

Operating Manual

ASpect LS Software for AAS



Manufacturer

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

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1 Software ASpect LS

ASpect LS is the control and analysis for the novAA and ZEEnit type atomic absorption spectrometers from Analytik Jena AG.

The following accessories are supported:

- Autosampler AS-F/AS-FD and AS 51s/AS 52s for flame technique
- Autosampler AS-GF and MPE 60 for graphite furnace technique
- Hydride systems HS60 modular and HS 55 modular
- Hydride systems HS60 / HS60A, HS55 / HS55A and hydride injector HS50 (hydride/Hg cold vapor technique)
- SFS 6 Injection Switch (flame technique)
- SSA 600 solid autosampler with or without liquid dosing

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

Software version described This document is based on the version ASpect LS 1.8.

Intended useASpect LS software exclusively serves to control the above mentioned atomic absorptionspectrometer types 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 LS.

ASpect LS and the devices 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 Starting ASpect LS

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

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

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

1.1.1 Quick Start window

After the software has been started and a user logged in (only if user administration is installed), the **Quick Start** window appears. After selecting the technique used, you can load a worksheet or switch to ASpect LS without any further default settings. You can also open the window from ASpect LS using the **File** | **Quick Start** command.

QUICK START 03.01.20	24 13:55:48										
Instrument ZEEni	t 700P	ASpe	ctLS Version: 1.7.0.0 analytik je								
OPERATOR: LAB.: TECHNIQUE:	SuStein TechCom Flame										
Worksheet		Last changed	Ву	DESCRIPTION							
Cu in aqueous so	olution	03.04.2020 14:56	Analytik Jena	Sample preparation:							
Mg in aqueous s	olution	03.04.2020 14:56	Analytik Jena	Measurement details: Flame: C2H2/air							
Na-Emission in a	queous solution	03.04.2020 15:18	Analytik Jena	Bumer: 50 mm Oxidant (aux.): off							
Zn in aqueous so	olution	03.04.2020 14:56	Analytik Jena	Calibration range: 0 - 2.5 mg/L							
				v							
Favorites Rece	ent Predefined All		, O all (4)	System check							
Simulation											
			Skip Quick Start	Exit OK							

window

_

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Configuration in the Quick Start 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 man- agement 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.
Technique	You can select different techniques depending on the configura- tion of the AAS device.
	Graphite furnace (Wall) Electrothermal atomization (EA) in the standard graphite tube The sample is in liquid form. Atomization of sample matter oc- curs at the wall of the graphite tube.
	Graphite furnace (Platform) Electrothermal atomization (EA) in a graphite tube with platform The sample is in liquid form. Atomization of the sample occurs on the platform of the graphite tube.
	Flame Atomization with burner/nebulizer system
	Hydride Determination of hydride-forming metals and mercury in a quartz cell, if necessary in combination with mercury enrichment.
	HydrEA Determination of hydride-forming metals and mercury with en- richment in the coated graphite tube
	Graphite furnace solid Electrothermal atomization (EA) in a graphite tube for solids The samples are transferred to the graphite tube on sample plat- forms using a solids autosampler (SSA 600 or SSA 6z).
Simulation	For trainings and demonstration purposes, you may operate AS- pect LS without an AAS device being connected.
	When enabled, all device functions (including data acquisition and analysis) are run in simulation mode.

Option/ button	Description					
System check	Establish connection between AAS device and PC (software)					
	Click this button to detect the spectrometer and accessories and configure them according to the selected atomization technique. For devices with lamp coding, the system checks which hollow cathode lamps (HCL) and super hollow cathode lamps (SHCL) are used in the lamp turret.					
Skip Quick Start	Switch to ASpect LS interface without selecting a worksheet					
Exit	Close the Quick Start window and exit Aspect LS					
ОК	Switch to ASpect LS interface after selecting a worksheet					

Worksheet table

The worksheet table shows the currently available worksheets that match the selected technique. The four tabs make it easier for you to find a worksheet:

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

1.1.2 Starting with a worksheet

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

- Install the accessories intended for the technique on the AAS device and then switch on the accessories and the AAS device.
- Start the software.
 - ✓ The **Quick Start** window appears.
- Select the atomization technique from the **Technique** list.
- Click on System check.
 - ✓ The device and accessories are initialized and connected to the PC/software. The device configuration is displayed in the field above. The system also checks whether the installed accessories match the selected technique.
- Enter the necessary details in the **Operator** and **Lab.** fields.
- Select the required worksheet in the worksheet table.
- Click on **OK**.
 - ✓ The ASpect LS 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.

See also

☐ Quick Start window [▶ 7]

1.1.3 Starting without a worksheet

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

- Install the accessories intended for the technique on the AAS device and then switch on the accessories and the AAS device.
- Start the software.
 - ✓ The **Quick Start** appears.
- Select the atomization technique from the **Technique** list.
- Click on System check.
 - ✓ The device and accessories are initialized and connected to the PC/software. The device configuration is displayed in the field above. The system also checks whether the installed accessories match the selected technique.
- Enter the necessary details in the **Operator** and **Lab.** fields.
- Click on Skip Quick Start.
 - ✓ The ASpect LS program 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 Lamps Lamps with an RFID chip are automatically detected in some device models and made available in the software.
- Specify the **Method parameters** (method development).
- Setting up a Sequence. The sequence specifies samples and actions in the intended order of execution. Some sample describing data, such as the name of the sample and its position on the sample tray may also be entered directly and are saved with the sequence.
- For routine analysis it is useful to create a sample information file. This file contains sample describing data such as sample name, dilution factor and sample tray positions. These data are needed if the concentrations are to be back-calculated to the original sample. Sample information files are text files; therefore, they can also 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 (export, print, etc.).

After the start of the **measurement** the result data are entered continuously in the main window. Detailed result presentation (individual values, signal curves) is accessible by selection of the corresponding table cell. The results obtained last are always appended to the end of the table; overwriting of results is not possible.

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

1.1.4 Lamp turret, mounting

- Open the window **Spectrometer** | **Control** by clicking on Δ in the toolbar.
- Click on Lamp turret to open that window.

The window **Lamp turret** shows the current stocking of the 6 lamp or 8 lamp turret. For devices with a lamp coding unit the stocking of the lamp turret for lamps with RFID chip is established automatically on initialization.

For devices with 8 lamp turret, super hollow cathode lamps (S-HCL) can be used on positions 5 to 8. For devices with a 6 lamp turret, only lamp position 6 can be fitted with an S-HCL if it is equipped with the necessary power supply. Super hollow cathode lamps cannot be used in the ZEEnit 700 Q.

	Lamp	turret								×	
M	ounting	J Lamp his	story	Code lamps							
	Pos	Туре	cod.	Elements	Max. curr. [mA]	Max. Boost [mA]	Recmd. curr. [mA]	Recmd. b [mA]	oos	Aliç adj.	
	1	MHCL	-	Cr;Mn;Fe;Co;Ni;Cu;Zn	10.0		-				
	2	MHCL	-	Cd;Pb	10.0		-			*	
	3	HCL	-	Dy	10.0		-			*	
	4	MHCL	-	Na;K;Cr;Hg	10.0		-			*	
	5	HCL	-	Au	10.0	-	-		-		
	6	6 MHCL - Ca;Tl;Pb;Bi			10.0		-	*			
	7	MHCL	-	Rh	10.0	-	-		-	*	
	8	HCL	-	Mg	10.0	-	-		-	*	
	<									>	
	(Change		Register lamp	Unregiste	er lamp		Initiali	ze		
		Delete ta	ble	L	amp alignment	E	Energy				
	(change lan	ıp		Align	0					
									Close	9	

Table area

Column	Description
Pos	Position of the hollow cathode lamp in the lamp turret
Туре	Lamp type
cod.	Only appliances with coding unit
	If a coded lamp is stocked on the lamp position, then the entry receives a star ("*"). The lamp parameters are established automatically in this case and they cannot be changed manually.
Elements	The elements to be analyzed with this lamp
Max. curr.	Maximum possible lamp current
Max. Boost	Maximum possible boost current for S-HCL
Recmd. curr.	Recommended lamp current for coded lamps
Recmd. boost	Recommended boost current with coded S-HCL
Alignment / adj.	If marked with "*", the lamp was adjusted (see section "Adjusting The Lamps" below).
Alignment / Value	Adjusted value of the lamp, required for customer service

Buttons Buttons Description Change Change the parameters for the marked lamp position. This Select lamp/element window appears. Note for coded lamps: The lamp parameters of coded lamps are established automatically and cannot be changed. **Register** lamp Only appliances with coding unit Identify the lamp with the selected lamp position. For coded lamps the parameters are established and entered. **Unregister lamp** Delete all lamp parameters of the selected line. Initialize Move the lamp turret into the basic state. On initializing the lamp information is transferred to the program. Delete table Delete all positions without confirmation prompt. change lamp Switch off the currently selected lamp and move to the lamp change position in the lamp turret. The lamp can then be replaced once it has cooled down sufficiently. Lamp Adjustment For lamps the optical axis can differ from the mechanical axis. In the result the possible energy maximum does not come to the recipient. During the automatic adjustment the lamp turret is turned until the energy maximum is reached. Newly fitted lamps should thus always be adjusted. The adjustment of HCL and SHCL occurs automatically when you press the **Align** button. The adjustment value is permanently stored and the lamp is marked with "*" in the column **Alignment**/**adj**. The adjustment must only be repeated on replacing the lamp. Following changing of a deuterium hollow cathode lamp, this must also be adjusted in accordance with energy maximum. Adjustment is performed in the **Spectrometer** window. Selecting non-coded lamps Lamps are not coded on the ZEEnit 700 Q, novAA 400 and older device types. There is no feedback from the lamp turret to the PC. To avoid measurement errors, always load the lamp turret according to the positions entered. Specify the non-coded lamps in the lamp turret in the Select lamp/element window. Use the Δ icon to open the **Spectrometer** window and switch to the **Control** tab. Click on **Lamp turret** to open that window. Mark the position of the lamp turret in the table in which you place a lamp or whose ▶ placement you wish to change.

• Click on **Change** to open the **Select lamp/element** window.

İ	Sele	ct lar	np/e	leme	ent																			-	_		×
Lamp type HCL										~	Ma	ax. la	mp	curre	nt (m	IA]:		10.0	•	Max	Boos	t [mA]:		0.0			
		Li	Be											В	С	Ν	0	F	Ne		Dy	n. D	yspros	iva sium (E	Dy)		
		Na K	Mg Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Al Ga	Si Ge	P As	S Se	CI Br	Ar Kr								
		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te		Xe								
		Fr	Ra	La Ac		Та	VV	Re	Us		PI	Au	пg		PD	DI	PO	At	Rn								
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu										
				111	Га		мр	гu	AIII	UIII	DK		LS		IVIU	110	LI										
																			Ŷ								
																						(Ж		(Cancel	

• Enter the following values:

Value	Description
Lamp position	Show the position in the lamp turret
Lamp type	Select the lamp type
	The selection is based on the lamp position and the lamp types available at the position. S-HCL and S-MHCL are only available on the positions 5 to 8 for the 8 lamp turret and only on position 6 for the 6 lamp turret.
	none Position does not contain a lamp.
	HCL Single-element hollow cathode lamp
	MHCL Multi-element hollow cathode lamp
	S-HCL Single-element super hollow cathode lamp
	S-MHCL Multi-element super hollow cathode lamp
Max. lamp current	For setting the maximum lamp current
Max. Boost	Only for S-HCL and S-MHCL
	For setting the maximum boost current
Elements	Click the element symbol in the periodic table to select the lamp element:
	Blue buttons indicate selectable elements. Gray (inactive) but- tons indicate elements that cannot be analyzed with the AAS technique. Green element buttons define selected elements.
	For M-HCL and S-MHCL several elements can be selected. Click on the element symbol again to cancel the selection. Selected el- ements are shown in the adjacent table.

- Press OK to close the Select lamp/element window and return to the Lamp turret window.
 - \checkmark The lamp specification is entered into the table of the Lamp turret.

See also

- B Check lamp energy (novAA 400 P/ZEEnit) [▶ 107]
- B Check lamp energy (novAA 800) [▶ 109]

1.2 Closing ASpect LS and switching off the analyzer

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

- Select the menu item File | Exit.
- If, at this time, method, sequence or sample information data have not yet been saved, you will be prompted to save the data.
- Depending on the accessories installed and the atomization technique used, further notifications about software-based actions will be given:
 - Flame: Extinguish burning flame
 - Hydride system: Flush hydride system
 - ✓ After processing the actions, ASpect LS is closed. Switch off the analyzer at the mains switch.

1.3 General information on operation

1.3.1 The workspace

When you close Quick Start, the main window of ASpect LS opens with the settings for the atomization technique selected.

Bearbeiten	Aktionen Ansicht Methodene	ntwicklung Routin	e Syster	n Extras ? 2							
≊ × I	C Meth: Cr_prepro	grammed	¹ Sequ:	*Fl sequence prepro	Prober	unbenan	nt		6	3	3 analytikjen
Se	equenz/Ergebnisse Seque	nz Ergebnisse	Übersio	ht							
Ē	Nr. Typ / Name	Pos.	Nr.	Name	Linie	Ext/Ems	SD(Ext./Ems)	RSD%	Datum	Zeit	Einzelwerte(Ext./Ems
meter	1 Nullabgleich	1	1	AspectLS_SW-Tes	5 [.]			3	81.08.2010	11:36	
	2 KalNull1	1	2	Nullabgleich	Cu 324	0.00000		3	31.08.2010	11:37	
·	3 KalStd.1	4	3	KalNull1	Cu 324	-0.00566	0.00067	11.8 3	31.08.2010	11:37	-0.00613 -0.00518
ne	4 KalStd.2	4	4	AspectLS_SW-Tes	S'			3	31.08.2010	11:38	
	5 KalStd.3	4	5	Nullabgleich	Cu 324	0.00000		3	31.08.2010	11:39	
·. [6 KalStd.4	4	6	KalNull1	Cu 324	-0.00388	0.00032	8.2 3	31.08.2010	11:40	-0.00355 -0.00418 -0.0
de	7 KalStd.5	4	7	KalStd.1	Cu 324	0.02018	0.00078	3.9 3	31.08.2010	11:41	0.01931 0.02040 0.020
	8 KalStd.6	4	8	KalStd.1	Cu 324	0.01986	0.00052	2.6 3	31.08.2010	11:42	0.02022 0.01927 0.020
•	9 Kalib. berechnen		9	KalStd.2	Cu 324	0.05817	0.00064	1.1 3	81.08.2010	11:43	0.05759 0.05886 0.058
eber	10 Probe 001		10	KalStd.3	Cu 324	0.12305	0.00097	0.8 3	81.08.2010	11:44	0.12354 0.12366 0.12
	11 Probe 002		11	KalStd.4	Cu 324	0.24665	0.00225	0.9 3	31.08.2010	11:45	0.24406 0.24782 0.248
	12 Probe 003		5 12	Kalib. berechnen	Cu 324			3	81.08.2010	11:46	
-ID	13 Probe 004		13	Nullabgleich	Cu 324	0.00000		3	81.08.2010	11:46	
	14 Probe 005		14	KalNull1	Cu 324	-0.00075	0.00073	97.5 3	31.08.2010	11:47	0.00009 -0.00111 -0.0
	15 Probe 006		15	KalStd.1	Cu 324	0.02512	0.00058	2.3 3	31.08.2010	11:48	0.02564 0.02522 0.024
nz	16 Probe 007		16	KalStd.2	Cu 324	0.06388	0.00096	1.5 3	31.08.2010	11:49	0.06295 0.06382 0.064
r _	17 Probe 008		17	KalStd.3	Cu 324	0.12803	0.00024	0.2 3	31.08.2010	11:50	0.12778 0.12808 0.128
-	18 Probe 009		18	KalStd.4	Cu 324	0.15459	0.12101	78.3 3	31.08.2010	11:51	0.01789 0.19787 0.248
tion	19 Probe 010		19	KalStd.4	Cu 324	0.18408	0.08697	47.2 3	31.08.2010	11:53	0.08816 0.20629 0.25
	20 Probe 011		20	Kalib. berechnen	Cu 324			3	31.08.2010	11:53	
	21 Probe 012		21	Kalib. berechnen	Cu 324			<u>e</u>	31.08.2010	11:53	
	22 Probe 013		22	Kalibrierfunktionen				3	31.08.2010	11:53	
.	23 Probe 014		23	0.1ppm Cu	Cu 324	0.00333	0.00141	42.1 3	31.08.2010	11:54	0.00495 0.00264 0.002
	24 Probe 015		24	QC-Std.1	Cu 324	0.00841	0.00133	15.9 3	31.08.2010	11:55	0.00795 0.00737 0.009
n	25 Probe 016		25	QC-Std.1	Cu 324	0.00386	0.00061	15.9 3	31.08.2010	11:57	0.00315 0.00417 0.004
	26 Probe 017		26	QC-Std.4	Cu 324	0.15394	0.07848	51.03	31.08.2010	11:59	0.07625 0.15239 0.233
	27 Probe 018		27	QC-Std.4	Cu 324	0.23642	0.00292	1.2 3	31.08.2010	12:00	0.23305 0.23791 0.238
neet	28 Probe 019		28	Nullabgleich	Cu 324	0.00000		3	31.08.2010	12:01	
	29 Probe 020		29	AspectLS_SW-Tes	S			3	31.08.2010	12:03	
			30	Nullabgleich	Cu 324	0.00000		3	31.08.2010	12:04	
			31	QC-Std.4	Cu 324	0.07520	0.00052	0.73	81.08.2010	12:05	0.07522 0.07571 0.074
			32	QC-Std.4	Cu 324	0.08478	0.00097	1.1 3	31.08.2010	13:09	0.08529 0.08538 0.083
	<pre></pre>	>	< 1	Kloule is all to be	0 204	0 00000		h	1 00 0010	10.10	>
024			Ext./E	ms/Zeit Konz.1 Ko	onz.2 QC-Erg	g. Fehler	Einzelw. Prol	oen-ID E	Energie Eir	nst. Be	enutzerdefiniert

Elements on the workspace

No. Description The title bar provides information about the software version, the connected device, 1 the technique, and the worksheet (if loaded). The **menu bar** is used to access all program functions of the software. 2 3 The toolbar contains the buttons for starting and pausing measurement sequences, and displays the currently loaded method, sequence and sample ID file. Click the 📫 button behind the fields to load the data record. You will also find the buttons for opening the cookbook 🐻 and for creating a new worksheet 🛅 4 This icon toolbar gives you access to the most important windows (functions) of the software. When one of the windows is opened, the corresponding icon turns red. If several windows are open, clicking on the icon again brings that window to the front. 5 The main window shows the sequence and the measurement results. 6 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 [> 82]

1.3.2 Use help

You can get help on the operation of ASpect LS via the menu command **?**|**Help topics F1**. While working with Aspect LS windows and dialogs, you can activate context-sensitive help by pressing function key **F1**.

The program displays brief information (tooltips) about buttons on the toolbar and icon bar when you move the mouse pointer over them.

1.3.3 Overview of the menu bar, toolbar and icon bar

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

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

Toolbar

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

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

lcon bar

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

Button	Description
₫	Check spectrometer functions
5	Open flame window
\bigcirc	Open furnace window
Hy	Open Hydride system window
łtł	Open method window
围	Specify autosampler
Ū	Open sample information data window
	Open sequence window
R	Open window with calibration
00	Open window with quality control data
E	Open the data management

Button	Description
lì	Manage worksheets, open saved worksheets

1.3.4 Frequently used control elements

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

General buttons

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

Button	Description
ОК	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
•••	
ē	Open the Print window. From this window, you can print out the con- tents of the active document window or export it to a file.

Tables

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

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

In input fields, the following functions are additionally available:

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

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

Buttons accessible in tables

Button	Description
t≡	Moves the selected table row up by one position Note : A table row must be completely selected in order to move it. To do this, click on the number of the relevant row in the first column of the table.
t≡	Moves the selected table row down by one position
↓=	Transfers the value of the selected cell to all following table rows of the same sample type
	If the inc. (increment) checkbox is ticked this value will be incre-

If the **inc.** (increment) checkbox is ticked this value will be incremented automatically, e.g. Sample001, Sample002, etc.

Ì≡ Seq	uence					_	-		×
		_							
	Туре	Pos	Name	Name(2	Elements		Spe	ecifics	^
1	Autozero	43			all				
2	Cal-Zero1	43			all				
3	Cal-Std1	45			all				
4	Cal-Std2	46			all				
5	Cal-Std3	47			all				
6	Cal-Std4	48			all				
7	Compute calib.								
8	Sample	1	Sample 001		all				
9	Sample	2	Sample 002		all				
10	Sample	le 3 Sample 003 all							
11	Sample	4	Sample 004		all				
12	Sample	5	Sample 005		all				
< 10	00 i.u	**	00.011					>	
Rov	Row Samples t= t= Append Insert Delete Sequence<-QC sample ID								
 0	🗅 Open 🔁 Save 🖶 OK Accept Cancel								

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:

lcon	Description
Ð	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.
[Q]	Deactivates the zoom mode and resets the graph to the original scale
Т	Activates the text mode
1	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 but- ton to move existing text.
K	Activates the selection mode in signal or spectral plots
, ▲	Clicking the left mouse button adds labels to the measuring points.

Function keys

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

Using the printer

The software uses the default printer set up under Windows.

2 Managing worksheets

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

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

Open the **Manage Worksheets** window by clicking on **b** in the toolbar or via the menu command **Method Development** | **Manage Worksheets**.

Manage Worksheets						- 🗆	×
Worksheet	Last changed	Ву	Technique	Favorite	Inactive	New	
Cr in aqueous solution	03.04.2020 14:55	Analytik Jena	Flame			Prefill	
Cu in aqueous solution	03.04.2020 14:56	Analytik Jena	Flame			Change	
Mg in aqueous solution	03.04.2020 14:56	Analytik Jena	Flame			Delete	
Na-Emission in aqueous solution	03.04.2020 15:18	Analytik Jena	Flame	⊻			_
Zn in aqueous solution	03.04.2020 14:56	Analytik Jena	Flame				
						Load	
0 -11/5)	1	Descriptio	n:			1	
Show active worksheets only Show current technique only		Sample prep Elem./Wave Measuremer Flame: C2H2 Burner: 50 m Oxidant (aux Calibration ra	varation: xlength: Zn 213.86 nm tt details: 2/air mm .); off ange: 0 - 1.25 mg/L		~		
ē						Close	

Elements in the Manage Worksheets window

Buttons/ options	Description
New	Create new worksheet
Prefill	The loaded sequence and method are already populated
Change	Edit selected worksheet
Delete	Delete selected worksheet
Load	Load selected worksheet for a measurement
	Note: Only worksheets that match the currently set atomization tech- nique can be loaded.
Show active work- sheets only	Hide all worksheets marked as Inactive in the table
Show current tech- nique only	Show all worksheets in the table that use the currently set atomiza- tion technique
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	Last change to the worksheet
Ву	This operator made the last change. The name of the operator is taken from the Quick Start.
Technique	Atomization technique used

Table column	Description
Favorite	If activated, displays the worksheet on the Favorites tab in the Quick Start window.
Inactive	If activated, this worksheet will not be displayed in the Quick Start.
	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.

Name:	Pb in Fo	00	od	d											\bigstar	Favorite
Method:	Pb in Fo	00	od	d								1	-†			nactive
	16.10.2019	9 1	10:	0:34												
Sequence:	Pb in Fo	00	od	d								1	-†			
	19.10.2019	9 1	16:	6:56												
Sample ID:	Load Sa	am	mp	nple ID fil	e										\sim	
	File:)	olic	lic\Docu	ments	(Analy	ytik Jei	na\A	Spect	.S\us	er\Pro	ben2()-02-2	27.csv	Ľ	
	Usev	wil	vild	dcards *	and?	to lo	ad the	lates	st mato	hing f	ile					
Results file:	Always	cr	crea	eate new	v file (a	ppen	ıd time	starr	ıp)						\sim	
	Folder:	Γ	(5	(Standa	rd)										\sim	
	Name:		Pł	Pb in apr	oles										_	
	C:\Lleem\P	L. Dub	ublic		ente) Ar	oshtik		inectl	S/EA/	DECIII		in anal				
	C. YUSCIS VI		CIDIIC					pecit		LJUL	1340					
Elements:																
Last changed:	03.01.202	024	24 1	15:30												
Description:	Sample	e p	pre	reparatio	on:											^
	Elem./W	Na	ave	velength	n: Pb 2 ails:	83.31	nm									
	Modifier	er: N	: NH	VH4H2P	04											
	Sample Temper	e vo erat	vol atur	olume: 20 ture: 800/	0 μL 1600 °	С										
	Calibrati	tio	on	n range:	0 - 10	µg/L										v
													0	K		Cancel

Elements in the window New Worksheet

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.					

Field/option	Description
	Open folder containing Sample ID files After loading the worksheet, the folder containing the sample ID file is opened. Click on 🗂 and select the folder.
	Load Sample ID file A sample ID file is automatically loaded when the worksheet is loaded. Click on 🗋 and select the file. You can also define a file mask using the "*" and "?" wildcards.
Results file	Optionally, you can define settings for saving the results:
	none Measurement starts with the Start measurement window in which the name of the results file and the storage location are specified.
	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, the worksheet will not be displayed in the Quick Start.

Specifying a worksheet

▶ To create a new worksheet, click on in the icon bar to open the Manage Work-sheets 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 specify if you want to save a results file and if you want to use a sample ID file and then edit the description.
- Exit the window with **OK**.
 - ✓ The new worksheet appears in the Manage Worksheets window and can be loaded.

See also

B Starting a measurement routine [▶ 77]

2.2 Editing a worksheet

You can edit all settings in an existing worksheet.

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

2.3 Deleting a worksheet

You can delete a worksheet.

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

2.4 Loading a worksheet

You can load a worksheet when you start ASpect LS in **Quick Start** or in the **Manage Worksheets** window.

- Click on bi in the icon bar to open the Manage Worksheets window.
- Enable the **Show current technique only** option.
- Select the worksheet in the table and click on Load
 - \checkmark 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.

See also

Starting with a worksheet [▶ 9]

3 Methods

Methods store the parameters required for an analysis.

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

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

The **Method** window is opened by clicking on **iii** in the icon bar. The last active method is displayed. If no method has been loaded since Aspect LS was started, the window displays contain the default settings or are empty.

3.1 Creating, saving and loading methods

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

3.1.1 Creating a new method

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

- Select the menu command File | New Method.
 Alternatively, click on iii is there is no active method.
- Select one of the three options in the **New Method** window:
 - **Based on default parameters:** Open the **Method** window with default settings for calibration and statistics only.
 - Based on current parameters: Open the Method window with the currently set method parameters.
 - Based on saved method: Select a method in the Open Method database window.
- Confirm 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 method parameters using the **OK** or **Accept** buttons.
 - ✓ You can now save the method or use it for the next analysis. For the analysis, create a sequence based on the method and optionally fill in a sample ID table. Then start the measurement.

3.1.2 Save methods

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

Elements in the Save Method window

Save method					
Name: Pb in Food				c	Cat: KK
Name	Vers.	Date	Time	Cat.	Operator
Cd in Food	2	13.12.2023	12:55	KK	SuStein
Cr for ZEEman test	1	12.03.2020	13:44		SuStein
Mg in Food	1	27.02.2020	11:40		User
Pb in Food	1	16.10.2019	10:34	KK	Analytik Jena
TI in Food	1	16.10.2019	10:26		Analytik Jena
Sort by Name/Vers. Current version only Save calibration data	ing	Descriptio	ın:	0	K Cancel
Ontion D	escrintic	n			
option D	courptit				
Name	Aothod n	200			

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 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 is displayed for methods with the same name.
Save calibration	Save any available calibration curves with the method
data	The calibration curves can be used for further analyses.
Description	Optionally enter further explanations for the method
	Click on to open a list with predefined comments. You manage these comments in the Data Default descriptions window.

Saving a method

- ▶ In the Method window, click on Save or select the menu item File | Save | Method.
 - ✓ 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.

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

See also

- Creating predefined notes [▶ 164]
- Configure general settings of the user management [> 177]

3.1.3 Load a method

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

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

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

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

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 **iii**.

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

Button	Description
Open	Open a saved method
Save	Save the current method parameters
ē	Print method parameters
0	View properties of the method
ОК	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)

.

The element lines are specified in the **Method** | Lines window. You may choose a maximum of 200 different lines. This selection loads the data from the cookbook with the default settings for atomization of the elements.



Elements in the Method | Lines window

Line	table	parameters

Column	Description
No.	Number of element line
Elem.	Element icon of the element to be analyzed
Wavel.	Wavelength of analysis line in nm
	After clicking on this table cell, another line of the same element can be selected.
Linedescr.	Line designation
	You can choose a free name, which serves to clearly identify the analysis line.
Optic. mode	Optical working mode for flame and hydride technique:
	Single-beam The light is directed through the sample chamber, the lamp drift is cor- rected by an automatic autozero directly before measurement.
	Double-beam Double beam In the measurement of the reference signal the light on the sample chamber is guided past and used for correction of the lamp drift.
	Emission Measurement of the emission signal of the element in the flame
Lamp	Lamp type used:
	HCL Single-element hollow cathode lamp
	S-HCL Super hollow cathode lamp with one element
	MHCL Multi-element hollow cathode lamp

Column	Description
	S-MHCL Super hollow cathode lamp with several elements
Current	Set lamp current (not for the Emission operating mode)
Boost	Set boost current (only for S-HCL)
Slit	Set slit width

Use the **Append** button and **Insert** to add a new analysis line to the list at the end of the list or at the selected position in the list. Use **Delete** to remove a selected line from the list.

Insert element lines into the list 🕨

st In the **Method** | **Lines** window, click on **Append** to open the **Select element/line** window.

ł	Sele	ct ele	men	t/line	e																		—		×
	Sele	ectE	lem	ent		Cr							M	ax. Ia	amp	curre	ent (m	nA]:	1	0.0	► M	ax. Boost [mA]:	15.0 🗘	
Elements													Elem.	Line [nm]	Туре	Sens. [%]									
		Li	Be											В	С	Ν	0	F	Ne		Cr	357.9	P	100	
		Na	Mg											AI	Si	Ρ	S	CI	Ar		Cr	427.5	3	27	
		к	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		Cr Cr	425.4 360.5		24	
		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	T	Xe		Cr	429.0			
		Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn						
		Fr	Ra	Ac																					
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu								
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr								
		_	_																		Sortk				
		Cr35	/																0			-y Element	(Line	
																	_								
	Default parameters from: Cookbook													De	select	t									
-																									
																						OK		Cancel	

The window contains a periodic table and a line table. In the periodic table, the selectable elements are depicted as blue buttons. Elements for which a lamp is present in the lamp turret are marked in bold. The line table contains the following columns:

Column	Description
Elem.	Element symbol
Line	Wavelength in nm
Туре	P = Primary line, S = Secondary line, * = own line
Sens.	Analysis sensitivity of the line
	The sensitivity of the primary line is equivalent to 100%.

- By enabling the **Element** or the **Line** option, the line table is sorted increasingly by either the chemical symbol or the wavelength.
- If you click on an element in the periodic table (darker buttons are selectable elements), only the lines of the selected element are displayed in the line table.
 Alternatively, enter the element symbol in the Select Element field.
 Clear the Select Element field to display the full list of elements in the line table.
- To select, click on the rows of the desired lines in the line table one after the other. The selected lines are displayed below the periodic table.
- To undo the selection of a line, click on it once more in the line table. Use the **Deselect** to deselect all lines previously selected.

- You can choose between two parameter presets to develop methods further. To do this, in the **Default parameters from** list field, enable the **Cookbook** option or the **Method DB** option.
- Confirm the selection with **OK**.
 - ✓ The selected elements/lines are transferred to the **Method** | **Lines** window.

Note: You can select several lines with varying sensitivity for an element.

See also

■ Cookbook [▶ 167]

3.2.2 Specify the analysis parameters of the signals (Method | Evaluation window)

In the Method | Evaluation window, specify the type and form of the signal analysis.

₽₽₽ M	ethod												×
Lines	Evalu	ation	Furnace	Sample transport	Calib.	Statistics	QCS	QCC	Ou	tput			
No.	Elem.	Lineo	descr.	scr. Background		S Med.FS [T]	Limit Std.No.	Intmode		Read time [s]	Smooth		
1	Cd	C	d228 Z	eeman 2-field mode	0.80	0.45	3	Area		4.7	strong		
										t≡	t≡	J= □inc.	
	Open		□	Save	• ()		OK			Accept	С	ancel	

The following line parameters can be defined:

Column	Description
No.	Number of element line
Elem.	Element symbol
Linedescr.	Line designation
Int.mode	Mean Absorbance (emission) averaging over the emission time.
	Area Calculation of the peak area of the absorbance (emission) over the integra- tion time
	Height Calculation of the peak height (largest value after smoothing) of the ab- sorbance (emission) during the integration time
	Select Mean for sufficiently high sample volumes available (flame tech- nique, rarely hydride technique). The Area and Height options are used for atomization of a defined sample volume (graphite tube technique, hydride technique or in flame technique in conjunction with an injection module).
Background	no background No background correction, switch off deuterium HCL

Column	Description
	D2 background Measurement of the background radiation for elimination of the non-spe- cific absorption, switch on deuterium-HCL
	only D2 background Background measurement only, but no sample measurement, switch on deuterium HCL
	The special background corrections for the Zeeman AAS are described in the section below.
Ems WD	Only for flame emission measurements with the integration type Mean
	Wavelength difference (in nm) to analysis line, with which the emission background is measured
	In order to be able to measure samples with a high emission background (e.g. salts), there is the possibility of detecting the background next to the analysis line and subtracting it from the measured emissions.
Smooth	Smoothing of the measurement value peak
AZDK	Autozero drift control When switched on, during the autozero phase (AZ) of the furnace pro- gram, the energy fluctuation of the lamp is tested

Background corrections specifically for Zeeman AAS (graphite tube and HydrEA technique) **Note**: Only Zeeman 2-field mode is available with the ZEEnit 700 Q. It is enabled by selecting the **Zeeman** option.

Option	Description
no background	No background correction, deuterium HCL or Zeeman magnet is off
Zeeman 2-field mode	Background correction by means of Zeeman 2-field mode, Zeeman magnet on
or Zeeman	In the Max.FS column, set the maximum field strength in Tesla.
Zeeman 3-field mode	Background correction by means of Zeeman 3-field mode, Zeeman magnet on
	You must set the maximum field strength in the Max.FS column and the mean field strength in Tesla in Med.FS .
Zeeman dyn. mode	Background by means of Zeeman dynamic mode, Zeeman magnet on
	You must set the maximum field strength in the Max.FS column and the mean field strength in Tesla in Med.FS . In the Limit column, enter the number of the standard with the limit concentration.
only Zeeman back- ground	Measure background only, no sample measurement, Zeeman magnet on
D2 background	Measurement of the background radiation for elimination of the non- specific absorption by means of deuterium HCL
	Deuterium HCL on. Zeeman magnet off

You can optimize the parameters for the Zeeman background correction automatically in the **Spectrometer** | **Field strength opt.** window.

See also

- Background corrections for Zeeman AAS ZEEnit 700/650 P [▶ 113]
- Background correction for Zeeman AAS ZEEnit 700 Q [▶ 116]

3.2.3 Specifying flame parameters (Method | Flame window)

Burner parameters and gas flows for flame technique are adjusted in the **Method** | **Flame** window.

ίŤ.	/lethod						—	×
Line	Evaluation	Flame Sample	transport Calib.	Statistics QCS	QCC Outpu	t		
FI S	ame craper: xidant (aux.):	before each sar	nple 🗸	Burner// Type: Burne Nebu	Nebulizer r angle [deg]: lizer rate [mL/min]	mm 🗸		
N	o. Linedescr.	Flame	C2H2/air [L/h]	C2H2/N2O [L/h]	Burner height [mm]			
	1 Cr357	C2H2/N2O	100	190	4 t=	tī ti		
	Open	F I Save	a c		ОК	Accept	Cancel	
	- F							

Line-independent settings

The line-independent parameters are the same for all element analyses with the current method. First, adjust those parameters that apply to the complete method and that cannot be varied for the analysis of individual elements/lines.

Option	Description
Scraper	Only for acetylene-nitrous oxide flame
	The scraper is activated for the automatic analysis process with the 50-mm burner and acetylene/nitrous oxide flame. The automatic cleaning process can take place at different times.
Ox. control	off
	Operation without auxiliary oxidant
	on Operation with auxiliary oxidant
	When working with auxiliary oxidant, optimize the flame parameters manually.
Туре	Selection of the burner type used
Burner angle	Angular position of the burner relative to the optical axis
	The burner angle must be set manually on the burner (normally it is set to 0°). The entry of the value is optional. It only serves to complete analysis method and report data.
	Value range: 0 –90°
Nebulizer rate	Aspiration rate of the nebulizer
	The aspiration rate is a nebulizer-specific value. The entry of the value is optional. It only serves to complete analysis method and report data.
	Value range: 1.0 – 9.9 mL/min

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

See also

□ Optimizing the flame [▶ 121]

3.2.4 Entering the furnace program (Method | Furnace window)

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

it Μ	ethod												—		×
Lines	Evaluation	Furnac	e Sa	imple tr	ansport	Calib.	Statist	ics (QCS	QCC	Output				
Furnace parameters overview Platform															
No	Linedescr	Tot.	Dry.	Pyrol.	. Atomize			Ini	Drotr	Enr	١	Modifier			
INO.	Linedesci.	#	#	Temp.	Temp.	Ramp	Gas	nŋ.	Fleu.	LIII.	#1	#2			
1	Cd228	8	3	600	0 1700 1500 Stop					Pd/Mg(NO3)					
1													>		
										Clas	on furnesse		-		
	Edit furnace	program			Ac	cept furn	ace pro	gram		To	an iumace	2450			
										-	inp. [CJ.	2450	<u> </u>		
	Modif. <u>E</u>	xtras								Ra	amp [°C/s]:	500			
Hold [s]: 4															
	Open	C+	Save	ə		i			OK		Accep	ot Ca	ancel		

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

The following furnace program parameters are listed:

Column	Description								
Linedescr.	Name of element line								
Tot.	Total number of furnace program steps								
Dry.	Number of drying steps in a furnace program								
Pyrol. Temp.	Pyrolysis temperature in °C								
Atomize	Detailed display of temperature data during the atomization phase:								
	Temp. End temperature of atomization phase								
	Ramp Temperature variance during atomization phase in °C/s								
	Gas Feed of inert gas								

Column	Description
Inj.	Not selected Sample is injected before start of furnace program.
	Marked with an asterisk * The sample is injected at a later point in time.
Pretr.	Thermal preparation
	Sample and modifiers will be thermally prepared if this item was marked.
Enr.	Enriches the sample if selected.
Modifier	Additionally involved modifiers. For each measurement, a maximum of five additional modifiers can be selected.

Buttons

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

"Clean furnace" as an additional sequence action

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

Option	Meaning	
Temp.	Specified end temperature for bake-out process	
Ramp	Rate of temperature change	
Hold	Holding time at end temperature	

See also

Specifying measurements and actions in a sequence [69]

3.2.4.1 Editing a furnace program

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

Furnace	2								-		
nace pi	rograi	m Modif.Extras P	lot								
			Temp.	Ramp	Hold	Time	G	as			1
Step * Name	[°C]	[°C/s]	s	s	int.	Add.	– Inj.	E/P			
1		Drying	80	6	20	28.3	Max	Stop			
2		Drying	90	3	20	23.3	Max	Stop			1
3		Drying	110	5	10	14.0	Max	Stop			1
4		Pyrolysis	350	50	20	24.8	Max	Stop			1
5		Pyrolysis	600	300	20	20.8	Max	Stop			1
6		AZ*	600	0	6	6.0	Stop	Stop			
7		Atomize	1700	1500	4	4.7	Stop	Stop			
8		Clean	2450	500	4	5.5	Max	Stop			
2										>	
Row								Total time:		180 s	
A	ppen	d Insert		Delete		Delete ta	ble	↑ -:			
_			<u> </u>								
Co	okbo	ook program	Check	program							
Meas	start	delav [s] [.]	0.0								
			0.0	•							
🗌 Mini	mum	cooling time (redu	ced cleaning	temperatur	e)						
			•								
											_

Tabular display

The table lists all steps belonging to the current furnace program with the associated settings for temperature, holding time, gas supply, use of modifiers, and enrichment/ thermal pretreatment.

Option Description				
Append	Insert a new row at the end of the list			
Insert	Insert a new row before a selected list place			
Delete	Delete selected rows			
Delete table	Delete entire furnace program table			
t≓	Copy the parameters in a row to all subsequent rows			
Meas start delay	Optionally enter a time delay capture of the measurement signal			
	By default, acquisition of the measuring signal will begin as the At-omize furnace program step starts. A time setting will delay the start- ing point of signal acquisition by the preset amount of time. The func- tion is used to start the measurement only after the atomization tem- perature has been reached on the temperature plateau.			
Cookbook program	Load furnace program from the cookbook for the selected analysis line			
Check program	If the furnace program contains errors of a kind that renders program execution impossible, the faulty step will be displayed in a message box. The program cannot be launched in this case. Correct the faulty step (or change the furnace program that precedes this step).			
	As part of a program start, the furnace will be checked for potential thermic overheat situations (if all basic conditions are known). If the settings for temperature or time are found to be excessively high, a "Thermal furnace overheating" error message will appear during the program startup routine – the furnace program will be abandoned in this case. You should then correct the steps with the highest furnace temperature and the longest holding time.			
Transfer drying	For analysis of several lines			
step(s)	Accepts and transfers the settings made for drying parameters to the furnace programs for all analysis lines			

Control buttons and input fields

Option	Description		
Transfer cleaning step(s)	For analysis of several lines		
	Accepts and transfers the settings made for graphite tube baking to the furnace programs for all analysis lines		
Minimum cooling time (reduced cleaning tempera- ture)	The bake-out temperature and the resulting cooling time are a crucial factor for the analysis time of a sample. The bake-out temperature is set to at least 2450 °C as standard. The preset bake-out temperature can also be higher for elements that are difficult to atomize. This temperature is sufficient to remove most of the sample and matrix residues from the graphite tube. For samples with a suitable matrix, which usually require a lower atomization temperature, the bake-out temperature and thus the required analysis time can be reduced. By enabling this option, the bake-out time is automatically set to the value of the atomization temperature plus 150 °C.		

Specifying parameters for individual furnace program steps

Program steps

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

- Use the New, Insert or Delete buttons to adapt the furnace program to your requirements.
- To edit, click a desired one of the table cells.
- A list will open in this cell if preselections are limited. Numbers must be edited directly in the field.

Step	Description		
Drying	Evaporation of solvent in the sample		
Pyrolysis	Thermal pretreatment in which the sample is thermally decomposed without administration of oxygen		
Ash	Thermal pretreatment in which the sample is thermally decomposed using an appropriately selected additive gas (for example, oxygen)		
AZ	Autozero: Measures optical zero state (absorbance = 0)		
Atomize	Release of analyte atoms		
Clean furnace	Removal of residual sample matter		

Temperature parameters	Parameter	Description			
	Temperature	End temperature of this step			
		Value range for novAA 400 P and ZEEnit series: Maximum temperature up to 3000 °C in steps of 1 °C Minimum temperature not less than 20 °C above cooling water tem- perature (preferably 35 °C) of circulation cooler			
		Value range for novAA 800: Maximum temperature up to 2600 °C in steps of 1 °C Minimum temperature not less than 20 °C above cooling water tem- perature (preferably 35 °C) of circulation cooler			
	Ramp	The heating rate intended to achieve target (end) temperature			
		Value range for novAA 400 P and ZEEnit series: 1 3000 °C/s in steps of 1 °C/s; FP (Full Power), NP (No Power) are possible limit rates			
		Value range for novAA 800: 1 1100 °C/s in steps of 1 °C/s; FP (Full Power), NP (No Power) are possible limit rates			
	Hold	The time for which a target (end) temperature is to be maintained			
Gas supply

Parameter	Description
	Value range: 0 999 s less heating time
Time	Total duration of a step (sum of heating time plus hold time), is auto- matically calculated
Option	Description
int.	Flow of protective gas
	novAA 400 P and ZEEnit series
	Stop: No inflow, effective 2 s before step change
	Min: Minimum inflow rate (0.1 L/min Ar)
	Max: Maximum inflow rate (2.0 L/min Ar)
	novAA 800
	Min: Minimum inflow rate (0.1 L/min)
	Med: Medium inflow rate (0.5 L/min Ar)
	Max: Maximum inflow rate (2.0 L/min)
Add.	Flow of additive gas, e.g. air, nitrogen, etc.
	novAA 400 P and ZEEnit series
	Stop: No inflow, effective 2 s before step change
	Max: Maximum inflow rate (0.5 L/min)
	novAA 800
	Min Minimum inflow rate (0.2 L/min)
	Med Medium inflow rate (0.5 L/min Ar)
	Max: Maximum inflow rate (0.7 L/min)

Injection step/thermal pretreatment

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

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

See also

B Optimizing atomization temperature [▶ 126]

3.2.4.2 Specifying matrix modifiers, enrichment, and pretreatment

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

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

G Furnace				×
Furnace program Modif.Extras Plot				
Modifier	after			
Name	Vol. Pos Sample			
#1 NH4H2PO4 ~	5 🔹 85 👻			
☑ #2 Pd/Mg(NO3)2	5			
□ #3				
□ #4				
∐ #5				
Enrichment				
off 🗸 🗸	Cycles 0			
Thermal pretreatment	Warm up delay [s] 0			
Preheat sample				
	OK	Ca	ncol	
Line. Cd228 V	UK UK	Ca	ncel	

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

Matrix modifiers

Up to five modifiers can be specified for analysis of a given element line. These can be activated by clicking on the relevant modifier checkbox.

In order to prevent errors due to carryover effects, analytical components are recorded in the following standard order:

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

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

Enter the following parameters for the modifiers:

Option	Description
Checkbox	Use modifier for the analysis
Name	This list field contains the names of typically used modifiers.
	Select a name from this list or enter this name directly at the input field.
Vol.	Enter volume to be taken (1 to 50 μ L)
Pos	Specify position of modifier on sample changer

Option	Description
after sample	Autosampler will pick the particular modifier up, after the sample was picked up, i.e. the sample will be injected into the graphite tube be- fore the sample if this box is active.
Pretr.	Thermal pretreatment of modifier

Enrichment

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

The following enrichment modes can be specified:

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

Thermal pretreatment

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

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



NOTICE

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

If the temperature of the thermal pretreatment is higher than 300 $^{\circ}$ C, the graphite furnace must be cooled to below 300 $^{\circ}$ C in an additional step before the remaining components are added.

Pipetting into the hot furnace (above 300 $^{\circ}$ C) will destroy the tip of the tube! There will be no error message with higher temperatures!

Solid analytics using the SSA 600 solids autosampler

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

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

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

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

3.2.5 Specify Hydride and HydrEA systems (Method | Hydride window)

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

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

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

👬 Method						_	×
Lines Evaluation Hydride Sample transport	Calib.	Statistics	QCS	QCC	Output		
Mode Hg without enrichment (contin.) FBR mode Cell temp.['C]: Pump speed level: System cleaning after sample Cleaning with acid at action Cleaning with reductant+acid	Oper Loa AZ v Rea AZ v Purg Hea Coo	ation times d time vait time inction time vait time ge time 1 ge time 2 it time colle	[s] ctor ctor		14 * 10 * 20 * 10 * 10 * 10 * 10 * 45 *	Gas flow [L/h]	
Pos. reductant 28 🗘 Wash times	i	[O	<	Ассер	Plot ot Cancel	

Mode

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

Option	Description
Hydride (continu- ous)	Operation with autosampler or manual The reaction takes place in the reactor under continuous conditions (HS 60 A / HS 60 HS / 60 modular).
Hydride (batch)	Manual mode The sample is pipetted into the reaction beaker (max. 30 mL). The beaker is to be clamped gas-tight to the head of the batch module. With the first channel of the component pump, the reductant is

Option	Description
	pumped into the reaction beaker. The fast and partly vigorous reac- tion liberates metal hydride or atomic Hg vapor (HS 55 A / HS 55 / HS 55 modular).
FBR mode	For continuous mode only, recommended for Hg analysis
	Fast Baseline Return (FBR) After the maximum absorption has been reached, the direct argon gas flow purges the cell free during Wash time 2 thus causing a fast return of the signal to baseline level.

Cell temperature / Pump speed level

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

System cleaning

For continuous operation

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

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

Operation times

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

Option	Description
Load time	Time in which the sample pump loads the sample tube up to the two- valve assembly with sample. This time is needed only for the first measurement of a new sample.
AZ wait time	Time directly preceding the baseline adjustment (AZ = auto zero).
Prewash time	Time for purging the beaker with argon before the reaction (for hy- dride formers) The prewash time is used to purge off air in order to prevent an oxy- hydrogen reaction in the following reaction.
Reaction time	Time in which the sample pump pumps sample into the reactor. This is the crucial parameter for the supplied sample volume and the measuring sensitivity.
Pump time	Time in which reductant is pumped into the beaker in order to start a reaction.
Wash time 1 3	Times used to convey the reaction gas by means of the argon flow. The transport paths are different in the individual phases for the vari- ous operating modes. The transport paths can be graphically displayed.
Heat. time collector	Time in which the collector heating is on in order to release the en- riched Hg.
Cool. time collector	Time in which the collector is ventilated in order to cool it down for a new enrichment cycle.
Gas flow	Defines the argon flow flowing in the phases displayed left of it. The adjusted gas flow applies until a new gas flow can be entered. The gas flow can be switched over with varying frequency for the different operating modes. The gas paths for the individual phases are illustrated in the graphic of the analysis process on the hydride system. The gas flows are adjustable in three steps from 5 to 15 liters/hour.

Batch parameters

Option	Description
Sample volume	Enter the volume in mL of the sample in the beaker
Enrichment cycles	For the batch operation with Hg enrichment on the collector
	Define the number of beakers, the content of which is enriched

Present gas flows and analysis procedures of the hydride/HydrEA system graphically Click on **Graphic for** to open the graphic presentation of the gas paths for the individual phases of the analysis process.

<mark>†††</mark> Plot				—		×
Graphic for:	Parameters: Gas flow: 0 + s 0 + L/h	Take up sam Take up redu Take up was Sample valve Reagent tran	nple uctant sh sol. e to reactor isport			
Gas paths and flows React. GLS Batch	< Ar Coll. Cell > >	Autozero Delay time Measuremen Heat collecto Cool collecto	nt or or			
Phase Load Sample pump	AZW AZ React		Purge1	Purg	e2	
Reagents Measurement Collector						
Time [s]:	10 15 20 25 30	35 40 45	50 55	60	65	<u>-</u>

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

Element	Description
Graphic for	If sample statistics has been activated, the different processes can be displayed for the first, the next and the last measurement.
Gas paths and flows	This flow diagram shows the gas paths of the hydride system. The React. (reactor), GLS (gas/liquid separator), Coll. (gold collector), Batch (batch module) and Cell (cell) and Furnace modules are shown with their connecting hoses (for argon and reaction gas). In the process graph, click on the phase whose gas flow you want displayed. The gas path is marked in red and the argon flow displayed numerically in L/h.
Parameters	Display and edit the operation times, measuring times and the corre- sponding gas flows of a selected phase. Click on the corresponding phase. The name and the numerical value of the operation or measuring time / gas flow is displayed and can be changed. The process graph will be updated accordingly when you change a parameter.
Line	Toggle displayed line data

See also

Method parameters for autosampler for flame and hydride/HydrEA technique [▶ 44]

B Hydride system [▶ 132]

3.2.6 Specify parameters for autosampler (Method | Sample transport window)

The view in the **Method** | **Sample transport** window adapts to the atomization technique and the autosamplers used.

3.2.6.1 Method parameters for autosampler for flame and hydride/HydrEA technique

The following autosamplers are available for the flame technique:

- AS-FD / AS-F
- AS 52s / AS 51s

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

- Use of the autosampler
- Wash mode and controlled cleaning
- Automatic dilution during the analysis
- Use of SFS 6 injection switch or HS 50 hydride injector

∰† Method	- 🗆 X
Lines Evaluation Flame Sample transport Calib. Sta	tistics QCS QCC Output
Accessories Use autosampler Use injection switch Use hydride injector HS50 Injection time [s]: Load time [s]: Dilution if conc. exceeded	Wash after sample Wash time [s]: 15 Mixing cup cycles: 1 Controlled cleaning Control limit (Abs):
in mixing cup V Mixing cup level [mL]: 5	AZ sol. pos.: 19 ★ (0=wash sol.) Delay time [s]: 15 ★ Techn. parameters
🗂 Open 📑 Save 🖶 🛈	OK Accept Cancel

Using accessories

Option	Description
Use autosampler	Use the connected and initialized autosampler.
	If deactivated the sample is supplied manually without autosampler.
Use injection switch	The SFS 6 Injection switch can be used in combination with an au- tosampler or in manual mode. The SFS 6 ensures reproducible condi- tions in the flame. It permanently draws in purging and carrier solu- tion, which allows the burner to be kept at a constant temperature. Small sample volumes can be measured in a reproducible manner and gaged against a carrier solution. The injection module can also be used for processing time constant signals (mean integration).
	Injection time During this time, the valve of the SFS 6 opens the sample path to at- omize the sample and transport the aerosol to the burner. The time depends on the highest concentration to be expected. Typical values: 0.5 to 2.0 s.
	Load time The time needed to fill the sample aspiration path between sample cup and injection module with new sample.
Use hydride injec- tor HS50	The hydride injector HS 50 is a purely pneumatic batch system for manual operation. It consists of batch installation and cell holder with quartz cell. The reductant solution is transported pneumatically from the supply bottle into the reaction tank. The quartz cell is heated by the flame.

	0				
	Option	Description			
		The HS 50 works with the region or height signal evaluations.			
		The measurement procedure is divided into the following parts: Pre- wash – Autozero – Reaction/Integration.			
		Reaction time During the reaction phase reactant is transferred to the reaction beaker. The measurement signal acquisition starts at the same time the reaction time starts. The integration time has to be set in a way to acquire the total signal.			
		Prewash time During the prewash time, the reaction beaker is purged of air. The prewash phase is omitted for the determination of Hg because the ar- gon flow is necessary in order to transport the Hg out of the sample.			
		Sample volume Sample volume used			
	Delay time	This time is required to transport the sample to the atomization unit (e.g. flame or reaction chamber in the hydride system). The time is essentially determined by the length of the sample tubes. This time is needed to convey the sample to the flame.			
Dilution if concentration ex- ceeded	lf using the AS-FD and in the method, you car lution when the conce	AS 52s autosamplers, you can dilute samples automatically. Here n define the fill level in the mixing cup and activate automatic di- ntration is exceeded.			
	Dilution if concentration the concentration excer 10 %, the sample is dil termined as part of a p luted solution state. The mixing cup is filled up can edit the 10% limit	on exceeded checks the measured concentration of the samples. If eeds the measuring range of the calibration curve by more than luted in the mixing cup. Required volumes are mathematically de- orogram sequence, depending on the absorbance value for undi- ne calculated analyte volume is added to the mixing cup and the to the defined fill level with diluent from the supply bottle. You value in the Options Calibration window.			
	List / Option	Description			
	Dilution if conc. ex- ceeded	none No automatic dilution is carried out if the concentration is exceeded.			
		in mixing cup Dilution is carried out as described above if the concentration is ex- ceeded.			
	Mixing cup level	The mixing cup is filled to this volume with diluent.			
	Note : Individualized di dow.	ilution factors can be set for each sample in the Sample ID win-			
Washing and controlled clean- ing	While a measurement sequence is running, you can specify washing steps to clean the various sample paths inside the system and its accessory units.				
	If the concentration of by more than 10%, the tem (hydride techniqu measurement. During the cleaning results. Th highly concentrated sa activated.	the sample exceeds the measuring range of the calibration curve e burner/nebulizer system (flame technique) or the hydride sys- e) can be washed to remove contamination from the previous the wash, the absorbance/emission is measured in order to check he automatic controlled cleaning is recommended after measuring imples, especially when the Dilution if conc. exceeded mode is			

	Option	Description						
	Wash	off Wash mode switched off. No washing performed automatically. Between each sample Washing after each sample, but not within a statistical series Time in which the rinsing agent is aspirated in the wash cup. Includes washing of tube path and burner-nebulizer system.						
	Wash time							
	Mixing cup cycles	Number of rinse cycles for the mixing cup In a rinse cycle the mixing cup is filled with wash li then emptied again.	quid / diluent and					
	Controlled cleaning	Will automatically trigger controlled cleaning on ex concentration level if active.	ceeding specified					
	Control limit (Abs)	The signal level must have returned to this value d cycle before the diluted samples or samples with lo are measured.	uring the rinsing ower concentrations					
Autosampler wash sequence	To perform washing of autosampler arm dips pump provides wash pump rate is greater to hydride system. The of jector SFS6 and the b off into the waste bot	ed situation. of the sample aspiration path and the burner-ne s the cannula into the wash cup of the autosamp liquid from a storage bottle for the duration of t than the aspiration rate of the nebulizer or the p complete sample path is cleaned (cannula, samp urner-nebulizer system). Surplus amounts of wa ttle.	ebulizer system, the oler. A membrane he dipping. Its oump rate of the ole tube, sample in- ash liquid will flow					
	The mixing cup of the AS 52s or AS-FD is cleaned by filling with wash liquid/diluent and draining it again in one single cycle.							
Delay time	The delay time is required to transport the sample to the atomization unit (e.g. flame or reaction chamber in the hydride system). The measurement delay time must be adapted depending on the aspiration length between sample and nebulizer.							
	Set the time in the Delay time field. If you define a pseudo measurement in the Method Statistics window, use the following times. If you do not activate a pseudo measurement, extend the specified times by 3 s.							
	Accessories / with act	tivated pseudo measurement	Time					
	Short aspiration capillary, working manually 8 s							
	Standard aspiration capillary, working manually 12 s							

	Autosampler without	ut injection module 18 s				
	Autosampler with in	njection module 20 s				
Other buttons / options	Option/button	Description				
	AZ sol. pos.	Position of reference solution on the autosampler tray				
		Note : You define all other sample positions in the sequence or the sample ID.				

Open the Autosampler | Techn. parameters window

Here you can specify further parameters for the autosampler, such as the immersion depth in the sample cups and the dosing speed.

18 s

Injection module SFS, working manually

Techn. parameters

See also

- B Sample ID window [▶ 73]
- Specifying measurements and actions in a sequence [69]
- General settings for calibration and blank correction [▶ 172]

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

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

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

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

- Use of an autosampler
- Wash modes
- Automatic dilution during the analysis

The **Use autosampler** option must always be activated for the graphite tube technique for solution analytics.

††† Me	thod											-	-	×
Lines	Evaluation	Furnace	Sample transp	ort Calib.	Sta	atistics	QCS	QCC	Outpu	ıt				
	cessories) Use autosa ution if conc. (none iluent position	mpler exceeded	8	7		-Was Be Was ⊡ C Con	h tween ru sh cycle controlle trol limit	uns s: d cleani (Abs):	ing	Tec	0.00	2 * 2 *		
	pen	🗗 S	ave	e ()			Oł	<	A	ccept	1	Canc	el	

Use autosampler for automatic dilution

In connection with the autosampler, automatic sample dilution can be carried out. Individualized dilution factors can be set for each sample in the **Sample ID** window. In the method, you specify the dilution mode and position of the diluent.

You can also specify parameters for automatic dilution when the concentration exceeds the limit. If the value for concentration is found to exceed the measuring range as determined by the respective calibration graph by more than 10 %, the sample will be diluted. The maximum dilution factor is limited by the smallest volume to be injected reliably (2 μ L). You can change the 10% limit value in the **Options** | **Calibration** window.

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

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

Specify washing steps

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

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

Controlled cleaning

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

Option	Description
Controlled cleaning	Will automatically trigger controlled cleaning on exceeding specified concentration level if active.
Control limit (Abs)	The signal level must have returned to this value during cleaning be- fore the diluted samples or samples with lower concentrations are measured.

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

Autosampler

Washing the autosampler	After receiving the samples or other liquids, the pipettor tube is automatically cleaned with the washing liquid in the diluent cup (deionized water, slightly acidified with 0.1 N HNO ₃). Here the cleaning liquid is pumped from the storage bottle through the dosing tube and into the wash cup of the autosampler.
Parameters for dipping depth and dosing speed	The parameters of the autosampler regarding the immersion depth in the various cups and dosing speeds are selected in the Autosampler window. Click on the Techn. param- eters button to open it.
	See also
	\square Technical parameters of the autosampler for the graphite furnace technique [> 146]
	Specifying measurements and actions in a sequence [> 69]
	Sample ID window [> 73]

■ General settings for calibration and blank correction [▶ 172]

3.2.6.3 Method parameters for autosampler for graphite furnace technique (solid analytics)

Note: The analysis of solids using graphite furnace technology cannot be carried out with the novAA 800 or the ZEEnit 700 Q. The corresponding settings are therefore not available for these devices.

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

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

HT Method					—		×
Lines Evaluation Furnace S	Sample transport Calib.	Statistics QCS	QCC	Output			
Autosampler SSA6/SSA6Z manual ma SSA600 automatic mode SSA-600 with liquid piper	ode e tter	Sampler tray Single tray (42 Double tray (82)	2 pos.) 34 pos.)				
Mode One-platform mode Batch mode Batch (special position 42) Number of platforms: 3		Getting sample weight O Weigh Weigh with confirmation O No weighing					
Workflow for time critical Speed Speed level:	samples 2 🗘	Installation site: very disturbed Controlled cleaning Control limit (Abs): 0.0010 OK Accept Cancel					
Option	Description						
SSA6/SSA6Z man- ual mode	Use manual aut If using the mar tion options nee weighed and the on the Solid tab	osampler SSA nual SSA 6 auto ed to be specifi eir sample ma	6 (z) osamp ed. All ss valu	ler, no further sa samples must be es entered in the	mple tr e indivio e main v	anspo dually vindov	rta w
SSA600 automatic Automatic solids autosampler SSA 600 without liquid dosing mode							

_

Option	Description
SSA-600 with liq-	Automatic solids autosampler SSA 600 with integrated dosing auto-
uid pipetter	matics for liquid components (standards or modifiers)

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

Option	Description
Mode	One-platform mode The analysis is performed with only one platform, which is always reloaded. This platform is located in tray position 1. During the analysis procedure, all necessary steps (taring, dosing, weighing, liquid dosing) are performed with this platform.
	Batch mode Several platforms are used during the analysis. Analysis may run auto- matically, depending on your pre-settings.
	Batch (special position 42) Several platforms are used during the analysis. Analysis may run auto- matically, depending on your pre-settings. For samples requiring no weighing, for example Cal-Zero or liquid standards, position 42 on the sample tray is used. For this reason, an empty platform must be placed in this position as pipetting destination of sample is necessary.
	Number of platforms For Batch mode and Batch (special position 42) Number of platforms used and available number of sample positions
Workflow for time	Behavior of the autosampler during sample preparation and dosing
critical samples	If activated, the platforms are only loaded with samples directly be- fore the measurement. This prevents samples from volatilizing during longer waiting periods on the sample tray or from "creeping" across the platform due to high adhesion, as is the case with oils for exam- ple. This mode requires the operator to be present at all times.
	When deactivated, all available platforms are prepared before the start of the measurement. All actions that require the user's presence (sample loading or manual pipetting of modifiers) are performed in combination. The AAS device can work through the samples in this mode without the constant presence of the operator.
Speed	The speed of the SSA600 movements can be set in three levels. Recommended level: 2
Sampler tray	Number of trays placed one on top of the other.
Getting sample weight	Weigh Once a dosed solid substance has been weighed, the initial weight is adopted without a preliminary query for acceptance of this weight.
	 Weigh with confirmation The weighing result is displayed after each weighing of the solid. The operator can signal acceptance of the initial sample weight by pressing the green key (key on the autosampler or OK in the weighing window on the screen). On actuation of the orange key (key at autosampler or Repeat in the weighing window on the monitor screen), the platform will return into dosing position, dosing will be altered and weighing will subsequently repeat.
	No weighing Samples are not weighed. Therefore, no concentration analysis mea- surements are possible. The result can only be evaluated qualitatively.

Option	Description
Installation site	Depending on the interfering factors (especially vibrations), set the precision of the built-in microbalance If the weighing time seems too long, you can shorten it by changing the setting for place of installation. This will be at the expense of pre- cision. The settings can be defined in 4 gradations from very dis- turbed to very quiet .
Controlled cleaning	If activated, controlled cleaning takes place automatically if the con- centration is exceeded.
	If samples are analyzed that cause the working range of the calibra- tion curve to be exceeded by more than 10%, the graphite furnace and sample platform are baked out to remove contamination from the previous measurement. The absorbance is measured during cleaning. Cleaning is ended when the control limit is reached.
	Note: Controlled cleaning can also be defined as part of a sequence, independently of a concentration exceeded situation.
Control limit (Abs)	Absorbance value to which the signal level must have fallen during cleaning before the next sample is measured.

See also

Solid analysis with graphite furnace technique [> 91]

3.2.7 Specify calibration parameters (Method | Calib. window)

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

łŤ	Meti	hod								×
Line	es	Evaluation	Flame S	ample tra	insport Calib.	Statistics QCS	QCC Ou	utput		
C	alibr	ation mode			Blank cor	rection				
S	Stand	dard calibrat	ion	\sim	Absorba	nce corrected	\sim			
S	td. pi	rep.								
p	rep.	by sampler		\sim						
١	No.	Linedescr.	Mix.vol. [mL]	AM Pos	Calib. func.	Intercept	Weighting	Check	Unit	
	1	Cr357	5	0	automatically	calculate	none	none	mg/L	
		Stocks		Concentra	ations			tΞ	t≘ t≟	
									inc.	
E	h Or	0.0	Flag	21/0	– 0		OK	Accort	Concol	
	JOF			ave			UN	Accept	Cancer	

For a calibration a maximum of 65 standards can be used.

Calibration mode

Option	Description
No calibration	The results of sample measurements are exclusively presented in ab- sorbance or emission. Calibration is not necessary for these measurements. No further en- tries are required on the Calib. tab. The sequence list should, logically, only consist of samples.
Standard calibra- tion	Calibration is performed with samples of known concentration. Samples of unknown concentration are measured against this calibration.
Method of addi- tions	Different quantities of a known sample are added to the unknown sample and the resulting substance measured. The concentration of the unknown sample results from the performed regression.
	The standard addition process is not available for solid analysis in a graphite tube.
Method of addi- tions 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.
	Variab. weighs per add. For solid analytics / addition calibration Determine the number of different solid sample weighed portions per addition series.

Standard preparation

Option	Description
manually	The standard solutions are already prepared.
prep. by sampler	Only for autosamplers AS-52s or AS-FD
	The reference solutions are prepared in the mixing cup of the au- tosampler by mixing different proportions of stock solutions and dilu- ent.
	In this case, adjust the following volumes for preparing the standard solutions in the line table:
	Mix.vol. Total filling volume in the mixing cup (value range: 1 to 20 mL)
	Sample part Only with addition method: Proportionate sample volume (incre- ments of 0.5 mL).
	With the addition method, the fraction of the sample solution of a measurement series is always the same. The proportionate sample solution must be smaller than the total fill volume. The difference volume is filled up with stock solution and diluent solution. The sample volume/total volume ratio is the correction factor for the concentration to be computed.
by variation of vol-	Only graphite furnace technique
ume	Different volumes of the stock solution, or quantities of the reference sample, are brought to atomization so achieving different degrees of concentration (relative to the sample volume / weight).
by dilution	Only graphite furnace technique
	Defined volumes of the stock solution, and the missing volume of diluent for the sample volume, are brought into the graphite tube in a transfer step and thus a grade of concentration is reached (relative to the sample volume / weight).
	In this case, adjust the following volumes for preparing the standard solutions in the line table:

Option	Description
	Vol. Total volume pipetted into the graphite tube (1 to 50 μ L).
	Max. add. vol. Only with addition method Maximum amount of stock solution to be added If the addition solutions are prepared by dilution, this is the sum vol- ume of the addition volume and the diluent volume.

Blank correction

Only with Method of additions and Method of additions calib.

Option	Description
Absorbance cor- rected	For each standard addition, the blank is measured and the deter- mined absorbance value is subtracted from all measured values be- fore calculating the regression line. This method was customary for a long time; with many real samples however, it may lead to incorrect results.
Concentration cor- rected	First, a separate standard addition is carried out for the blank solution using the same concentration additions as for the sample. The result- ing concentration is automatically subtracted from all other concen- trations determined by standard addition.

Line-specific calibration parameters

Line-specific calibration param- The line-specific calibration parameters are set in the table:

Table column	Description				
No.	Sequence of selected line in the table				
Linedescr.	Name of the analysis line				
Volumes	Depending on atomization technique and calibration process various volumes must be set (see above "Preparing the standards").				
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 ra- tional 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.				

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.

Table column	Description
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 All calibration points are taken into account with the same weighting
	1/conc Give greater consideration to calibration points with smaller concen- trations
	1/SD Give greater consideration to points with smaller deviations within the multiple repeated measurements of a standard (requires: mean statistics activated).
	1/(SD*conc) Combination of the calculation methods 1/conc and 1/SD
Check	The software allows automatic checking of determined calibration curves against a prediction range calculated on the basis of a manually selected statistical certainty.
	none Uses all measured and non-deleted calibration points for the calcula- tion of the curves. Calibration points are neither labeled nor elimi- nated.
	Elim .outliers If calibration points are outside the calculated prediction range, out- liers 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. Then, another E-Test is performed for the calibration point now.
	 All calibration points lying outside the new prognosis range, that have not been eliminated as outliers are marked by "?" in the table and brown color in the graph.
Unit	Unit of concentration of each element

See also

 \square General settings for calibration and blank correction [\triangleright 172]

3.2.7.1 Specifying stock standards

If you produce the standard concentrations automatically with an autosampler, you must specify stock standards from which the individual standards are then generated by dilution. To do this, you must specify the stock standards before completing the calibration

table, and you can use multiple stock standards with different elements and concentrations. If you use stock standards more often, you can manage these in the database in the **Data** | **Insert stock standard** | **Stock std/QC samples** window.

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

See also

■ Managing databases for stocks and QC samples [▶ 163]

3.2.7.2 Entry of concentrations for manually prepared standards

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

Cal	ibratio	on table								
	Cal-Z	ero:	1	Cal	standards:	5				
		Туре	Pos	Rec	Cr [mg/L]					
		Cal-Zero1	1	REC	0					
		Cal-Std1	2	-	1					
		Cal-Std2	2	-	2					
		Cal-Std3	2	-	3					
		Cal-Std4	2	REC	4					
		Cal-Std5	2	- 🗸	5					
	<									>
								t≣ f≣	:	÷ ↓=
										inc.
										ОК

Standard types

Calibration table for standard methods with manually pre-

pared standards

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

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

Calibration method	Standard types				
	Cal. standards: Calibration standards				
Method of addi-	Cal. standards: Calibration standards				
tions	Add. standards: Addition standards				
Method of addi- tions calib.	Add. standards: Addition standards				

Standard table

Column	Description
Туре	Standard type
	The standards are numbered according to the selected number.
Pos	When using the autosampler Enter the position of the standard on the sample tray of the autosam- pler.
REC	Only with standard method Define the corresponding standard as recalibration standard.
Elements	Concentration of the individual elements in the standard

Completing the calibration table

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

3.2.7.3 Entry of concentrations for calibration standards prepared automatically with autosampler

With the flame technique, the calibration standards are prepared automatically by mixing with the autosampler. For graphite tube technique, a calibration series is accomplished by volume stepping or volume thinning inside the graphite tube.

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

Calibration table for standard methods with automatically prepared standards

librati	on table									
Cal-Z	Zero: 1	•	Cal. s	tandards		5 🛊				
	Туре	Pos	Pr [%]	eparation Vol.[μL]	Stock	Rec	Cr [mg/L]			
1	Cal-Zero1	1	0	0	0	REC	0			
2	Cal-Std1	2	10	500	1	-	1			
3	Cal-Std2	2	20	1000	1	-	2			
	Cal-Std3	2	30	1500	1	-	3			
	Cal-Std4	2	40	2000	1	REC	4			
	Cal-Std5	2	50	2500	1	-	5			
<										>
Deact	ivate standards with C	trl + mou:	se click or (λtrl + space				t≡	t≣	→ → → inc. OK

Standard types

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

Calibration method	Standard types					
Standard calibra- tion	Cal-Zero : Calibration standards without analytes Multiple calibration zero standards can be entered, e.g., if the ele- ments being analyzed are present in different solvents. In this case the concentration of the respective element line must be set to "0", the other columns remain blank.					
	Cal. standards: Calibration standards					
Method of addi-	Cal. standards: Calibration standards					
tions	Add. standards: Addition standards					
Method of addi- tions calib.	Add. standards: Addition standards					

Standard table

_

Table column	Description
Туре	Standard type
	The standards are numbered according to the selected number.
Pos	Position of the stock standard or zero value on the sample tray
Preparation	% : For flame technique Percent by volume of the stock component in the solution
	Vol. : For flame technique Volume of the stock component in µL. The value is calculated from the vol% entered and the Mix.vol. defined in the line table of the Method Calib. window.
	Vol. : For graphite furnace technique This volume is injected into the graphite furnace.
	Stock Number of the stock standard in the stock table
REC	Only for standard methods
	Define standard as recalibration standard
Element	Calculated concentration of the individual elements in the standard

Completing the calibration table

- In the Method | Calib. window, click on Concentrations.
- ✓ The Calibration table window appears.
- Use the various list fields above the table to set the number of standards as required for a selected calibration method.
 Maximal number of standards: 65.
- For flame technique: Enter the volume percentage for each standard in the table.
- For graphite furnace technique: For each standard, enter the volume that is injected into the graphite furnace.
- For each standard, enter the number of the stock standard.
- If lines in a standard are not to be used for calibration, deactivate them:
 Click on the line field and press the space bar. To reactivate, repeat the process.
- Click on **OK** to confirm the settings.

See also

B Specifying stock standards [▶ 54]

3.2.8 Specify statics parameters (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.

¦†† Me	ethod										—	×
Lines	Evaluation	Flame	Sample transpor	Calib.	Statistics	QCS	QCC	Outpu	t			
S	Statistics Sigma st Median s	atistics			Confi © ©	dence ir off absolut relative	nterval c e	alculati	on			
	Calib.std. QC Pre-runs			3 4 3 4 3 4 3 4 4 7 7 7 7	9	dence (6	sigma)		~			
[🗌 Grubbs ou	tlier test										
)pen	C+	Save	e ()	(Ж		Accept	(Cancel	

Statistics

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 devia- tion and the relative standard deviation are calculated.
Median statistics	Calculate median and range (R)
	Error statistics according to the median method:

Option	Description
	 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. The mean value of the two measured values in the middle of the sorted list.
	As the smallest and largest individual measured values do not influ- ence the measurement result, the median statistics are suitable for the elimination of outliers.

Replicates

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

Grubbs outlier test

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

Option	Description
Deactivated	All values of the statistics series are used to determine the mean value.
Activated	Outliers are eliminated and excluded from the calculation of statistical quantities. The thus found mean values in the result table are marked by "!".

Confidence interval calculation

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

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

Confidence level

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

3.2.9 Specify quality control samples (Method | QCS window)

In the **Method** | **QCS** window, you can specify the quality control (QC) samples. This involves the insertion of control measurements, with samples in predetermined positions during measurement. These control measurements should yield known results. It is ei-

ther 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 the QC charts serves to monitor quality over a long period of time. The QC charts are saved with the method and continued for any further measurement with the method.

†† Me	thod							×
Lines	Evaluation	Flame Sample trans	port Calib. Statisti	cs QCS QCC (Output			
Type N	C std.3 QC std.3	∨ Name: Delete	QC-Std.3	Reaction:	reca	ıl. + rerun	~	
No.	Linedescr.	Exp. conc.	Low. deviation [%]	Up. deviation [%]	QC chart	React!	Unit	
1	Cr357	3	10	10	+	+	mg/L	
	QC samples	overview				t≡ f:	∎ ↓ ≒ ⊡ inc.	
[1] 0	pen	🖿 Save	e ()	ОК	Accep	ot	Cancel	

Elements in the Method | QCS window

Option	Description
Туре	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/Change	Define a new QC sample or modify an existing QC sample
Delete	Delete selected QC sample
Unit	Concentration unit of the QC sample
QC samples over- view	Open a list with line-specific parameters of all QC samples
Line table	The table displays the parameters of the QC sample selected in the Type list box.

Types of QC samples

You can specify the following QC sample types:

Option	Description
QC sample	Define a sample as a QC sample
	The concentrations of the QC sample may either be loaded from the database or typed in directly.
	from database Select the relevant QC sample in the adjacent list box. You can man-
	age the database of QC samples in the Data Stock std/QC samples window.

Option	Description
	enter manually Enter the concentrations of the QC sample directly into the line table Max. number of QC samples: 50
QC std.	Define a standard as QC sample
	Any standard defined in the calibration table can be used as a QC standard.
	Possible number of QC standards = number of standards in the cali- bration table (max. 65)
QC blank	Define the blank sample as a QC sample
QC spike	Define a spiked sample as a QC sample
	In recovery/addition, the measurement results of a defined concen- tration 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 con- centration). After measuring the sample and QC stock, the concentra- tion difference of both is compared with the expected concentration increase (Exp. conc. increase) specified here and the recovery rate is calculated. When using the flame technique, the solution with added stock solution must have been pre-mixed.

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

Option	Description
QC trend	The measured concentration value is stored when the quality control sample appears for the first time in the analytical procedure. When the QC sample appears the next time, the concentration difference is formed and evaluated. It is advisable to measure these QC samples at the beginning and at the end of a sample measurement 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	limit	is	ex-
ceeded					

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

QC sample type	Procedure
QC sample QC std.	flag The measured value is marked in the sample table. The measuring program continues with the next sample.
UC Spike	recal. + continue A recalibration is performed. The QC sample is then measured again. If the QC sample is now within the range, the measurement is contin- ued with the next sample, otherwise the measuring program is stopped.
	cal. + continue A new calibration is performed. The QC sample is then measured again. If the QC sample is now within the range, the measurement is continued with the next sample, otherwise the measuring program is stopped.

QC sample type	Procedure
	recal. + rerun A recalibration is performed. The QC sample is then measured again. If the QC sample is outside the range, the measuring program is stopped. If it is within the range, all samples are measured again after the last QC sample or the last (re)calibration. If the QC sample is again outside the permissible error limits, the measurement program will be stopped.
	cal. + rerun A new calibration is performed. The QC sample is then measured again. If the QC sample is outside the range, the measuring program is stopped. If it is within the range, all samples are measured again after the last QC sample or the last (re)calibration. If the QC sample is again outside the permissible error limits, the measurement program will be stopped.
	Next line The current measuring program is aborted and the measuring pro- gram 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 The current measuring program is aborted.
QC blank	flag
	next element
	Stop
QC trend	No reaction
QC matrix	

Line-specific parameters of the CC sample types in the line table.

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

Entering parameters of QC samples In the **Method** | **QCS** window, click on **New/Change** and create a new parameter set for a QC sample or edit the selected parameter set. The **Add/modify QC sample type** window appears.

- Select the QC sample type in the **Type** list.
- Only QC samples: If several QC samples are defined, define a consecutive number in the adjacent list box.
- Only **QC std.**: Select the number of the standard in the list box according to the order in the calibration table.
- Enter the line-specific parameters in the table.
 - \checkmark Define further QC samples in the same way.

3.2.10 Specify quality control (Method | QCC window)

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

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

You may choose various control options with different reactions simultaneously.

<mark>∔††</mark> Met	thod						—		×
Lines	Evaluation	Flame Sample trans	port Calib. Statisti	cs QCS QCC	Output				
Type Ne	QC std.3	✓ Name:Delete	QC-Std.3	Reaction	reca	ıl. + rerun	~]	
No.	Linedescr.	Exp. conc.	Low. deviation [%]	Up. deviation [%]	QC chart	React.!	Unit		
1	Cr357	3	10	10	+	+	mg/L		
(QC samples overview inc.								
Cţ) Ot	pen	Save	e ()	ОК	Accep	ot	Cancel		

Types of quality control

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

Reactions if error limits are exceeded

Option	Description
none	Do not perform the control in question
flag	Marks the corresponding sample, calibration or recalibration in the sample table, if the error limits are exceeded.

Option	Description				
repeat + continue	Only with RSD/RR% check				
	Repeats the measurement of the respective sample, if the serial preci- sion limit was exceeded, before the next sample is measured				
cal.+cont.	Only with Calib. check and Recal. check				
	If the error limits for the calibration or the recalibration factor are ex- ceeded, perform a new calibration and then continue the measure- ment with the next sample				
next element	Only with 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 with Calib. check and Recal. check				
	Stops the measurement of the currently running method, if the error limits were exceeded				

Control of the graphite furnace

Only for graphite furnace technique

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

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

Line-specific parameters of quality checks

In the table, enter the line-specific parameters of the various quality checks. You may define for every analysis line, whether it shall be considered for the check. If one or several of the checked lines exceed the error limit, the reaction chosen above will be released.

Quality check	Parameter	Meaning
RSD/RR% check	RSD/RR% <	The system will respond as selected 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	R²(adj.) >	The coefficient of determination R ² (adj.) must be larger than or equal to the specified value. Other- wise, the system will respond as selected.

Quality check	Parameter	Meaning
		R² ! If the lines are marked by "+", R ² (adjust) 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 cali- bration factors are outside these specified limits.
		Rec. ! For lines marked with "+", the recalibration factor will be checked.

See also

Specify statics parameters (Method | Statistics window) [> 58]

3.2.11 Specify results output (Method | Output window)

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

- Specify the number of decimal places for the display and printout of absorbance and concentration separately for each element in the table.
- The print sequence of the order in the table.

ł	Met	hod										—	×
Lir	es	Evaluation	Flame	Sample transport	Calib.	Statistics	QCS	QCC	Output				
_													
	No	Linedescr		Dec. places		Dec	. place	s		Signif	figure	s	
	INU.	Lineuesci.		Abs./Ems			Conc.			C	onc.		
	1	Cr357		5			4				4		
			-							tΞ	t≘	τΞ	
												inc.	
(<u>•</u> •) O	pen		Save	ē (D	(ЭК	A	Accept		Cancel	

4 Sequences

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

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

4.1 Creating, saving and loading sequences

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

4.1.1 Creating a new sequence

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

- Select the menu item **File** | **New Sequence**.
- ▶ Alternatively, open the window with the current sequence parameters by clicking on ■ or using the menu item Method Development | New Sequence.
 - ✓ 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 in the database. This allows you to reuse the sequence for later measurements. Sequences are saved in the database in the **Save sequence** window. You can save additional data with the sequence to categorize sequences and make them easier to find.

quence	ave sequence					
	Name: sequence name				С	at:
	Name	Vers.	Date	Time	Cat	Operator
	Cu 20-03-03	1	03.03.2020	13:44	PV	SuStein
	Cu, Zn, Cd	1	22.11.2023	12:02	PV	SuStein
	FI sequence prepro	2	23.11.2023	15:45		SuStein
	Sort by Name/Vers. Sort Dure a sing		Description	n:		
	Current version only					~
					0	K Cancel

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 is displayed for sequences with the same name.			
Description	Optionally enter further explanations for the sequence			
	Click on to open a list with predefined comments. You manage these comments in the Data Default descriptions window.			

Saving a sequence

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

See also

Creating predefined notes [> 164]

4.1.3 Loading a sequence

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

- Open the sequence database window with one of the following alternatives:
 - In the toolbar, click on the folder icon ¹ next to the Sequ field.
 - Select the menu item File | Load analysis sequence.
 - Open the **Sequence** window by clicking on \blacksquare and then click on **Open**.
- Optionally, you can limit the displayed sequences by selecting a category in the **Cat.** field. To display all sequences, delete the entry in this field.
- Enable the **Current version only** option if only the latest versions of the sequences are to be displayed.
- 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 of an analysis.

Click on \blacksquare to open the **Sequence** window.

}≡ Seq	luence					—		×
	Туре	Pos	Name	Name(2	Elements	Spe	cifics	^
1 2 3	Autozero Cal-Zero1 Cal-Std1	43 43 45			all all all			
4 5 6	Cal-Std2 Cal-Std3 Cal-Std4	46 47 48			all all all			
7 8 9	Compute calib. Sample Sample	1	Sample 001 Sample 002		all all			
10 11 12	Sample Sample	3 4 5	Sample 003 Sample 004 Sample 005		all all all			-
Rov	N				Samples t= .	t≡	1 <u>−</u>	~
	Append Ins Delete table Fro	sert m seque	Delete	0	Sequence<-QC sample ID		inc. Types	
[1] 0	🗂 Open 📑 Save 🖶 OK Accept Cancel							

Table of sample and action sequences

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

Table column	Description
Туре	Sample type or analysis step.
Pos	Sample position on autosampler tray (if used).
Name	Sample name This entry is optional. For calibration and QC samples this sample name is transferred from the method if a sample name was specified there. For analysis samples, the names can be transferred from the sample information file.
Name(2)	Additional designation for sample identification (optional).
Elements	Only for multi-element methods
	Select elements / element lines that are analyzed in a sample or for which special actions are performed.
	Copy all Columns All elements/element lines specified in the method are determined (default setting).
	Element symbol Only the specified elements will be determined, e.g. Cu, Pb.
	Element symbol + index (when analyzing several lines of an ele- ment) Only the named element lines are determined, e.g. Cu1, Cu2.
	not element symbol The named elements are not determined, e.g.not Cu, Pb.
	not element symbol + index The named element lines are not determined, e.g.not Cu1, Pb2.
Specifics	For multi-line methods, you can optionally set whether an action should be performed for each line, each element or only for the last line in the method.

Buttons

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

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

See also

B Sample information data [▶ 73]

Specifying measurements and actions in a sequence 4.3

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.

O Samples	Calibration mode Std. prep.: Number of std.:	e:	Standa prep. by 5	rd calil y samp	oration oler	
O Reag. blank	Amount	3	xxx			
	Line	f(x)	f(x=0)	w(x)	Check	Unit
 Calibration Recalibration Peak pick Special action Load method 			T		-	mg/L
)K		Acc	at a	Cancel

tions

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

Option	Description
Samples	Measure the number of samples specified under Number.
QC	Measure a QC sample and evaluate it as specified in the method

Option	Description
	After activating the option in the list, select one of the QC samples specified in the Method QCS window. The parameters of the QC sample are displayed in the opposite field.
Reference	Only flame technique
	Always define the reference sample as the first measurement in the sequence. Distilled water is used as the reference.
Blank	Measure the blank sample without analytes
QC blank DL	Measure a blank sample to determine the limits of detection and quantitation according to the blank method
Autozero/Automax	Carry out AZ-measurement (Autozero) for absorbance measurements or measurement of the maximum value for emission analyses.
Calibration	Measure the standard samples with known concentration of the ana- lyte and calculate the calibration according to the specification in the method
Recalibration	Measure the standard sample intended for recalibration and calculate a recalibration
Sample-addition	For the calibration process Method of additions calib.
	Add this sample and determine the calibration curve and sample con- centration
Blank-addition	For the calibration process Method of additions calib. and the blank correction Concentration corrected
	Add this blank sample and determine the blank
Peak pick	Determine actual line maximum of the spectral line and its deviation from the table value (offset)
	The device wavelengths are corrected according to the established line maximum and a device autozero is executed. For long measure- ments, this function can be used to correct any drift of the spectrome- ter.
Special action	These actions do not directly affect the measurement of the samples (see below).
Load method	Load a saved method to start another analysis within a sequence

Special actions

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

Option	Description
Flame on / Flame off	Only flame technique
	Extinguish/ignite flame
Clean furnace	Only graphite furnace technique
	Additional bake-out step to clean the graphite furnace. The graphite tube is heated to a predefined temperature once. The parameters for this bake-out step are specified in the New Method Furnace window.
Format tube	Only graphite furnace technique
	Formatting the graphite tube
Clean system	For hydride technique
	Also clean system The parameters for this step are specified in the Method Hydride window.
Load system	For hydride technique

Option	Description
	Following a new installation or cleaning of the hydride system as should occur daily at the end of work, the tubes must be loaded with reagents before starting the analyses. Therefore this action should oc- cur in the sequence before the first measurement.
Lamp off	Switch off hollow cathode lamp
Idle time	Wait for the entered time and then continue with the analysis
Pause	Stop the analysis
	The sequence can then be continued by clicking on $lacksquare$.
Веер	Generate a beep from the PC to notify you of an action, e.g. to indi- cate the end of calibration
Repeat/While	Repeat a part of the sequence up to the While special action
	As an abort criterion a number of loop cycles or a time in minutes can be specified. The entries in the results file are supplemented with a counter or date and time according to the abort criterion.
	For an online measurement, the autom. option must be activated. This prevents the prompt for sample metering during the manual mode.
Show Cal. plots	Display the calibration curve during the running sequence
Compute calib.	Recalculate the calibration function
Clean collector	For hydride/hydrEA technique
	Heat gold collector to remove analyte residues
Clean system	For flame technique
	Washing the sample path
Clean	Perform controlled cleaning for solution analysis
	The parameters are specified in the Method Sample transport win- dow.

Specifying a sequence

- Open the **Sequence** window by clicking on **E**.
- Click on **Append**.
 - ✓ The Edit sequence window with the measurements and actions available for the current method 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.
- Optionally, enter the elements to be analyzed in the **Elements** table column.
- When using the autosampler: Specify the position of the samples on the autosampler. The positions of standard samples and QC samples are taken as a default setting from the method. You can edit these positions here.

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

Usual sequence for a measurement routine A usual sequence contains the measurements in the order:

- 1. For flame technique: Reference measurement
- 2. Calibration

3. Number of samples

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

See also

- B Specifying flame parameters (Method | Flame window) [▶ 32]
- B Specify Hydride and HydrEA systems (Method | Hydride window) [▶ 40]
- Specify parameters for autosampler (Method | Sample transport window) [43]
- Entering the furnace program (Method | Furnace window) [> 33]
5 Sample information data

The sample information data (sample IDs) include the specific data for the analysis samples and QC samples, such as sample name, position on the autosampler, weight, dilution or concentration unit. Sample names and positions can be sent 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 LS.

Open the Samples ID window by clicking on **I** in the toolbar or via the menu item **Method Development** | **Sample ID**.

5.1 Creating, saving and opening sample information data

Creating a new sample ID set	•	In the toolbar, click on I or select the menu commands Method Development Sample ID or File New Sample Information File .
		✓ The Sample ID window appears.
		Specify the settings for samples and QC samples.
		Click on OK or Accept to activate the data records.
		✓ The sample IDs are activated and will be used for the next analysis. You can also save the sample ID for a later analysis.
Saving sample IDs		In the Sample ID window, click on Save or select the menu item File Save Sample information .
	►	Save the data record in the standard window Save as .
		✓ The sample IDs are saved in CSV format. You can load the data for further analy- ses or edit it in a spreadsheet program or text editor.
Open sample information data		You can open a sample ID file using one of the following alternatives:
		 In the toolbar, click on the <u>icon next</u> to the Samples field.
		- Select the menu item File Open Sample Information File.
		– In the Sample ID window, click on Open.
	►	Choose the file in the Open standard window.
		✓ The sample IDs are displayed in the Sample ID window and can be used for the next analysis.

5.2 Sample ID window

In the **Sample ID** window, you can specify the samples and QC samples. In addition to the name and position on the autosampler, you can enter parameters important for the analysis. Open the **Sample ID** window by clicking on **1**.

Sampl	mple ID le inform	ation OC some	lo informatio									o x
	Pos	Name	Pre-DF	Unit	Wt. [a]	Vol. [mL]	Name(2)	AS-DF	3lank corr	Sample type	Elements	•
1	1	Sample 1 Sample 2	1.000 1.000	mg/L mg/L		100.00 100.00		1.00 1.00	off off	Sample Sample	all all	
3	3	Sample 3 Sample 4	1.000	mg/L mg/L		100.00		1.00	off off	Sample Sample	all all	
5 6 7	5 6 7	Sample 5 Sample 6 Sample 7	1.000	mg/L mg/L mg/l		100.00		1.00	off off	Sample Sample Sample	all all all	
8	8 9	Sample 8 Sample 9	1.000	mg/L mg/L		100.00 100.00		1.00	off off	Sample Sample	all all	
10	10	Sample10	1.000	mg/L		100.00		1.00	off	Sample	all	
R	Rows t≡ t≡ t≡ Append Insert Delete Number: 9											
Sample ID->Sequence From sequence row 1 Sequence -> Sample ID 1												
🗂 Open 📑 Save 👼 Close												

Sample information

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

Column	Description
Pos	Position of sample on autosampler
Name	Sample name
	This entry is optional. Maximum number of characters: 20
Pre-DF	The predilution factor is the factor by which the original sample has been diluted before it is placed in the autosampler or fed to the spec- trometer when working without autosampler. The factor is necessary to calculate the concentration of the original sample (Conc.2 in the results table).
Unit	Concentration unit of sample.
Wt.	Initial weight (for solution analytics only)
	This mass (in g) of the original sample was brought into solution in the sample pretreatment. The initial weight is necessary to calculate the concentration of the original sample (Conc.2).
	Note: For solid analytics, known sample initial weights must be speci- fied in the Solid results window or weighed before the measurement of unknown sample weights.
Vol.	The initial weight was dissolved in this volume (in mL) of the solvent. This value is required for the calculation of the concentration of the original sample (Conc.2).
Name (2)	Additional sample name The entry is optional. Maximum number of characters: 20
AS-DF	Dilution factor of the autosampler.
	Note: The dilution mode used here is defined in the Method Sample transport window.
Blank corr.	Blank correction
	off No blank correction is performed.
	on For calculating the concentration of the original sample, the blank

For calculating the concentration of the original sample, the blank value measured last in the sequence is subtracted.

Column	Description
	Note: You specify the procedure for blank correction in the Options Calibration window.
Sample type	Selection of the sample type Blank or Sample
	The sample data of the sample ID is assigned to the sample order in the sequence according to the sample type, i.e.
	1st blank value in sample ID = 1st blank value in sequence
	2nd blank value in sample ID = 2nd blank value in sequence
	1st sample in sample ID = 1st sample in sequence
	2nd sample in sample ID = 2nd sample in sequence etc.
Elements	Only multi-element methods
	Elements or element lines to be analyzed from a sample
	all All elements/element lines specified in the method are determined (default setting).
	Element symbol Only the named elements are determined, e.g. Cu, Pb.
	Element symbol + index (when analyzing several lines of an ele- ment) Only the named element lines are determined, e.g. Cu1, Cu2.
	not element symbol The named elements are not determined, e.g.not Cu, Pb.
	not element symbol + index The named element lines are not determined, e.g. not Cu1, Pb2.

Buttons

Button	Description
Append	Insert number of new rows at the end of the list
Insert	Insert number of new rows at the selected place in the list
Delete	Delete the selected row
Number	Input field for the number of rows to be inserted or deleted
Delete table	Deletes the complete table of sample information
Sample ID->Se- quence	Transfers sample names and positions on autosampler to the se- quence list. Define the first row of the information to be transferred in the sequence list in the From sequence row input field.
Sequence -> Sam- ple ID	Transfer sample names and positions in the autosampler from the se- quence list to the sample information table. Define the first row of the information to be transferred in the sequence list in the From se- quence row input field.

QC sample information

The QC samples are shown on this chart analogous to **Sample information** charts. In addition, the **Type** column contains information about the QC type. The **Unit** column is omitted because the unit is defined in the method. Blank correction is not available for QC samples.

Button

Button	Description
QC sample ID->Se-	Transfers QC sample names and positions on autosampler to the se-
quence	quence list.

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

See also

- Specify parameters for autosampler (Method | Sample transport window) [43]
- General settings for calibration and blank correction [172]
- Frequently used control elements [▶ 18]

5.3 Specifying information data for samples and QC samples

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

- Open the **Sample ID** | **Sample information** window by clicking on **I**.
- 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 all rows are the same, you can click on ↓ to copy the entry of a selected cell to all subsequent cells of the column. If the inc. (increment) option is activated, the value is increased by 1 each time the information is transferred to the next row. This makes it easy to fill spaces in the autosampler or to number sample names consecutively.
- You can copy text from the input fields to the clipboard and paste it again. To do this, use the key combinations Ctrl+C and Ctrl+V or use the context menu commands after right-clicking on the table cell.
- When all information has been entered, in the From sequence row field enter the row of the sequence from which the sample information is transferred to the sequence. Click on Sample ID->Sequence to apply the information.
- Specify the QC sample information in the same way in the Sample ID | QC sample information window.
 - \checkmark The sample information will now be used for the next analysis.

6 Performing analyses and calculating results

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

lcon	Menu item Routine	Function
	Run sequence	Start an analysis process
	Run Selected Se- quence Row F6	Execute the selected line in the sequence. Several rows can be marked using the mouse in combination with the Ctrl- and/or Shift-Key.
\times	Stop	Stop the analysis process immediately
		The stop function should be used only with the flame technique. For hydride-/hydrEA technique and graphite tube technique sample residue remains in the system or graphite tube with direct stop and it can lead to contamination.
	Break	For hydride/hydrEA technique and graphite furnace technique
		Register a program interruption when executing a hy- dride or furnace program
		After this request was detected, the button is grayed out. The current sample measurement is processed to com- pletion, then the analysis is stopped.
	Continue	Continue a stopped routine
C	Reprocess	Reprocesses the results, if the original data, e.g. the cali- bration function or the method, have changed.

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

6.2 Starting a measurement routine

After you have selected the method, the sequence and possibly the sample information data, the system has all information necessary to start the analysis process.

The AAS must have been prepared for the technique to be applied:

- Flame technique: The flame has been ignited and burns longer than the specified warm-up time.
- For graphite technique: The furnace is ready.
- Hydride technique: The cell is pre-heated.
- Autosampler: Samples have been prepared and placed onto the tray.
- HCL is switched on and burns for at least 20 min.

Saving analysis results during the analysis process

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

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

art measurement Sequence:					
Results file					
Name:	Current method:				
Results	AspectLS_SW-Test1				
Folder:	Version: 2 from: Posults				
(Standard)					
Description:	Continue with:				
	AspectLS_SW-Test1 Version: 2				
 New file/list Append to file/list 					
Switch off lamp/flame after e	ror stop				
"Attach date/time to the results filename	" is active ("Options"). OK Cancel				
Option	Description				
Name	Enter the file name for the result database				
	New file/list If activated, a new file name must be entered. The program checks if the file name exists already. Existing files cannot be overwritten.				
	In the Options Analysis sequence window, if the Attach date/time to the results filename option is enabled, this information is auto- matically appended to the results name. A message about the en- abling of this option appears in this window.				
	Append to file/list				
	New results are appended to an existing results file. Use •••• to open the selection dialog. Choose an existing results file from the displayed list.				
Folder	Choose the save path for the results file				
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.				
Switch off lamp af- ter error stop	When the measurement is stopped because of an error the HCL is automatically switched off.				
OK	Start measurement				

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

The result database is saved with the extension ".tps".

Start measurement

- Start the measurement routine using menu command Routine | Run sequence or by clicking on .
- In the Start measurement Sequence window, select a file name for the results file. You may optionally save the result to a new file or append it to an existing file. Overwriting of an existing file is not possible.
 - ✓ After you select the file name, the measurement routine will start according to the settings made in the method and the sequence. If you use an automatic sampler, the measurement runs automatically. In the case of manual sample feed without autosampler, follow the prompts for the provision of samples displayed on the screen.



Displays during the analysis process

NOTICE

With multi-element methods, the sequence is processed according to the order of the elements or element lines in the method. The sequence is first processed completely for the first element before the sequence starts again with the second element. In the sequence, the measurement of certain elements can be excluded or agreed for individual samples. Waiting times can also be inserted depending on the element

While the measurement is running, the results are displayed in real time in the main window. In addition, the following windows can be opened.

- Signal plot: Measurement signal curve
- Bar graph: Measured values in a bar graph
- Report window: Current flame status or furnace status
- **Sample conc. in calibration curve**: Position of the determined sample concentration in the calibration curve

You define these display windows in the **Options** | **Analysis sequence** window. The display windows can also be closed or opened during the measurement:

- While the measurement is running, you can click on Display windows and activate or deactivate the desired windows.
- Use the View | Open Results Windows F7 menu command to open the display windows.
- Use the View | Close Results Windows F8 menu command to hide the display windows.

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:

··· •·· •	
- Not measured/exe	cuted yet.
0 Just being measur	ed.
+ Already measured	/executed.

Additionally, in the symbol bar at the side large buttons are displayed during measurements:

Option	Description
oisplay win- dows	Open and close display windows
Activate scraper	The scraper cleans the burner head between two measurements within a statistics series of a sample.
Show method	Open method window
	The method can only be read, but not edited.
Sequence Samples	Show sequence window
	The sequence can be extended while the measurement is running. The sequence window includes a Sample ID button that allows you to edit further sample ID data.
Extinguish flame	Stop the analysis process immediately and extinguish the flame

See also

- Creating predefined notes [▶ 164]
- B Sequence window [▶ 67]
- B Options for analysis sequence [▶ 171]

6.3 Interrupt, stop and resume measurement routine

A running measurement routine can be interrupted and then resumed. However, when using the graphite furnace technique and the hydride technique, the currently running sample measurement should be finished first and only the analysis process stopped. This procedure is to prevent sample residues from being deposited in the graphite tube or hydride system. With the flame technique, the measurement can be stopped at any time.

- ▶ Use **Routine** | **Stop** or click on **X** to stop the analysis process immediately.
- Use Routine | Break or to register an interruption in the analysis process. After this request was detected, the button is grayed out. The currently running hydride program or furnace program will be finished first. Then, the analysis process will be stopped.
- Use Routine | Continue or by to resume a stopped/interrupted routine. The Continue sequence dialog box opens where the action status prior to the interruption is output.

If the method is changed, activate the **Continue with modified method** option. This results in a new method entry in the results file and another version of the method is saved.

The measurement can be continued as follows:

Option	Description
First statistical run	Continue with current sample, current line and first statistics mea- surement (reset statistics)
From table row ->	Continue with current line and adjacent table position
next element	Continue with next line and first place in the table

6.4 Repeating actions of the sequence

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

- In the main window on the Sequence or Sequence/Results tab, select the rows with the actions to be repeated.
- In the Start measurement window, select a file name to which the result of the repeated measurement shall 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.
 - ✓ After you selected the file, the selected action will be repeated.

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

6.5 Reprocessing analysis results

Each time the evaluation conditions are changed, e.g. change of the calibration function, method changes, etc., the results must be reprocessed to let the changes take effect. Likewise, it is possible to change sample information data, such as sample names and dilution factors, and have them taken into account for the presentation of analysis results. The options for the reprocessing are specified in the **Reprocess results** window.

C	Reprocess results		×						
	Start data Name:								
	C:\Users\Public\Documents\Analytik Jena\ASpectLS\FL\RESULTS	Α							
	✓ Modified sample information data ☐ Allow QC chart entries								
	Reprocess entries								
	from to								
	1 - 3 - Update result plots								
	Folder:								
	(Standard)								
	Name								
	New file/list Append to file/list								
	Description: (Select)	\sim							
		^							
		Ť							
	ОК	Cancel							

Options in the Reprocess results window

Option	Description			
Name	Name of original file with analysis results.			
Modified sample information data	ample information data were changed and shall be updated in re- processing.			
Allow QC chart en- tries	nter reprocessed values on the QC charts if QC charts are specified in ne method			
Reprocess entries	Reprocesses the entries in the result list covering the rows specified in the by and to fields.			
Update result plots	Update the display windows during reprocessing			
Folder	Choose the save path for the results file			
Name	Enter the file name for the results file			
New file/list	New file name entered. The program checks if the file name exists al- ready. Existing files cannot be overwritten.			
Append to file/list	Append the reprocessed values to the existing file			
Description	This additional note is saved with the reprocessed analysis results. The entry is required if the optional 21 CFR Part 11 compliance mod- ule is installed. User-defined descriptions can be selected from the list.			

Performing reprocessing

- Click on Conservation of the menu command Routine | Reprocess.
 The Reprocess results window opens.
- Specify the options and select a file name.
- Click on **OK**
 - \checkmark The reprocessing is performed.

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

See also

■ Creating predefined notes [▶ 164]

6.6 Evaluating measurements parallel to running analyses

No further evaluation of results can be carried out during measurement operation, but another program instance of the application can be opened in offline mode. In this mode, there is no communication with the device. 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 LS in the second instance by menu command File | Start Offline Program Instance.
- Open the results file of the running measurement using menu command File | Open Results.

The results measured so far will be loaded in the result window.

- Further results of the running measurement can be loaded via menu command View | Reload results list (if new results are measured by the online program instance or by clicking on .
 - ✓ The results display is updated. You can edit the results further, e.g., by opening the sample details or selecting a different calibration function.

See also

- Displaying details of single values of samples [> 88]
- Calibration [▶ 97]

6.7 Displaying results and analysis progress in the main window

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

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

≊ × I	IF C Meth: AspectLS	SW-Test1	Cu 2	0-03-03	C1) Sample	: untitled		6						lytikjen
S	equence/Results Sequence	e Results (Overview											ielect columns.
ž	No. Type / Name		Pos.	No.	Name	Line	Conc.2	SD2	Unit	Conc.1	Unit	Abs.	RSD%	Rem.
meter	1 Autozero	43		32	QC-Std.4	Cu 324			ma/L	0.7907	ma/L	0.08478		QCI->cal
	2 Cal-Zero1	43		33	Nullaboleich	Cu 324			mg/L		mg/L	0.00000		
?	3 Cal-Std1	45		34	KalNull1	Cu 324				0	ma/L	0.00468		
ne	4 Cal-Std2	46		35	KalStd.1	Cu 324				0.2	ma/L	0.02264		RSD!
	5 Cal-Std3	47		36	KalStd.1	Cu 324				0.2	ma/L	0.02551		RSD!
t i	6 Cal-Std4	48		37	KalStd.2	Cu 324				0.5	ma/L	0.06205		RSD!
od	7 Compute calib.			38	KalStd.2	Cu 324				0.5	mg/L	0.06416		RSDI
	8 Sample 001	1		39	KalStd.3	Cu 324				1	mg/L	0.12861		RSD!
6	9 Sample 002	2		40	KalStd.3	Cu 324				1	mg/L	0.12949		RSD!
npler	10 Sample 003	3		41	KalStd.4	Cu 324				2	mg/L	0.25315		RSD!
	11 Sample 004	4		42	KalStd.4	Cu 324				2	mg/L	0.26100		
	12 Sample 005	5		43	Kalib. berechnen	Cu 324								R ² (adj.)!
e ID	13 QC-Std.4	48		44	QC-Std.4	Cu 324			mg/L	1.965	mg/L	0.25642		#KOR QC
				45	10ppm Cu	Cu 324	6.714		mg/L	6.714	mg/L	1.0156		>KAL
				46	10ppm Cu	Cu 324	10.54	225.4	mg/L	10.54	mg/L	0.07637		RSD!
nce				47	10ppm Cu	Cu 324	10.95	34.51	mg/L	10.95	mg/L	0.07926		#KOR RS
,				48	QC1_2ppm Cu	Cu 324	-0.1894	18.17	mg/L	-0.1894	mg/L	0.00174		<kal qc<="" td=""></kal>
-				49	QC1_2ppm Cu	Cu 324	1.381	0.3666	mg/L	1.381	mg/L	0.17834		RSD! QC
tion				50	QC1_2ppm Cu	Cu 324	0.5446	0.0030	mg/L	0.5446	mg/L	0.07035		QCI->rec
				51	Nullabgleich	Cu 324			mg/L		mg/L	0.00000		
				52	AspectLS_SW-Tes									
				53	Nullabgleich	Cu 324			mg/L		mg/L	0.00000		
				54	QC2_2ppm Cu	Cu 324	2.128	0.0117	mg/L	2.128	mg/L	0.27882		QC!->ca
				55	Nullabgleich	Cu 324			mg/L		mg/L	0.00000		
				56	QC2_2ppm Cu	Cu 324	1.349	0.4947	mg/L	1.349	mg/L	0.17439		RSDIQC
				57	QC2_2ppm Cu	Cu 324	0.5935	0.0097	mg/L	0.5935	mg/L	0.07650		QC!->ca
				58	Nullabgleich	Cu 324			mg/L		mg/L	0.00000		
eet				59	AspectLS_SW-Tes									
				60	Nullabgleich	Cu 324			mg/L		mg/L	0.00000		
				61	KalNull1	Cu 324				0	mg/L	0.00456		
				_										

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** (presentation of measurement results)
- **Overview** (summary of the measurement results)
- Solid (preparation of the solid samples for analysis)

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

6.7.1 Sequence/Results tab

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

See also

- Sequence tab [> 83]
- Results tab [▶ 84]

6.7.2 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:

lcon	Description		
-	Not measured/executed yet.		
0	Just being measured.		
+	Already measured/executed.		

After the measurement, a selected sample can be measured again. To this end, you must have marked the sample row in the sequence. Then, click on the toolbar.

6.7.3 Results tab

All measurement results and statistical evaluations are listed on the **Results** tab. 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.

Abs./Time table

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

Column	Description
No.	Number in analysis sequence
Name	Sample name
Line	Element line
Abs./Ems	Mean or median of the measured single absorbance/emission values
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)
RSD%	Relative standard deviation (mean value statistics)
Date/Time	Date and time of sequence start
Single values(Abs./ Ems)	Single values of absorbance measurements (emission measurement)

Conc.1 table

The table shows the analyzed concentrations of the samples as supplied to the AAS.

Column	Description				
No.	Number in analysis sequence				
Name	Sample name				
Line	Element line				
Unit	Concentration unit				
Conc.1	Analyzed concentration of sample				
SD1	Standard deviation of Conc.1 (mean statistics)				
RSD%	Relative standard deviation of Conc.1 (mean statistics)				
R	Range of Conc.1 (median statistics)				
R%	Relative range of Conc.1 (median statistics)				
Cf	Confidence interval				
DF	Dilution factor if concentration is exceeded				
	If the concentration is exceeded, you can activate automatic dilution with the sample changer in the Method Sample transport window. The dilution factor of this automatic dilution is taken into account in the calculation of Conc.1 .				
Rem.	Marking of events during the measurement				
Abs./Ems	Mean or median of the measured single absorbance/emission values				
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)				
Date/Time	Date and time of sequence start				
Single values(Abs./ Ems)	Single values of absorbance measurements (emission measurement)				

Conc.2 table

The table shows the concentrations of the original sample. In calculating **Conc.2**, the sample information data (see **Sample ID** table below) are considered:

Pre-dilution

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

Column	Description				
No.	Number in analysis sequence				
Name	Sample name				
Line	Element line				
Unit	Concentration unit				
Conc.2	Concentration of original sample taking sample information data into account				
SD2	Standard deviation of Conc.2 (mean statistics)				
RSD%	Relative standard deviation of Conc.2 (mean statistics)				
Cf	Confidence interval of Conc.2				
Rem.	Marking of events during the measurement				
Abs./Ems	Mean or median of the measured single absorbance/emission values				
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)				
R(Abs.)	Range of absorbance values (median statistics)				
Single values(Abs./ Ems)	Single values of absorbance measurements (emission measurement)				

QC Res. table

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

Column	Description			
No.	Number in analysis sequence			
Name	Sample name			
Line	Element line			
QC (for calibration	R²(adj.)			
functions)	Slope			
	Char.conc.: Characteristic concentration			
QC (for QC samples,	Conc.1			
not for QC blank)	Nominal val.: Concentration setpoint			
	Recovery : Recovery rate For QC samples and QC standard, the recovery rate of the concentra- tion is determined. For QC-Stock, QC-Trend and QC-Matrix, the recov- ery rate of the concentration increase caused by the spiking is deter- mined.			
QC (for blank detec-	SD: Standard deviation of the blank measurements			
tion limit)	LOD: Limit of verification			
	BG: Limit of determination			
Rem.	Marking of events during the measurement			
SD(Abs.)	Standard deviation of absorbance values (mean value statistics)			
Date/Time	Date and time of sequence start			
Single values(Abs./ Ems)	Single values of absorbance measurements (emission measurement)			

Error table

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

Single values table

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

Sample ID table

The table contains the sample information data.

Column	Description				
No.	Number in analysis sequence				
Line	Element line				
Туре	Sample type (e.g., Sample, Blank, QC sample)				
Pos	Position of sample on autosampler				
Pre-DF	Predilution factor This is the factor by which the original sample has been diluted be- fore it is placed in the autosampler or fed to the device when working without autosampler. The factor is required for the calculation of the concentration of the original sample.				
Wt.	Only for solution analytics				
	Initial weight in grams Mass of the original sample in grams, which was dissolved in solution (in mL). The mass is necessary to calculate the concentration of the original sample (Conc.2).				
Vol.	Volume of solvent used to dilute the weighed sample portion (in mL). This value is required for the calculation of the concentration of the original sample (Conc.2).				
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 (Conc.2) , the blank concentration determined last in the sequence was subtracted.				
	Note: In the Options Calibration window, select whether Conc.2 or Conc.1 of the blank is used for the blank correction.				

Energy set. table

Not for novAA 800

The table contains an overview of the set device parameters.

Column	Description			
No.	Number in analysis sequence			
Name	Sample name			
Line	Element line			
РМТ	Voltage of the photomultiplier in V			
HC ampl. level	Amplification of the hollow cathode lamp signal			
BC ampl. level	Amplifier stage of the background signal			
D2 current	Current of the deuterium lamp			

User defined table

In this table, you can select the parameters for the results output and their order.

- Click the **Select columns** button in the top right corner of the tab.
- 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 **F** and **t** in the list. Several simultaneously selected parameters are moved as a block.
- After returning to the main window the results are displayed. You can change the width of the table columns by moving the mouse pointer to the table line in the table header (the pointer changes to a double arrow) and 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.

Solids Table

This table is displayed when analyzing solids using the graphite furnace technique.

Column	Description				
No.	Number in analysis sequence				
Name	Sample name				
Line	Element line				
Norm.abs.	Mean value of the standardized absorbance (absorbance / weighed portion)				
SD	Standard deviation of the conc. 1 (mean value statistics)				
RSD%	Relative standard deviation of the conc. 1 (mean value statistics)				
Mass	Mean absolute analyte mass				
Unit	Absolute unit of the analyte				
Hum.[%]	Relative moisture of the sample				
Wt.	Weights for all individual amounts				
Date/Time	Date and time of sequence start				
Single values(Abs./ Ems)	Single values of absorbance measurements (emission measurement)				

See also

Overview of markings used in the display of values [185]

6.7.4 Overview tab

The results of the analysis are summarized on the **Overview** tab. You can choose from the following outputs:

Column	Description				
Conc.1	Analyzed concentration of sample				
Conc.2	Concentration of original sample taking sample information data into account				
Abs(RSD/R)	Standard deviation or median of the individual absorbance values				
Abs./Ems	Mean or median of the measured single absorbance/emission values				
SD	Standard deviation of Conc.1 (mean statistics)				
RSD	Relative standard deviation of Conc.1 (mean statistics)				
LOD	Limit of verification				
LOQ	Limit of determination				
Recovery(Nominal val.)	Recovery rate (setpoint)				
R²(adj.)	Corrected coefficient of determination R ²				

By activation of the respective check boxes, the following sample types can be displayed:

- Samples
- QC samples
- Cal-Std
- Other

Click on 🖶 to open the **Print Overview** window, from which you can start the printout of the data displayed in the current overview.

See also

Print functions [> 155]

6.7.5 Solid tab

Not available for novAA 800 and ZEEnit 700 Q

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

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

See also

Solid analysis with graphite furnace technique [> 91]

6.8 Displaying details of single values of samples

For each measurement in the main window, the individual values of the statistics measurement can be shown in the **Single values** window.

- Open the **Single values** window by double-clicking on the corresponding sample row in the results table.
- Alternatively, right-click on the sample row and click on **Detail results** in the context menu or select the sample row and choose the menu command **View** | **Detail results**.

Si	ingle	values - [QC	2_2ppm Cu]			
(Cu	324	No.: Type: Name:	57 QC : QC2_	sample2 S 2ppm Cu	Abs.: SD: RSD:	0.07650 Date: 31.08.2010 0.00123 Time: 14:00 1.6 1.6 1.6
	No.	Rem.	Abs.	Conc.1 mg/L	Abs. BG	0.100)
	1		0.07544	0.5851	-0.00632	0.075	5 bitterholide as bits as blocks when the del the
	2		0.07623	0.5914	-0.00686	0	In advantage and a second and the second and the second
	3		0.07784	0.6042	-0.00637	G 0.050	
						0.025	5
						0.000	A A A A A A A A A A A A A A A A A A A
						0	0.0 0.5 1.0 1.5 2.0 2.5 3.0
	<				>		Time [s]
		Delete		✓ Overla	pped		Q 2 T
		• •					OK Cancel

Sample data

The following sample data is displayed in the upper part of the window:

Field	Description				
Tield	Description				
Pb 283 (example)	Analyzed element line				
No.	Number of measurement in the result table				
Туре	Sample type				
Name	Sample name				
Abs.(Ems)	Absorbance or emission value (averaged over all single values)				
SD	Standard deviation (mean value statistics). This parameter is dis- played independently of the statistical method chosen for the mea- surement (mean/median).				
RSD	Relative Standard Deviation (mean value statistics). This parameter is displayed independently of the statistical method chosen for the measurement (mean/median).				
Date/Time	Date and time of the measurement selected in the table				

Single value display

The measured single values of the samples (statistic runs) are shown in the table.

Column	Description			
No.	Number of single value within the sample measurement			
Wt.	For solid analytics			
	Weighed portions of individual samples.			
Abs.	Calculated absorbance of single value			
	For solid analysis: normalized absorbance			
Conc.1	Analyzed concentration of the sample as it was supplied to the AAS. Pre-dilutions and weighed portions were not yet taken into account.			
Abs. BG	Absorbance of the background			
Rem.	Empty: The single value is included in the calculation of the sample mean.			

	Column	Description
		MAN The value was manually excluded from the calculation of the sample value
		KOR The value was automatically excluded from the sample value calcula- tion due to the Grubbs outlier test.
Delete/reactivate individual sample values	If desired, you average. Afte change to tak To this er Click on D sults repr Click on R Note: By activ detected and	a may manually exclude a single value from the calculation of the sample r deleting or reactivating a single value, recalculation is necessary for the e effect. nd, mark the single value to be excluded in the table. Delete to exclude the value from the calculation of the sample mean for re- ocessing. Reactiv. to include the selected individual value in the calculation again. vating the Grubbs outlier test option, outliers among single values can be eliminated automatically during the analysis.
Graph	In the graph r function of tir posed.	ight of the table, the signal curve of the marked single value is shown as a me. If you activate the Overlapped option, all curves are displayed superim-
	The following	J functions are available for the graphics:
	lcon	Description
	€	Enlarge graphic section / Zoom
	୍ର	Reset graphic to original size
	т	Insert note in the graphic
	1	Click on the button and draw a frame in the graphic with the mouse. You can write a note in this frame.
Copying signal values to the clipboard	You can copy the clipboard sheet prograr	the signal values of the sample displayed in the Single values window to using the key combination Ctrl+C . You can insert the data into a spread- n (e.g. Excel or Origen) and generate graphics for publications.
Change sample line	You can switc row buttons:	h between the rows of the sample table in the main window using the ar-
	lcon	Description
	•	Display values of the previous sample in the sample table
	•	Display values of the next sample in the sample table
Replace standard	Only for calib	ration standards and samples with addition calibration

An outlier in the calibration can be replaced by a re-measured standard value by activating the **Replace with entry number** option and specifying the line number of the remeasured standard. A recalculation is required for the change to take effect.

See also

■ Replacing calibration standards by re-measurement [▶ 100]

6.9 Solid analysis with graphite furnace technique

Solid analysis in the graphite tube is available for the following devices:

- ZEEnit 700 P
- ZEEnit 650 P
- novAA 400 P

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

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

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

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

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

6.9.1 Functions on the Solid tab

	Seq.		T	News	1.1		Wt	Tare	0	Std.			
NO.	Row	Pos.	Type	Name	Line	#	[mg]	[mg]	Dos.	Mod.			
1	1	1	Cal-Zero1		Pb 283	1							
2	2	2	Cal-Std1		Pb 283	1							
3	3	3	Cal-Std2		Pb 283	1							
4	4	1	Cal-Std3		Pb 283	1							
5	5	2	Cal-Std4		Pb 283	1							
6	6	3	Cal-Std5		Pb 283	1							
7	8	1	Sample	Sample 001	Pb 283	1	2.016	49.886					
8	8	2	Sample	Sample 001	Pb 283	2	2.000	50.094	*				
9	8	3	Sample	Sample 001	Pb 283	3	2.092	49.476	*				
10	8	1	Sample	Sample 001	Pb 283	4	2.059	49.960	*				
11	8	2	Sample	Sample 001	Pb 283	5	2.100	50.660	*				
12	9	3	Sample	Sample 002	Pb 283	1							
13	9	1	Sample	Sample 002	Pb 283	2							
14	9	2	Sample	Sample 002	Pb 283	3							
15	9	3	Sample	Sample 002	Pb 283	4							
16	9	1	Sample	Sample 002	Pb 283	5							
17	10	2	Sample	Sample 003	Pb 283	1							
18	10	3	Sample	Sample 003	Pb 283	2							
19	10	1	Sample	Sample 003	Pb 283	3							
20	10	2	Sample	Sample 003	Pb 283	4							
21	10	3	Sample	Sample 003	Pb 283	5							
22	11	1	Sample	Sample 004	Pb 283	1							
23	11	2	Sample	Sample 004	Pb 283	2							
24	11	3	Sample	Sample 004	Pb 283	3							
						F	repare sar	nples					1
	Measure	row(s)	Prepa	are re-measurement	from		Tai	re		Dosin)	Weigh	

Table elements

The table contains the following entries:

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

Column	Description				
Pos	Designates the positions of sample platform on the SSA 600 tray. Po- sitions range from 1 to 42 in single-tray mode and from 1 to 84 in double-tray mode.				
	Note: Positions are assigned by the software! Samples must be distributed according to predefined positions.				
Туре	Type of the sample which needs to be placed, or has already been placed onto this platform.				
Name	Name of sample				
Line	Analytical line				
#	Number within the statistics measurement				
Wt.	Mass of the sample in mg				
	If the entry "" is found in this column, the sample is not to be weighed and contains only liquid components (e.g. liquid standard).				
	Note: Before determination of the weighed portion the tare of the sample platform must be established.				
Tare	Mass of the empty platform in mg				
	For samples not to be weighed, this entry will also be "".				
Dos.	Sample was dosed onto the platform, unless there is a "*" marker				
Std. Mod.	If marked with "*", this element indicates that liquid components (standards or modifiers) are dosed onto the platform				
Pretreat.	Only if thermal pretreatment is defined in the method				
	If marked with "*", thermal pretreatment was carried out for the plat- form				

If known, the following settings can be directly entered at the sample table:

- Weighed portion if sample preparation occurred on external scales
- Deadweight (tare)
- Marking for completely dosed sample platform
- Marking for pipetted modifiers
- Marking for thermal pretreatment

Buttons for sample preparation	Button	Description
	Tare	Determines the weight of an empty platform for marked tray positions
		This is accomplished by transferring the respective position contents onto the scales and returning them onto their positions after weigh-ing. The determined weight is entered in the Tare column.
	Dosing	Transfers the platforms of marked positions successively into dosing position
		A dialog window appears with details regarding the sample that needs to be dosed. Depending on what options were selected, more preparations can be made before or after this sample for marked posi- tions. If a table already contains entries, related preparations will be skipped. Compliance with this order: Tare - Dosing - Weighing - (Dos- ing) - (Weighing) - Mod./Std Pipetting is compulsory.
		with tare Weight of empty platform is determined in advance.
		with weighing After dosing, the dosed sample is weighed.
		with Mod./Std. pipetting After weighing, the platform is taken to the liquid dosing station.

Button	Description
	If the Weigh with confirmation option is configured in the Method Sample transport window, the Dosing and Weigh steps can be re- peated as often as required. If all three options are enabled, this se- quence may be used to run a complete sample preparation procedure. On completion of this sequence, the tray will contain filled platforms that are completely prepared for analysis. If one of the preparatory steps was not carried out, this step will be requested as part of the an- alytical procedure.
Weigh	Weigh dosed platforms
Load/Save	Save and reload weighing and dosing data of selected rows
	When changes are made to the sequence or method, the sample table is recreated on the Solid tab. The existing entries will be lost. You can save and restore data using the Load/Save function.
Std./Mod.	Only for SSA 600 without liquid dosing
	Successively transfers the platforms of marked positions into the posi- tion for dosing of liquid analytical constituents (liquid standards, mod- ifiers)
	Displays a dosing screen for liquid dosing. This screen shows the liq- uids and volumes to be dosed.
Prepare	Burn out the platforms of the selected position
	Place the platforms into the furnace, trigger and run burn-out pro- gram and return the platforms to the tray as soon as the furnace has cooled down.
	During thermal pretreatment, the appropriate modifiers are first pipetted onto the platforms. Then the furnace program is run down to the E/P step. After the furnace has cooled down, the platforms are transported back to the tray.
	If the with tare option is selected, the platforms are weighed and their weight entered in the Tare column.

Re-analyzing samples and correcting weight entries

Measure row(s) Newly determine an element in a sample or measure a sequence vidually in the method development. Note: For row measurement of the sample sequence the start muture interview.	indi- st
Note : For row measurement of the sample sequence the start mu	st
always occur with statistic run 1 or the following run of the last m sured statistic run.	cu
Prepare re-mea- surementCreates the current Solid tab of the statistics run to be remeasure from the entries for remeasuring selected in the results table. After this these sample platforms can be correspondingly dosed and 	d ?r
Re-measure single val.Start measurement of the samples selected with Prepare re-mea surement.	-
Delete entriesFor selected table rows, delete all entries in columns starting with umn Wt.	col-

See also

- Re-analyze samples for solid analysis [▶ 95]
- Method parameters for autosampler for graphite furnace technique (solid analytics)
 [▶ 49]

6.9.2 Measuring solids samples

Manual solid analysis	If the samples are placed in the graphite tubes with the help of the manual autosampler SSA 6(z), the weighed portion must be determined on a separate scale. Enter the weights manually on the Solid tab.
Automatic solids analysis for non-time-critical samples	For non-time-critical samples, many preparation steps can be combined. The processing of non-time-critical samples is specified by deactivating the Workflow for time critical samples option in the Method Sample transport window.
	When using the SSA 600 with automatic liquid dosing, the dosing of modifiers and stan- dards can take place during the processing of the sequence and does not have to be pre- pared manually. Up to four standards and three modifiers can be placed on the SSA 600. If more standards or modifiers are needed, they have to be pipetted manually. During thermal pretreatment, the modifiers are automatically applied to the platforms using the liquid dosing unit and then prepared for analysis in the graphite furnace.
	Automatic analysis without operator intervention requires a sample platform for each individual measurement:
	Total number of sample platforms = number of analytical samples x number of analyti- cal lines x number of sample measurements in a statistical series
	If the number of samples exceeds the number of platforms defined in the method, the platforms are re-dosed after processing.
	 Create a method and a sequence.
	Switch to the Solid tab in the main window.
	 The Pos column shows the assignment of samples on the autosampler trays. The assignment is determined by the software and cannot be changed.
	Start the processing of the sequence row by clicking on .
	Prepare the sample platforms according to the program instructions. Place the samples and pipette liquid components if necessary.
	 The measurement starts when all samples have been prepared or the number of sample platforms defined in the method have been filled.
	If there are still samples left after the first measuring run, select the corresponding sample rows in the sequence with the mouse. Hold down the Shift or Ctrl key to se- lect several rows.
	Resume the measurement with and append the results to the existing ones by ac- tivating the Append to file/list option in the Start measurement window.
	Prepare the sample platforms again according to the program instructions. Then the measurement starts automatically.
	 Continue until all the samples have been processed.
Automatic solids analysis for time-critical samples	Samples that volatilize easily or "creep" out of the platform due to high adhesion and wet the edge and handle of the platform require rapid processing of the platform after sample application. If you would like to analyze such samples, enable the Workflow for time critical samples option in the Method Sample transport window.
	 Create a method and a sequence.
	Start the processing of the sequence row by clicking on .
	Follow the sample preparation instructions on the screen. A sample is prepared and measured. This is followed by a prompt to prepare the next sample platform until all samples have been processed.

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

See also

Method parameters for autosampler for graphite furnace technique (solid analytics)
 [▶ 49]

6.9.3 Save data of previously prepared samples

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

- Select the samples that have already been prepared. The samples must be in a contiguous block.
- Click on Load/Save to open the Load/Save SSA600 table window.

Load/Save SSA600 table	
Save Save 1 Save 2	
Save selected entries	
Load starting from row 1	•
Close	

- Select one of the two **memories**.
- Click on Save selected entries.
- Click on **Close** to close the window.
- After the Solid table has been rebuilt in the main window, reopen the Load/Save SSA600 table window.
- Select the memory.
- In the list field, enter the row number of the table from which the data block is to be inserted.
- Click Load starting from row.
- Click on **Close** to close the window.
 - ✓ The data block is inserted into the **solids** table starting from the specified row. Check whether you need to resort the platforms.

6.9.4 Re-analyze samples for solid analysis

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

Re-analyze a sample

Switch to the **Results** tab in the main window.

- Double-click on the sample with the outlier to open the **Single values** window.
- Mark the outlier in the table.

- Click Mark for re-measurement. • Close the **Single values** window. In the same way mark all additional outliers of other samples. Switch back to the Solid tab. Click Prepare re-measurement. ✓ The table to be processed is created. Here the individual values and other entries present are deleted where appropriate as the table is newly structured. If necessary the data should be saved beforehand. Prepare the samples in accordance with the platform assignment for the analysis. Start the measurement by clicking on Re-measure single val. ✓ On the **Results** tab, sample results reprocessed based on the re-measured outliers are appended to the end of the table. Re-analyze an element in a • Select all individual measurements of the sample element in the solids table. sample Click Measure row(s). Enter a new file name in window **Start measurement** or append the data to the existing file. Start the measurement with **OK**. Measure the solid table by row In method development, the solids table can be processed row-by-row. The measure-(method processing) ment of an element of a sample must be started with Run #1 or the run which follows the last measured statistics run. Select the individual measurements of the sample element in the solids table. Click Measure row(s). ▶ Enter a new file name in window **Start measurement** or append the data to the existing file. Start the measurement with **OK**.

See also

Save data of previously prepared samples [> 95]

6.10 Washing the system

Wash steps are started for the various systems via the Routine | Wash menu item. In addition, rinse commands are accessible in the respective technique-specific windows such as for autosampler and hydride system.Flame techniqueThe sampler tube is immersed in the rinse position and rinses the cannula. If the Injection Switch has been selected as accessory unit, the switch will open. This is to ensure that the sample path is rinsed, too. The rinse pump is continuously delivering fresh wash solution.Hydride technique / HydrEAThe hydride system is rinsed with acid (or reductant, if necessary). The wash parameters for the hydride system are specified in the Method | Hydride window.

Selection fiel tion window

7 Calibration

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

Open the **Calibration** window by clicking on *L* in the toolbar or via the menu command **Method Development** | **Calibration**.



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

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

in the Calibra-	Option	Description
	Line	Select the element line whose calibration is displayed
	Calibration function	Display of the calibration function used (set in the Method Calib. window).
		The calibration function is specific for every element line.
		You may select a new calibration function from the list box. The cali- bration is then recalculated accordingly.

See also

B Specify calibration parameters (Method | Calib. window) [▶ 51]

7.1 Showing the calibration curve

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

Color markings

Measuring points have been marked in the following manner:

Color	Description
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	Description
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

Notes on the prognosis or con- fidence range	The position of the prognosis range depends on the selected statistical certainty. It is a measure of the "quality" of the calibration, from which also the statistical certainty of the measurement of the analytical samples depends in the end. Besides, the prognosis range serves to identify suspected outliers among the calibration points. The confidence level is selected in the Method / Statistics window. The prediction or confidence band is selected in the Options Calibration window.
Enlarge the calibration graph	After clicking on 🔍, you can enlarge a section of the calibration curve by holding down the left mouse button. Click on 🔀 to reset the enlargement.
Insert remark	A text field for a remark can be inserted in the graph.
	$lacksim$ Click on and hold ${f T}$ to drag the frame for the text field on the graph.
	• Enter the text in the input window.
	\checkmark The text is displayed on the graph.
	You can edit text after double-clicking on an existing text field.
Print calibration graph	Click 🖶 to print the calibration curve and calibration data.
	See also
	Specify statics parameters (Method Statistics window) [> 58]
	Constant softings for salibration and blank correction [1, 172]

7.2 Displaying calibration results

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

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

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

To exclude individual calibration standards from the calculation, select the standard in the table with a mouse click and then click on Delete std.. The measurement is only marked as deleted and can be reactivated at any time.

Display of calibration data – Parameters tab This tab shows the calibration data as far as their calculation makes sense.

Parameter	Description
R²(adj.)	Coefficient of determination
Slope	Slope of calibration curve
Method SD	Method standard deviation
Char.conc. / Char.mass	Characteristic concentration or mass (concentration or mass neces- sary to absorb 1% of the available light energy in the atomizer – equal to an absorbance value of approx. 0.0044)

Residuals tab

Limit of detection and quantification limit of the current calibration – LOD/LOQ tab The graph on the **Residuals** tab shows the deviations of the calibration points from the calculated calibration curve and the limits of the prediction band.

The limits of detection and the limits of quantitation of the AAS can be determined based on the current calibration results.

In this area, values of the blank method and the calibration curve method will be displayed only if the AAS has been calibrated already.

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

Calibration graph method

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

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

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

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

Calculation instructions for the blank method:

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

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

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

If required, you can vary the factors and measurement repetitions in the **Options** | **Calibration** window.

See also

- Specifying measurements and actions in a sequence [69]
- □ General settings for calibration and blank correction [▶ 172]

7.3 Modifying a calibration curve

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

- changing the calibration function used
- disabling/enabling standards

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

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

The program recalculates the calibration curve and displays the modified curve.

The modified calibration parameters are applied to the results, if you activate menu command **Routine** | **Reprocess** or click on **C** on the toolbar.

See also

Reprocessing analysis results [> 81]

7.4 Replacing calibration standards by re-measurement

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

- Provide the new standard to be measured. When using an autosampler, set the standard to the position specified in the sequence.
- Select the relevant standard in the sequence and start the measurement of the sequence row by clicking on .
 - ✓ The value of the newly measured standard appears at the end of the sample table.
- Double-click on the standard to be replaced.

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

See also

■ Reprocessing analysis results [▶ 81]

8 Quality control

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

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

In the **Method** | **QCS** window, define the type of QC samples and their parameters and in **Sequence** define the integration of the QC sample within the measurement series.

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

Open the **QC** window by clicking on **b** in the toolbar or via the menu command **Method Development** | **QC**.

See also

- Specifying measurements and actions in a sequence [> 69]
- B Specify quality control samples (Method | QCS window) [▶ 59]

8.1 Displaying QC charts

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

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

Graph area

Options/views

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

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

Option	Description
Number	Number of the measured value in the QC series
Value	Measured value (converted according to the presentation type of the QC chart) \ensuremath{QC}
Date / Time	Measuring time
Operator	Displayed when working with User Management indicating the 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

8.2 Parameters of QC charts

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

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

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

Graphic setting

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

Option	Description
Point size	The individual points are displayed as circles. Choose a higher point size for larger circles.
Connect points	Connects the points on the graph with each other by a line.

See also

Specify quality control samples (Method | QCS window) [▶ 59]

Chart type

8.3 Entries and limits of the QC charts

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

Option	Description
Entry scheme	all values Enter each QC check performed.
	1 value/day Enter only the last QC check of the day.
	2 values/day Enter only the first and last QC checks of the day.
	Definition of "day": 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. pe-	Only for Control chart (process control chart)
riod	The previous period is a number of QC chart entries used to calculate the control (C) and warning (W) limits. The preparation period always contains the older chart entries. If set to 0 (no prep. period), all en- tered QC data will be included in the calculation of control and error limits.
Exclusion limits for	Only for target value chart
target value charts Factor	The exclusion limits are calculated from the limits specified for the quality control samples multiplied by the factor (default is 1).

Renewing charts

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

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

9 Controlling and monitoring spectrometer and accessories

9.1 Spectrometer

The **Spectrometer** window is used to test spectrometer functions and method development. The following data can be adjusted or viewed and the following actions performed:

- Checking the lamps
- Stocking of the lamp turret
- Start up behavior of lamps and D2HCL (deuterium hollow cathode lamp)
- Lamp spectrum
- Optimization of the Zeeman magnetic field

Open the **Spectrometer** window with the menu command **Method Development** | **Spectrometer** or by clicking on **A**.

All specifications and optimizations in this window are carried out for the optical parameters defined on the **Control** tab and the element line selected there.

9.1.1 Set the optical parameters on the spectrometer

Set the optical parameters of the spectrometer in the **Spectrometer** | **Control** window:

- Wavelength (element line)
- Slit width
- Lamp current
- Type of background correction
- Optical operating mode
- Lamp preheating

☆ Spectrometer		– 🗆 X
Control Energy Energy scan	Spectrum	
Optical parameters Position: Wavelength [nm]: Slit width [nm]: Current [mA]: Optical mode: Background correction:	1 - MHCL (Cr.Mn;Fe;Co;Ni;Cu;Zn) 324.8 Cu Element manual 0.8 2.0 Boost current [mA]: 0.0 Single-beam Image: Compare the second	Data Source: Cu324 V Transfer to method
Pre-heated lamp Position: none Current [mA]: 0.0	Boost current [mA]: 0.0	Lamp turret
		Close

Select data

The data to be displayed or edited is selected in the **Source** list:

Option	Description	
Element line	Select element line from the current method	

Option	Description	
Instrument	Display data from the last analysis setting	
	The data does not have to match the element lines set in the method.	

The optical parameters are updated according to the selected data. Other elements and their lines that are not included in the method can be selected from the periodic table with the elements available in the lamp turret by clicking on **Element**.

Set the optical parameters

The parameters of the selected element line are displayed and edited in the **Optical parameters** group.

Option	Description
Position	Display of the position of the set lamp and the lamp type
	If the element is available in several lamps of the turret, the first lamp available in the turret is approached after clicking on Set . If a different lamp is required, this can be selected in the Position list.
Wavelength	Display of the selected line
	After activating the manual option, the wavelength information can be edited, e.g., to take into account a peak position determined during the spectrum scan.
Slit width	Select the spectral bandwidth of the monochromator
Current	Display of the lamp current used
Boost current	Display of the boost current for super hollow cathode lamps
Optical mode	Selection of operating modes: Single beam, double beam or emission mode
Background correc- tion	Selection of background correction
	The selection of Zeeman modes is only available for Zeeman AAS.

Click on **Set** to set the selected line and the optical parameters. The lamp turret is moved to the required position and the spectrometer is set to the wavelength. A peak search and a zero adjustment are also carried out. If both were carried out correctly, the indicator lamp lights up green, otherwise it turns red.

Click on **Transfer to method** to transfer the edited data to the method. It is recommended to save the edited method.

Pre-heated lamp

For the method processing a further lamp can be pre-heated in order to shorten the waiting times which are linked with the start up behavior of the lamps.

Option	Description	
Position	Set the lamp position of the lamp to be pre-heated	
Current	Lamp current of the lamp	
Boost current	Boost current if a super hollow cathode lamp is preheated	

This setting is also defined by clicking on Set.

Select lamp/element button

Click on Select lamp/element to open the window for loading the lamp turret.

See also

- Lamp turret, mounting [> 11]
- Background corrections for Zeeman AAS ZEEnit 700/650 P [> 113]
- Background correction for Zeeman AAS ZEEnit 700 Q [> 116]

9.1.2 Check lamp energy (novAA 400 P/ZEEnit)

The **Spectrometer** | **Energy** window is used to monitor and control the lamp energy for the optical parameters set on the **Control** tab.

🛧 Spectrometer	– 🗆 X
Control Energy Energy scan Spectrum	
Energy levels HCL: 57.0 D2HCL: 63.0	Parameters AGC Peak pick
Cu 324.75	Transfer to method PMT [V]: 300 D2HCL current [mA]: 0.9 Boost current [mA]: 0.0 🗘
Start Delete	Lamp alignment Align 0 Energy
	Close

Energy levels

Option/button	Description
HCL	Current energy level of the line radiator at the photo multiplier in % numerical and graphic
	In addition to the blue current level the graph also shows the gray measured maximum level (i.e. the highest value attained by adjust- ment). Display for HCL, S-HCL and emission signal.
D2HCL	Current energy level of the background radiator D2HCL The current level is shown graphically with a red bar.
Start	Start measurement (e.g., for lamp adjustment)
Delete	Delete measurement values
Stop	Stop measurement

Parameter

Option	Description
РМТ	Current voltage of the receiver (photomultiplier) in volts Value range: max. 600 V
D2HCL current	Average lamp current of the deuterium hollow cathode lamp Value range: 5 to 35 mA

The energy adaptation between the HCL lamp and the background radiator D2HCL occurs via two separate amplifier settings.

Option	Description
AGC	Voltage of the photomultiplier and the D2HCL current, equalized to a 65 to 75% energy level
Peak pick	Determine actual line maximum of the set spectral line and its devia- tion from the table value (offset)

	Option	Description
		The window Peak pick appears in which the offset is shown graphi- cally and numerically. The device wavelengths are corrected according to the established line maximum and a device autozero is executed.
	Transfer to method	Transfer parameters to the method
Burner setting for flame tech- nique	The burner height car The increase and decr	n be varied using the arrow keys on the Burner drive input field. rease of the signal is symbolized by the bar next to it.
Adjusting the HCL	The HCL is adjusted a alignment group.	utomatically after clicking on the Alignment button in the Lamp
	The adjustment runs a turret window.	according to the same algorithm as the adjustment in the Lamp
	Option	Description
	Optical mode	Optical operating mode used
	Background correc- tion	Type of background correction
	РМТ	Voltage of the photomultiplier
	D2 current	Current of the deuterium HCL (if used for background correction)
	D2 gain	Gain of the signal of the deuterium HCL (if used for background correction)
	Burner drive	Burner height in flame technique
	 tion, from the eler Click AGC. ✓ The voltage of nal of line radia correction the tween 65 and are updated. 	nent to be measured, from AAS and allow to be nebulized. the photomultiplier is automatically set in such a way that the sig- ator lies between 65 and 75 %. If you are working with background current of the D2HCL is then set such that its signal also lies be- 75%. If the intensities of both radiators are equalized, all displays
Adjusting D2HCL	The D2HCL (deuteriun window.	m hollow cathode lamp) is adjusted in the Spectrometer Energy
	In the Spectromet lect the only D2 bar rameters.	er Control window, go to the Background correction list and se- ackground option. Then click on Set to adjust the spectrometer pa-
	• Change to the Ene	ergy tab.
	 Click on AGC to sta the D2HCL current 	art the calibration of the voltage of the photomultiplier PMT and t with the aim of setting the energy level to 65 to 75%.
	 Start the energy m 	neasurement by clicking on Start .
	 Set the energy leve Note: The gray hig and can be deleted 	el (red bar) to a maximum value. ghlighted bars indicate the last maximum to have been reached d using the Delete button.
	 With focus adjuant ally and then ti 	usting: Move the lamp holder slightly in the axial direction manu- ighten the locking screws.
	 With axis adjus hardware secti 	stment: Adjust the fine adjustment screws on the D2HCL (see on of the Operating Manual).
- Continue depending on any error messages or the D2 current:
 - Click on Manual amplification setting.
 - If an error message indicates too little energy for the D2HCL, first check the D2HCL current. If it does not stand at 35 mA after the control, enter the value 35 mA and repeat the control by clicking on AGC.
 - If the D2HCL current is already at 35 mA, raise the BC amplification by one step (steps from 0 to 4) and repeat the control by clicking on **AGC**.
 - If an error message shows too much energy for the D2HCL (too little energy for the HCL), raise the HC amplification by one step (steps from 0 to 4) and repeat the control by clicking on AGC.

Option AGC

- Lamp turret, mounting [> 11]
- B Set the optical parameters on the spectrometer [▶ 105]

9.1.3 Check lamp energy (novAA 800)

The **Spectrometer** | **Energy** window is used to monitor and control the lamp energy for the optical parameters set on the **Control** tab.

A Spectrometer	– 🗆 X
Control Energy Energy scan Spectrum	
Energy levels	Parameters
Cu 324.75	AGC Peak pick
HCL: 163119	Transfer to method
D2HCL: 125047	
	Burner height[mm]: 5 🖶
Start	Lamp alignment Align 0 Energy
	Close

Energy levels

Option	Description
HCL	Current energy level of the line source (HCL or emission signal)
D2HCL	Current energy level of the background source D2HCL
Start/Stop	Start/stop determination of the energy level
	If the lamps light up green, the energy level is OK. If the lamps light up red, the lamp must be readjusted.

Parameters

Description
Autozero

Option	Description
	The dark signal of the HCL is determined.
Peak search	Determine actual line maximum of the set spectral line and its devia- tion from the table value (offset)
	The window Peak search appears in which the offset is shown graph- ically and numerically. The device wavelengths are corrected accord- ing to the established line maximum and a device autozero is exe- cuted.
Transfer to method	Transfer parameters to the method
D2HCL current	Lamp current of the D2HCL
	The value cannot be changed.

Burner setting for flame tech- nique	The burner setting can be varied using the arrow keys on the Burner height input field. The signal change is symbolized by the bar next to it.
Adjusting the HCL	The HCL is adjusted automatically after clicking on the Alignment button in the Lamp alignment group.
	The adjustment runs according to the same algorithm as the adjustment in the Lamp turret window.
Adjusting D2HCL	The deuterium hollow cathode lamp (D2HCL) is adjusted manually. Please also observe the notes on adjustment in the novAA 800 operating manual.
	In the Spectrometer Control window, press the Element button to open the Select element/line window.
	• Select an element line in the wavelength range 190 to 350 nm. Click on OK to close the window.
	Select the only D2 background option from the Background correction list.
	• Approach the spectrometer parameters using Set .
	• Change to the Energy tab.
	Press the Start button to begin the energy measurement. Wait until the D2HCL has started.
	Set the energy level to a maximum value:
	 With focus adjusting: Move the lamp holder up or down slightly before tightening the securing nuts (items 1, 3, 5 in the figure).
	 With axis adjustment: Adjust the adjustment screws (item 2 in the figure).
	• Stop the adjustment process by clicking on Stop and click Close to exit the window.
	✓ The D2HCL is adjusted.



- 1, 3, 5 Fixing nuts of the lamp holder
 - 4 Attachment screws for the safety bracket of the lamp holder
- 2 Adjusting screws

■ Lamp turret, mounting [▶ 11]

9.1.4 Investigating lamp drift

In the **Spectrometer** | **Energy scan** window the drift behavior of the active lamp and the deuterium lamp, if it was specified for the background correction, are shown graphically and evaluated.

The red line marks the energy flow of the D2HCL and the blue line marks the energy flow of the active lamp. The signal colors can be chosen in the **Options** | **View** window.

For the assessment of the drift behavior the following parameters are displayed:

Option	Description
Ints.	Intensity of the lamp radiation for HCL and D2HCL
Drift [%/min.]	Ratio of the mean value of 10 values a minute ago and the mean value of 10 values at the current point in time
Range	Difference of the largest and smallest measurement value in the last minute



■ View options [▶ 168]

9.1.5 Record lamp spectrum and determine peaks

In the **Spectrometer** | **Spectrum** window, you can record a lamp spectrum. The peaks are recorded in the selected wavelength range for the optical parameters set on the **Control** tab.

You can correct the peak offsets found for the active hollow cathode lamp on the **Con-trol** tab and transfer them to the method.



Define the scan settings

In the **Parameters** area, you define settings for the spectrum scan:

Option	Description
Start	Start wavelength of the spectral range to be taken up
End	End wavelength of the spectral range
Speed	Scan speed of the monochromator: slow , medium (not novAA 800) or fast .
	With the speed slow the best signal-noise ratio is attained through the longer integration times.
Signals	Selection of the displayed lamp spectra (can only be selected for D2 HCL background correction if the D2HCL is switched on).
	HCL Only signal of the active HCL
	D2HCL Only signal of the D2HCL
	both Signals of the active HCL and D2HCL

Use the buttons to start the spectrum scan:

Button	Description
Start/Stop	Start deletes the current display and starts the measurement. The button changes to Stop and can be used to interrupt the measurement.
Continue	Continue interrupted measurement.

The result is presented graphically and numerically. The signal colors can be chosen in the **Options** | **View** window.

Line/option	Description
Red line	Signal of the D2HCL
Blue line	Signal of the active HCL
Green vertical	Cursor for the numerical display of wavelength and intensity value
	The cursor can be moved with the [<] and [>] keys under the graph.
HCL	Numerical values of wavelength and intensity at the cursor position for the HCL.
D2HCL	Numerical values for D2HCL

See also

■ View options [▶ 168]

Set the optical parameters on the spectrometer [105]

9.1.6 Background corrections for Zeeman AAS ZEEnit 700/650 P

For the **Zeeman AAS devices**, the background correction can be set in the **Method** | **Evaluation** window by means of the Zeeman magnetic field. The following operating modes for the Zeeman magnetic field can thus be selected:

- Zeeman 2-field mode
- Zeeman 3-field mode
- Zeeman dyn. mode

The optimum field strengths for the Zeeman 2 field and Zeeman 3 field modes can be found by means of an optimization program.

Optimizing the Zeeman magnetic field For the measurement in the graphite tube technique with background correction in the static 2 field or 3 field modes with a ZEEnit series spectrometer there are optimization programs which automatically pass through a measurement series with different field strengths from a given start to a given end value. The measured values so obtained are output in tabular form, the measurement peaks can be read from the graphs displayed during the measurement.

With this information determine the optimum field strength for your analysis problem and transfer this value into the method. For the optimization, a sample should be used that is as representative as possible of the samples to be analyzed.



The automatic optimization of the field strengths occurs in the **Spectrometer** | **Field strength opt.** window.

Parameters for optimizing the 2 field mode

In the 2 field mode the maximum field strength is varied during the measurement series.

Parameter	Description
Start	Start value for the variation of the maximum field strength (0.01 to 1.00 T)
End	End value for the variation of the maximum field strength (0.01 to 1.00 T)
Step width	Step size for the variation of the maximum field strength (0.05 to 0.25 T)

Parameters for optimizing the 3 field mode

In the 3 field mode the medium field strength is varied during the measurement series. The maximum field strength is thus fixed.

Parameter	Description
Start	Start value for the variation of the medium field strength (0.05 T) $$
End	End value for the variation of the medium field strength ($0.01 - (Max-0.05 T)$)

Parameter	Description
Step width	Step size for the variation of the maximum field strength (0.05 – 0.25 T) $$
Max. field strength	Maximum field strength (0.05 to 1.00 T)
Parameter	Description
Sampler pos.	The sample for optimization is in this position on the autosampler.

Buttons	for th	ne or	otim	ization
Duttons	101 0	10 01	Juni	12001011

Buttons	Description
Start	Start measurement series
Transfer to method	Transfer found parameters into the method
Save	Save results of the optimization
Load	Load saved optimization results

Display of the optimization parameters The graph shows both absorbance curves for the measurement signal (blue curve) and for the background (red curve). In the selection list it is possible to choose between **Height** and **Area** of the signal evaluation.

The following values are displayed in the table area:

Parameter	Description
No.	No. of the optimization step
Field str.	Value for the field strength
Abs. Height/Area	Absorbance value for the evaluation of the signal height or area
backgr. Height/ Area	Background absorbance value for the evaluation of the signal height or area
Zeeman Factor	Zeeman-Factor (Abs/(Abs. + backgr.))

The Zeeman dynamic mode

ASpect LS supports a special dynamic mode in the standard calibration method for the spectrometers of the ZEEnit series. This unites the advantages of the stationary 2 field and 3 field Zeeman modes:

- In the lower concentration range, the better sensitivity of the 2-field operating mode can be exploited
- In the upper concentration range, higher concentrations can be measured at the cost of sensitivity in the 3-field mode, in the course of which the well-known Zeeman rollover-effect is shifted to the higher concentrations.

For this, the magnetic field is operated in three states as in the stationary 3-field mode. Only two absorbance values, however, are recorded:

- Absorbance difference between the switched-off magnetic field and the magnetic field with the maximum field strength (H-value / high sensitivity (high))
- Absorbance difference between the magnetic field of medium field strength and the magnetic field of maximum field strength (L-value / low sensitivity (low))

Both values (L-value and H-value) are recorded and saved in the active integration mode (area or height) at each measurement. The values of the alternative integration mode are not saved, that means that you have to decide on one of the two integration modes before the measurement.

Representation of the H and L values in the tables and graphs

The two values are shown in the tables in the same way as in the other Zeeman operating modes of area and height values.

The L-value peak and the H-value peak are shown in the result graphs. The background is depicted for maximum field strength.

	The single-peak graph is split into two graphs, one above the other, with different ab- sorbance scales, while all other graphs use a common coordinate system for L and H val- ues.
Calibration of the H and L val- ues	During the calibration, calibration curves are calculated for the L values and the H values (H curve and L curve).
	In the process, it is possible to take calibration points with higher concentrations into ac- count, but only for the L curve. The delete H value button in the calibration table is there for that purpose. Once both calibration curves have been calculated, the user can define a limit concentration.
	If the H value of the sample lies below the absorbance in the sample measurement that corresponds to the H curve value of the limit concentration, the H value and the H curve are used in the concentration calculation. If it lies above this value, the L value and the L curve are used in the concentration calculation.
	The form of the curve (linear, non-linear) is selectable for the H curve, while a non-lin- ear calibration curve is always calculated for the L curve.
Recalibration of the H and L values	The recalibration standard is to be chosen so that it lies close to the limit concentration. During the recalibration, a common recalibration factor is calculated for both curves and used for the concentration calculation.
	See also
	Background correction for Zeeman AAS ZEEnit 700 Q [> 116]

9.1.7 Background correction for Zeeman AAS ZEEnit 700 Q

For the ZEEnit 700 Q, the background correction can be set in the **Method** | **Evaluation** window by means of the Zeeman magnetic field.

The optimum field strengths for the Zeeman field can be determined using an optimization program. The optimization program automatically runs through a series of measurements with different field strengths for a selected sample, from a specified start value to a specified end value. The measured values are displayed in a table.

With this information, determine the optimum field strength for your analysis task and transfer this value into the method. For the optimization, a sample should be used that is as representative as possible of the matrix composition to be analyzed.

The automatic optimization of the field strengths occurs in the **Spectrometer** | **Field strength opt.** window.



Parameters for optimization

For optimization purposes, the maximum field strength is varied during the measurement series.

Parameter	Description
Start	Start value for the variation of the maximum field strength (0.01 to 1.00 T)
End	End value for the variation of the maximum field strength (0.01 to 1.00 T)
Step width	Step size for the variation of the maximum field strength (0.05 to 0.25 T)
Parameter	Description
Sampler pos.	The sample for optimization is in this position on the autosampler.

Buttons for the optimization

Button	Description
Start	Start measurement series
Transfer to method	Transfer found parameters into the method
Save	Save results of the optimization
Load	Load saved optimization results

Display of the optimization parameters

The graph shows both absorbance curves for the measurement signal (blue curve) and for the background (red curve). In the selection list it is possible to choose between Height and Area of the signal evaluation.

The following values are displayed in the table area:

Parameter	Description
No.	No. of the optimization step
Field str.	Value for the field strength
Abs. Height/Area	Absorbance value for the evaluation of the peak height or area
backgr. Height/Area	Background absorbance value for the evaluation of the peak height or area

Parameter	Description
Zeeman Factor	Zeeman-Factor (Abs/(Abs. + backgr.))

Perform optimization A prerequisite for optimization for a specific element line is that the loaded method contains this element line.

- In the Spectrometer | Control window, go to the Source list field and set the line from the method and in the Background correction list field, select the Zeeman option.
- Change to the **Field strength opt.** tab.
- Place a representative sample on the autosampler and enter the position in the Autosampler pos. field.
- You can vary the settings in the **Field strengths** group.
- Click **Start** to start the optimization.
 - ✓ The optimization runs automatically.

You can transfer the parameters directly to the method at the end of the optimization (**Transfer to method** button). You can choose whether to transfer the parameters of the selected table row or the found optimum. You can save the results generated during optimization using the **Save** button.

9.1.8 Adjusting the spectrometer

The spectrometer can be adjusted by the software. A preheated lead hollow cathode lamp is required for the adjustment, the lines of which are used to adjust the spectrometer.

- Start the adjustment using the menu command Actions | Spectrometer alignment.
- In the Spectrometer alignment window, start the automatic adjustment by clicking on Start. A progress bar indicates the progress of the adjustment.
- At the end of the adjustment, save the correction values found by clicking on **Save**.
 - ✓ The new correction values for the spectrometer are used for each subsequent measurement.

9.2 Flame

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

Open the Flame window using the menu command Method Development | Flame or by clicking the sicon.



NOTICE

If a specially equipped AAS device has been configured to use LPG during installation, the software will display LPG as the fuel gas. It is not possible to use LPG with nitrous oxide as an oxidizer.

9.2.1 Testing flame functions

The Flame | Control window contains the following functions:

- Ignite/extinguish flame
- Switch air or nitrous oxide as oxidant
- Display of gas pressures and gas flows
- Activate scraper
- Setting the gas flows

👲 Flame o				- 0	×
Control Manual optimization	Automatic optimization				
Status Flame: C2H2/ Burner: 50 mr Siphon: OK	air Fuel: M Nebulizer: Air: N2O:	ОК 1.2 ОК ОК	Actual fuel flow Fuel: Oxidant: Oxidant (total): Fuel/oxidant	45 L/h 402 L/h - L/h 0.112	
Function tests Test air Test N2O Test fuel End test	Flame Ignite flame Air> N2O Extinguish flame	Settings C2H2/air: C2H2/N2O: Oxidant (aux.): Burner height:		45 ÷ L/h 210 ÷ L/h 0 × L/h 8 * mm	1
				Close	

Status

Орион	Description
Flame	Status display of the flame:
	off: The flame is not burning.
	C2H2/air: The acetylene-air flame is burning.
	C2H2/N2O : The acetylene-nitrous oxide flame is burning.
Burner	Attached burner head:
	100 mm : 100 mm single-slot burner
	50 mm: 50 mm one-slit burner
	Error: No burner head present or is not recognized.
Siphon	The level of the mixing chamber siphon, through which non-atom- ized liquid is discharged, is monitored. The siphon must always be filled sufficiently to prevent backfiring of the flame, particularly that of the nitrous oxide flame.
	OK : The siphon is filled with liquid up to the overflow.
	Error: The level of the siphon is insufficient.

Pressures

Option	Description
Fuel	Status of fuel pressure at device inlet "-" – No fuel pressure detected
Nebulizer	Operating pressure at nebulizer.
Air	Status of the air inlet pressure

Option	Description
	The status is only displayed when the air supply is open.
N20	Status of the N_2O inlet pressure
	The status is only displayed when the nitrous oxide supply is open.

Current gas flows

Option	Description
Fuel	Fuel flow
Oxidant	Oxidant flow through nebulizer
Oxidant (aux.)	Auxiliary oxidant Displayed only if auxiliary oxidant is activated in the method.
	Air : 75 / 150 / 225 NL/h
	N2O : 60 / 120 / 180 NL/h
Fuel/oxidant	Fuel/oxidant flow ratio

Test functions

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

Option	Description
Test air	Open solenoid valve in air path
	Prerequisite: Air inlet pressure and fuel gas are present.
	Displays nebulizer pressure, oxidant flow and total oxidant (when the auxiliary oxidant is activated).
Test N2O	Only active with acetylene-nitrous oxide flame and 50 mm one-slit burner.
	Open the solenoid valve in the nitrous oxide path
	Prerequisite: Nitrous oxide inlet pressure and fuel gas are present.
	Displays nebulizer pressure, oxidant flow and total oxidant (when the auxiliary oxidant is activated).
Test fuel	Set target gas flow (proportional valve) Displays fuel gas flow for the acetylene-air flame (with Test air) or the acetylene-nitrous oxide flame (with Test N2O).
	Test air or Test N2O must be activated before this test.
End test	Finishes the test function

Flame/Scraper

Buttons	Description
lgnite flame	 Ignite acetylene-air flame Ignition arm swings out; filament lights up. Acetylene target gas flow (proportional valve) is adjusted when nebulizer pressure and oxidant flow have reached their setpoints. If the flame does not ignite within 10 s, the ignition attempt is aborted. If the flame is burning, the Extinguish flame button becomes active.
Air> N2O	 Switch from acetylene-air to acetylene-nitrous oxide flame Oxidant valve (3/2 solenoid valve) switches from air to nitrous oxide. Fuel gas flow for acetylene nitrous oxide flame (proportional valve) is set. The button changes to N2O> air.
N2O> air	Switch from acetylene-nitrous oxide to acetylene-air flame

Buttons	Description				
	 Oxidant valve (3/2 solenoid valve) switches from nitrous oxide to air. Fuel gas flow for acetylene-air flame (proportional valve) is set. The button changes to Air> N2O. 				
Extinguish flame	 Extinguish the flame When the acetylene-nitrous oxide flame is burning, switch to the acetylene-air flame and wait a few seconds. The fuel gas flow (proportional valve) is shut off. After a few seconds of waiting (to expel the fuel gas from the mixing chamber and burner), air (solenoid valve) is shut off 				
Scraper	Only 50 mm burner with mounted scraper and acetylene-nitrous ox- ide flame				
	Activate scraper for cleaning the burner head				

Settings

In the **Settings** field, you can edit the gas flow settings:

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

See also

Specifying flame parameters (Method | Flame window) [▶ 32]

9.2.2 Optimizing the flame

For the analysis, the flame can be optimized for every element line with respect to:

- Fuel gas flow
- Burner height
- Total oxidant flow, if the use of auxiliary oxidant has been chosen in the method.

You may optimize the flame manually by changing the parameters and observing the signal level, or you may have the parameters searched automatically by the application. In both cases, you may transfer the found parameters to the method at the push of a button.

Manual flame optimization Manual flame optimization is carried out in the Flame | Manual optimization window.

🗄 Flame	– 🗆 X				
Control Manual optimization	Automatic optimization				
Line Cu 324	✓ Set 0.9				
Parameters to be optim	ized 0.8				
Fuel [L/h]:	0.7				
	75				
Burner height [mm]:					
Ovident (our) [] (b]:					
Oxidant (aux.) [L/n].	0.2				
	0.1				
Oxidant (total) [L/h]:	0.0				
Fuel/oxidant	- 0.00 0 10 20 30 40 50 60 70 80 Time				
	Absorbance Maximum				
Stop	AZ 0.5948 0.6005				
Acceptiva	lues				
	Close				
Option	Description				
Line	Choose the element line for which the flame shall be optimized				
	You may choose among the analysis lines defined in the method.				
Set	Move the monochromator to the selected analysis line				
Fuel	Adjust the fuel gas flow				
Burner height	Set the burner height to the optical axis of the beam path				
Oxidant (aux.)	Set auxiliary oxidant flow:				
	Air: 75 / 150 / 225 NL/h				
	N20: 60 / 120 / 180 NL/h				
Oxidant	Oxidant flow in L/h				
Fuel/oxidant	Ratio of fuel gas flow				
Start	Starts the measurement. The signal is continuously recorded				
	The button label turns into Stop .				
AZ	Start autozero measurement				
Stop	End the measurement				
Accept values	Transfer the determined flame parameters for the set element line into the method				
Graph	Display of signal curve Ordinate expansion is possible via the input fields at the Y-axis.				

Perform manual optimization

Note: There is a small delay between the modification of the parameters and the signal response.

Maximum absorbance value during the current measurement

Current absorbance value

- Ready the test solution. Instructions for the appropriate test solution can be found in the cookbook. The test concentration given there causes an absorbance of approx. 0.1. Use 2 to 3 times concentration for optimization.
- From the Line list, choose the desired element line.

Absorbance

Maximum

- Click on **Set** to move the monochromator to the wavelength of this line.
- Immerse the tube of the nebulizer into the zero solution.
- Start the AZ measurement by using **AZ**.
- Immerse the nebulizer sample tube into the sample solution.
- Start the measurement with **Start**.
- Vary the Fuel setting by means of the arrow buttons and watch the signal change in the graph and in the Absorbance field. Adjust the fuel rate until absorbance is maximal.
- Change the **Burner height** setting until you have found the maximum extinction level.
- When using the flame with auxiliary oxidant, vary the Oxidant (aux.) parameter until again you obtain the maximum signal level.
- Repeat steps starting with the **Fuel** setting until you can no longer notice a relevant increase of the signal level.
- Stop the measurement with **Stop**.
- Click on Accept values to transfer the found parameters for the selected element line to the method.

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

Automatic flame optimization Automatic flame optimization is carried out in the **Flame** | **Automatic optimization** window.

> The used optimization algorithm changes the settings for fuel flow and burner height with the aim to obtain an increase in the signal level. This algorithm takes into account the interactions between the two parameters (fuel flow and burner height). The optimization procedure will be stopped if in three successive steps no further increase in signal level is achieved. This means that either the maximum signal level was reached or the change of the parameters is of no effect on the signal level.

	5	•					5					
🗴 Flam	e									_		\times
Control	Manual o	optimization	Automati	c optimization								
Line	(Cu 324		~				Position:		1	•	
Line	Step	Param Gas flow	neters Burn.heigh	Fuel/oxidant	Signal	^						
Cu 324	4	75	8	0.000	0.7100		1.00	- 1.1				
Cu 324	1 5	85	8	0.000	0.8100							
Cu 324	1 6	95	8	0.000	0.9100		g 0.75					
Cu 324	F 7	105	8	0.000	0.9100		an					
Cu 324	1 8	95	7	0.000	0.8600		50 50					
Cu 324	1 9	95	9	0.000	0.9400		۵.50 <u>م</u>					
Cu 324	F 10	95	10	0.000	0.9500		~					
Cu 324	11	95	11	0.000	0.9400		0.25					
Cu 324	12	90	10	0.000	0.9000							
Cu 324	13	100	10	0.000	1.0000		0.00					
Cu 324	14	105	10	0.000	0.9500		1	6 11 16	21	26	31 36	
Cu 324	15	100	10	0.000	1.0000	¥			Step			
	Start	AZ	2				De	elete cept values	(🗂 Loa	id ve	
										C	Close	

Option	Description
Line	Select the element line for which the flame is to be optimized
	The wavelengths set in the method are available for selection.
Position	Position of the test sample on the autosampler
All lines	Establish the flame parameters automatically for all element lines in the method
Start	Start measurement and record signal continuously
	The button changes to Stop .
Stop	End the measurement
AZ	Determine autozero
Delete	Delete determined values
Load	Loads optimized flame parameters
Save	Save optimized flame parameters
Accept values	Transfer the determined flame parameters for the set element line into the method
Table	Display of found parameters.
Graph	Display of signal curve

Perform automatic optimization

- From the Line list box, choose the desired element line.
- Immerse the nebulizer sample tube into the sample solution.
- Click **Start** to start the optimization.
 - ✓ The **Automatic optimization** dialog window opens.
- If appropriate, activate following settings:

Option	Description
Set optimized val- ues automatically for the current method.	This setting has to be activated for automatic optimization because only the parameters from the last optimization are available after the procedure is completed.
Automatically save optimization data	If activated, enter the desired file name in the field File name .

For single line optimization: If not arranged prior to the optimization, following successful optimization transfer the parameters for the element line into the method with Accept values.

9.2.3 Extinguish the flame

- In the Flame | Control window, click on Extinguish flame.
- While a sequence is running, click on Extinguish flame in the toolbar on the lefthand side of the main window

9.3 Furnace

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

- Parameters of the furnace programs used in the method
- Selection of modifiers

- Optimization of the atomization and pyrolysis temperatures during method development
- Coating of the graphite tube for the hydrEA technique
- Graphical representation of furnace program
- Checking the furnace functions
- Position of the furnace (only novAA 800)

Open the **Furnace** window using the menu command **Method Development** | **Furnace** or by clicking the \bigcirc icon.

See also

■ Optimizing atomization temperature [▶ 126]

9.3.1 Viewing the furnace program

The line-specific furnace program is displayed in the **Furnace** | **Furnace** program window. The furnace program is created in the method. If the **Furnace** window is opened via the toolbar, the entries are deactivated and the parameters can only be viewed.

	Furnace	2										×	
Fı	irnace pi	rogra	m Modif.Extras	Optimization	Plot Co	ntrol							
				Temp.	Ramp	Hold	Time	G	as				
	Step	^ Name		o * Name	[°C]	[°C/s]	S	S	int.	Add.	Inj.	E/P	
	1		Drying	80	6	20	28.3	Max	Stop				
	2		Drying	90	3	20	23.3	Max	Stop				
	3		Drying	110	5	10	14.0	Max	Stop				
	4		Pyrolysis	350	50	20	24.8	Max	Stop				
	5		Pyrolysis	900	300	10	11.8	Max	Stop				
	6		AZ*	900	0	6	6.0	Stop	Stop				
	7		Atomize	1750	1500	5	5.6	Stop	Stop				
	8		Clean	2350	500	4	5.2	Max	Stop				
	<										>		
									Total time:		169 s		
				Check	k program								
	Meas	start	delay [s]:	0.0									
			doidy [o].	0.0									
	Line:		Mg285	✓				OK	(С	ancel		

The parameters on display are:

Column	Description
Step	Sequential number of working step
*	No function was assigned to this field so far.
Name	Name of furnace program step
Temp.	Target temperature in program step
Ramp	Heating rate in program step
Hold	Holding time of target temperature within program step
Time	Total duration of working step
Gas	Supply internal gas (Int.mode) and additive gas (Add.). Possible states:
	Stop No supply

Column	Description
	Min Minimal supply rate (only internal gas flow)
	Max Maximum supply rate
lnj.	Injection step Sample will be injected into furnace on completion of this step.
E/P	Working step for enrichment or thermal pretreatment of individual components.

■ Editing a furnace program [▶ 34]

9.3.2 Viewing matrix modifiers, enrichment and pretreatment

In the **Furnace** | **Modif.Extras**, window you can view the following line-specific parameters:

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

The settings are defined in the method. If the **Furnace** window is opened via the toolbar, the entries are deactivated and the parameters can only be viewed.

See also

Specifying matrix modifiers, enrichment, and pretreatment [> 38]

9.3.3 Optimizing atomization temperature

In the **Furnace** | **Optimization** window, the optimum pyrolysis and atomization temperature for an element line is determined and set by carrying out a series of measurements with increasing step end temperatures.

Once optimized, furnace parameter settings for atomization and pyrolysis can be saved and loaded to other methods.

Surnace							—		×
Furnace program Modif.	Extras Optimization Plot	Control							
Settings Optimize: Step number: Start temp. [*C]: Step width [*C]: End temp. [*C]: Sampler pos.:	Pyrolysis 5 5 700 ÷ 50 ÷ 1100 ÷	1.00. 0.75. (atpunize) 0.50.							
Start	Delete Save	0.25	750	1000	1250 1	500	1750	2000	
Pyrolysis temp	Load berature->Method	□ y-scale	20	Te	emperature [°C] 0	1750]°C >		
Line: Mg285	✓ ()				ОК		Ca	incel	

Parameters and control buttons

Option	Description
Optimize	Selects parameter for optimization: Pyrolysis or Atomize
Step number	Number of the selected step in the furnace program
Start temp.	The lowest end temperature of the furnace program step to be opti- mized within the measurement series
Step width	The temperature of the program step is increased by this amount from measurement run to measurement run
End temp.	Highest end temperature of a furnace program step to be optimized as part of a series of measurements
	Note : Available for selection are only such parameters which make sense for the particular furnace program.
Sampler pos.	Position of the sample in the autosampler with which the optimiza- tion (pyrolysis/atomization) is carried out
Start/Stop	Automatically create a sequence for the optimization measurement
	Start/stop optimization
Delete	Delete determined values
Save	Save optimized furnace parameters
Load	Load optimized furnace parameters
Atomization tem- perature- >Method / Pyroly- sis temperature- >Method	Transfer obtained values into current furnace program

Results display

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

Graphic representation is facilitated by **Furnace | Optimization** window tools. Available for displaying are the particular autozero value and the measured extinction value:

Option	Description
Red line	Background signal that depends on pyrolysis or atomization tempera- ture

Option	Description
Blue line	Specific absorption depending on pyrolysis or atomization tempera- ture
Vertical cursor	Optimum pyrolysis and atomization temperature selected by the oper- ator
y-scale	If this checkbox was set, y-axis scaling will be such that the back- ground signal can be depicted in the best possible manner. An opti- mized scaling can be separately selected for pyrolese and for atomiza- tion.
A->H/H->A	Switches the graphic between signal area (A) and signal height (H).
	Shifts vertical lines for pyrolese or atomization temperature (depend- ing on what step was selected for optimization) to the left or the right, thus defining a desired optimal furnace temperature.

Performing optimization

Parameter	Optimization goal
Pyrolysis tempera- ture	No specific absorption losses and minimal background signal
Atomization tem- perature	A constant specific absorbance

- Create a method for the current analysis line and save it.
- Open the **Furnace** window in the method and where appropriate adapt the furnace program.
- In the Furnace | Optimization window, enter the optimization parameters (optimized temperature, Start temp., Step width, End temp., position of the sample on the autosampler).
- Prepare sample on autosampler.
- Click **Start** to start the optimization.
 - The optimization runs automatically. The measurement results are displayed in the main window and shown graphically in the Furnace | Optimization window. To display individual sample readings, click onto a measurement point of the graphic or use a double click onto the sample line in the results window.
- Use the < / > buttons to move the vertical cursor over the graphic area or use arrow keys as necessary to adjust optimal temperature. Transfer the value to the furnace program using Atomization temperature->Method / Pyrolysis temperature->Method.
- Repeat this procedure for all other analytical lines included in the current method.

9.3.4 Graphical representation of furnace program or graphite tube coating

The **Furnace** | **Plot** window contains the following functions:

- Graphical representation of furnace program
- Monitoring execution of current furnace program
- Coating graphite tube with iridium layer for HydrEA technique

neee program		
nace program		
Graphical representation of fur-	The furnace program	is displayed as a graph in the temperature-time coordinate system.

Option	Description
Black line	Programmed temperature-versus-time graph

Option	Description
Red line	While a test is running, the black line in the already completed fur- nace program part is overlaid with a red line designating the actual temperature/time graph.
Inj.	The injection step is marked with an "Inj." identifier above the dia- gram.
Green bar	An enrichment phase will be marked by a green horizontal bar.
Yellow-brown bar	Autozeroing (AZ*) is marked by a yellow-brown vertical bar.
Light pink bar	The integration step (measured value acquisition) is marked by a light pink vertical bar.

run

Testing furnace program in trial Execution of the current furnace program is checked in a test run. During this test run, temperatures and times are displayed in the graph. No sample is injected, autozero and integration are not performed.



The plot shows the various steps of a furnace program. The red line indicates the actual furnace temperature during program execution.

During program execution, the following values are output for digital display:

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

Coating the graphite tube

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

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

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

9.3.5 Further furnace functions

The Furnace | Control window contains the following functions:

- Information relating to the graphite tube
- Formatting the graphite tube
- Baking out the graphite furnace
- Open/close graphite furnace
- Indication of current cooling water temperature
- Configure the circulation cooler

5										
Generation Furnace										×
Furnace program	Modif.Extras	Optimization	Plot	Control						
Graphite furn Type: Heat cycles Life time:	ace : Ret Form:	Platform 9 0 set			Furnace Open furn Cooling water temp Furnace LED	ace p. [°C]:	30			
Clean furnac Temp. [°C]: Ramp [°C/s] Hold [s]:	e2	2450 500 5	Start	T	emperature for LE Test Water flow Inert gas Add. gas	D switch-off: W: Tra	ater coole ansforme	3(er er temp	00 👤	
auto	Ор	ermanent				Test				
Line: Mg	j285	× •	•			ОК		Car	ncel	

Graphite tube data

The **Graphite furnace** area contains information about the graphite tube, which is entered when the tube is changed and then automatically updated. If you are using a new tube, set the values to 0.

Option	Description	
Туре	Tube type according to setting in the window Quick Start	
Heat cycles	Number of heating cycles of this tube	
Life time	Statistical ratio for thermal strain exposure of graphite tube as a product of control parameters and step times of currently active furnace program.	
	This numerical ratio can always be estimated only for a particular type of job.	

Option	Description
	Note : Before removing a graphite tube which is still in a state fit for operation, you are recommended to record its operating data from the Graphite furnace area in order to be able to restore these values for automatic subsequent updating after the tube has been installed again.

Formatting the graphite tube

Formatting the graphite tube performs the following functions:

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

Formatting must be performed in each case:

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

Option	Description
FF%	Formation factor determined as part of formation
Formate	Start formatting
	The Formate window appears, which displays the currently measured furnace data. Nine temperature levels $(300 - 1500 - 300 - 1500 - 300 - 1000 - 2000 - 2400 °C)$ are run and the test temperatures in the tube are measured. On completion of the last step, the formation factor will appear and the data obtained for tube temperature recalibration will be saved.

Recirculating chiller

Configure the circulation cooler.

Option	Description
auto	The circulation cooler switches automatically to keep the cooling wa- ter temperature within the operating range.
permanent	The circulation cooler is constantly switched on to ensure maximum cooling capacity.

Baking out the furnace

Bake-out is a single-step cleaning program. The gas flow is permanently set to maximum flow. Current parameter settings which can be modified here will be saved with the method.

Option	Description
Temp.	Temperature of baking out (cleaning)
Ramp	Heating rate
Hold	The time for which baking lasts
Start	Triggers a baking (cleaning) process, displays the Clean furnace win- dow that reports currently measured furnace data.

Further furnace functions

С

Option	Description
Cooling water temp.	Current cooling water temperature
Furnace LED	Turns the furnace camera on if active. A special window with a graphite tube image will be imposed onto the screen. Sample injection can be monitored.

Option	Description
	The furnace camera is delivered with permanently On presetting. The option for this is located in the Options Analysis sequence window.
	Note: The furnace camera is not available for all AAS device types.
Open furnace	Open graphite furnace
	Graphite tube can be retrieved or installed.
Close furnace	Close graphite furnace
Temperature for LED switch-off	Furnace temperature from which the LED of the illumination unit is switched off. At the same time the furnace camera is switched off and the measurement value acquisition is prepared.

Furnace test

The furnace is checked for sensor errors. If one of the error states listed here appears, every measurement will be aborted (on the screen a corresponding error message will be displayed).

Start the error test with **Test**. If the test was successful, the indicator will turn green; if the test fails, it will turn red.

See also

B Options for analysis sequence [▶ 171]

9.3.6 Setting the furnace position (novAA 800)

Only for novAA 800

In the **Furnace** | **Position** window, the height of the graphite furnace relative to the beam path can be adjusted if the furnace should cut the beam path.

G Furnace	—		×
Furnace program Modif.Extras Optimization Plot Control Position			
Alignment Height [mm] 💽 Energy HCL: 163142 Reset Save			
Line: Pd247 V • OK	Ca	ancel	

- Use the arrow keys in the **Height** input field to change the position of the furnace in the beam path and observe the changes in the energy of the HCL.
- Use the **Save** button to permanently save the newly set furnace height.
- Click on **Reset** if you want to reset the furnace height to the preset height.

9.4 Hydride system

You can perform the following functions in the **Hydride system** window:

- Check the status of the hydride system
- Test various functions of the system for errors
- Re-initialize the hydride system
- Load the system tubes with reagents before the start of analysis

	 Flush the system, e.g. after the end of the analysis for cleaning Open the Hydride system window using the menu command Method Development Hydride or by clicking the Hy icon.
Initializing the hydride system	 The hydride system is always initialized at the beginning of work with the AAS. Reinitial-ization may be necessary if the connection to the AAS has been interrupted. In the Hydride system window, click on Initialize.
	\checkmark Communication between the hydride system, the AAS and the PC is established.
Loading the hydride system	Loading of reagents is necessary before start of analysis, following a new installation or following cleaning of the hydride system.
	In the Hydride system window, click on Load system.
	\checkmark The tubes of the hydride system are loaded with reagents.
Flush hydride system	The hydride system can be flushed with acid or reductant to remove residues from the system. The associated parameters are specified in the Method Hydride window.
	In the Hydride system window, click on Clean system.
	\checkmark The hydride system is flushed.
	See also

B Specify Hydride and HydrEA systems (Method | Hydride window) [▶ 40]

9.4.1 Checking the functions of the hydride system

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

Hy Hydride system	- 🗆 X
Control Error test	
Pumps Speed level:	Gas flow Valve2 Valve3 Valve4 (20 L/h) (6 L/h) (25 L/h) Cell Cell 8
gas path	Heating on Target Actual
● GLS -> cell	Temp.[°C]: 150 🗘 0
 GLS -> exhauster Gas -> cell Gas -> exhauster Gas -> exhauster 	Sample valves Sample to waste Sample to reactor
GLS -> collector -> cell Gas -> collector -> cell Gas -> collector -> exhauster Batch -> cell Batch -> exhauster	
 Batch -> collector -> exhauster 	Bubble sensor O Start
Load system Clean system	Initialize Close

Control of the pumps

This function switches the pumps on and off.

	Ontion	Description					
	Components nump	The component nump transports the reagents of the hydride system					
	Sample numn	The sample pump transports the liquid analysis sample					
	Sumple pump						
	Note : If neither of the two valves 3 or 4 is activated when one of the two pumps is switched on, valve 3 is automatically switched on to prevent backflow of the liquid. When the sample pump is running, the component pump is also activated to prevent liquid blockage in the gas-liquid separator.						
Control of the gas paths	In the gas path area, sequence can be swite	all paths of argon gas flow which are meaningful for the analysis ched by means of magnetic valves (magnetic valve groups).					
	The Gas -> valve 2 -> gas paths that do not	The Gas -> valve 2 -> cell option is used to switch a large gas flow directly to the cell for gas paths that do not go to the cell. This opens valve 2.					
Valves in the gas flow	These functions can b	be used to switch the valves in the gas path.					
	Valve2 switches the g	gas flow through the tip of the batch module on and off.					
	Valve3 switches 6 L/I	h argon to the set path.					
	Valve4 switches 25 L	/h argon to the set path.					
Checking the cell	Ontion	Description					
	Cell height	Adjust the cell height in the beam path					
	Heating on	Switch on the cell heating					
		The function can be used for pre-heating the cell. The cell is heated to the temperature in the Target field. After switching the cell heater on and off, the temperature value is displayed in the Actual field.					
Switching sample valves	In the Sample valves sample path to either	area, the solenoid valve pair (V6, V7) can be used to switch the waste or the reactor.					
Heating the gold collector	Only for Hg/hydride s	systems with enrichment					
	In the Collector area,	you can show and edit the gold collector settings.					
	Option	Description					
	off	Switch off the heating and cooling of the gold collector					
	Heating on	Switch on the heating of the gold collector					
	Cooling on	Switch on the fan of the gold collector					
		The gold collector is cooled down.					
	Heat value	Parameters for the bake-out temperature of the gold collector					
		Value is preset by the manufacturer and should only be changed if the thermal properties of the gold collector heating have changed. A higher value corresponds to a higher cleaning out temperature.					
	Set	Save displayed heating value as the new value in the hydride system					
Clean bubble sensor	Only for HS 60 and H The bubble sensor giv	S 60 modular ves a signal if liquid has entered the gas path after the gas-liquid					

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

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

9.4.2 Testing the hydride system for errors

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

Hy Hydride system			—		×
Control Error test					
Hydride system Type: HS60 M Version: V T0 4.0	!] :	50]	
Error					
Gas pressure					
● +24 V					
Safety relay					
Transformer temperature					
Collector temperature					
Gold collector heating time					
Cell temperature					
Cell heating time					
Line frequency					
Bubble sensor					
Cell temperature sensor					
Load system Clean system Initialize				Close	e

Connected hydride system

Option	Description
Туре	Connected and initialized hydride system
Version	Version of the hydride system firmware
Line frequency	The measured line frequency 50 or 60 Hz is displayed. Deviations of 2 Hz above and below are tolerated, otherwise the fault report "line frequency" is issued.

Fault test

The results of the test are indicated by green (for successful test) and red (negative test result) indicator lamps. The error test is started with the Test button.

A negative test result can have the following causes:

Option	Description
Gas pressure	Argon gas pressure is not present
+24 V	Operating voltage +24 V is not present
Safety relay	Safety relay not switched on
Transformer temperature	Transformer is too hot or the sensor is defective
Collector temperature	Gold collector is too hot or the sensor is defective

Option	Description
Gold collector heating time	Gold collector temperature cannot be reached
Cell temperature	Cell is too hot or the thermoelement is defective
Cell heating time	Set temperature of cell cannot be reached
Line frequency	Line frequency neither 50 not 60 Hz
Clean bubble sensor	Liquid is located in the gas path after the gas-liquid separator
Cell temperature sensor	The temperature sensor in the cell is defective

9.5 Autosamplers for flame technique

The software supports the following autosamplers for the flame technique:

- AS-F and AS-FD
- AS 51s
- AS 52s

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

The following functions are available in the **Autosampler** window:

- Show connected autosampler type
- Adjusting the autosampler
- Also rinse the autosampler
- Reinitialize the autosampler
- Perform a self-test

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

Open the **Autosampler** window using the menu command **Method Development** | **Autosampler** or by clicking the \blacksquare icon.

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

- In the Autosampler window, click on Initialize.
 - ✓ Communication between the autosampler, the AAS and the PC will be established.

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

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



NOTICE

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

Before installing the autosampler, switch off the AAS device and disconnect the mains plug from the socket. Otherwise, a short circuit can cause communication errors or damage the interface.

9.5.1 Specifying autosampler for flame technique

The **Autosampler** | **Parameters** window provides setting options and display functions for the following parameters:

- Autosampler type
- Washing parameters
- Setting options for controlled cleaning
- Function for mixing cup washing

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

😬 Autosamp	oler						—		×
Parameters	Techn. paramete	rs Function tests	Positions	Add reagent	t				
Autosa	ampler		Speci	al functions —					
Туре	e .	AS-FD 🗸	-Wa	sh mix cup —					
Tray:		139 Pos. 🗸	Ve	olume [ml]:	5	•	Sta	irt	
Versi	ion: 1	2.599							
Wash									
after	sample	~							
Wash Mixing	time Wash cup [s] g cup cycles:	: 15 • 1 •							
Contro	lled cleaning								
⊡ Co	ntrolled cleaning								
Contro	ol limit (Abs):	0.005							

Autosampler

Option	Description
Туре	Selection / display of the connected type of autosampler
	"-": No autosampler selected
	AS 51s / AS-F: Autosampler for flame, hydride and HydrEA tech- niques without dilution function
	AS 52s / AS-FD: Autosampler for flame, hydride and HydrEA tech- niques with dilution function
Sampler tray	"-": No tray attached
(AS-F / AS-FD)	139 Pos. Tray with 129 positions for 15 mL Sarstedt sample cups on the outer track and 10 positions for 30 mL Sarstedt cups on the inner track

Option	Description
	54 Pos. Tray with 54 positions for 50 mL Sarstedt sample cups
Sampler tray	n_n
(AS 51s / AS 52s)	No tray attached
	87 pos. Tray with 77 positions for 15 mL Sarstedt sample cups on the outer track and 10 positions for 30 mL Sarstedt cups on the inner track
	49 pos. Tray with 49 positions for 30 mL Sarstedt sample cups
	30 Pos. Tray with 30 positions for 50 mL Sarstedt sample cups
Version	Version number of autosampler software

Wash

Option	Description
Wash mode	off Wash mode is switched off. No washing performed automatically.
	Between each sample Washing after each sample, but not within a statistical series
Wash time	During this time, rinsing solution is aspirated from the mixing cup.
Mixing cup cycles	Number of wash cycles for the mixing cup
	Fills mixing cup with wash liquid/diluent solution and drains it again in one cycle.

Control	led	C	leaning
Control	icu	C	cunnig

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

Special functions

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

Option	Description
Wash mix cup	Wash mix cup separately outside a sequence measurement
	Volume Enter volume for cleaning
	Start Start the wash cycle

9.5.2 Technical parameters of the autosampler for the flame technique

In the Autosampler | Techn. parameters window, specify the following parameters:

- Immersion depth of the cannula in the various cups
- Working speed of the dosing unit
- Alignment of autosampler arm in relation to sample cups

🚟 Autosampler					– 🗆 X
Parameters Techn. parameter	ters Function	tests Positions Add rea	agent		
Action Take up Dispense Take up Wash Dispense	Type AS-FD AS-FD AS-FD AS-FD AS-FD AS-FD	Location Sample cup Special cup Mix cup Mix cup Wash cup Add reagent	Depth mm 112 100 30 112 114 15	Speed Level 6 10 6 	Table Speed: 6 Depth [mm]: 112 Depth at pos.: 1 Set
Wash	nitialize			Ok	Cancel

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

Сир	Action
Sample cup	Samples are taken up by a dosing unit or aspirated by a nebulizer (flame technique) or peristaltic pump (hydride technique)
Special cup	Take up or aspirate special samples
Mix cup	Dispense analyte and diluent solution, and take up samples after dilu- tion
Wash cup	Flush cannula and intake path
Add reagent	Programmed addition of reagent to the sample

Elements of the actions table	Column	Description
	Action	Available action options:
		Take up Take up sample from cup for dispense into mixing cup or dispense into flame
		Dispense Dispense sample into the mixing cup
		Wash Take up wash solution
	Туре	Connected autosampler type
	Location	Cup to which a given action refers
	Depth	The depth to which the cannula submerges in units of 1 mm
	Speed level	Working speed of the dosing unit
		Greater values cause the dosing unit to work faster, with smaller val- ues it will work more slowly. Recommended values:
		Taking samples: Average speed levels
		Dispense into the mixing cup: One of the two highest levels, so that fast injection to ensure thorough mixing takes place. Besides, the complete mix up is supported by a fixed wait time before the take up from the mixing cup (or sample cup).

Column	Description
	The taking of diluent and of the separating air segments is carried out at a fixed speed.

Table subarea

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

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

See also

Setting the immersion depth and dosing speed of the autosampler [140]

9.5.3 Setting the immersion depth and dosing speed of the autosampler

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

- Open the Autosampler | Techn. parameters window by clicking on **E**.
- Select the table row whose parameters you want to change.
- For the specification of sample and mixing cups, in the **Depth at pos.** field, set the position on the tray, at which you want to test the immersion depth.
- Only AS-GF and MPE 60/2: If dilution in sample cups is activated in the Method |
 Sample transport window, set the position of the mixing cups.
- Activate the **Set** checkbox to move the sampler arm to the specified cup position.
- Watch the movement of the sampler arm and vary the **Speed** and **Depth** until you achieve the desired result.

See also

- Technical parameters of the autosampler for the flame technique [> 138]
- Technical parameters of the autosampler for the graphite furnace technique [146]

9.5.4 Functional test of the autosampler for flame technique

In the Autosampler | Function tests window, the autosampler functions can be checked.

🐱 Autosamp	bler			—		×
Parameters	Techn. parameters	Function tes	sts Positions Add reagent			
Tracker O Cup © Waa O Mixi O Tub Pipetter Speed	/Rotator no sh position ng position e position	1 ×	Dipping arm Depth [mm]: 0 Pumps Wash pump Mix cup pump	Error test Version: [Tracker/Rotator Tray ident. Pipetter (drive)	12.599	
Volume	e [μL]:	0	Test programs	Pipetter (volume Test	÷)	
Ta	ke up Dispe ve to bottle Reset	nse	Test program 1 Test program 2 Test program 3 Start	Adjust sampler		
Was	h Initial	ize		ОК	Cancel	

Tracker/Rotator

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

Option	Description
Cup no	Drives to the cup position selected from the corresponding list box
Wash position	Move to wash cup
Mixing positions	Only for autosamplers with dilution function
	Drives to the mixing cup

Pipettor

Only for autosamplers with dilution function

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

Option	Description
Speed	Dosing rate
	Level 1 – minimum dosing speed
	Level 12 – highest dosing speed
Volume	Pipetting volume to be taken up
Valve to bottle	Switch the valve to the bottle
	The valve switches the flow between the diluent bottle and the sam- ple. In switching, you must hear the valve click.
Take up	Take up the set volume at the set dosing speed
Dispense	Dispense the set volume at the set dosing speed
Reset	Reset volume settings

Dipping arm

The autosampler arm is lowered by the value **Depth** at the position selected for **Tracker/Rotator**.

Pumps

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

Option	Description
Wash pump	Pump for feeding the wash cup

Option	Description
Mix cup pump	Pump for draining the mixing cup

Test programs

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

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

Error test

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

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

Error	Description
Wash bottle level	Reports excessively low fill level of storage bottle (bottle empty).
Diluent bottle level	Reports excessively low fill level of storage bottle (bottle empty).
Tracker/Rotator	Swivel drive of sampler arm and rotary drive of tray are defective
Tray ident.	Sample tray not detected
Pipetter (drive)	Dosing unit error
Pipetter (volume)	The volume taken up by the dispensing unit was too large

See also

Adjusting the autosampler [▶ 142]

9.5.5 Adjusting the autosampler

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

Alignment position The autosampler arm can be adjusted to the following positions:

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

Adjusting the positions

Customized options are provided for adjusting the positions.

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

Adjusting the autosampler

- Place a sample cup on position 1 of the sample tray.
- Open the Autosampler | Function tests window by clicking on . Click on Adjust sampler.
- Select a position for adjustment.
- Adjust the immersion depth so that the position of the sampler arm relative to the cup can be well assessed.
- Adjust the position of the autosampler arm with the buttons.
- Additionally with **Tray**: Adjust the position of the sample tray.
- Accept the new parameters of the position by clicking on **Save** in the firmware of the autosampler.
- Repeat the previous steps for the positions that have not yet been adjusted.
 - \checkmark The new positions are permanently stored in the autosampler firmware.

See also

- Functional test of the autosampler for flame technique [▶ 140]
- Functional test of the autosampler for graphite furnace technique [150]

9.5.6 Position overview of the autosampler for flame technique

The **Autosampler** | **Positions** window displays the sample tray positions used in the current sequence. The display modes **all positions** or **only special positions** can be selected for the display.

Note:

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

9.5.7 Supply of reagents for sample

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

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

9.6 Autosamplers for graphite furnace technique

The software supports the following autosamplers for the graphite furnace technique:

- AS-GF autosampler without mixing cup
- MPE 60 autosampler with mixing cup
- MPE 60/1 autosampler without mixing cup

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

You specify the parameters directly relevant for the analysis (occupancy on the sample tray or dilution) in the method, the sequence and in the sample ID.

Open the **Autosampler** window by clicking the \mathbf{E} icon or by using the menu command **Method Development** | **Autosampler**.

The Autosampler window contains the following functions:

- Show connected autosampler type
- Adjusting the autosampler
- Also rinse the autosampler
- Reinitialize the autosampler
- Perform a function test
- Display sample allocation
- Perform reagent addition

You specify the parameters (allocation on the sample tray, dilution, mixing and rinsing steps) that are directly relevant for the analysis in the method, sequence and sample identification.
Initializing the autosampler The autosampler is always initialized at the beginning of work with the AAS in the **Quick** Start. Reinitialization may be necessary if the autosampler has lost its orientation, e.g. due to a mechanical impact. In the **Autosampler** window, click on **Initialize**. ✓ Communication between the autosampler, the AAS and the PC will be established. Wash sample tube Wash liquid is pumped through the sample tube via the dosing unit and dispensed into

the wash cup.

- In the Autosampler window, click on Wash.
 - The sample tube is washed.



NOTICE

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

Before installing the autosampler, switch off the AAS device and disconnect the mains plug from the socket. Otherwise, a short circuit can cause communication errors or damage the interface.

9.6.1 Specifying the autosampler for graphite furnace technique

The Autosampler | Parameters window provides setting options and display functions for the following parameters:

Autosampler type

Wash mode

- Washing parameters
- Setting options for controlled cleaning
- Function for mixing cup washing

The Wash and Controlled cleaning parameters are taken from the current method. Conversely, however, changes in the Autosampler | Parameters window do not affect the entries in the method.

Autosampler	Option	Description	
	Туре	Selection / display of the connected type of autosampler	
		"-": No autosampler selected.	
		AS-GF/MPE 60: Autosampler for graphite tube technique	
	Sampler tray	"-": No tray attached	
		89 Pos. : For MPE 60 Tray with 77 sample cups (V = 2 mL), 4 special sample cups (V = 5 mL) and 8 special sample cups (V = 2 mL)	
		108 Pos. : For AS-GF Tray with 100 sample cups (V = 1.5 mL) and 8 central cups for diluents, special samples, standards, modifiers etc. (V = 5 mL)	
	Version	Version number of the autosampler firmware	
Wash	Ontion	Description	

off

Wash mode switched off. No washing performed automatically.

Between each sample

Washing after each sample, but not within a statistical series

	Option	Description
		Between runs Washing after each measurement, including within a statistical series
		Between components The autosampler is washed after transfer of each component into the graphite tube (modifier, standard, sample, etc.).
	Wash cycles Wash cup	Number of wash cycles per wash, 1 to 5
Controlled despine	0	
Controlled cleaning	Option	Description
	Controlled cleaning	Cleaning check if concentration is exceeded
		The cleaning progress is checked by repeated measurement.
	Control limit (Abs)	The signal level must have returned to this value before the diluted samples or samples with lower concentrations are measured.
Washing MPE 60 mixing cup	On the MPE 60 autos Option	ampler with dilution function, the mixing cup can be washed. Description
	Wash mix cup	Wash mixing cup separately outside the measurement
		Volume Enter volume for cleaning
		Start Wash the mixing cup
	Mixing cup cycles	Number of rinse cycles for the mixing cup In a rinse cycle the mixing cup is filled with wash liquid / diluent and then emptied again.

9.6.2 Technical parameters of the autosampler for the graphite furnace technique

In the Autosampler | Techn. parameters window, specify the following parameters:

- Depth of immersion of cannula / dosing tube into the various cups
- Working speed of the dosing unit
- Alignment of autosampler arm in relation to sample cups
- Automatic depth adjustment for volume decrease during the analysis
- Alignment of the autosampler to the graphite tube

🖬 Autosampler — 🗆 🗙						
Parameters Techn. parameters Function tests Positions						
Action Take up Take up Inject sample Dispense special Automat. depth correct Sample cup Align sampler to fit	Type AS-GF AS-GF AS-GF AS-GF ion s urnace Camera	Location Sample cup Special cup Graphite furnace Graphite furnace	Depth mm 52 -0.9 -0.9	Speed Level	Table Speed: 3 • Depth [mm]: 52 • Depth at pos.: 1 • Set	
Wash	nitialize			Ok	< Cance	

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

Option	Description		
Sample cups	Take up samples through dosing unit		
Special cups	Take up special samples		
Mix cup	Dispense analyte and diluent solution, and take up samples after dilu- tion		
Graphite furnace	Inject samples or special samples into the graphite tube		

Option	Description
Action	Take up Take up sample from the sample cup, special cup or mixing cup
	Dispense Dispense sample into the mixing cup
	Inject sample / Dispense special Inject sample or special sample into the graphite tube
Туре	Connected autosampler type
Location	Cup to which a given action refers
Depth	The depth to which the cannula submerges in units of 1 mm
Speed level	Working speed of the dosing unit
	Greater values cause the dosing unit to work faster, with smaller val- ues it will work more slowly. Recommended values:
	Taking samples: 3
	Dispense into the mixing cup: 9
	Injection into the graphite tube: 1

Table subarea

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

Option	Description
Speed	Speed of dosing unit

Option	Description	
Depth	Set immersion depth of the cannula	
	The immersion depth is measured from the highest position of the sampler arm.	
Depth at pos.	Position of special or sample cup at which the immersion depth is measured	
Set	If activated, the sampler arm moves over the cup for which the posi- tioning 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 sampler arm moving above the cup.	

Automatic depth correction

Option	Description	
Automat. depth correction	Automatically adapts the depth, to which the dosing tube will im- merse into sample or special cups, to a new volume.	
Sample cups	Only active if Automat. depth correction is active.	
	Opens the Sampler positions, volumes and depths window for set- ting deviating cup geometries and volumes for individual cups. The settings are taken into account during automatic depth adjustment	

Additional functions	Option	Description
	empty mixing cups	Only MPE 60/2 and AS-GF
		The button is active if sample cups have been defined as mixing cups in the Method Sample transport window. Clicking on the button releases these positions for reuse.
	Open furnace / Close furnace	Open and close furnace to change furnace tube
	Align sampler to furnace	Start software-assisted alignment of the autosampler to the graphite furnace

See also

- Setting the immersion depth and dosing speed of the autosampler [140]
- Automatic depth adjustment with autosampler for graphite furnace technique
 [148]
- Aligning the autosampler to the graphite furnace [▶ 150]

9.6.3 Automatic depth adjustment with autosampler for graphite furnace technique

The automatic adjustment of the immersion depth of the dosing tube into the sample and special cups prevents unwanted contamination of the dosing tube. To draw in a sample volume, the dosing tube will dip into a sample cup just as much as necessary to accomplish this. As total volume removal increases, the immersion depth will automatically be corrected.

The immersion depths for sample cups or special cups set in the **Autosampler** | **Techn. parameters** window initially apply to all cups on the sample tray.

Fill volumes or cup sizes at variance with standard cups can be separately specified and duly considered for automatic depth correction.

In the Autosampler | Techn. parameters window, activate the Automat. depth correction checkbox.

- Click on Sample cups.
 - ✓ The **Sampler positions, volumes and depths** window opens.

Sampler positions, volumes and depths				
	Special cups 101 - 108	Sample cups 1 - 100		
Position:	101	1		
Volume [µL]:	0	0		
Depth [mm]:	0.0	0.0		
Diameter [mm]:	18.5	12.0		
	Delete volumes	Delete volumes		
Maximum dipping depths (auto	Maximum dipping depths (auto adjustment)			
Sample cups	Depth[mm]: Position:			
○ Special cups	65 📮 1	Reset		
Set Save OK				

• Specify the following parameters for individual special and sample cups:

Option	Description
Position	Set cup position on the tray, for which the three displayed values: vol- ume, depth and diameter apply.
	Make the settings for each cup that is to be changed.
Volume	Displays the amount of sample volume already retrieved from a cup or allows input of lacking sample volume balance into a cup not com- pletely filled.
	The value is updated by the program after each sampling.
Depth	Displays additional depth corresponding to the sample volume al- ready taken.
	This value is recalculated after each sample take-in sequence. The to- tal immersion depth is the sum of the specified immersion depth (Depth column on Techn. parameters tab) and the additional depth displayed here.
Diameter	Indicates the cup diameter.
	On this basis, the depth is calculated according to the removed vol- ume.
Diameter	For cups with dimensions at variance against those of standard cups
	Allows you to specify a diameter for each cup individually if selected.
Delete volumes	Resets volume values for all special cups or sample cups to 0.
Reset	Reset all volumes and depths for all cups to 0 and the diameters to the values last saved with OK .

Maximum immersion depth (auto adjustment)

A maximum allowed immersion depth can be specified in order to prevent the dosing tube from hitting the cup bottom and getting twisted.

Option	Description
Sample cup	Applies settings for maximal immersion depth to sample cups if marked.
Special cup	Applies settings for maximal immersion depth to special cups if marked.

Option	Description
Depth	Defines the maximal allowed immersion depth of the autosampler into a sample cup or special cup
	Note: Please note that the autosampler will at once dip down to the new depth level if the Set checkbox is selected! Make sure that the autosampler path is not blocked. Then save the current immersion depth by clicking on Save .
Position	Sample tray position at which the dipping depth settings are tested
Set	The dosing tube will dip into a cup that was specified via Position and to a depth that was set via Depth . The immersion depth can be visually checked.
Save	Save the changed immersion depth for the cup type

9.6.4 Aligning the autosampler to the graphite furnace

The fine alignment of the autosampler to the graphite furnace is software-supported. The autosampler is aligned in such a way that the dosing tube can optimally dispense the samples in the graphite tube without touching the dosing insert. The injection depth for the sample is set in the same process.

- Open the **Autosampler** | **Techn. parameters** window by clicking on **E**.
- Click on Align sampler to furnace.
 - $\checkmark\,$ The wizard for aligning the autosampler starts. Follow the further instructions on the screen.

9.6.5 Functional test of the autosampler for graphite furnace technique

You can test the functions of the autosampler in the ${\bf Autosampler}\,|\,{\bf Function}\,{\bf tests}$ window.

Tracker/Rotator

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

Option	Description
Cup no	Approach selected sample cup
Wash position	Move to wash cup
Mixing positions	Only autosampler with dilution function
	Drives to the mixing cup
Tube position	Start up graphite furnace

Pipettor

This test checks the dosing unit.

Ontion	Description
option	Description
Speed	Adjust the pipetter speed
Volume	Adjust the pipetting volume to be taken up
Take up	Take up the set volume at the specified dosing speed
Dispense	The set volume is dispensed at the specified speed
Valve to bottle	The valve switches the flow between the diluent bottle and the sam- ple. In switching, you must hear the valve click.
Reset	Reset volume setting

Dipping arm

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

Test programs

• Enter the depth by which the autosampler arm is lowered in the **Depth** field.

Tests are provided to test the autosampler with pre-configured, dry running test programs. The cups approached in the test must be empty! When the test programs are finished, you are informed of the test success.

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

Program	Description
Test programs 1	 Aspirates volume from position 1 Aspirates volume from position 41 Discharges volume into graphite tube Washes dosing tube two times
Test programs 2	 Only for MPE 60 Aspirates diluent solution from waste bottle Aspirates volume from position 10 Discharges volume into mixing cup Aspirates volume from mixing cup Discharges volume into graphite tube Purging the dosing tube Drains mixing cup Washes and drains mixing cup
Test programs 3	Immerse in every position

Error test

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

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

Option	Description
Wash bottle level	Reports excessively low fill level of storage bottle (bottle empty).
Waste bottle level	Fill level of waste bottle is too high (bottle is full).
Tracker/Rotator	Swivel drive of sampler arm and rotary drive of tray are defective
Tray ident.	Sample tray not detected
Pipetter (drive)	Dosing pump error
Pipetter (volume)	The volume taken up by the dispensing unit was too large

Adjusting the autosampler

The autosamplers are supplied factory-adjusted. In rare cases, readjustment may be necessary. Click on **Adjust sampler** to open the window for readjusting the autosampler.

See also

Adjusting the autosampler [▶ 142]

9.6.6 Position overview for autosamplers for graphite tube technique

The **Autosampler** | **Positions** window displays the sample tray positions used in the current sequence. The display modes **all positions** or **only special positions** can be selected for the display.

Note:

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

9.7 Solid autosampler SSA 600

To run automated solid analytical procedures, the SSA 600 is applied. The type of autosampler is identified during device initialization in the **Quick Start** window. The **Solid sampler parameters** window contains the following functions:

- SSA 600 function test
- Alignment of SSA 600 to graphite tube furnace

The solids sampler SSA 600 can be operated with or without liquid dosing, therefore the function test and adjustment is based on the autosampler specified in the method.

- Using the icon **iii** open the window **Method**.
- On the Lines tab, select an analysis line and on the Sample transport tab, enable the option of the installed autosampler, e.g. SSA-600 with liquid pipetter.
- Activate the settings with **Accept**.
- Open the **Solid sampler** window by clicking on **E** or via the menu command **Method Development** | **Autosampler**.

Control buttons in autosampler window

Buttons	Description
Reset	Take up sample platforms which are on various positions of the au- tosampler and transport back to the sample tray.
Initialize	Reinitialize the autosampler
	The autosampler is always initialized at the beginning of work with the AAS in the Quick Start . Reinitialization may be necessary if the autosampler has lost its orientation, e.g. due to a mechanical impact or due to pressing the stop button on the autosampler. Communica- tion between the autosampler, the AAS and the PC will be estab- lished.
Align	Start a routine to align the SSA 600 to the graphite tube furnace



NOTICE

Connect autosampler only to AAS in deenergized state!

Do not connect the autosampler when the AAS is in power-on condition. Failure to comply may result in faulty communication of even destruction of the interface.

9.7.1 Function test of solid sampler

You can test the functions of the connected autosampler in the **Solid sampler** | **Function tests** window. The following options are available:

Option	Description
Status/Buttons	Display SSA 600 status and button on the SSA 600 that was actuated since the latest query in appropriate color (green, orange, red).
	Using Update , the status can be queried again and the button display be updated.
Move to position	Move to the position selected in the Pos list field. No platform is taken up or put down.
Rotate tray	Rotate the sample tray to the selected position

Option	Description
Transport	Means that SSA 600 transports a platform from a given position to the next starting and target position. If Take-up platform is activated, the gripper picks up a platform. If Put-down platform is activated, the gripper places the platform at the target location.
Gripper	Open and close gripper
	Lower the cannula
Balance	Determine the weight of a platform located on the tray at the set position (Pos).
	Weighing with tare Before weighing the platform, the scale is tared. #1 indicates the tared weight. #2 contains the weight of the platform (also with dosed sample as may be the case).
	Internal calibration During this calibration, the internal calibration curve of the scale is determined again. To do this, first reset the scale, determine the zero point and then weigh an internal weight. The values obtained for zero-point and internal weight will provide the input for determina- tion of the scales calibration graph.
Loop	The autosampler transports two platforms (positions 1 and 2) back and forth between the sample tray, the scale and the furnace. The number of transports can be entered in the Cycles field.

9.7.2 Alignment of solid sampler

The **Solid sampler | Alignment** window contains the following functions:

- Check and adjust the movement to individual positions
- Align the autosampler to the graphite furnace
- SSA 600 with dosing unit: Automatic depth correction for taking in matrix modifiers and special liquid samples.
 - Test of liquid dosing

Option	Description
Alignment position	Selection of the position on the autosampler
Adjust position	Alignment of the gripper to the set adjustment position
Open gripper/Close gripper	Open and close gripper with software control, e.g. for changing the gripper tips

Only autosamplers with liquid dosing:

Lower cannula	Lower the cannula
Automat. depth correction	Settings for the automatic depth adjustment for the liquid dosing
Wash	Wash dosing tube with the pre-set and with 🗗 confirmed number Wash cycles .
Test liquid dosing	Check liquid dosing
Change dispenser syringe	Move the piston of the dosing unit downwards for the change

Monitoring & aligning individual positions

- Select a desired position from the **Alignment position** table.
- Click Move to in the Adjust position group to move the autosampler to the selected position. Put a platform up in this position and check the position of the platform.

	Use control buttons in this group to make positional corrections as necessary.
	Save all modified setting by clicking the Save button.
Align gripper to the graphite tube furnace	The gripper of the autosampler must be aligned to the furnace using the software. To do this, you need the adjustment aid included with the autosampler.
	In the Solid sampler Alignment window, click on Align.
	 When the adjustment routine is complete, the autosampler is aligned with the furnace.
	A detailed description of the adjustment procedure can be found in the "SSA 600 Solids Sampler" operating manual.
Washing the system	Only for SSA 600 with liquid dosing
	When cleaning the system diluent is taken from the supply bottle and pumped through the entire path via the dosing device to the dosing tube and dispensed into the wash cup.
	• Enter the number of repetitions in the Wash cycles input field.
	Save the entry with the 🔁 icon.
	Start the wash process with the Wash button.
Automatic depth correction for dosing unit	Typically, depth correction occurs automatically when working with the SSA 600, i.e. as the volume that is drawn from autosampler cups increases, the immersion depth will be matched accordingly. Starting volumes other than those which were set via Method can be corrected in this window. The settings are made in the same way as for the autosam- pler for the graphite tube technique.
	See also

Automatic depth adjustment with autosampler for graphite furnace technique
 [148]

10 Data management

This section provides information on the following topics:

- Print functions
- Management of methods, sequences and sample IDs
- Management of device-specific files
- Definition of units for concentrations and contents
- Management of frequently used stock solutions and QC samples

10.1 Print functions

The software has a large number of output formats for data output. In addition to output to the printer, the data can be exported to Excel, PDF, HTML, XML or text format or saved as bitmap or scalable graphics using the print function.

Report templates are used for the output of analysis results and window contents. 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

The software offers different possibilities to print results data:

- Print the complete record. The complete record of an analysis contains the method parameters, the calibration and analysis results with individual sample values (statistic runs). A report may be printed of the current results in the main window and the saved data.
- Print current results. In this printout only the data of the main window are printed. Here you can choose between a complete and a compact printout.
- Print selected data from the **Overview** tab. For this printout you can select the analysis lines and results in a dialog window.

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

- ▶ Open the **Data** | **Reports** window by clicking on **E**.
- Alternatively, open the window with the menu command **Extras** | **Data** or the menu command **File** | **Print** | **Report**.
 - ✓ The name of the current file, file information (Description field) and all method versions used for creating the current results file are displayed.

Data		- 🗆 X
Reports Data managem	ent Units Stock std/QC samples Default descriptio	ons
Results data for print ou	t or export - current data	Theory (1994) in the later Accel folge (1975)
C:\Use\ReportTest	Daten.tps	A BARE TRAC
Description:		Annual Control and Annual And Annual An Annual Annual Annu
Instrument:	ZEEnit 700 No.:	
Technique:	Flame	
SW version: Description:	1.1	
	¥	
Use compact repo	rt	72-17-55 × 5-57-8.
Select method param	eters for print out: none all	
No. Name	Vers. Date Time Created	
2 testrep2	1 05.12.2011 8:42 AJSERVICE	
3 testrep	2 05.12.2011 8:22 AJSERVICE 3 05.12.2011 8:22 AJSERVICE	Report templates
T tostiep		🖶 Print
		Class
		Close
lf you want to pr the desired file.	int a saved file, use 📫 to open the defa	ult Open window and sele
lf you want to pr	int the shortened compact report activa	ate the option Use compac
report.		
Select all method	l versions to be printed in the table	
Make the selecti	on by clicking with the mouse and holdi	na down the Shift or Ctrl ke
Use the all butto	n to select all versions and the none but	tton to remove all selection
Click on Print to	open the ASpect LS Report window.	
If necessary char	have the output format in the Direct to lis	st and set special parameter
of the output for	mat with Options .	
Start the printou	t with Start.	

Note: Use the Preview setting for the printout. When you click on Start, the pages to be printed are first displayed in the print preview. This allows you to check whether all the required data is output before printing.

Print current results

The results tabs displayed in the main window can be printed.

- Activate the tab in the main window, the content of which you wish to print.
- Start the printout using the menu command **File** | **Print** | **Active Window**.
 - ✓ The **Results report format** window opens.
- Click on complete output if you want to print the results with the signal diagrams.
 Select compact output for printing the results in a compact overview.
- Continue as described above for "Print complete record".

Note: If you activate the checkbox in the **Results report format** window and then click on **complete output** or **compact output**, this window will no longer appear the next time you print the results and the last results report type will be used automatically. You can reset this setting in the **Options** | **View** window.

Print selected data • Change to the **Overview** tab in the main window.

Click on at the bottom of this tab or select the menu item File | Print | Active Window.

✓ The **Print** / **Overview** window appears.

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

See also

■ View options [▶ 168]

10.1.2 Print further analysis parameters and settings

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

- Method
- Sequence
- Result data and results overview
- Sample ID
- QC (Quality Control charts)
- Calibration
- Autosampler positions

The printing of the parameters occurs from the respective window.

- On the Aspect LS workplace, activate the window, the content of which you want to print.
- ▶ Start printing the parameters with a click on 🖶 in the window.
- Alternatively, select the menu command File | Print | Active Window.
 - ✓ The ASpect LSReport window opens.
- 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 Adapting report templates

Use report design mode	The report templates installed by default can be individually adapted. For a better over- view report views can be edited with real values.
	• Activate the menu command File Report Design Mode.
	Open the window whose report template you want to change.
	Open the menu command File Print Active Window.
	✓ The report designer opens.
	Make the desired changes and save the changed report template.
	• Link the report stylesheet with the corresponding print contents (see "Managing Report Stylesheets below).
Short introduction to the report designer	The individual components of the report template are called Objects . A table can thus consist of an object each for the header, the list values and a graph.
	These objects again contain the information to be printed and carry the associated lay- out characteristics such as fonts, alignment, make up, 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 charac- teristics.
	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 can 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 with which further settings can be changed.
	You will find further information on the operation and functions of the report designer in the handbook "Designer.pdf" on the ASpect LS-CD.
The Report Templates window	The templates are edited in the window and assigned to the Aspect LS 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.
	_

- ▶ Open the **Data** | **Reports** window by clicking on **E**.
- Use **Report templates** to open the window of that name.

For the following windows a report template must be available:

Name	Description
Method/Results	Full report
Results	Content of the Results tab in the main window
Method	Method parameters in the window Method
Calibration	Calibration of the analysis in the window Calibration
QC chart	Data of the QC charts in the window QC
Sample ID	Sample information in the window Sample ID Sample Information
QC sample infor- mation	Information data of the QC samples in the window Sample ID QC sample information
Sequence	Sequence order in the window Sequence
Results (Overview)	Content of the Overview tab in the main window
Sampler pos.	Assignment of the autosampler in the window Autosampler Posi- tions
SSA600 table	Content of the Solid tab in the main window

Change assignment

You must assign a new/edited report template to the corresponding print function again.

- Mark the window, the report stylesheet for which has been changed, in the list.
- Click **Change** to open the dialog box for assigning the files.
- If only one report template is to be assigned, activate the Use report template file (*.lst) option and select the desired file by clicking on ¹/₂.
- If several templates are offered at the same time at the start of printing, activate 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**.

The new report template is displayed in the Report templates window.
 Editing a report template
 Mark the window, the report stylesheet for which has been edited, in the list.
 Use Edit to open the report designer window.
 Restore default settings
 You can restore the settings according to the program installation.
 Click on Default settings.

See also

Importing report templates [▶ 162]

10.2 Management for all file types

The following data types are generated in ASpect LS:

- Methods
- Sequences
- Results files
- Report templates
- Worksheets

The above data types are organized in the **Data** | **Data management** window. The window appears after you click on \equiv or select the menu item **Extras** | **Data management**.

10.2.1 Managing methods and sequences

Methods and sequences are stored separately in a database. The method database is saved as "method.tps". The database containing the sequences is called "sequ.tps". In the text of this section, methods and sequences will hereafter be referred to as "data records".

Elements in the database window

When saving, opening, deleting, importing and exporting methods and sequences, database windows are opened, that have identical elements.

Save method Name: Pb in Food Cat: KK Name Vers. Date Time Cat. Operator Cd in Food 2 13.12.2023 12:55 KK SuStein Cr for ZEEman test 1 12.03.2020 13:44 SuStein Mg in Food 1 27.02.0201 11:40 User Pb in Food 1 16.10.2019 10:34 KK Analytik Jena Tl in Food 1 16.10.2019 10:26 Analytik Jena
Name: Pb in Food Cat: KK Name Vers. Date Time Cat. Operator Cd in Food 2 13.12.2023 12:55 KK SuStein Cr for ZEEman test 1 12.03.2020 13:44 SuStein Mg in Food 1 27.02.2020 11:40 User Pb in Food 1 16.10.2019 10:34 KK Analytik Jena Tl in Food 1 16.10.2019 10:26 Analytik Jena
Name Vers. Date Time Cat. Operator Cd in Food 2 13.12.2023 12:55 KK SuStein Cr for ZEEman test 1 12.03.2020 13:44 SuStein Mg in Food 1 27.02.2020 11:40 User Pb in Food 1 16.10.2019 10:34 KK Analytik Jena Tl in Food 1 16.10.2019 10:26 Analytik Jena
Name Vers. Date Time Cat. Operator Cd in Food 2 13.12.2023 12:55 KK SuStein Cr for ZEEman test 1 12.03.2020 13:44 SuStein Mg in Food 1 27.02.2020 11:40 User Pb in Food 1 16.10.2019 10:34 KK Analytik Jena Tl in Food 1 16.10.2019 10:26 Analytik Jena
Cd in Food 2 13.12.2023 12:55 KK SuStein Cr for ZEEman test 1 12.03.2020 13:44 SuStein Mg in Food 1 27.02.2020 11:40 User Pb in Food 1 16.10.2019 10:34 KK Analytik Jena Tl in Food 1 16.10.2019 10:26 Analytik Jena
Cr for ZEEman test 1 12.03.2020 13:44 SuStein Mg in Food 1 27.02.2020 11:40 User Pb in Food 1 16.10.2019 10:34 KK Analytik Jena TI in Food 1 16.10.2019 10:26 Analytik Jena
Mg in Food 1 27.02.2020 11:40 User Pb in Food 1 16.10.2019 10:34 KK Analytik Jena Tl in Food 1 16.10.2019 10:26 Analytik Jena
Pb in Food 1 16.10.2019 10:34 KK Analytik Jena TI in Food 1 16.10.2019 10:26 Analytik Jena
Tl in Food 1 16.10.2019 10:26 Analytik Jena
Sort by Description:
Description.
Name/Vers.
Decreasing
Current version only
✓ Save calibration data
OK Cancel
- OK Calcel
Ontion / display Description
Option/display Description
Name Entry or display of the name of the selected meth

	Option/display	Description
	Cat.	Additional property for searching the method/sequence in the data-
		base A maximum of three digits can be entered as the category name. You can limit the display of the list by entering the category name in the Cat. field. If you want to display the records of all categories, clear the entry in the Cat. field.
		Note : When using the optional 21 CFR Part 11 compliance module, you can define categories for methods with which the methods are marked as approved for use. In this case, only these methods can be used for measurement with the appropriate user authorization.
	List of records	Stored records with name, version, date, time, category and operator
	Sort by	Sort the list according to various properties
		Sorting can be done in ascending or descending order, depending on the option selected.
	Description	Enter or display additional notes, e.g. on the use of the records
		You can create predefined notes in the Data Default descriptions window.
	Current version only	If several versions of a method/sequence with the same name have been created, only the method/sequence with the highest version number is displayed.
	In the software, met other version is crea	hods/sequences with the same names are not overwritten, but an- ted and the version number is increased by 1.
	The databases also p methods or sequenc	provide functions for importing, exporting or deleting individual es from the respective databases.
	Note: Hold down the records in the databa	e Ctrl or Shift key while selecting with the mouse to select multiple ase window.
Open the data management	• Open the Data	Data management window by clicking on 🔳.
	 Select the record 	type you want to edit in the Type list. Method or Sequence .
Exporting data records	Using the export fun You may export seve tensions: Method da	action, you can make records available to other devices/computers. eral data records to a common file. Export files get the following ex- ata records - ".met", sequence data records - ".seq".
	• Click on Export to	o open the database window.
	 Select the data re 	ecords and click on Export .
	 Enter a file name The database win 	e in the standard Save as window and click on Save . ndow with the exported files is displayed.
	• Click on Close to	close the database window.
Importing data records	Using the import fur your database. An in records you want to	nction, you can load data records from other devices/computers into nport file can contain several records from which you select the load.
	• Click Import to o	pen the Select file to import window.
	 Select the file to This will open the and category of t the name of the 	be imported and click on Open . e database window with the presentation of name, date of creation he data records contained in the file. In the title bar of the window, import file is displayed.

	In the database window, select the data records you want to import and click Import. The records are imported into the database. If a method/sequence with the same name already exists, a new version of the record is created. In the database window, the current versions of the available data records appear.
	 Click on Close to close the database window.
	\checkmark The imported records can now be used in the software.
Deleting data records	Using the delete function, you can permanently delete data records from the database.
	 Click on Delete to open the database window.
	 Select the records you want to delete.
	Click Delete .
	✓ The database window is updated, displaying only the remaining data records. For data records of the same name, the version number is reduced by 1.
Deleting records via the File menu	Alternatively, you can open the database window for deleting records using the menu item File Delete Method or File Delete Sequence . Then, proceed as described above.
	See also

Configure general settings of the user management [> 177]

10.2.2 Managing results data

	Results data are stored in a database during the measurement. A new database file is created each time a sequence is started, but you can also append measurements to an existing file that already exists. Results data is saved with the extension TPS.
	Open the Data Data management window by clicking on E.
	In the Type list select the option Results .
Importing results data	You can import results data into the software. During this process, the data is placed in the results folder of the active atomization technique within the file structure of the software.
	In the Quick Start window, select the atomization technique for which data is to be imported.
	In the Data Data management window, click on Import. The Select results files window is displayed.
	 Select the TPS files and click on Open.
	• Select a subfolder for the results memory and click on OK .
	\checkmark The TPS files are copied to the results folder of the active atomization technique.
Exporting results data	Use this command to copy one or more results files to another folder.
	In the Data Data management window, click on Export. The Export window is displayed with an overview of existing TPS files. The files are listed with name, size and time of the last change.
	 Select the TPS files.
	Click on Export to open the Find folder window.
	• Select the target folder and click on OK .
	\checkmark The TPS files are copied to the target folder.

Deleting results files

You can permanently delete results data.

- In the Data | Data management window, click on Delete. The Delete results files window is displayed with an overview of available results databases.
- Select the TPS files.
- Click on **Delete** and confirm the subsequent prompt to delete the files with **OK**.
 - ✓ The data are permanently deleted.

Searching for results of individ- 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 menu command Extras | Search Sample. The Search for sample window is displayed.
- Enter the sample name in the Sample input field.
 If the entered string is part of the name, enable the Substring search checkbox.
- You can limit the time of the measurement by activating the **Date** checkbox.
- Click on Start.
 All results which contain samples with the sample name entered are displayed in the table.
- In order to open one of the displayed result files, select the file in the list and confirm with **Open**.
 - ✓ The results are displayed in the main window.

10.2.3 Importing report templates

Templates for print reports that were created externally must be imported into the software via data management.

- In the Type list, select the option Report templates and click on Import.
- ▶ In the **Open** window, select the report file LST and click on **Open**.
 - ✓ The report template is imported into the software. Now assign the report template to the print content in the **Report templates** window.

10.2.4 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. Worksheets have the extension WST.

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

Importing a worksheet

- Click on Import.
- In the Import Worksheet window, click on Import. Optionally, you can activate the including sequence and method(s) option for the import of methods and sequences beforehand.
- Select the worksheet in **Import Worksheet** and click on **Open**.
 - ✓ The worksheet is imported.

Exporting a worksheet

• Click on **Export**.

- In the Export Worksheet window, select the worksheet by clicking with the mouse. Activate the including sequence and method(s) option to export methods and sequence.
- Click Export.
- In the Save as window, enter a folder and a name for the export file and click Save.
 The worksheet is exported.

Deleting a worksheet

- Click Delete.
- ▶ In the **Delete** window, select the worksheet and click on **Delete**.
 - ✓ The worksheet is deleted.

10.3 Specifying units of measurements

In the **Data** | **Units** window, the units available for the entire application are managed. Preferred variants are available (for solutions: mg/L, μ g/L, ng/L, g/L and for solid samples: mg/kg, μ g/kg, ng/kg). These units cannot be changed by the operator. Units deviating from these can be freely defined.

▶ Open the **Data** | **Units** window using the **≡** icon.

The table contains the overview of the available units.

Option	Description
Unit	Name of the unit (max. 10 characters)
Comment	Remarks on the unit (max. 20 characters)
Factor	Factor 1 corresponds to 1 $\mu g/L$ or $\mu g/kg$, factor 1000 corresponds to 1 ng/L or ng/kg
	The factor must be entered for units you have entered yourself.
Туре	solid: Unit related to solid sample
	liquid: Unit related to liquid sample (solution)

Use the buttons to manage your own entries.

Button	Description
Append	Insert new row at the end of the list
Insert	Insert row above the selected row
Delete	Only delete custom units. The preferred units cannot be deleted.
Save	Save changes and entries

10.4 Managing databases for stocks and QC samples

The databases for frequently used stock standards and QC samples are managed in the **Data** | **Stock std/QC samples** window. You can add, delete or edit entries in the database. The stock standards and QC samples are available in method development.

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

Option	Description
Name	Name of the standard (max. 20 characters)
Unit	Name of the unit (max. 10 characters).
Elements and con- centrations	The element concentrations are to be entered in the format element symbol concentration; in the given example e.g. Fe 0.5; Cu 10; Co 0.005. Alternatively, click on Concentrations to open the window of the same name in which you can assign the concentration to each ele- ment.

Use the buttons to manage the entries:

Append	Insert new row at the end of the list	
Insert	Insert row above a selected row in the list	
Delete	Delete the selected row	
Save	Save the lists of the stock standards/QC samples	
Concentrations	Opens the input window for the entry of the element(s) and concen- tration(s) of the selected standard	

10.5 Creating predefined notes

User-defined notes can be defined for the following operations:

- Saving a method
- Saving a sequence
- Starting reprocessing
- Start measurement

The user-defined notes can be inserted by clicking on ... next to the **Rem.** field in the corresponding windows. Frequently used notes are already stored in the software.

Create comment

- Select the process from the Select category list.
- Click Edit to open the list of comments.
- Create a new comment by clicking on New. Enter a title in the Name field under which the comment can be selected. In the Text field, enter the actual comment.
- You can edit a comment by clicking on Change or remove it from the selection list by clicking on Delete.

10.6 Exporting data to ASCII/CSV format

You may save measurement results both automatically and manually in ASCII/CSV format. For both export formats, the parameters for the decimal separator, and the result columns to be exported are defined in the **Options** | **ASCII/CSV export** window.

Automatic continuous data export port 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 desired results table.
- Holding the ctrl or shift key depressed, choose the samples by mouse clicks on the respective row.
 - Select all sample rows with the menu command Edit | Select All Ctrl+A.
- Use the menu command **Edit | Save Selection** to open the standard **Save as** window.
- Enter the file name and confirm it with OK.
 The data will be saved in the CSV format which can be read by MS Excel and other programs.

See also

- Export options [▶ 170]
- B Options for continuous ASCII export [▶ 170]

10.7 Using the Windows clipboard

Copying results to the clipboard The application lets you copy the results of selected samples directly to the Windows clipboard thus making them accessible to other Windows applications.

The commands for this can be found in the **Edit** menu.

	Menu item Edit				
	Copy visible Col- umns only Ctrl+C	Copy the visible sample results from the current table			
	Copy all Columns	Copy the sample results from all tables			
	Column Titles	If activated (check mark), the copy action includes the column headers.			
	 Select the samples Holding the ctrl or spective row. 	s from the desired table of the results list. shift key depressed, choose the samples by mouse clicks on the re-			
	 Select all sample r 	ows with the menu command Edit Select All Ctrl+A.			
	• Activate the menu command Edit Column Titles if you want to copy the title bar.				
	• Activate the desire	ed menu command to copy the results to the Windows clipboard.			
Copying graphics as screen- shots	Graph window and graphs of calibration curves, absorbance signals or emission signals can be copied to the clipboard as a screenshot.				
	 Click on the right mouse button on the graph. 				
	• Select the Copy graphic menu item in the context menu if you only want to copy the graphic.				
	Select the Copy window menu item if you want to copy the entire window.				
	✓ The selected of dows application	bject is copied onto the clipboard and is available for other Win- ons.			
Copying signal values to the clipboard	You can copy the sign	als of the individual samples (statistics runs) to the clipboard.			
	Open the Single v corresponding san	alues window by double-clicking with the left mouse button on the nple row in the results table.			

• Copy the data to the clipboard with "Ctrl "+"C".

 \checkmark The data is now available to other Windows applications, e.g. Excel.

11 Cookbook

The cookbook gives a complete overview about the definable elements for the atom absorption spectrometry and the appliance settings and analysis notes recommended by Analytik Jena. When creating a method these data can be loaded as default setting element and technique specifically. The database of the cookbook can also be called up separately.

• Open the cookbook with the **o** icon in the toolbar or use the menu command **Method Development** | **Cookbook**.

Cookbook			
Technique: Flame (Abs)	Element	Ba 👻	
Performance: Ba Charact. concentration Check concentration ("0.1 Abs.") Typical value (±30%) for 50mm-burner and C2H2/N2	[mg/L/1%Abs] : [mg/L] : O flame	0.25 5.0	
SpectrometerMain line[nm] : 553.6Alternat. line[nm] : 455.4Slit width[nm] : 0.2HCL current[mA] : 6.0	Atomizer: Flame Flame C/O-Stoichiometric Fuel flow [NL/h] Usable burner height [mm] Alternative flame	: C2H2/N2O : 0.65 : 225 : 5 - 8 : C2H2/Air	
< > ē		Close	

Display and operating elements in the cookbook window

Option	Description	
Technique	Choice of atomization technique used	
Element	Selection list of the elements to be analyzed with the selected tech- nique	
	About gives general information on analyses with the selected atom- ization technique.	
Window display	Information on the analysis	
	Scroll between the window pages	

12 Options – Customizing ASpect LS

In the **Options** window, you can choose the following settings, which apply to the complete operation of ASpect LS:

- View options
- Save paths of files
- Parameters for data export
- General measurement settings
- General settings for calibration

The options selected in this window remain set after exiting and restarting ASpect LS. The **Default settings** button resets all options to default values.

• Open the **Options** window using the menu command **Extras** | **Options**.

12.1 View options

n the Options View window, you can define the functions visible on the workspace	2.
---	----

🔹 Opt	tions					—		×
View	Folders	ASCII/CSV export	Continuous ASCII export	Analysis sequence	Calibration			
- Disp ☑ : ☑ :	blay Show tooll Show icon I left O top	bar bar ⊖right ⊖bottom	☐ Hide event wir ☑ Hide results w ☑ Display tooltip ☐ Allow screens ☑ Use PrtScr key	ndows indows automatically s aver y for hardcopy (instea	ad of F5)			
Sign Si Bi L-	als ignal ackground signal (dy	d n. mode) Ask for re	esults report type (compac	t or complete) when	printing]		
	Defa	ultsettings		ОК	Accept		Cancel	

```
Elements in the Options | View window
```

Option	Description		
Show toolbar	Show toolbar		
Show iconbar	Show toolbar and select toolbar position		
	The position of the toolbar can also be changed by dragging it with the mouse. The setting is not saved.		
Hide event win- dows	Do not show the event windows (e.g. delay time)		
	Instead of this, the messages appear in the status bar of the main window.		
Hide results win- dows automatically	Hide results window when sub-windows (e.g. Method window) are opened		
	After closing the sub-windows the result windows are displayed again.		

Option	Description		
Display tooltips	Show small help texts (tooltips) above all icon buttons and for the column titles in the Method , Sequence and Sample ID windows		
Allow screensaver	Turn on Windows screen saver during input pauses		
Use PrtScr key for hardcopy (instead of F5)	By default, the screen printout is triggered with F5 . The PrtScr/Print button is used for the Windows clipboard function. If this option is enabled, the PrtScr/Print button starts the printout or the screenshot.		
	This function becomes active only after restarting ASpect LS.		
Lock application af- ter [min]:	Only available if the optional 21 CFR Part 11 compliance module is installed		
	The screen is locked if no input is made in the PC within the specified time. The screen is enabled again when an authorized user logs in.		
	In flame mode, the permanent presence of a user is required to extin guish the flame in good time if it changes. Activation of this functior is not recommended for flame technique.		
Signals	The button opens the color selection dialog. Predefined or new signal colors can be selected.		
Ask for results re- port type (compact or complete) when printing	When printing analysis results, the query dialog for the protocol type is displayed again.		

See also

Print analysis results [▶ 155]

12.2 Storage paths

The save paths selected for the program and the files during installation are displayed in the **Options** | **Change data directory** window.

Option	Description		
Program	Installation path of executable files		
Work directory	Directory for user data		
	The working directory contains further subfolders and is defined dur- ing installation or through settings in User Management.		
Temporary data	Directory for temporary application files.		
Sample informa-	Default path for opening and saving sample information files		
tion	This path may be changed. When opening and saving the sample in- formation data a deviating path can be selected.		
Export/Import	Default path for the export and import of method and sequence data		
	This path may be changed. When exporting and importing a deviat- ing path can be selected.		
Results	Folder for results files		
	This default folder may contain additional subfolders for result stor- age. These folders are available for saving results files at the start of measurements.		
Application data	List for data in which ASpect LS stores necessary data		

The **Add** button creates new subfolders for saving results below the **Results** folder. You can delete or rename empty folders.

12.3 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 forms of data export, automatic and manual.

Configuration

Option	Description	
Decimal separator	Separator for decimal numbers	
List separator	Separator for the elements of a list	

In the **Results fields for export** field, you may define which columns of the result table are exported to the ASCII file. **all** exports all columns of the selected and non-selected tables of the result list, **only selected fields** opens a list in which you can choose the columns to be exported.

12.4 Options for continuous ASCII export

In the **Options** | **Continuous ASCII export** window, you can activate the export of results data during the analysis run. The export file is updated respectively after the output of a new line in the process and result 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. The data is stored in the default path for export/import **(Options | Folder** window).

File name	Description
Method name.csv	The CSV file is given the name of the method. The file is saved in the default path Export/Import (Options Folder window).
Results file name.csv	The CSV file is given the name of the result file. The file is saved in the default path Export/Import .
other	You may freely define file name and save path. Click on the button opens the file selection dialog for the selection of an existing file.
Create separate file for each sample (result row number and sample name is appended to file- name)	A separate file is created for each sample. The file name is appended with the row number of the results list and the sample name. Charac- ters that are not allowed are replaced by underscores (e.g. Test method-001 QC 1 mg_L.csv).
Export path	The ASCII files are saved in this path.

Exporting the signals

The time-resolved absorbance or intensity signals (peaks) can also be exported as CSV files.

Use the **Continuous export of signals (CSV)** option to activate the signal export. The file name is generated based on the schema "ListRow-SampleName-LineName-RepeatMeasurement", e.g. 0007-sample-Al309-02.csv. In the **Export path** field, you can select a path for saving the signal files.

12.5 Options for analysis sequence

In the **Options** | **Analysis sequence** window, you define generally valid settings for the analysis procedure.

Stop after following errors	Action	Description
	Invalid calibration function	If activated, the analysis sequence will be stopped if the calibration function could not be calculated.
Additional error checks	Function	Description
	Monotony of cali- bration points	The calibration points will be tested for monotony. The monotony test serves to determine if higher standard concen- trations also lead to higher measured values.
	Autosampler level	Not for AS-GF and AS-F/AS-FD
	sensors	The fill level of the autosampler and the waste bottle is monitored.
	Autozero drift check	The drift of the absorbance values is checked during the autozero process.
Display windows	By activating the correst during the analysis pro Autosampler adjust-	sponding options, you can have various display windows shown cess. Description
	ment window	
	Signal Plot	If activated, a window is displayed during the analysis process show- ing the curve of the measured signal (e.g. absorbance curve) as a function of time.
	Scaling of max. sig- nal value	Set the maximum of the measured value axis for the displays of the signal curve.
		auto: Automatic axis scaling
		Alternatively, this setting can also be made using the View Scale (Abs) menu function.
	with furnace pro- gram	The temperature curve of the furnace program is also displayed in the signal curve.
	Bar graph	Measured values are displayed with absorbance or emission result as a bar chart.
	Graphical peak over- view	Peaks of the individual measurement are displayed one after the other.
	Report window	If activated, a window is displayed during the analysis process show- ing status information on the used atomizer (flame, graphite tube furnace, hydride system).
	Sample conc. in cali- bration curve	The Sample conc. in calibration curve window with the current calibration and, if already measured, recalibration curve is displayed.
		After the measurement of the sample, the calculation of the uncor- rected concentration from absorbance/emission data is illustrated by red auxiliary lines. If addition calibration is used, the converted cali- bration curve is displayed.
	Furnace Camera	Continuously shows the image of the furnace camera with the image of the graphite tube until the temperature set in the furnace control is reached. This allows you to directly watch as a sample droplet is deposited and drying.

Autosampler adjust- ment window	Description
	Note : The furnace camera is not available as standard for all AAS device types.
Option	Description
Attach date/time to the results filename	Current PC/time at the start of measurement are automatically appended to the name of the result file
Min. lamp pre-heat-	Sett the automatic lamp preheating time
ing time (routine)	If no preheating time is set, the preheating time itself must be ob- served.
Beep after end of	Only for graphite furnace technique
cooling phase	A beep will sound as soon as the graphite tube has completely cooled down.
Take-up compo-	Only for graphite furnace technique
nents during cooling phase	While the graphite tube is cooling down, the autosampler is used to take the next sample. This option may be used to accelerate a measuring sequence.
Stop after trans- former overheating	Only for graphite furnace technique
	The program will not continue if the transformer overheats.
	Interrupts a running program on detecting a transformer overheat situation if disabled. Resumes the interrupted program after the transformer has cooled down.
Formation required	Only for graphite furnace technique
after opening fur- nace	Always format the graphite tube after the furnace has been opened
Continuous export also during repro- cessing	Automatically export the results after a recalculation
Do not update time- stamp when repro- cessing	After recalculating the results, the original measurement times are retained
Clean mixing cham- ber when flame is extinguished	For flame technique only
	Wash the mixing chamber when extinguishing the flame
Burn-in time acety-	For flame technique only
lene/N2O flame [min]	Set the stabilization time of the acetylene-nitrous oxide flame

12.6 General settings for calibration and blank correction

In the **Options** | **Calibration** window, you can make basic settings for the calibration and blank correction. All checkboxes are deactivated in the default settings.

Options for calibration	Option	Description
	Correlation coeffi- cient	Select the ratio for the calibration curve's goodness of fit
		R: Correlation coefficient
		R ² : Coefficient of determination
		R ² (adjust): Adjusted coefficient of determination

Miscellaneous

	Option		Description
	Show predict stead of conf interval	ion in- idence	If enabled the prediction band for the calibration is displayed. The confidence band is provided as default.
	auto compare quadratic ins of rational fu	es with tead nction	"auto" indicates the automatic selection of the calibration function. If enabled the quadratic function is used for the comparison. The de- fault setting is the broken rational function.
	Compute slop mean concen tion instead c	oe for tra- of 0	If enabled the slope of the calibration graph is calculated for the mean concentration of the calibration range. As default the slop is calculated for 0 concentration.
	>CAL if the u standard is ex	pper x-	By default, ">CAL" is displayed when the upper standard is exceeded by 10%.
	ceeded by [%)] 	You can adjust the percentage value here. If the Dilution if conc. ex- ceeded option is activated in the Method Sample transport window, dilution is performed automatically from this percentage value of the overrun.
Options for blank correction	For blank corr 1 -based or Co	ection yc nc. 2 -ba	ou can choose between two different calculation methods: Conc. sed.
	In the Conc. 2 calculation, the original concentration of the blank (Conc2 _{BV}) is first calculated based on the sample IDs of the blank. Conc2 _{BV} is taken into account when determining the Conc. 2 of the sample.		
	In the Conc. 1 -based calculation, the blank concentration (Conc1 _{Blank}) determined directly from the sample is used to calculate the sample concentration. This method can be used if the sample ID data (e.g. dilutions) do not strongly influence the concentration of the blank solutions and therefore no sample ID data is entered for the blanks.		
	Calculation ex Conc. 1 -b Conc. 2 -b	ample fo ased: Coi ased: Coi	r liquid original sample with predilution: $nc2_{Sample} = (Conc1_{Sample} - Conc1_{Blank}) * DF_{Sample}$ $nc2_{Sample} = (Conc1_{Sample} * DF_{Sample}) - Conc2_{Blank}$
	Conc1 _{Sample}	Concentra sample ID	tion of the sample without taking into account the information in the
	Conc2 _{Sample}	Original co	oncentration of the sample
	Conc1 _{Blank}	Concentra sample ID	tion of the blank without taking into account the information in the
	Conc2 _{Blank}	Original b	lank
	DF _{Sample} I	Dilution fa	actor of the sample
	The default setting for blank correction is the Conc. 2 -based method. If you want to revert to the shorter Conc. 1 -based method without taking into account the sample ID of the blank value, activate the Blank correction based on Conc1 option.		
Limits of detection/quantifica- tion	You can edit the factors and number of repeat measurements for the limits of detection/ quantification. The calculated limits of detection/quantitation are displayed in the Cali- bration 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 Cal- ibration window and in the printouts of the calibration and results/blank measure- ments.		
	To edit the fac default setting	ctors and gs are pro	measurement repetitions, click on LOD and LOQ . The following ovided:
	Parameter		Value
	Factor LOD		3

Parameter	Value
Factor LOQ	9
Replicates	11

See also

Specify calibration parameters (Method | Calib. window) [▶ 51]

13 Optional FDA 21 CFR Part 11 Compliance module

The optional FDA 21 CFR Part 11 Compliance module for ASpect LS 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 LS 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 LS, open the menu item System | User management.
- Alternatively, you can open the user management outside of ASpect LS via the Windows menu **ASpect LS** | **User Management**.
- Enter the login data of a user with user administration 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 pro-file.

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 result 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).
Passwd. protect.	Active: User login requires a password.
	Not active: User login is possible without a password.

Option	Description
	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	Create 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 win- dow 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 administration has a new feature for setting up the user levels. While the available authorizations of user levels were fixed in previous versions of the user administration, 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	 6 user levels are created by default in the user administration. The user levels can be freely configured and supplemented with additional user levels. By default, one administrator level and 5 user levels are preset: Administrator level (level 0) The administrator has full rights in the user administration. By default, the administrator has no rights in ASpect LS. Level 1
	 Users at this level have all authorisations for ASpect LS for method development and routine and can configure the software. Level 2 to 4
	Users of these levels have graduated authorisations for analysis operation, whereby the following applies: Level 2 > Level 3 > Level 4. They do not have authorisations to configure ASpect LS.
	 Users at this level have authorisations for logging into the user administration and ASpect LS minimal authorisations, 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 levels 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 users want 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 in- terval (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 meth- ods (categories) (ME004)	You can assign the Cat. (category) characteristic to the methods when saving and thus identify methods for use. In the 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 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 LS.

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 LS User Management window, select the menu item Extras | Settings....

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 at- tempts	Shows the number of invalid login attempts (max. 10).
	If this is exceeded, ASpect LS terminates after a waiting period and must be restarted for another login. An entry (warning) is added to the audit trail file.
Disable account af- ter failed login at- tempts	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 let- ters 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 differ- ent	Only passwords which are different from the respective user name will be accepted. This policy equally applies to changes in password.
User must change password at next login is active	By default, new users must change their password the first time they log in.
Password expires in	After the time limit has expired, the user is prompted to change the password when logging in. The password is then extended by a term as set in Policies. This value is then acknowledged as a template that can be modified for other single users (max. 999 days).
Minium password	Minimum number of characters for newly created passwords
length:	Number of characters: 3 to 10

For server-based login, activate 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 AS- pect LS locally.
Allow local login for AJService ac- count	Activating this option enables AJ Service personnel to carry out main- tenance on the device without additional support from the adminis- trator.

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 di-	Setting the working directory
rectory	

ASpect LS

Option	Description
	The working directory contains a database of methods and sequences and the results files. The working directory was defined during the in- stallation of ASpect LS 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 pro- gram.
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 meth- ods	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) autho- rization is deactivated for a user, this user cannot start a sequence if the associated method is not marked with one of the specified cate- gories.

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

See also

B Save methods [▶ 26]

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 administration 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 con- figurations 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 ex-	Password will remain valid for unlimited time if this box is active.		
pires	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 work- ing directory	A separate working directory is set for the user according to the fol- lowing 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, as opposed to removing it, prevents the user name from being reas-signed 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 LS User Management** window.
See also

Configure general settings of the user management [> 177]

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**.
 - \checkmark The changes are applied and take effect the next time the user logs on.

See also

B Creating a new user account [▶ 180]

13.2 Changing a password

This function is only available for local login to ASpect LS 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 LS, select the menu item System | Change password. The Change password window appears.
- Enter the old password and the new password twice and confirm by clicking on **OK**.
 - ✓ If the entry is correct, the **Password is changed!** message appears.

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 LS and user management. To view the audit trail, permissions must be granted in the user account.

You can open the audit trail in ASpect LS 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
- 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
Туре	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
Date/Time	Date and time of the event (PC clock)

	Table column	Description	
		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 Management	Designates the user in login state at the moment of an event.	
	Source	Differentiation according to events in the user management or in AS- pect LS	
	Description	Detailed information on the selected event	
Selecting a view	If you have opened to events in both ASpe display to events in	the audit trail in the User Management window, you will see the ct LS and the user management. In the View list, you can restrict the ASpect LS or administrative events.	
	If you have opened to only events in ASpect	the audit trail in ASpect LS with the menu item System Audit Trail , ct LS 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 work-sheets. Click on Deactivate filter to remove the restrictions of the set filter.		
Updating an audit trail	Click Refresh to refr were added while th	esh the audit trail entry list. This may be necessary if further entries ne audit trail is open.	
Printing the audit trail	You can print the au printed.	dit trail. If you have filtered the entries, only the filtered entries are	
	 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. 		
	\checkmark The audit tra	il is output in the selected output format.	
Exporting the audit trail	You can export the a the audit trail has be the filtered entries a	audit trail entries to a CSV file. The export function is only available if een opened in the user management. If the filter is activated, only are exported.	
	Click on Export t	o 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 LS. 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". This file contains the check-sums of the result file.

A file may be signed by more than one user.

See also

- \square Configure general settings of the user management [\triangleright 177]
- Configuring user levels [▶ 176]

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 menu item **System | Sign off results**.
- 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 [▶ 180]
- Configure general settings of the user management [> 177]

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
Status	The signature state may take on one of the following meanings:

Option	Description
	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 cor- rupt.
Invalid (T The result newly calc variances.	Invalid (TPS data) The results file 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
> KAL	The mean value is larger than the working range of the calibration curve.	Mean values	Sequence and results window
< KAL	The mean value is smaller than the working range of the calibra- tion curve.	Mean values	Sequence and results window
< LOD	The value is smaller than the limit of detection.	Mean values	Sequence and results window
< LOQ	The value is smaller than the limit of quantitation and larger than the limit of detection.	Mean values	Sequence and results window
RSD !	The mean value is outside the range of the specified relative standard deviation.	Mean values	Sequence and results window
RR!	The mean value is outside the range of the specified relative range.	Mean values	Sequence and results window
Factor!	Limit of recalibration factor for the calibration curve was ex-	Calibration curve	Sequence and results window
R²(adj.)	The quality of regression R ² (adj.) of the calibration curve falls be-	Calibration curve	Sequence and results window
	low the specified value.		Calibration curve window
MAN	The value was manually excluded from the calculation of the mean value.	Single values	Individual sam- ple values win- dow
KOR	The value was automatically ex- cluded from the calculation of mean values by the Grubbs outlier test	Single values	Individual sam- ple values win- dow

14.2 Storage locations of the ASpect LS files

The folders used to store files differ depending on the installation options and the version of Windows you are using. The folders used by default are listed below. The folders used by the current installation are displayed in the **Options** | **Folder** window.

Working directory (and subfolders)

Drive:>User>Public>Documents>Analytik Jena>ASpect LS

Туре	Folder	Files
Results	C:\User\Public\Documents\Analytik Jena\ASpectLS\ <technique>\Results</technique>	*.tps – result data
Method and sequence data	C:\Users\Public\Documents\Analytik Jena\ASpectLS\ <technique>\meth</technique>	*.tps

Туре	Folder	Files
Optimization results (e.g. optimization of the furnace program)	C:\Users\Public\Documents\Analytik Jena\ASpectLS\ <technique>\opt</technique>	*.tps
Default parameters	C:\Users\Public\Documents\Analytik Jena\ASpectLS\ <technique>\tables</technique>	*.dat
Sample ID files, unit files and exported files (CSV)	C:\Users\Public\Documents\Analytik Jena\ASpectLS\user	*tps; *.csv
Report templates	C:\Users\Public\Documents\Analytik Jena\ASpectLS\user\Reports	*.lst – template; *.jpg- preview file
Options and adjustment values	C:\Users\Public\Documents\Analytik Jena\ASpectLS	*.cfg; *.ini
Worksheets	C:\Users\Public\Documents\Analytik lena\ASpectLS\Worksheets	*.wst

Application data (and subfolders)

Drive:>ProgramData>Analytik Jena>ASpectLS

Туре	Folder	Files
Device data and prede- fined comments	C:\ProgramData\Analytik Jena\ASpectLS	*.dat;*.tps
User management and audit trail data	C:\ProgramData\Analytik Jena\ASpectLS\UserMgmt	usrlrv.tps – user database; Evntlog*.tps audit trail

Program

Drive:>ProgramData>Analytik Jena >ASpectLS or Drive:>Program Files (x86)>Analytik Jena >ASpectLS

Туре	Folder	Files
Devices and system configuration	C:\Program Files (x86)\ASpectLS	ASpectLS.ini

Technique: FL – Flame; EA – Graphite furnace; EAS – Solid graphite furnace; HS – Hydride; HF – HydrEA

Before a complete restore (application and data), the ASpect LS installation must also be executed.

Information on the display of folders and file name extensions: Some folders may be hidden folders, and the display of file name extensions may also be switched off. In Windows Explorer, select **View** to show hidden files, folders, and extensions.

See also

Storage paths [▶ 169]