select all sample rows using the **Edit** | **Select All** menu item.
- Select the **Edit** | **Save Selection** menu item.
- In the **Save as** default window enter a file name. Confirm your entry by clicking on **OK**.

  ✓ The software exports the results in ASCII/CSV format with the file extension ".csv".
- If you select the **Edit** | **Copy visible Columns only** or **Copy all Columns** menu item the software copies the data to the clipboard. You can transfer the data to an open Excel file using the Ctrl+V key combination.

Data format

The software separates the entries in the text file using the specified list separator. Each line ends with a newline character (CR/LF).

- The export file begins with header data containing information about the device, the software version used, and the date and time the file was created.
- The date is formatted according to the setting in the Windows Control Panel. The (short) date format is used.
- A blank line is followed by the list of fields to be exported.
- The header data is generated only once. The header data is followed by the measured values.

Example of an export file:

```
Instrument: PQ 9200 #10587200262BB0101 Tech: ICP-OES
SW-Version: ASpect PQ 1.3.2.2007 Created: 29.10.2024 14:04

Nr.;Name;Linie;Typ;Einheit;Konz.1;SD1;RSD%;VB;VF;Einheit;
Konz.2;SD2;RSD%;VB;100%
norm.;QC;QC;QC;Bem.;Ints.;SD(Ints.);RSD%;Datum;Zeit;
Norm.Ints.;SD;RSD%;Masse;Einh.;Feuchte[%];RHF[%];Einw.[mg];
Fehler;Pos;Vor-VF;Einw. [g];Vol. [mL];Ges.einw.
[g];Name(2);AS-VF;BW-
Korr.;Faktor;Einzelwerte(Ints.);;;Untergrund(Ints.);
    1;Sample1;Co237.863;0;µg/L;1968;47.49;
2.41;215.9;1;mg/L;1.968;0.0475;  2.41;0.2159;;;;;>
KAL;257059;6194;  2.41;29.10.2024;14:04;;;;;;;;;101;
1.000;;;;;    1;aus;
0.00;256411;251214;263551;20389;9786;27849;
    2;Sample1;Ni231.604;0;µg/L;1537;62.95;
4.10;93.89;1;mg/L;1.537;0.0630;
4.10;0.0939;;;;;;254729;10328;
4.05;29.10.2024;14:04;;;;;;;;;101;     1.000;;;;;    1;aus;
0.00;246002;252054;266131;4598;16546;33369;
    3;Sample2;Co237.863;0;µg/L;2289;17.01;
0.74;254.0;1;mg/L;2.289;0.0170;  0.74;0.2540;;;;;>
KAL;298914;2219;  0.74;29.10.2024;14:04;;;;;;;;;102;
1.000;;;;;    1;aus;
0.00;300902;299321;296520;27198;27379;28180;
    4;Sample2;Ni231.604;0;µg/L;1755;20.57;
1.17;108.4;1;mg/L;1.755;0.0206;  1.17;0.1084;;;;;>
KAL;290377;3374;  1.16;29.10.2024;14:04;;;;;;;;;102;
1.000;;;;;    1;aus;
0.00;294115;287557;289459;26485;9243;18241;
```

Fig. 1 CSV Export

12.2 Importing sample information files

You can generate sample information files (sample ID) in ASCII/CSV format using a LIMS or Microsoft Office applications and import them manually.

For a successful import, make sure that each line in the sample information file ends with a newline character (CR/LF).

Example of a valid sample information file:

```
Sample1;101;1.000000;mg/L;0.001;0;;100.000000;ID154-21;
1.000000;0;-1.000000;0.000000;alle
Sample2;102;1.000000;mg/kg(liq);0.001;2;5.6;100.000000;
ID154-22;5.000000;0;-1.000000;0.000000;Co
```

Fig. 2 CSV Import

Importing a sample ID manually

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

12.3 Results export fields

Field name	Description	Data type
No.	Number in the sequence list	Integer
Name	Name of the sample, standard or QC sample/standard	String, max. 20 characters

Field name	Description	Data type
Line	Element line	String, max. 10 characters
Type	Analyte or internal standard 0 = Analyte IS1 ... x = Internal standard	Integer
Unit1	Unit of concentration 1 (concentration of the analysis sample)	String, max. 10 characters
Conc.1	Concentration of the analyte in the sample/standard	Decimal number
SD1	Standard deviation of the conc. 1 (mean value statistics)	Decimal number
RSD%	Relative standard deviation of the conc. 1 (mean value statistics)	Decimal number
Cf	Confidence interval of Conc. 1	Decimal number
DF	Dilution factor for automatic dilution of the sample (taken into account for conc. calculation)	Decimal number
Unit2	Unit of concentration 2 (concentration of the original sample)	String, max. 10 characters
Conc.2	Concentration of the original sample	Decimal number
SD2	Standard deviation of the conc. 2 (mean value statistics)	Decimal number
RSD%	Relative standard deviation of the conc. 2 (mean value statistics)	Decimal number
Cf	Confidence interval of Conc. 2	Decimal number
100% norm.	Conc. 2 normalized to the percentage of the total concentration	Decimal number
QC	QC and calibration information	String, max. 30 characters
QC	QC and calibration information	String, max. 30 characters
QC	QC and calibration information	String, max. 30 characters
Rem.	Comments	String, max. 40 characters
Ints.	Mean value of the measured individual intensities	Decimal number
SD (Ints.)	Standard deviation (mean value statistics)	Decimal number
RSD%	Relative standard deviation (mean value statistics)	Decimal number
Date	Date of measurement	Windows setting for short date format, e.g., 2024-01-30
Time	Time of measurement	hh:mm, e.g., 14:29
Norm.Ints.	(not used in ASpect PQ)	/
SD	(not used in ASpect PQ)	/
RSD%	(not used in ASpect PQ)	/
Mass	(not used in ASpect PQ)	/
Unit	(not used in ASpect PQ)	/
Hum.[%]	(not used in ASpect PQ)	/
RHF[%]	(not used in ASpect PQ)	/
Wt. [mg]	(not used in ASpect PQ)	/

Field name	Description	Data type
Error	Error message if an error occurred during measurement	String
Pos	Position of sample on autosampler	Integer
Pre-DF	Pre-dilution factor. Factor by which the original sample was diluted before being placed on the autosampler or supplied to the spectrometer, if no autosampler is used. The factor is required for the calculation of the concentration of the original sample (**Conc. 2**).	Decimal number
Wt. [mg]	Initial weight in milligrams. The mass of the original sample which was dissolved in sample preparation (used in the calculation of conc. 2)	Decimal number
Vol. [mL]	Volume of solvent used to dilute the weighed sample portion in mL (used in the calculation of conc. 2)	Integer
Total wt. [g]	Total weighed portion of the sample and diluent in grams	Decimal number
Name(2)	Additional sample name	String, max. 20 characters
AS-DF	Dilution factor of the autosampler or dilution system	Decimal number
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.	0 | 1
Factor	(not used in ASpect PQ)	/
Single values(Ints.)	Individual values of the intensity measurements	String of decimal numbers separated by spaces, max. 1000 characters
Background(Ints.)	Background intensity at the element line	String of decimal numbers separated by spaces, max. 1000 characters

12.4 Fields of the sample information files

Field name	Description	Data type
Pos	Position of sample on autosampler	Integer
Name	Name of the sample, standard or QC sample/standard	String, max. 20 characters
Pre-DF	Pre-dilution factor. Factor by which the original sample was diluted before being placed on the autosampler or supplied to the spectrometer, if no autosampler is used. The	Decimal number

Field name	Description	Data type
	factor is required for the calculation of the concentration of the original sample (**Conc. 2**).	
Unit	Concentration unit of sample.	String, max. 10 characters
Factor	Unit factor Factor 1 corresponds to 1 µg/L or µg/kg, factor 1000 corresponds to 1 ng/L or ng/kg	String, max. 10 characters
Type	Unit type 0 = liquid 1 = solid 2 = liquid gravimetric	Integer
Wt. [mg]	Initial weight in milligrams. The mass of the original sample which was dissolved in sample preparation (used in the calculation of conc. 2)	Decimal number
Vol. [mL]	Volume of solvent used to dilute the weighed sample portion in mL (used in the calculation of conc. 2)	Integer
Total wt. [g]	Total weighed portion of the sample and diluent in grams	Decimal number
Name(2)	Additional sample name	String, max. 20 characters
AS-DF	Dilution factor of the autosampler or dilution system	Decimal number
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.	0 | 1
Sample type	Sample or blank 0 = sample 1 = reagent - blank	Integer
Elements	Elements or lines to be analyzed in the sample all = all elements of the method Element symbols separated by commas, e.g., Fe, Co, Ni	String, max. 10 characters

13 Optional FDA 21 CFR Part 11 Compliance module

The optional FDA 21 CFR Part 11 Compliance module for ASpect PQ 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

By default, 6 user levels are created in the user management. The user levels can be freely configured and supplemented with additional user levels.

If user management is installed and configured, the **System** menu item in ASpect PQ 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.

13.1 User management

13.1.1 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.

- In ASpect PQ, open the menu item **System** | **User Management**.
- Alternatively, you can open the user management outside of ASpect PQ via the Windows menu **ASpect PQ** | **User Management**.
- Enter the login data of a user with user management authorizations.
  - ✓ 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.

Details of the user profile

The following data is displayed for a user selected in the list:

Option	Description
User ID	Login name of user
User level	Assigned user level with user rights
Full name	Full name of user
E-signature	**Yes**: User is authorized to electronically sign results data. **No**: User has no authorization for electronic signature.
Status	**Active**: User name allowed for use (green circle). **Disabled**: User name is disabled and cannot be used (red circle).

Option	Description
Passwd. protect.	**Active**: User login requires a password. **Not active**: User login is possible without a password. Click on the padlock icon to open the **Modify user data** window. When the padlock is closed, password protection is activated.
Valid until:	**Indefinitely**: Password never expires. **Date/days**: User must change his/her password on expiry of specified term. The option is not displayed when logging in via Active Directory.

Buttons

Button	Description
New ...	Creating a new user The **Add user data** window appears.
Modify ...	Change user data for selected table row The **Modify user data** window appears for a selected user. The window can also be opened by double-clicking on the user.
Active users only	Show only active users
Audit trail	Open event report
Permissions	Assign user authorizations in the software
Exit	Exit the application

13.1.2 Configuring user levels

As of FDA 21 CFR Part 11 compliance module version 2.0, the user management has a new feature for setting up the user levels. While the available authorizations of user levels were fixed in previous versions of the software, you can now freely configure the user levels. In a list of software functions, activate or deactivate the functions that are to be accessible for a user level.

Number of available user levels

By default, 6 user levels are created in the user management. The user levels can be freely configured and supplemented with additional user levels.

- Administrator level (level 0)
  The administrator has full rights for user management and can configure user management, configure rights in the user levels, and create or block users. By default, the administrator has no authorization for ASpect PQ and cannot log in to the software.
- Level 1
  Users at this level have all authorizations for ASpect PQ for method development and routine and can configure the software.
- Level 2 to 4
  Users at these levels have graduated authorizations for analysis operation, whereby the following applies: Level 2 > Level 3 > Level 4. They do not have authorization to configure ASpect PQ.
- User level 5
  Users at this level have authorizations for logging into user management and ASpect PQ minimal authorizations, e.g., for auditing purposes.

Optionally, up to 4 further levels (6 to 9) can be created for special configurations.

Configuring user levels

▶ In the **User Management** window, click on **Permissions**.
  ✓ The **Change user permissions** window appears.

- In the Authorization/Levels matrix, you can enable a function in a level by ticking the checkboxes.
  If you right-click on a checkbox, you can use the context menu to set or remove all checkmarks in the level or apply the authorizations of another level.
- If you want to add additional layers to the matrix, click on **Configure**. Enable the **Additional user levels (max.4):** option and set the desired number in the list.
- If you want to reset the rights assignment to the default settings, click on **Configure**. Enable the **Reset permissions and levels to default** option. If additional user levels have already been assigned to users, you will be prompted to change the corresponding user profile.
- Each function authorization is assigned an ID. If a user wants to carry out an action for which they do not have authorization, this ID is displayed in the warning/error message. You can use the ID to clearly identify the missing authorization. If needed, activate the **Show column "ID"** option.

Notes on user rights

Individual user rights are linked to the general settings in the user management. You can access these settings in the **User Management** window via the **Extras** | **Preferences** menu item.

Permission	Description
Skip calibration interval (ME003)	In the user management settings, you can optionally define a validity period for the calibration. If you have activated this time period and the user does not have this permission, they cannot start a measurement.
Measurement with unreleased methods (categories) (ME004)	You can assign the **Cat.** (category) characteristic to the methods when saving and thus identify methods for use. In user management, you can specify up to 5 names for categories for which methods are marked as approved. If users have this permission, they can start a measurement with a non-approved method.

Information about the update

If you have already set up user management, the new user levels Admin and Level 1 to Level 4 are assigned to the users. Check whether the set authorizations meet your requirements and change the permissions in the levels. Pay particular attention to the fact that in the new installation, the administrator only has access to user management by default and no longer has permissions to use ASpect PQ.

13.1.3 Configure general settings of the user management

In the **Preferences** window, you can configure the user management in general with the following options:

- Registration and guidelines for the password
- Use of data directories
- Settings for the use of calibrations and methods
- Signatures

The settings apply to newly created user accounts and should therefore be made after installation, before user accounts are created.

- In the **ASpect PQ User Management** window, select the **Extras** | **Settings...** menu item.
  The **Preferences** window is displayed.
- Select the action group to be changed on the left-hand side.

- Perform the configuration.
  Click **Default settings** to restore the default settings for the selected action group.
  The settings of the other groups remain unaffected.
- Click on **OK** to apply the settings.

User access

You can configure the login locally via the user management or via a login server via Active Directory.

For local login, select the **Local (with user management)** option on the **User access** page and configure the general guidelines for new logins and passwords:

Option	Description
Number of login attempts:	Shows the number of invalid login attempts (max. 10). If this is exceeded, ASpect PQ 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	Block the user after exceeding the number of login attempts
Minium user name length:	Minimum number of characters for newly created user names (max. 10)
Enforce login with password	A password must be assigned to newly created user names.
Password with letters and numbers:	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 (max. 999 days). This value is then acknowledged as the default.
Minium password length:	Minimum number of characters for newly created passwords Number of characters: 3 to 10

For server-based login, enable the **Server-based (with Active Directory)** option and configure the following:

Option	Description
Domain name(s)	Domain name of the login server You can specify two servers.
Allow local login if login server not reached	If logging on via the server fails, users with the appropriate rights can log on locally in the user management via the Windows Start menu. Users must also be assigned a local password for this purpose. In the user management, authorized users can activate the **Local (with user management)** option so that it is possible to log in to ASpect PQ locally.
Allow local login for AJService account	Activating this option enables AJ Service personnel to carry out maintenance on the device without additional support from the administrator.

Folders

The working directory of the control and evaluation software and the directory for the audit trail file can be specified.

Option	Description
ASpect working directory	Setting the working directory The working directory contains a database of methods and sequences and the results files. The working directory was defined during the installation of ASpect PQ and can be changed here.
Audit trail	Setting the path of the audit trail file This path may be changed.
Folder with user database	Display of the user database path This path may only be changed with the help of 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.

Permissions (Details)

In this group, general settings for methods and calibrations are made that affect the authorizations in the user levels.

Option	Description
Calibration validity period [h:mm]:	Optionally specify the validity period of the calibration If the **Skip calibration interval** authorization is deactivated for a user (see User levels), the user cannot start a sequence after the validity period has expired. If the **Skip calibration interval** authorization is activated, the user can start the sequence. A message is displayed indicating that the validity period of the calibration has expired.
Method categories for released methods	You can enter up to 5 categories here to identify the methods as approved. You enter the categories in the **Cat.** field when saving the method. If the **Measurement with unreleased methods (categories)** authorization is deactivated for a user, this user cannot start a sequence if the associated method is not marked with one of the specified categories.

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

13.1.4 Creating a new user account

Only users with corresponding user rights are authorized to create a new user account. The rights for user management are assigned to the Admin level in the default settings for the user levels. 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 user This name will serve as a constituent 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 a password Capital lettering and small lettering are distinguished for passwords. 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 icon	**Closed**: Password protection is activated by assigning a password. **Open**: Password protection has not yet been activated.
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. This setting is hidden when logging in via the login server and Active Directory.
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 signature meanings of their user level are available.
Disable user ID	Deactivate the user account User names can be temporarily disabled. Disabling a user account 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 PQ User Management** window.

See also

Configure general settings of the user management [▶ 148]

13.1.5 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 [▶ 151]

13.2 Changing a password

This function is only available for local login to ASpect PQ or user management. When logging in via a login server, the passwords and their validity are managed there.

Depending on the specification in the user account, the user must change the assigned password at regular intervals when logging in locally.

- In **ASpect PQ**, select the **System** | **Change password** menu item. 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 was changed** message appears.

13.3 Viewing, printing and exporting the audit trail

The audit trail file records system events as well as all warning and error messages from ASpect PQ and user management. To view the audit trail, permissions must be granted in the user account.

You can open the audit trail in ASpect PQ 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
- Filter
- Refresh
- Print
- 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	Indicates the type of an event An audit trail keeps track of the following types of events and marks these with symbols: Info, Warning, Error, Login and Logout

Table column	Description
Date/Time	Date and time of the event (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 event is referenced (Windows system control)
User	Designates the user in login state at the moment of an event.
Source	Differentiation according to events in the user management or in ASpect PQ
Description	Detailed information on the selected event

Selecting a view

If you have opened the audit trail in the **User Management** window, you will see the events in both ASpect PQ and the user management. In the View list, you can restrict the display to events in ASpect PQ or administrative events.

If you have opened the audit trail in ASpect PQ with the menu item **System | Audit Trail**, only events in ASpect PQ are displayed.

Filtering the audit trail

By clicking on **Filter** you can search for registered users, entry types or time periods. You can also limit the search to actions relating to methods, sequences, results or worksheets. Click on **Deactivate filter** to remove the restrictions of the set filter.

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.

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 will open.
- Select the printout format from the **Direct to** list.
- Start printing by clicking on **Start**.
  ✓ The audit trail is output in the selected output format.

Exporting the audit trail

You can export the audit trail entries to a CSV file. The export function is only available if the audit trail has been opened in the user management. If the filter is activated, only the filtered entries are exported.

- 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.

13.4 Electronic signatures

Results data can be signed electronically in ASpect PQ. 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 and their assignment to an authorization level are created in the general settings of the user management. The setting that a user can sign a document is configured in the user account. A user can therefore sign a document if this function has been activated in their user account and if signatures are provided for their authorization level.

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.

See also

- Configure general settings of the user management [▶ 148]
- Configuring user levels [▶ 147]

13.4.1 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 may be changed. This makes signing by other users possible.
Password	Password of the user
Meaning	The meaning of signatures 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 **System** | **Sign off results** menu item.
- Enter user name and password.
- Select signature meaning.
- Click **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

- Creating a new user account [▶ 151]
- Configure general settings of the user management [▶ 148]

13.4.2 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

Option	Description
Status	The signature state may take on one of the following meanings: **Valid** Signature and results data are complete and correct. Calculated check sums of a file reveal no variance against the check sums contained in the signature file at the moment of signing. **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. **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

13.5 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 data medium.

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.

14 Annex

14.1 Overview of markings used in the display of values

Comment	Meaning	Values	Edition
> Cal	The mean value is larger than the working range of the calibration curve.	Mean values	Process and results window
< Cal	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** | **Analysis sequence** window) of the calibration curve falls below the specified value	Calibration curve	Process and results window Autosampler adjustment window **Calibration**
#MAN.	Sample single value or standard single value was manually excluded from the calculation of the sample means	Sample single values	Autosampler adjustment window **Sample single values**
#KOR.	Sample single value or standard single value was automatically excluded from the calculation of the sample means by Grubbs outlier test	Sample single values	Autosampler adjustment window **Sample single values**