

Operating Manual

Spectroquant[®] Prove plus

Spectroquant[®] Prove
Spectrophotometer 100 plus • 300 plus • 600 plus



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1 Spectrophotometers

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1.1 Photometry

When a beam of light is transmitted through a colored solution, then this beam loses its intensity, in other words a part of the light is absorbed by the solution. Depending on the substance in question, this absorption occurs at specific wavelengths.

Monochromators (e.g. narrow-band interference filters, lattices) are used to select the wavelength from the total spectrum of a tungsten-halogen lamp (VIS spectrum), a deuterium lamp (UV spectrum) or, respectively, a xenon lamp. The intensity of the absorption can be character-

ized using the transmittance T (or, respectively, T in percent).

$$T = I/I_0$$

I_0 = Initial intensity of the light

I = Intensity of the transmitted light

If the light is not absorbed at all by a solution, then this solution has a transmittance of 100%; a complete absorption of the light in the solution means 0% transmittance.

The measure generally used for the absorption of light is the absorbance (A), since this correlates directly with the concentration of the absorbing substance. The following connection exists between absorbance and transmittance:

$$A = -\log T$$

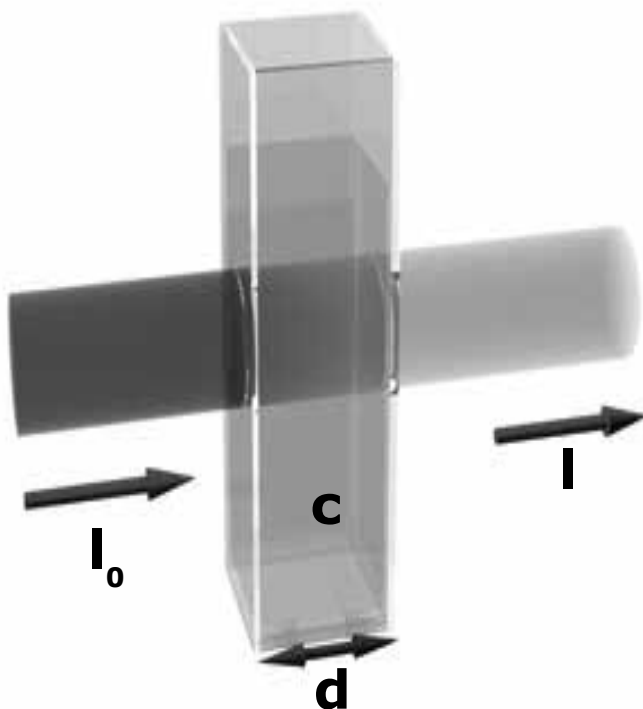
Experiments by BOUGUER (1698–1758) and LAMBERT (1728–1777) showed that the absorbance is dependent on the thickness of the absorbing layer of the cell used. The relationship between the absorbance and the concentration of the analyte in question was discovered by BEER (1825–1863). The combination of these two natural laws led to the derivation of Lambert-Beer's law, which can be described in the form of the following equation:

$$A = \epsilon_\lambda \cdot c \cdot d$$

ϵ_λ = Molar absorptivity, in $l/mol \times cm$

d = Path length of the cell, in cm

c = Concentration of the analyte, in mol/l



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1.2 The Spectrophotometers

The spectrophotometers that belong to the Spectroquant® analysis system differ from conventional spectrophotometers in the following important aspects:

- The calibration functions of all test kits are electronically stored
- The measurement value can be immediately read off from the display in the desired form
- The method for the test kits (cell tests and reagent tests) belonging to the Spectroquant® analysis system is automatically selected via the scanning of the bar code
- All cells formats used are automatically identified and the correct measuring range is selected automatically
- Instrument-supported AQA ensures that measurement results can be used as secure, reproducible, and recognized analytical results
- New methods can be downloaded from the internet site www.sigmaaldrich.com/photometer-service and permanently stored in the instrument

For technical data and instructions for use please refer to [section 6](#) and the Analytical Procedures and Appendices.

They can also be found in the internet.

2 Photometric Test Kits

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2.1 Basic Principle

By means of reagents, the component of a sample to be analyzed is converted into a colored compound in a specific reaction. The reagents or reagent mixtures contain – in addition to the reagent selective for a parameter to be determined – a number of auxiliary substances that are essential for the course of the reaction. These include, for example, buffers for adjusting the pH to the optimal value for the reaction, and masking agents that suppress or minimize the influence of interfering ions.

The color reactions are in most cases based on standardized analytical methods specifically optimized in terms of ease of use, a low working effort, and shorter reaction times. Furthermore, methods cited in the literature or developed by ourselves are also used. Details on the respective reference procedures are stated in the package insert or else in the parameter overview.

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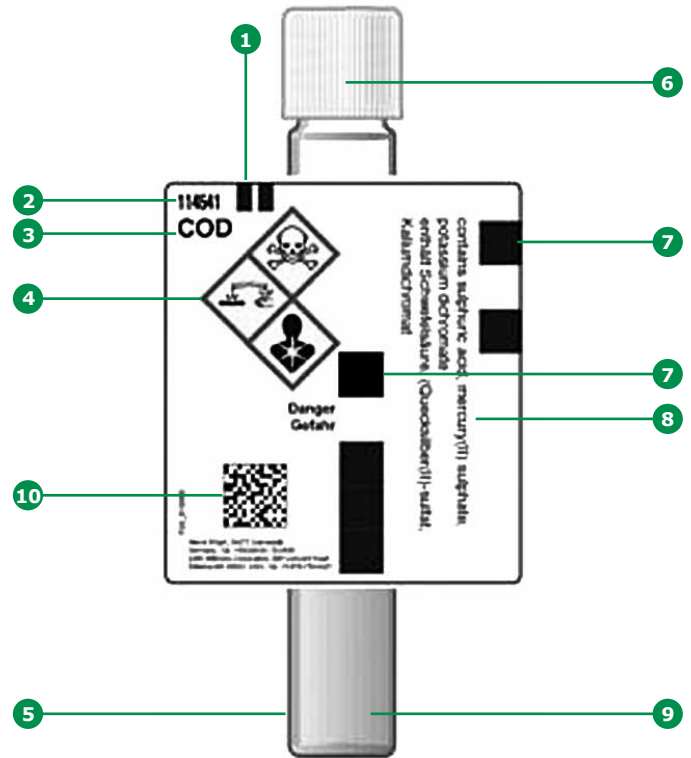
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2.1.1 Spectroquant® Cell Tests

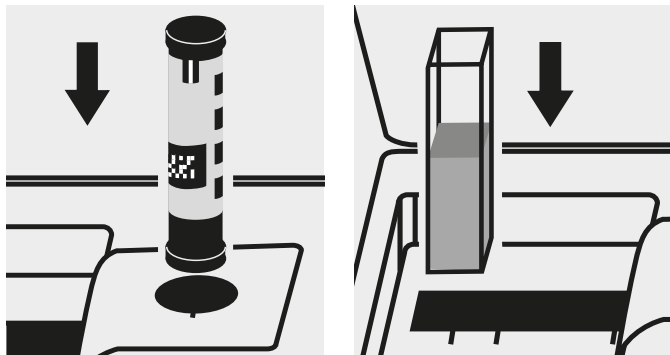


- 1 Identification mark for the correct insertion into the cell compartment of the spectrophotometer
- 2 Cat. No. of test kit
- 3 Designation of test kit
- 4 Risk phrases
- 5 Special cell in optical quality
- 6 Leakproof cap
- 7 Bar code for identification in the NOVA and Pharo photometers
- 8 Details regarding contents
- 9 Highly precise dosage of the reagent
- 10 2D barcode for identification in the Prove plus spectrophotometers

Additional reagent(s)

Certain cell tests, e.g. COD or nitrite, already contain all necessary reagents in the cells, and the sample must merely be added with a pipette. In other tests, however, for reasons of chemical compatibility it is necessary to separate the test into two or three different reagent mixtures. In such cases, besides the sample a metered reagent must also be added.

2.1.2 Spectroquant® Reagent Tests

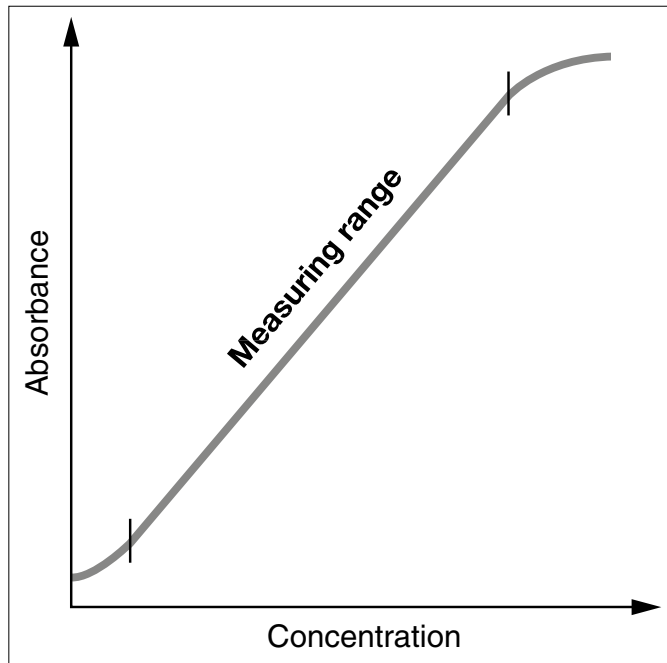


The principle behind the reagent tests is that the reagents necessary for the color reaction are combined in the form of liquid concentrates or solid-substance mixtures. A few drops of the reagent concentrate are added to the sample. This means that there is no need to dilute the sample, which in turn enhances the sensitivity of the detection. The procedure generally used in classical photometry by which the sample is made up to a defined volume in a volumetric flask is dispensed with.

The method is selected automatically by means of the scanning of the bar code by the AutoSelector. All cells formats used are automatically identified and the correct measuring range is selected automatically. Subsequently the result is automatically shown on the display.

2.2 Notes for Practical Use

2.2.1 Measuring Range



In photometry it is conventional practice to measure against the reagent blank value. Here the analysis is carried out "blind", i.e. without any analyte added. Instead of the sample volume, the corresponding quantity of distilled or DI water is used.

This **reagent blank value is prestored** in the spectrophotometers belonging to the Spectroquant® analysis system, which means that – due to the high batch reproducibility – it is possible to dispense with a separate measurement of the reagent blank. At the lower limit of the measuring range, the accuracy of the determination can be enhanced by performing the measurement against a separately prepared reagent blank. In some cases the intensity of the color of the solution and thus the absorbance can drop again when very high concentrations of the analyte are present (see package insert of test kit).

The intensity of the color of a solution, measured as the absorbance, is proportional to the concentration of the respective analyte only within a specific range. This measuring range (effective range) is electronically stored in the spectrophotometers for each individual test kit.

Below the specified measuring range, either a different cell or else another procedure must be used. The **lower limit of the measuring range** either takes the form of nonlinearity of the calibration curve, as shown in the figure, or else is given by the method detection limit. The **method detection limit** of an analytical method is the lowest concentration of the analyte in question that can be measured quantitatively with a defined degree of probability (e.g. 99%). The **upper limit of the measuring range** is the point at which the linear correlation between the concentration and the absorbance ends. In such a case the sample must be diluted accordingly so that it lies ideally in the middle of the effective range (least-error measurement).

2.2.2 Influence of pH

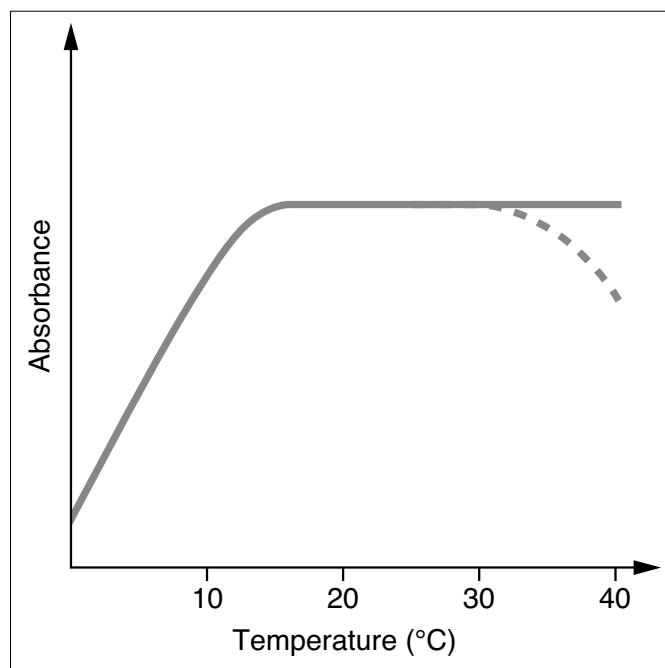
Chemical reactions follow an optimal course only within a certain pH range. The reagents contained in the test kits produce an adequate buffering of the sample solutions and ensure that the pH optimal for the reaction in question is obtained.

Strongly acidic (pH <2) and strongly alkaline (pH >12) sample solutions can prevent the pH from being adjusted to an optimal range, since under certain circumstances the buffering capacity of the test-kit reagents may not be sufficient. Any necessary correction is made by the drop-wise addition of diluted acid (reduces the pH) or diluted lye (raises the pH), testing the pH with suitable indicator strips after each drop is added. The addition of the acid or lye results in a dilution of the test solution. When up to five drops are added to 10ml of sample, the change in the volume can be neglected, since the resultant error is lower than 2%.

The addition of larger quantities should be duly considered by adjusting the sample volume accordingly.

The specified pH values for the sample solution and, wherever applicable, for the measurement solution are defined in the respective package inserts and in the Analytical Procedures and Appendices.

2.2.3 Influence of Temperature



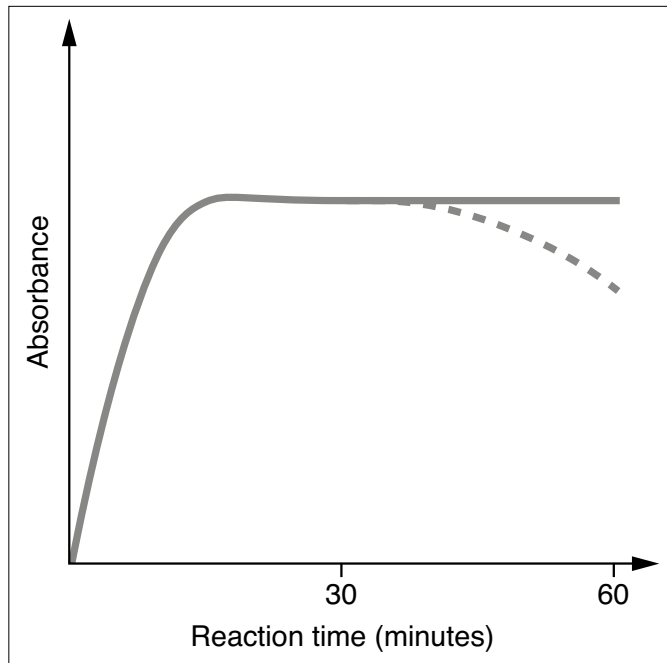
The temperature of the sample solution and the reagents may have an effect on the color reaction and thus on the measurement result. The typical temperature course is illustrated in the figure.

If the sample temperature is lower than 15 °C, false-low results must be reckoned with. Temperatures exceeding 30 °C generally influence the stability of the compound that is formed in the reaction. The optimal temperature for the color reaction is stated in the package inserts of the respective Spectroquant® test kits.

CAUTION

After thermic decomposition procedures, the determination of COD or total contents of nitrogen, phosphorus, or metal, a sufficient waiting time must be allowed for to permit the solution cool to room temperature.

2.2.4 Time Stability



Most of the color reactions require a certain time to reach the maximum color intensity. The solid curve in the figure at the right gives a schematic impression of a typical time course. The behavior of relatively instable color reactions with time is shown by the dotted curve. The reaction time specified in the working instructions refers to the period of time from the addition of the last reagent until the actual measurement. In addition, the package inserts for the individual test kits also state the time interval in which the measurement value does not change. The maximum time interval is 60 minutes; this time should not be exceeded, even in the case of stable color reactions.

2.2.5 Influence of Foreign Substances

Foreign substances in the sample solution can

- raise the measurement value as a result of an amplification of the reaction
- lower the measurement value as a result of a prevention of the reaction

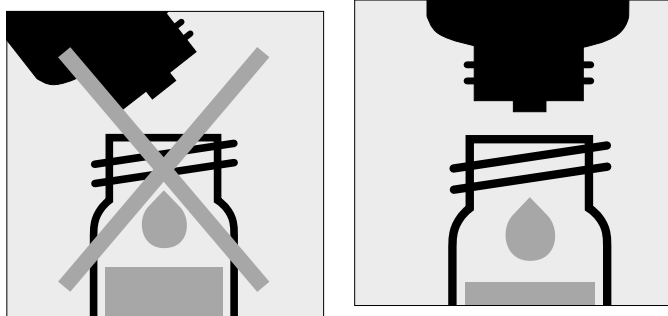
A quantification of these effects is stated in tabular form in the respective package inserts for the most important foreign ions. The tolerance limits have been determined for the individual ions; they may not be evaluated cumulatively.

Suitability for use in seawater

A tabular survey (see appendix 1) provides information on the suitability of the tests in connection with seawater and also on the tolerances for salt concentrations.

2.2.6 Dosing the Reagents

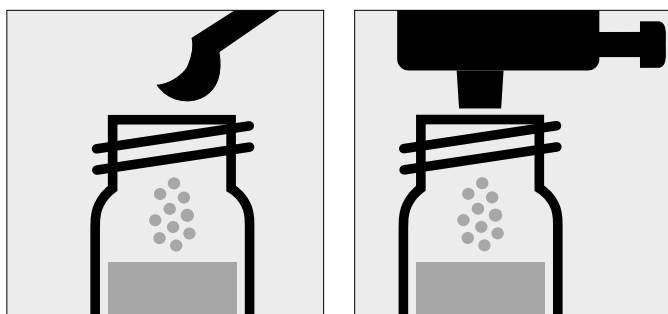
Small amounts of liquids are dosed by counting the number of drops from a leakproof bottle.



CAUTION

When using dropper bottles it is extremely important that the bottle be held vertically and that the drops be added slowly (approx. 1 drop per second). If this is not observed, the correct drop size and thus the correct amount of reagent are not achieved.

A positive-displacement pipette should be used for larger quantities of liquid or for the exact dosage of smaller reagent quantities. In these cases the reagent bottles are not fitted with a dropper insert.



Solid substances are dosed either with the dose-metering cap or with microspoons that are integrated into the screw cap of the respective reagent bottle. The dose-metering cap is used for solid reagents or reagent mixtures that are free-flowing. In all other cases the substances are dosed with the microspoon.

In this case it is necessary to add only level microspoonfuls.

To this end the spoon must be drawn over the brim of the reagent bottle.

At the first use replace the black screw cap of the reagent bottle by the dose-metering cap. Hold the reagent bottle vertically and, at each dosage, press the slide all the way into the dose-metering cap. Before each dosage ensure that the slide is completely retracted.

CAUTION

Reclose the reagent bottle with the black screw cap at the end of the measurement series, since the function of the reagent is impaired by the absorption of atmospheric moisture.

2.2.7 Shelf-life of the Reagents

The Spectroquant® test kits are in most cases stable for three years when stored in a cool, dry place. A few test kits have a lower shelf-life of 18 or 24 months or must else be stored in a refrigerator.

COD Cell Tests must be stored protected from light. The expiry date of the package unit is printed on the outer label. The shelf-life may become reduced when the reagent bottles are not reclosed tightly after use or when the test kit is stored at temperatures higher than those specified.

1 3 Sample Preparation

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Sample preparation covers all the steps necessary before the actual analysis can be performed.

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3.1 Taking Samples

The taking of samples is the first and **most important step** on the way to obtaining the correct analysis result. Not even the most exact method of analysis can correct any mistakes made in the taking of the sample. The objective of the sampling procedure is to gain a sample with a representative composition. The most important precondition for **gaining a representative sample** is the identification of the suitable sampling site. Here it must be borne in mind that the solution to be investigated can display varying concentrations in different places at different times.

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In sampling, a distinction is made between manual and automatic methods. In many cases a true picture of the average composition of the sample can be obtained only once several individual samples have been collected; this can be done manually or with an automatic sampler.

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Clean plastic or glass containers with a volume of 500 or 1000 ml are generally suitable for collecting samples. They should be rinsed several times, under vigorously shaking, with the water to be investigated, and then filled free of air bubbles and immediately closed tightly. The containers must be protected against the effects of air and heat and then be forwarded for the further analytical steps as soon as possible. In exceptional cases, preservation measures in the form of short-term refrigeration at +2 to +5 °C and chemical conservation can be taken.

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Further useful tips on suitable sample vessels for specific analytes and possible preservation and storage conditions can be found in EN ISO 5667-3, Water quality – Sampling – Part 3: Preservation and handling of water samples (ISO 5667-3:2018).

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Parameter	Preservation
COD	+2 to +5 °C max. 24 h or -18 °C max. 14 days
N compounds: NH ₄ -N, NO ₃ -N, NO ₂ -N	analyze immediately, only in exceptional cases +2 to +5 °C max. 6 h
P compounds: PO ₄ -P, P total	short-term storage, no preservation; with nitric acid to pH 1, max. 4 weeks
Heavy metals	short-term storage, no preservation; with nitric acid to pH 1, max. 4 weeks

3.2 Preliminary Tests

Correct measurement results can be obtained only within the measuring range specified for each individual parameter. When dealing with sample solutions of an unknown concentration, it is advisable to establish whether the sample concentration is indeed within the specified measuring range, ideally roughly in the middle of the range. Preliminary tests enhance the analytical reliability and make the determination of the necessary dilution ratios in the case of high concentrations easier. **MQuant® Test Strips** are very well suited for preliminary tests.

3.3 Dilution

Dilution of samples is necessary for two reasons:

- The concentration of the parameter under investigation is too high, i. e. it lies outside the measuring range
- Other substances contained in the sample interfere with the determination (matrix interference); false-high or false-low results may ensue

The following auxiliaries are absolute prerequisites for the dilution of the sample:

- Volumetric flasks of varying sizes (e.g. 50, 100 and 200 ml)
- Positive-displacement pipette
- Distilled or DI water

Only dilutions carried out with these auxiliary products are of sufficient reliability in the area of trace analysis, to which photometry belongs (for the simplified procedure see page 17).

An important aspect here is that once the volumetric flask has been filled up to the mark with distilled water the flask must be closed and the contents thoroughly mixed.

The dilution factor (D_F) resulting from the dilution procedure is calculated as follows:

$$D_F = \frac{\text{Final volume (total volume)}}{\text{Initial volume (sample volume)}}$$

The analytical result is subsequently multiplied by the dilution factor.

A calculation can be dispensed with when the dilution is programmed into the spectrophotometer. The dilution number (see the table) is entered and the measurement value is subsequently calculated correctly and immediately displayed.

All dilutions should be made in such a way that the measurement value lies in the middle of the measuring range. As a rule, the dilution factor should never be higher than 100. In the event that yet higher dilutions become necessary all the same, then this must be done in two separate steps.

Example

- Step 1: Make up 2 ml of sample to 200 ml with distilled water;
 $D_F = 100$, dilution number 1+99.
- Step 2: Take 5 ml of the above solution and make up to 100 ml;
 $D_F = 20$, dilution number 1+19.

The dilution factor for the total dilution is calculated by multiplying the individual dilutions:

$$D_{F_{\text{total}}} = D_{F_1} \times D_{F_2} = 100 \times 20 = 2000, \text{ dilution number } 1+1999$$

Simplified procedure

Dilutions up to 1:10 can also be prepared without volumetric flasks in a glass beaker, measuring the volumes of the sample and the dilution water using a previously calibrated positive-displacement pipette (see table for instructions).

Desired dilution	Volume of sample (ml)	Volume of distilled water (ml)	Dilution factor	Dilution number
1:2	5	5	2	1+1
1:3	5	10	3	1+2
1:4	2	6	4	1+3
1:5	2	8	5	1+4
1:10	1	9	10	1+9

3.4 Filtration

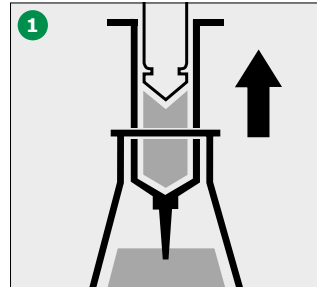
Strongly turbid samples require pretreatment before they can be determined in a spectrophotometer, since the effect of turbidity can result in considerable variations in the measurement values and in false-high readings. Care must be taken here to ensure that the substance to be determined is not contained in the suspended material, in which case a sample decomposition must be carried out.

Compounds that always occur in dissolved form (for example ammonium, nitrate, nitrite, chlorine, chloride, cyanide, fluoride, orthophosphate, and sulfate) permit a previous filtration, even when the sample solution is strongly turbid.

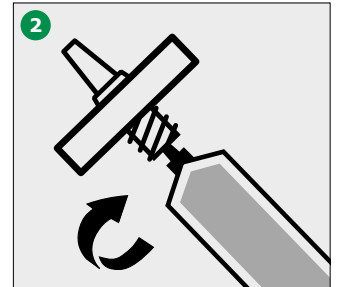
Weak turbidity is eliminated by the **automatic turbidity-correction** feature built into the spectrophotometer (see section 9.7.9); in such cases it is not necessary to filter the sample before analysis.

As a measure to distinguish between dissolved and undissolved water-borne substances, the water sample can be filtered through a simple paper filter. Following the recommendations stated in the reference methods, membrane filters with a pore size of 0.45 μm are required for fine filtration.

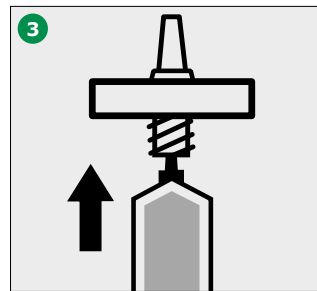
Procedure for Microfiltration



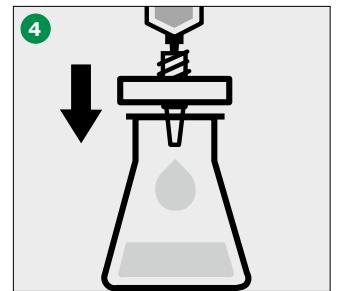
1 Draw out the liquid to be filtered with the syringe.



2 Screw the syringe tightly into the front side of the membrane filter attachment.



3 Hold the syringe upright and slowly depress the piston upwards until the membrane filter is fully wetted and free of air bubbles.



4 Filter the contents of the syringe into the intended glass vessel.

3.5 Homogenization

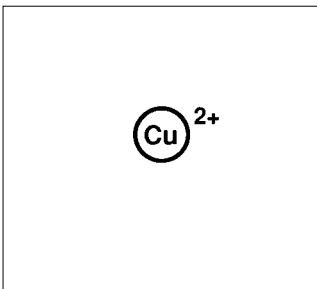
As a measure to ensure that a representative sample can be taken in the presence of suspended matter in the water sample in question, for certain parameters – e.g. COD and the total content of heavy metals – the sample must be homogenized. This must be carried out using a high-speed blender (2 minutes at 5000 – 20000 rpm and taking the sample while stirring).

3.6 Decomposition

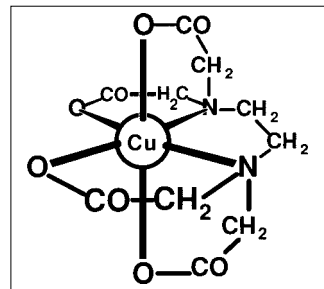
Water-borne substances can be present in the sample for investigation in a variety of forms: as the ion, bound more or less solidly in a complex, or as a solid substance.

The manner in which the sample is pretreated enables the three proportions to be distinguished from each other. This can be illustrated using a copper-containing wastewater sample as an example.

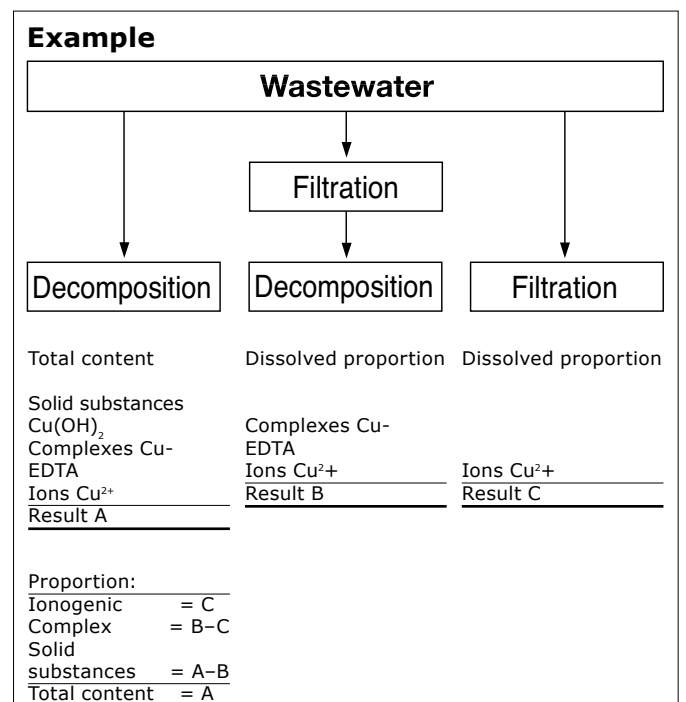
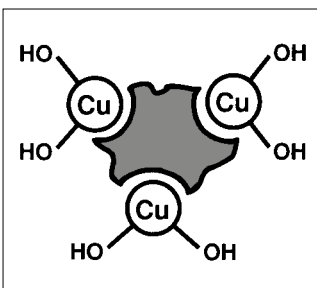
Ion



Complex



Solid substance



Decomposition converts the substance to be determined into an analyzable form. In most cases, decomposition agents take the form of acids in combination with oxidizing agents; in exceptional cases (e.g. in the determination of total nitrogen) an alkaline decomposition is more effective. The type of decomposition procedure used depends on the analyte to be determined and the sample matrix.

3 Sample Preparation – 3.6 Decomposition

The ready-to-use sample-decomposition products **Spectroquant® Crack Set 10 and 20** are suited for the preparation of the sample materials for the determinations stated in the table.

Determination of	Sample preparation with
Total phosphorus*	Crack Set 10/10C**
Total chromium* [= sum of chromate and chromium(III)]	Crack Set 10/10C
Total metal [= sum of free and complex-bound metal]	Crack Set 10/10C
Total nitrogen*	Crack Set 20

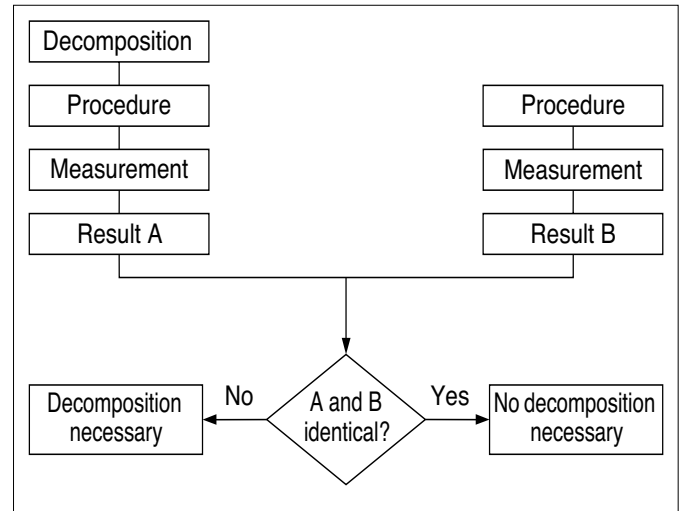
* The decomposition reagents are already contained in the packs of the respective cell tests.

** Decomposition cells are included in the pack; empty cells are required for the decomposition for Crack Sets 10 and 20.

The decomposition processes are carried out in the Spectroquant® thermoreactor (capacity: 12 or 24 decomposition cells) at 120 °C or, respectively, 100 °C. Details regarding the heating times and further treatment can be found in the package inserts contained in the Spectroquant® Crack Set packs.

In the event that the sample to be analyzed is a highly contaminated material (high proportion of organic substances) or water-insoluble samples, decomposition using concentrated acids and other agents is indispensable. Corresponding examples from the **collection of applications** for real samples are available on request.

The necessity for decomposition can be checked according to the following diagram.



For wastewater with a consistent composition, this check as a rule need be carried out only once. It is, however, advisable to check the result periodically.

4 Pipetting System

1

2

Positive-displacement pipettes permit

3

- an exact dosage of the sample volume
- a precise measurement of sample and reagent volumes and of the volumes of water for dilution purposes

4

Pipettes of varying volumes and also ones with a fixed volume are available.

5

Sources of error and hints on how to avoid them:

Closely follow the instructions for use contained with the pipette in question.

6

- Check the pipetted volumes
 - a) by weighing using analytical scales (weighing accuracy ± 1 mg), 1 ml of water at 20 °C = 1000 g ± 1 mg
 - b) using Spectroquant® PipeCheck; this is a photometric check of the pipette, and scales are not necessary (see section 5.2.3)
- Avoidance of spread effects by rinsing the pipette several times with the solution to be pipetted
- Always exchange the pipette tip
- Draw up the liquid slowly and depress piston completely to discharge the liquid

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5 Analytical Quality Assurance (AQA)

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The objective of analysis must always be to determine the true content of the analyte in question as accurately and precisely as possible.

4

Analytical Quality Assurance represents a suitable and indispensable method by which the quality of the user's own work can be assessed, errors in the measurement system diagnosed, and the comparability with the results obtained using the respective reference methods demonstrated.

5

6

Details regarding the necessity of AQA can be found in Memorandum A 704 of the German Association for the Water Sector, Wastewater, and Waste Materials (Deutsche Vereinigung für Wasserwirtschaft, Abwasser und Abfall e.V., DWA) and in the corresponding self-control/self-monitoring regulations of the German federal states (available in English).

7

8

Causes for errors can include:

- the working materials used
- the handling
- the sample under investigation

9

10

These errors have effects on both the accuracy and precision of the results obtained.

11

5.1 Quality Control at the Manufacturer

12

Spectrophotometers and photometric test kits possess specifications that are adhered to and above all else also documented by the manufacturer.

13

The **certificate for the spectrophotometer** enclosed with each device documents the quality of the measuring device.

14

15

16



Certificate of Final Inspection (full details)

Device Name: Spectroquant® Prove 600
 Serial no: 2005614705
 Software version: 1.4.5



Wavelength Accuracy*				
Equipment	Nominal value	Tolerance limit**	Actual value	Result
Holmium Oxide Liquid Filter Hellma 667-UV5	241.15 nm	240.0 - 242.4 nm	241.9 nm	P
	361.30 nm	360.1 - 362.5 nm	361.4 nm	P
	640.55 nm	639.4 - 641.8 nm	641.1 nm	P

Wavelength Precision / Reproducibility*				
Equipment	Wavelength	Nominal value	Actual value	Result
Holmium Oxide Liquid Filter Hellma 667-UV5	241.15 nm	±0.10 nm	0.01 nm	P
	361.30 nm	±0.10 nm	0.02 nm	P
	640.55 nm	±0.10 nm	0.06 nm	P

Photometric Accuracy*					
Equipment	Wavelength	Nominal value	Tolerance limit**	Actual value	Result
Neutral Density 1.0 Abs. Hellma 666-F4	440 nm	1.093 A	1.082 - 1.104 A	1.092 A	P
	546 nm	1.003 A	0.996 - 1.011 A	1.004 A	P
	635 nm	1.024 A	1.016 - 1.031 A	1.023 A	P
Neutral Density 2.0 Abs. Hellma 666-F203	440 nm	2.252 A	2.236 - 2.268 A	2.248 A	P
	546 nm	1.994 A	1.982 - 2.005 A	1.995 A	P
	635 nm	1.928 A	1.916 - 1.940 A	1.931 A	P

Photometric Precision / Reproducibility* @ 1.0 A				
Equipment	Wavelength	Nominal value	Actual value	Result
Neutral Density 1.0 Abs. Hellma 666-F4	440 nm	±0.003 A	0.000 A	P
	546 nm	±0.003 A	0.000 A	P
	635 nm	±0.003 A	0.001 A	P



Stray Light*				
Equipment	Wavelength	Nominal value	Actual value	Result
Potassium Chloride Hellma 667-UV1	198.00 nm	≤1.00 %T	1.00 %T	P
Sodium Nitrite Hellma 667-UV11	340.00 nm	≤0.10 %T	0.00 %T	P

Spectral Bandwidth***			
Equipment	Nominal value	Actual value	Result
Toluene in n-Hexane Hellma 667-UV6	±1.8 nm	1.1 nm	P

Selftest Hardware **P**

No visual flaws, no burrs, no loose parts and fastenings **P**

Date: 29/01/2020
 Inspector: gberg


- This document has been generated using electronic data processing and is valid without signature. -

Merck KGaA, 64271 Darmstadt, Germany
 www.analytical-test-kits.com

EMD Millipore Billerica, MA 01821 - USA

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The **certificate for the test kit**, available for each lot produced, documents the quality of the reagents contained in the test kit.



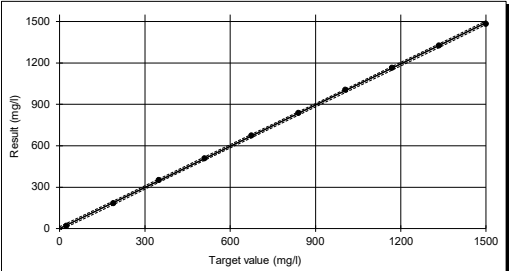
Lot certificate

Chargenzertifikat / certificado del lote


Spectroquant® COD Cell Test
Spectroquant® CSB-Küvettest
Spectroquant® Test en cubetas DQO

Cst.No. / Art.Nr. / Art. No.	114541.0001	n = 10	
Measuring Range / Messbereich / Intervalo de medida	25 - 1500 mg/l CSB / COD / DQO	Target value Sollwert Valor nominal (Standard / Patrón) mg/l COD/CSB/DQO	Result Messergebnis / Resultado (Standard / Patrón) mg/l COD/CSB/DQO
Lot no./ Charge-Nr. / Lote nro.	HC813858	25	19
Expiry date / Verwendbarkeit / Fecha de caducidad	2019/11/30	190	184
Standard / Standard / Patrón	Polysulfon hydrogen peroxide 1.02000 Lot 1824002	350	351
Photometer / Photometer / Fotómetro	Reference / Referenz / Referencia	510	508
Wavelength / Wellenlänge / Longitud de onda	675 nm	675	674
Cell / Küvette / Cubeta	905 nm	840	838
Tester / Prüfer / Verificador	10 mm (round / rund / redonda)	1.005	1.005
Date / Datum / Fecha	21 Standard	1.170	1.163
File / Datei / Fichero	2016/11/17	1.335	1.324
	1145410001_HCS13858_EN	1.500	1.483


Calibration Function / Kalibrierfunktion / Función de calibración ISO 8466-1 / DIN 35402 A51	Target value Sollwert Valor nominal	Lot value Chargenwert Valor del lote
Slope / Steigung / Pendiente	1,00 ± 0,05	0,99
Ordinate segment / Ordinatenabschnitt / Intersección en ordenadas		0
Reagent blank / Reag.blindwert / Valor en blanco del react. Tolerance +/- / Tolerancia	0,010 ± 0,010 A	0,010 A
Confidential interval (P=95%) Vertrauensbereich (95% Wahrscheinlichkeit) / Intervalo de confianza (95 % de probabilidad)	± 25 mg/l	± 12 mg/l
Standard Deviation of the Method Verfahrenstandardabweichung / Desviación estándar del procedimiento		± 4,9 mg/l
Variation Coefficient of the Method Verfahrensvariationskoeffizient / Coeficiente de variación del procedimiento	± 2,5 %	± 0,7 %



Merck KGaA, Darmstadt, Germany



Head of Lab. / Laborleiter /
Jefe de laboratorio



Quality control
Qualitätskontrolle / Control de calidad

Merck KGaA, 64271 Darmstadt, Germany, Tel.: +49 (0)6151 72-2440
 EMD Millipore Corporation, 400 Summit Drive, Burlington MA 01803, USA, Tel.: +1-978-716-4321
 Sigma-Aldrich Canada Co. or Millipore (Canada) Ltd., 2149 Winston Park, Dr. Oakville,
 Ontario, L6H 6J8, Phone: +1 800-365-1400

1/2

Calibration function:

The calculated function must agree, within specified tolerances, with the function electronically stored in the spectrophotometer.

Confidence interval:

Maximum deviation from the desired value over the entire measuring range; every measurement value can be affected by this deviation; this parameter is a measure for the accuracy.

Standard deviation for the procedure:

Measurement for the dispersion of the measurement values over the entire measuring range, expressed in ± mg/l.

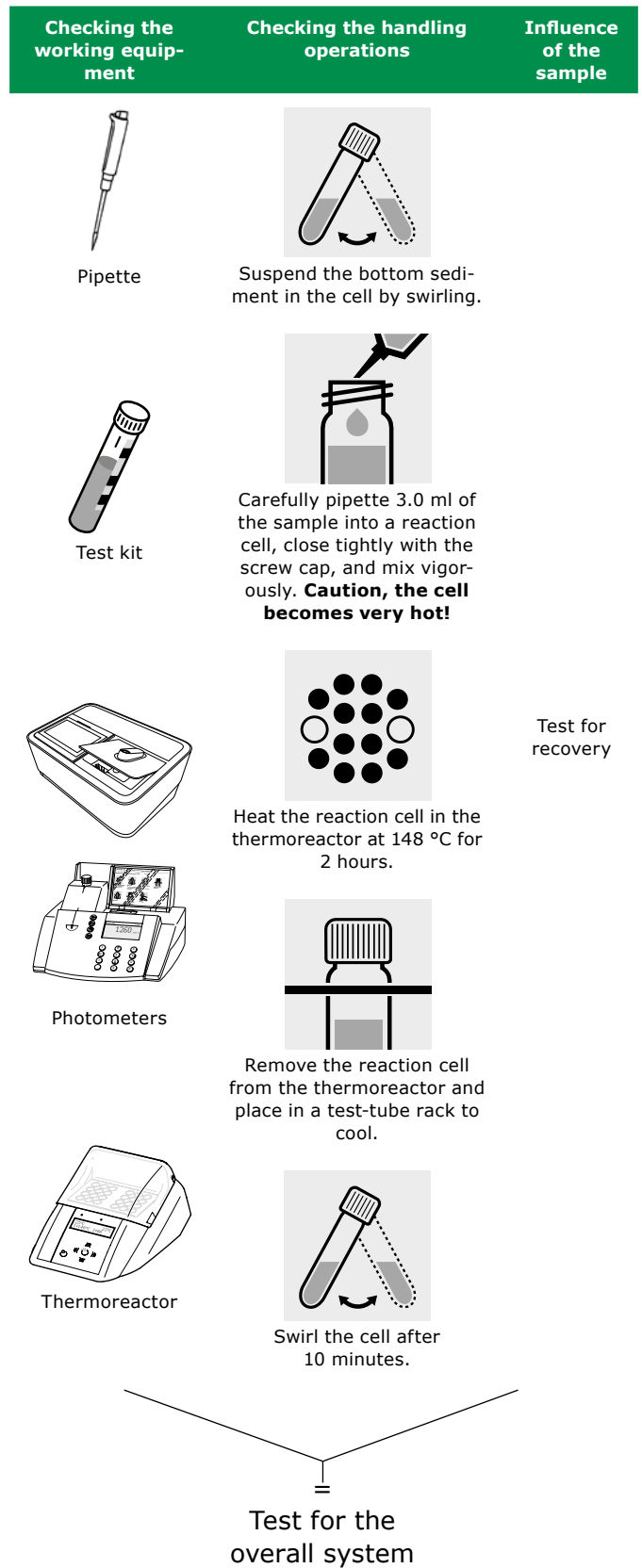
Coefficient of variation for the procedure:

Measurement for the dispersion of the measurement values over the entire measuring range, expressed in %. The smaller the standard deviation/coefficient of variation for the procedure, the more pronounced the linearity of the calibration curve.

5.2 Quality Control for the User

A complete check comprises the entire system, i. e. the working equipment and the mode of operation. The spectrophotometer offers an optimum degree of support in this regard, in the form of the different quality mode. The instrument, or the whole system (including reagents and all accessories) are checked, depending on which quality mode is selected. All checking operations can thus be supported by the spectrophotometer and the check values accordingly documented as per GLP (Good Laboratory Practice) recommendations (see section 9.11).

The following diagram provides an overview regarding internal quality-assurance aspects:



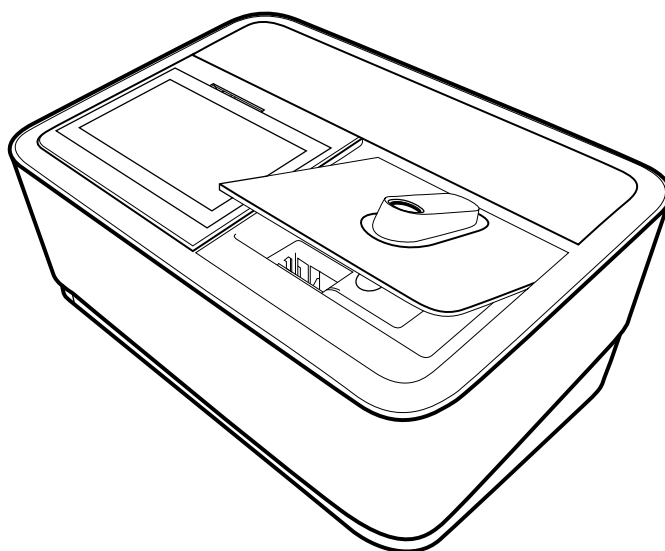
5.2.1 Checking the Spectrophotometer

As soon as the spectrophotometer is activated it runs a Self-Check. This means the hardware and the software of the spectrophotometer are checked and compared with internal standards.

The spectrophotometer itself is checked in the **AQA1 mode** with the **Spectroquant® PhotoCheck**: the pack includes round cells containing stable test solutions (**secondary standards**) for checking the spectrophotometer at the 445, 525, and 690 nm wavelengths. The test solutions are measured in a **reference spectrophotometer** monitored with **primary standards**, and the certificate stating the absorbance values is enclosed with the package unit. These desired values with the permissible tolerances are entered into the spectrophotometer or else handwritten into the control chart. For the measurement the cell is placed in the compartment for the round cell and identified by the spectrophotometer via the bar code, and the measured absorbance is compared with the desired value. The absorbance is shown on the display and can be entered into the corresponding control chart.

The measurement of four cells for a given wavelength tests – in addition to the wavelength accuracy – also the linearity of the absorbance over the effective range.

The verification of the instrument, as required by DIN/ISO 9000 or GLP, can be easily performed by using the **Spectroquant® PhotoCheck**. The PhotoCheck hence offers the possibility to check the instrument. All of the corresponding documentation required by these certification guidelines is done by the spectrophotometer automatically.



5.2.2 Checking the Overall System

3 The testing of the overall system includes checking the working equipment and checking the handling operations.

4 The **overall system** can be checked using standard solutions of a known content, preferably with the **Spectroquant® CombiCheck**; this corresponds with the **AQA2 mode** in the spectrophotometer.

5 **Spectroquant® CombiCheck** are ready-to-use standard solutions that in terms of the analyte concentration are finely adjusted to the individual test kits. They contain a mixture of several analytes that do not interfere with each other. The standard solution (R-1) is used in the same way as a sample. A double determination is recommended as a measure to diagnose any random errors.

6 **Standard solutions for photometric applications** are ready-to-use standard solutions that in terms of the analyte concentration are finely adjusted to the individual test kits. The standard solution is used in the same way as a sample. A double determination is recommended as a measure to diagnose any random errors.

7 In addition to the CombiCheck and the standard solutions for photometric applications, it is also possible to use **Certipur® standard solutions** for this checking procedure. These contain 1000 mg of the respective analyte per liter of solution.

They can be diluted to different final concentrations, which should preferably lie approximately in the middle of the measuring range of the respective test kit. The table presented in Appendix 2 provides an overview of the available CombiCheck and ready-to-use standard solutions.

Due to limited shelf-life characteristics, there are no CombiCheck or ready-to-use standard solutions available for certain parameters. Appendix 3 is a compilation of **standard working procedures** necessary to make your own solutions of a defined concentration. This allows the control of parameters where there are no simple-to-prepare solutions available.

If the test for the overall system shows that all requirements are fulfilled, the individual results are flagged as AQA2. If not, an error message is given and the individual components of the instrument have to be checked in detail.

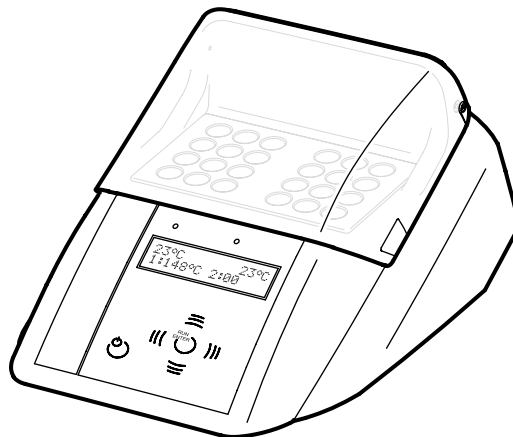
5.2.3 Checking the Pipettes



The **Spectroquant® PipeCheck** is used to check the pipettes. The pack contains cells filled with color-dye concentrates. After the addition of a predefined volume of water using the pipette in question, the cell is measured against a corresponding reference cell also contained in the pack. The difference in the absorbance values of the measurement cell and reference cell must not exceed the tolerances given in the package insert. If the tolerances are exceeded, the instructions given in the [section 4](#) must be followed accordingly.

5.2.4 Checking Thermoreactors

This is checked by means of the thermosensor.



The thermoreactor is preheated as described in the Instruction Manual. When the control lamp goes out, the temperature is measured in any one of the bores of the thermoreactor. The following desired temperatures must be achieved:

Block temperature 100 °C =
Desired temperature 100 ± 3 °C

Block temperature 120 °C =
Desired temperature 120 ± 3 °C

Block temperature 148 °C =
Desired temperature 148 ± 3 °C

The even distribution of the temperature over all bores can also be documented using the thermosensor.

5.2.5 Testing for Handling Errors

The user's own mode of operation must also be subjected to an exact analysis.

The following questions may serve as a guide:

- Is the test kit optimal for the measurement assignment in question?
- Is the test kit's measuring range suitable?
- Were the operating instructions for the test followed?
- Was the sample volume correct?
- Was the pipette handled properly?
- Was a new pipette tip used?
- Is the pH of the sample and measurement solution correct?
- Was the reaction time adhered to?
- Does the sample and reagent temperature lie within the correct range?
- Is the cell clean and free from scratches?
- Has the expiry date for the test kit been exceeded?
- Were suitable sample vessels used?
- Were the vessels used for the samples and preparation steps clean and free from detergent residues?

5.3 Determination of Sample Influences (Matrix Effects)

The influence of other substances contained in the sample may, under certain circumstances, be so great that their recovery rates lie in the region of several percent. It is recommended to check for any influence by using the addition solution contained in the **Spectroquant® CombiCheck** pack.

A defined quantity of the **addition solution** (R-2), which contains a known concentration of the respective analyte, is added to the sample and the recovery rate is determined. The following difference is then calculated:

Result (sample + addition solution) – Result (sample)

If the calculated difference is equal to the concentration of analyte of the addition solution that was added, the recovery rate is 100 %. In the case that the recovery rate lies outside a range of approx. 90 – 110%, a matrix interference is present.

5.4 Definition of Errors

It is obvious that measurement results as a rule may be associated with errors. This applies equally to standardized methods of analysis (reference methods) and to routine analysis. The discovery and the minimization of errors must be the objective here.

A distinction is made between systematic errors and random errors.

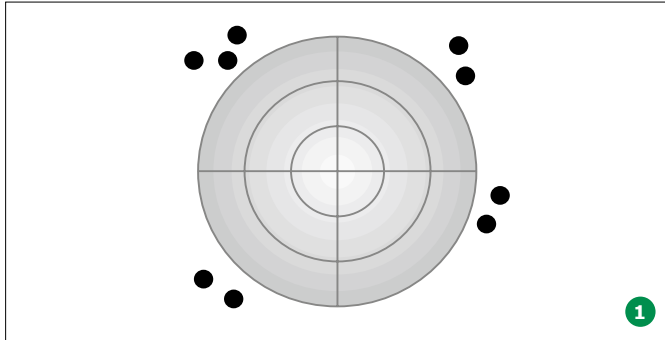
Systematic errors are present when all the results of an analysis deviate from the true value with the same algebraic sign. Examples here include: a wrong sample volume, a wrong pH, a wrong reaction time, a sample-matrix influence, etc. Systematic errors thus affect the **accuracy** of the method of analysis.

Accuracy = Deviation of the measured concentration from the true concentration

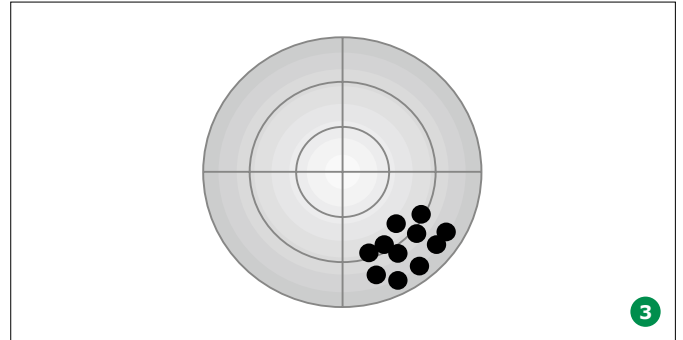
Random errors manifest themselves in the form of a wide range of deviation of the results of a given sample. These can be kept to a minimum by ensuring good operating techniques and multiple determination with calculation of the mean values. Random errors make the result of the analysis unreliable; they influence the **precision**.

Precision = Dispersion of the results among each other

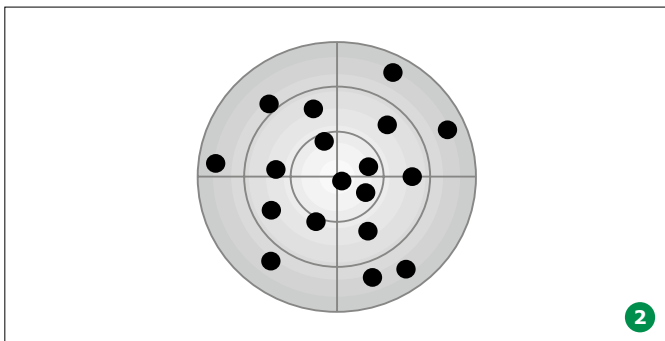
The following diagram illustrates the aspects of accuracy and precision:



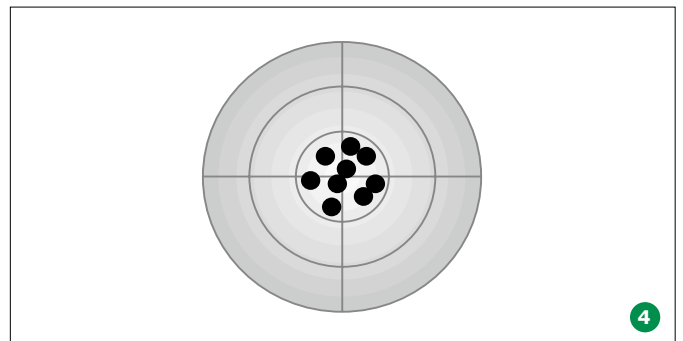
Accuracy: poor
Precision: poor
Major errors have been made!



Accuracy: poor
Precision: good
The high degree of precision mistakenly indi-



Accuracy: good
Precision: poor
Calculation of the mean values from at least three – or better even more – parallel determinations yields an approximation of the true value.



cates a correct value!
Accuracy: good
Precision: good
The ideal objective!

1 6 Overview

2

6.1 Scope of Delivery

- Spectrophotometer
- Power adapter
- Power connectors (3 pieces)
- Dust cover
- Zero cell
- Quick Guide (A4 format)
- Safety instructions
- Certificate of final inspection

4

5

6.2 Overview of the Instrument Packaging

The spectrophotometer is shipped in protective transport packaging.

CAUTION

Retain the original packaging including the inner packaging to protect the instrument against hard knocks if it has to be transported. Please note that damage caused by improper transport voids all warranty claims.

6

Front of the instrument

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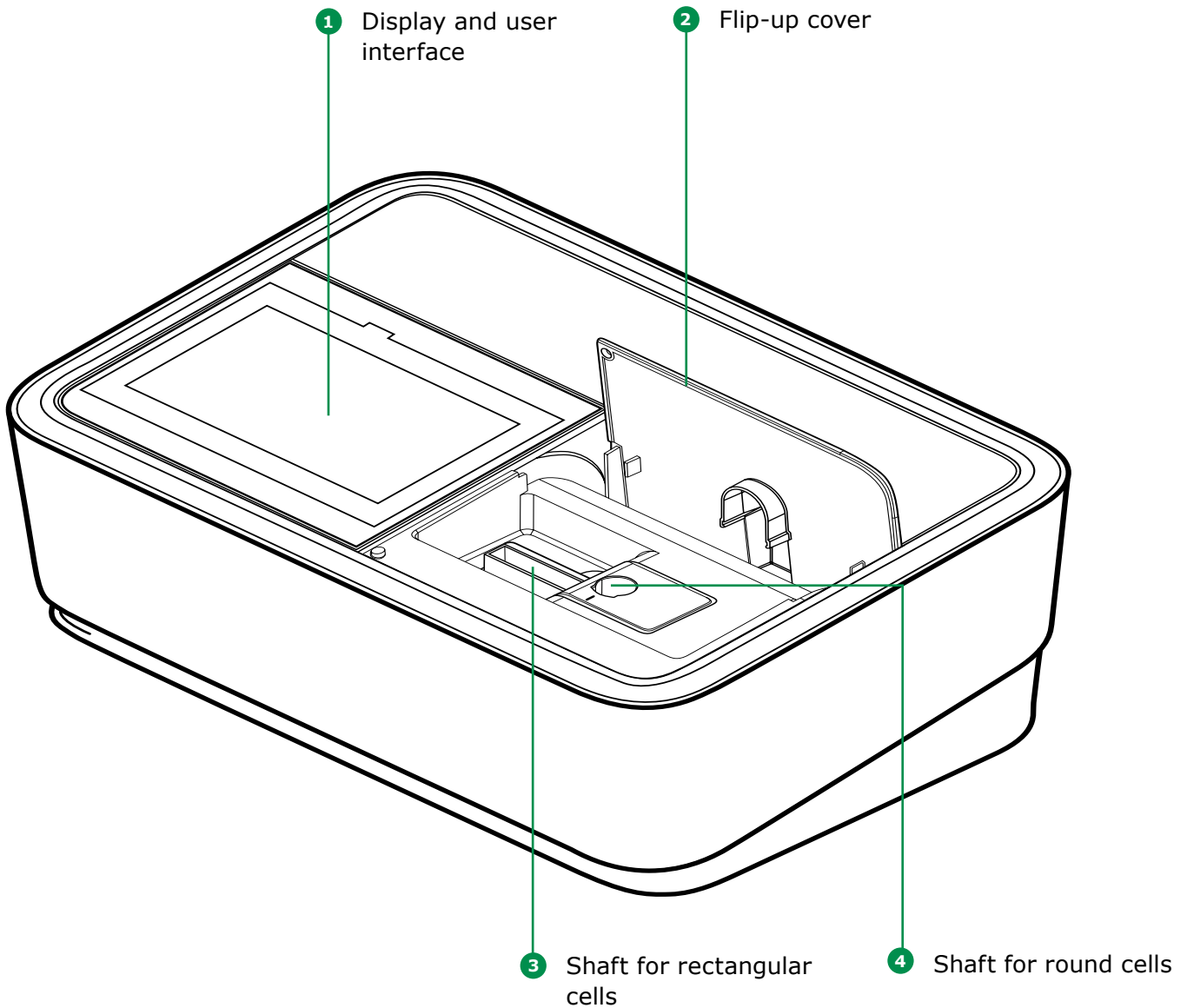
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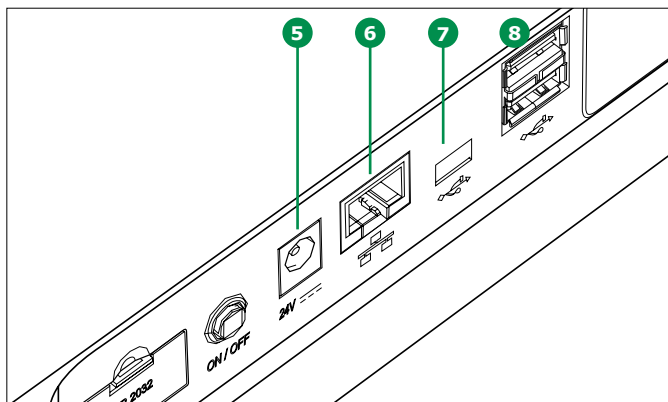
16



6.3 Display and User Interface

NOTE

The entire display is touch-sensitive. Make selections using a fingertip or special touch pen. Do not touch the display with sharp objects (e.g. the tip of a ballpoint pen).



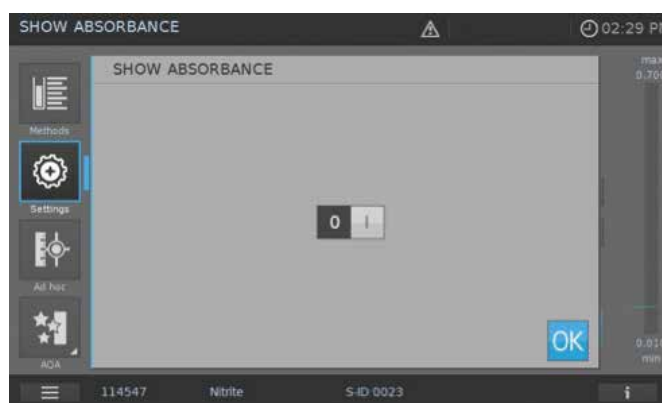
Ports at the rear of the instrument

- 5 Socket for plug-in power supply unit
- 6 LAN port
- 7 USB Mini B port
- 8 USB-A ports


NOTE

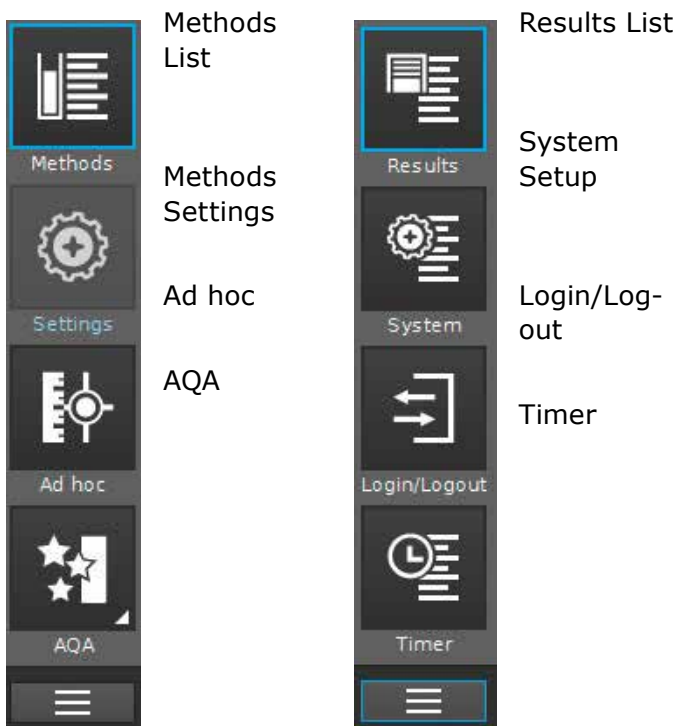
All connections comply with SELV.

- Do not place objects on the display, as doing so may scratch it
- Touch buttons, words or symbols to select them
- Scrollbars are provided to assist quick movement through long lists
- Touch the arrow in the scrollbar to scroll upwards or downwards through the list
- Following selection, the item is activated immediately
- Touching a main button outlines it in blue
- Selecting an item inverts it (with dark text being shown on a light background)
- Selecting a text inverts it (with dark text being shown on a light background), e.g. method-specific settings for concentration mode "Show Absorbance"
- "0" is OFF, "I" is ON – the active selection is displayed light grey with dark figure, in this case the Show Absorbance is ON

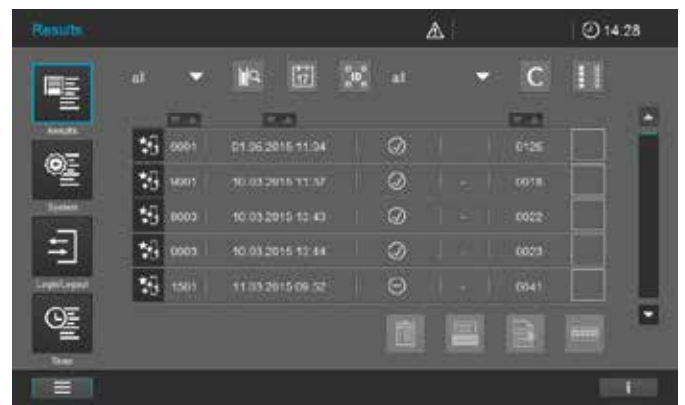
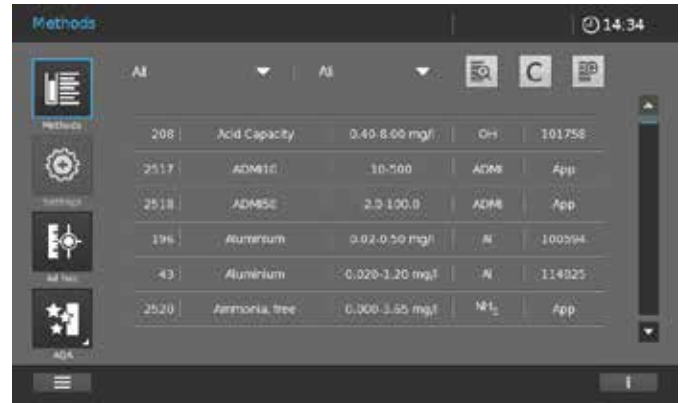


2 **Main menu navigation**

3 The main menu is always visible on the left: It consist of two pages with four smart icons each. To switch between the two pages push  at the bottom on the left.



"Methods" and "Results" are the most often used modes and they are at the top of the main menu navigation.




12 **NOTE**

The menu selected is always outlined in blue.




13 **NOTE**

Action buttons like "Start", "Save", "Print" give the following touch feedback:

- 14
-  Normal
Remains static

Active fields are always shown in bright color.

Pressed fields invert the color as long as the chosen action is performed.

- 15
-  Disabled
Draws 30% of the normal state

Inactive, disabled fields show faint color.

NOTE

The main menus "Settings (Method Settings)", "Ad hoc", "AQA", "System (Instrument Settings)", "Login/Logout", "Timer" open up a submenu. Example "Settings":

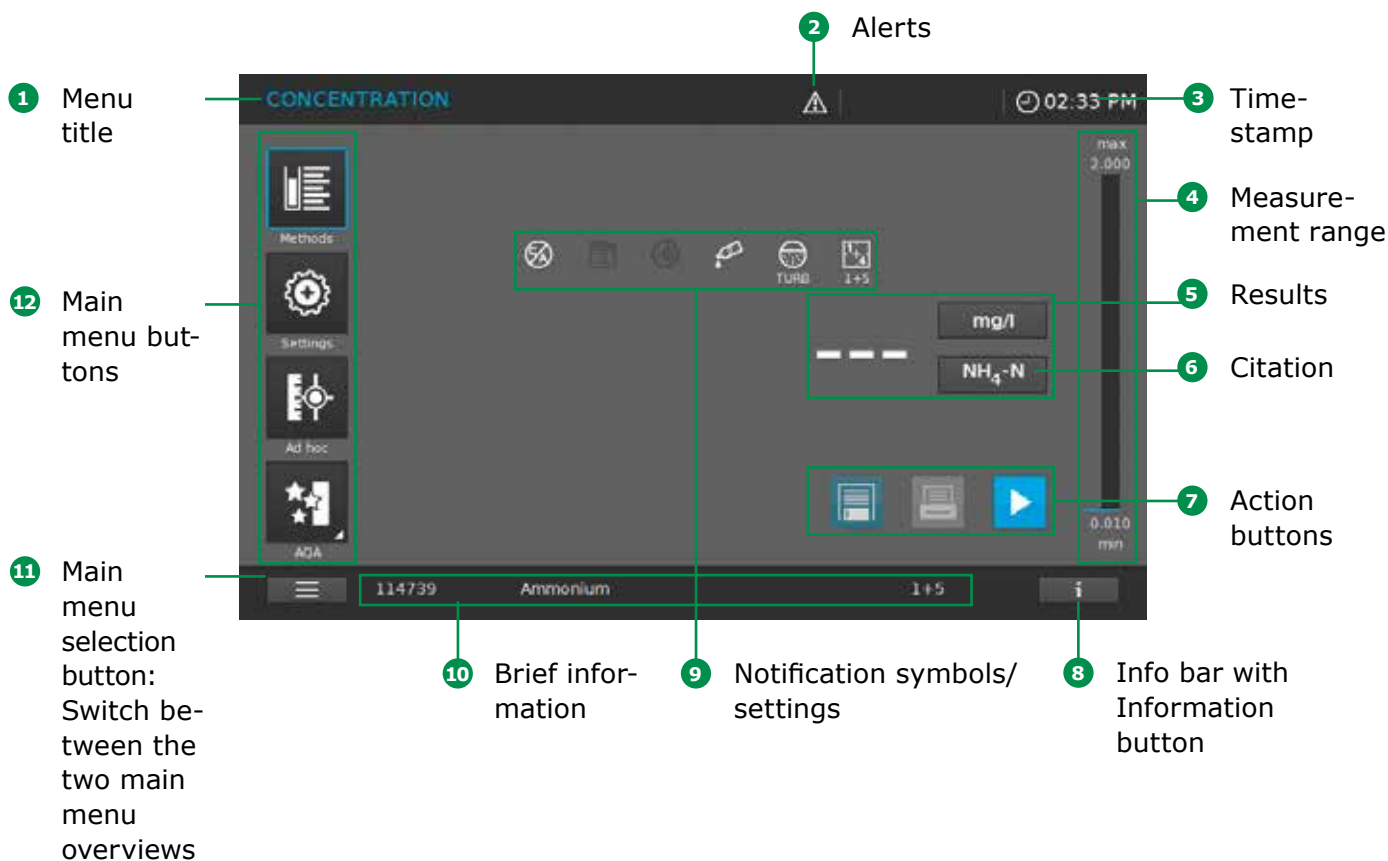


To leave these, the submenu has to be closed by touching the main menu button again, in this case:



The main menu "Methods" comprises two main overview panels arranged as shown below: the Concentration Measurement Overview and the Method List Overview.

Screen layout concentration measurement overview



Screen layout method list overview

1 Menu title

7 Focuses selected main menu button

2 Dropdown box (closed)

3 Dropdown box (closed)

4 Selection buttons

6 Name of method

5 Scrollbar

ID	Method Name	Range	Unit	App
208	Acid Capacity	0.40-8.00	mg/l	OH
2517	ADM10	10-500		ADM
2518	ADM50	2.0-100.0		ADM
196	Aluminium	0.02-0.50	mg/l	Al
43	Aluminium	0.020-1.20	mg/l	Al
2520	Ammonia, free	0.000-3.65	mg/l	NH ₃

Screen layout results overview

1 Menu title

7 Focuses selected main menu button

2 Filter menu

6 Result list

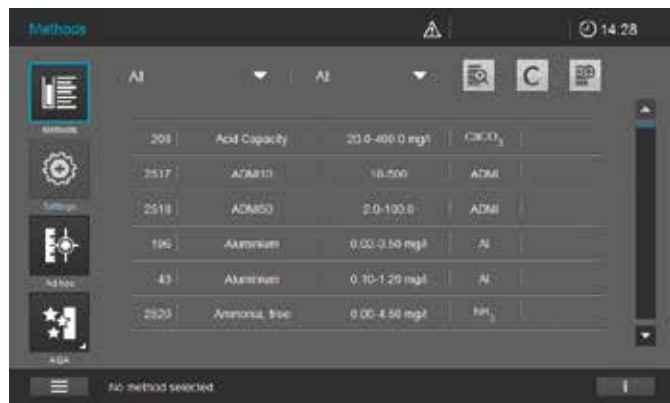
3 Selection buttons

4 Scrollbar

5 Action buttons

ID	Date	Time	Status	Value	App
9001	01.06.2015	11:04	✓	-	0126
9001	10.03.2015	11:37	✓	-	0018
9003	10.03.2015	13:43	✓	-	0022
9003	10.03.2015	13:44	✓	-	0023
1501	11.03.2015	09:52	⊖	-	0041

Main menu buttons



Method list



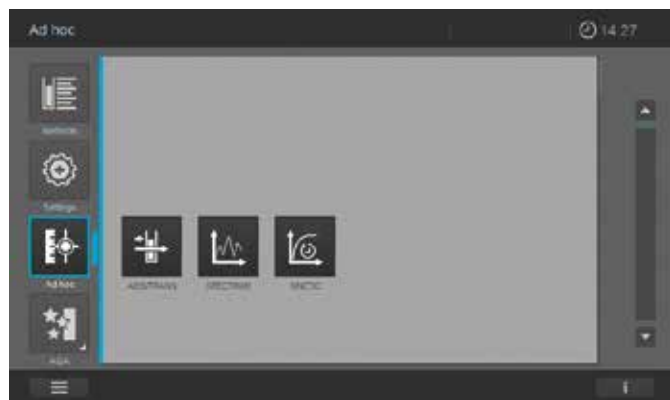
List of all methods, irrespective of mode



Settings



This button is used to activate method-specific settings (e.g. sample dilution, turbidity correction, zero adjustment, sample blank, reagent blank)



Ad hoc



For performing measurements (absorbance/transmission, spectrum, kinetics)
Allows measurements to be performed without the need to create methods

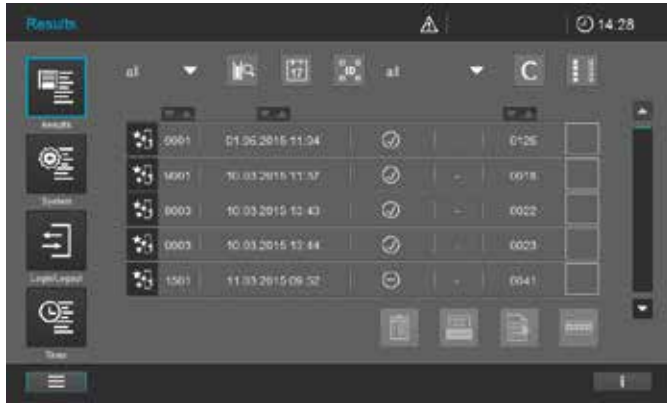


AQA



Overview and list of all Analytical Quality Assurance (AQA) modes

Main menu buttons

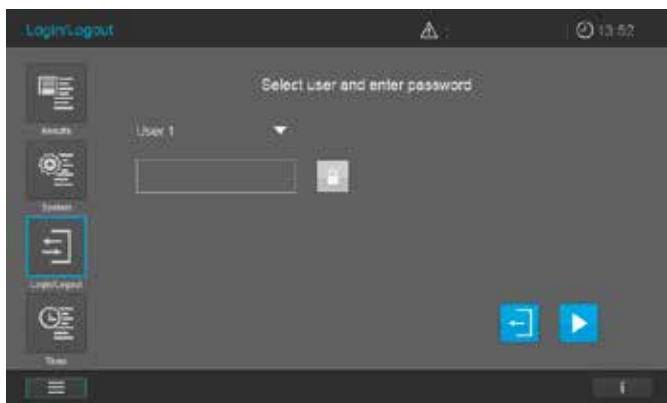


Results list

List of all stored results

System setup

This button is for optional instrument settings (e.g. date, time, updates etc.)



Login/logout

Check users in and out

Timer list

List of stopwatch functions



Overview of main buttons

Buttons	Description
	Method list List of all methods, irrespective of mode
	Settings This button is used to activate method-specific settings (e.g. sample dilution, turbidity correction, zero adjustment, sample blank, reagent blank)
	Ad hoc For performing measurements (absorbance/transmission, spectrum, kinetics) Allows measurements to be performed without the need to create methods
	Absorbance/Transmission Mode Ad hoc submenu: perform absorbance or transmission measurements
	Spectrum Mode Ad hoc submenu: record spectrum Method list: create methods -> Spectrum Mode
	Kinetic Mode Ad hoc submenu: perform kinetic measurement Method list: create methods -> Kinetic Mode
	AQA Overview and list of all Analytical Quality Assurance (AQA) modes
	AQA Status 1&2 AQA submenus: Status display of the period of validity and the outcome (passed/failed)
	AQA1 AQA submenu: List of AQA1 methods
	AQA2 AQA submenu: List of AQA2 methods
	Pipette check AQA submenu: List of pipette-checking methods
	Result list List of all stored results
	System setup This button is for optional instrument settings (e.g. date, time, updates etc.)
	Login/logout Log users in and out
	Timer list List of stopwatch functions

Overview of action & selection buttons

Action & Selection Buttons	Description
	Start button Start an action (e.g. measurement)
	Start zero Start zero adjustment for a method
	Apply
	Save
	Stop
	Close
	Logout User logout
	Search method
	Search/results list Search function, search criterion: method name, method number or item number
	Filter cancellation button Cancel all set filter options
	Edit For editing parameters
	Create method
	Print Print to pdf (USB device) or printer
	Export button All selected results are exported to an external memory device as .csv file
	Import button Updates/Methods are imported from an external memory device into the instrument
	Delete The selected items are deleted






7 Safety

This operating manual contains basic instructions that you must follow during the commissioning, operation and maintenance of the spectrophotometer. Consequently, all responsible personnel must read this operating manual carefully before working with the meter. Keep this operating manual in the vicinity of the meter.

This is a class A device. This equipment may cause interference in a residential installation. In this case the user is encouraged to perform appropriate measures to correct the interference.

Safety instructions

Safety instructions in this operating manual are indicated by the warning symbol (triangle) in the left margin. The signal word (such as "CAUTION") indicates the danger level. The following warning symbols are used:

Symbols	Description
	WARNING Hazardous area (general). The xenon lamp (UV/VIS) emits radiation in the ultraviolet region, which may cause damage to the eyes. Never look directly in the radiation of this light source without wearing proper eye protection. Protect your skin from the direct exposure to UV light.
	WARNING Dangerous electrical voltage.
 WARNING	WARNING Signifies instructions that must be followed precisely in order to prevent serious dangers to personnel.
CAUTION	CAUTION Signifies instructions that must be followed precisely in order to avoid minor injuries to personnel or damage to the instrument or the environment.
 CAUTION	CAUTION This is a cautionary notice with a warning symbol drawing your attention to the risk of (limited) harm to personnel.
NOTE	NOTE Signifies a notice drawing your attention to special characteristics.
	REFERENCE Used to indicate references to other documents.

Please pay attention to the separate safety instructions leaflet (part of delivery scope) and read it carefully.

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3 **7.1 Intended Use**

4 The intended use of the spectrophotometer consists exclusively of the carrying out of photometric measurements according to this operating manual. Observe the technical specifications of the cells in the operating manual. Any other use is considered to be unauthorized. The spectrophotometer was developed for performing water analyses in the laboratory.



6 **7.2 General Safety Instructions**

7 The spectrophotometer is built and inspected according to the relevant guidelines and norms for electronic instruments (see section 12). It left the factory in a safe and secure technical condition.

8 **NOTE**

9 The spectrophotometer must be opened, adjusted, or repaired only by specialist personnel authorized by the manufacturer. Noncompliance invalidates any claim under warranty.

10 **7.2.1 Function and Operational Safety**

11 The smooth functioning and operational safety of the spectrophotometer can only be guaranteed if the generally applicable safety measures and the specific safety instructions in this operating manual are followed during operation. The smooth functioning and operational safety of the spectrophotometer can only be guaranteed under the environmental conditions that are specified in the operating manual. If the spectrophotometer is moved from a cold environment to a warm environment, the formation of condensate can cause it to function incorrectly. In this event, wait until the meter reaches room temperature before using it again.

12 **Safe operation**

If safe operation is no longer possible, the spectrophotometer must be taken out of service and secured against inadvertent use.

Safe operation is no longer possible if the spectrophotometer:

- Has been damaged in transport
- Has been stored under adverse conditions over a lengthy period of time
- Is visibly damaged
- No longer functions as described in this manual

If you are in any doubt, contact the supplier of your spectrophotometer.



14 **7.3 Target Group and User Qualification**

15 The spectrophotometer was developed for use in the laboratory. Performing photometric determinations using test kits frequently involves the handling of hazardous substances. We presume that the operating personnel are familiar with handling hazardous substances as a result of their professional training and experience. In particular, the operating personnel must be able to understand and correctly follow the safety labels and safety instructions on the packages and test kit inserts.



7.4 Handling Hazardous Substances

When developing Spectroquant® test kits, the manufacturer works diligently to ensure that the tests can be carried out as safely as possible. Some dangers posed by hazardous substances cannot always be avoided, however.

WARNING

Improper handling of certain reagents can adversely affect your health. Always follow the safety labels on the packaging and the safety instructions on the package insert. The protective measures specified there must be carefully followed.

Safety data sheets

The chemical data sheets contain all the instructions needed to handle them safely, and give details of potential risks as well as actions to be taken preventively and if a danger is posed. Work safely by following these instructions.

1 8 Getting Started

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8.1 General Notes on Handling

The Spectroquant® Prove plus spectrophotometer is an optical precision instrument. It should always be handled with care, especially when in mobile use. Always protect the instrument from conditions that could damage the mechanical, optical and electrical components. Please note the following in particular:

- The temperature and humidity during operation and storage must be within the limits specified in the "Technical Data" section (see section 12)

The instrument must never be exposed to the following:

- Extreme dust, humidity and moisture
- Intense light and heat
- Fumes that are corrosive or contain high concentrations of solvents

In addition take care of the following:

- For measuring, the instrument must be placed on a flat surface
- Spilled liquid or other material should be removed immediately (see section 10.3)
- If a cell has broken in the cell holder, the cell holder should be cleaned immediately (see section 10.3)
- The cover should always be closed when the spectrophotometer is not in use
- When the spectrophotometer is being transported, the cell compartment must be empty

8.2 Initial Setup

Proceed as follows:

- Connect the power adapter (see section 8.2.1)
- Switch on the spectrophotometer (see section 8.2.2)
- Set the language (see section 8.2.3)
- Set the date and time (see section 8.2.4)
- Run the self-test (see section 8.2.5)

NOTE

For our Operating Manual and more information about the technical videos please visit: www.sigmaaldrich.com/spectroquant

8.2.1 Connecting the Power Supply

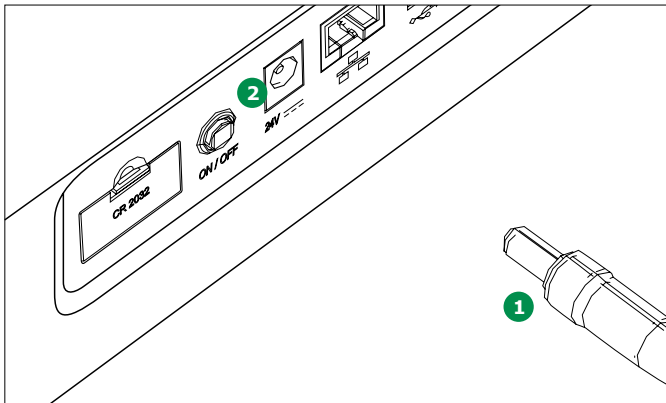
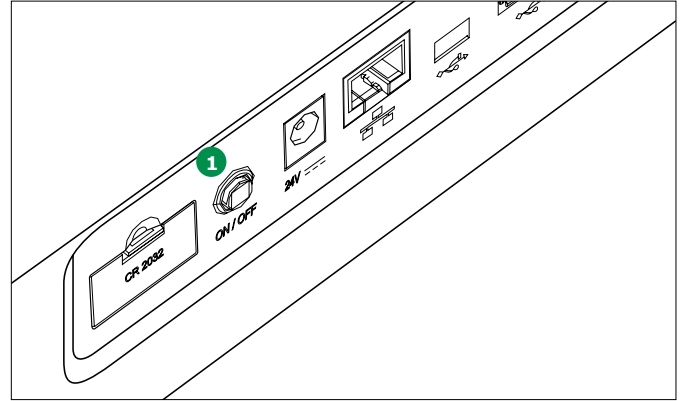
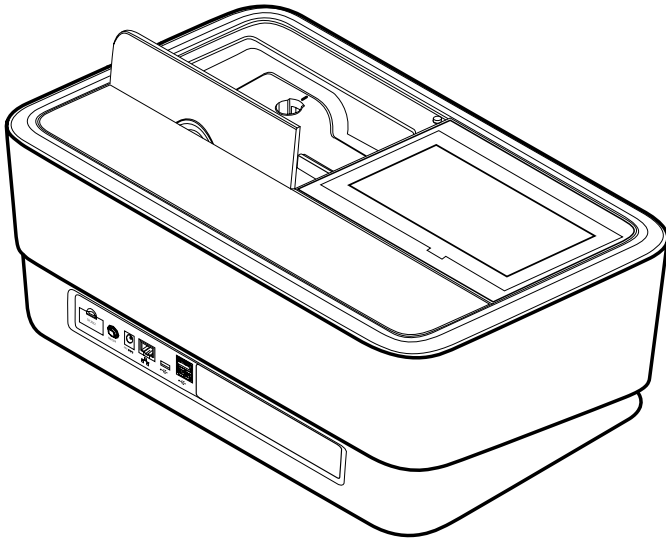
Power is supplied through the power adapter provided. The power adapter supplies the spectrophotometer with the required voltage and type of current (24 V DC).

CAUTION

The line voltage at the user location must fulfil the specifications stated on the power adapter (the specifications are also indicated in the operating manual). Only ever use the 24 V power adapter provided. Please note that damage caused by using a different power adapter than the one supplied voids all warranty claims.

8.2.2 First Power-on

After switching on the spectrophotometer for the first time you are automatically guided through the language, date and time setup procedures.



Connecting the power adapter:

1. Connect the miniplug **1** of the power adapter to the socket **2** of the spectrophotometer.
2. Connect the power adapter to a wall socket.

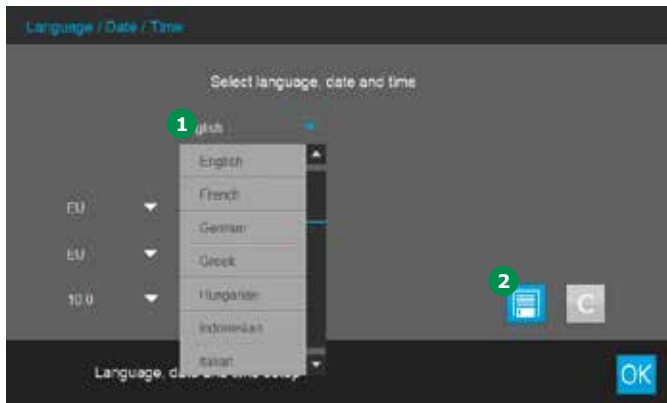
1. Press the ON/OFF button **1**. The spectrophotometer gives an audible signal (beep) and starts booting for approximately 2 minutes. You will see the following display:



2. The display switches to language setup (see section 8.2.3).

8.2.3 Language Setup

The software supports several languages. When you switch on the spectrophotometer for the first time, a list of language options is automatically displayed after the boot procedure.



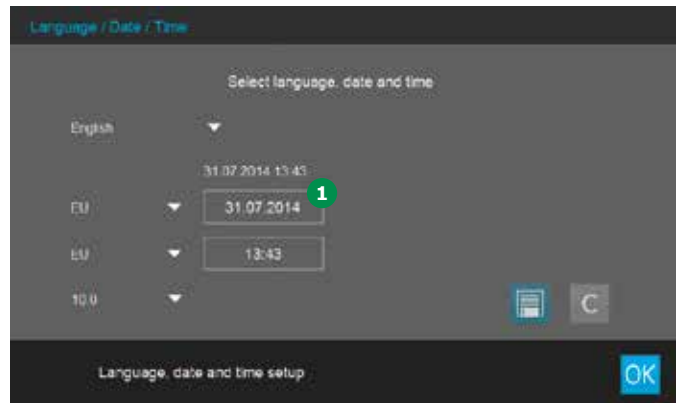
1. Select the desired language ①.
2. Tap on the Save button ② to confirm.

NOTE

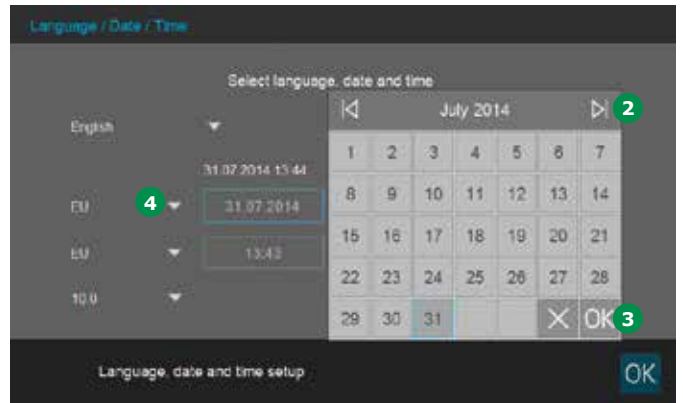
The saving process of changing the language requires some seconds.

8.2.4 Date, Time and Country-specific Settings

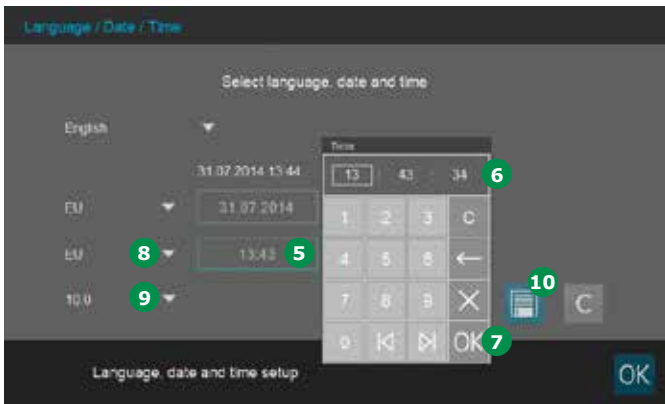
During initial setup, having set the language option you are automatically guided through the date and time setup procedure.



1. Tap on the Date format button ①.
2. The calendar view pops up ②. You can now enter the date.



3. Tap on OK ③ to confirm.
4. Tap on the Arrow button ④ to choose the country-specific basic date setting. The date format can be set and displayed for EU and US.

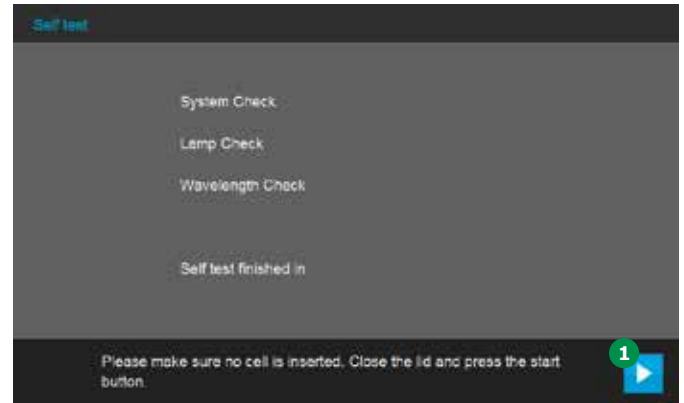


5. Tap on the Time format button **5**. The numeric key panel **6** pops up. Now you can enter the time.
6. Tap on OK **7** to confirm.
7. Tap on the Arrow button **8** to choose the country-specific basic time setting. The time format can be set and displayed for EU and US.
8. Tap on the Arrow button **9** to choose the decimal separator "."/"/," used in your country.
9. Tap on the Save button **10** to confirm.

After initial setup is complete, you can change the date and time at any time in the setup/date/time menu (see section 9.2.3).

8.2.5 Self-test

Following language, date and time setup the spectrophotometer performs a self-test.



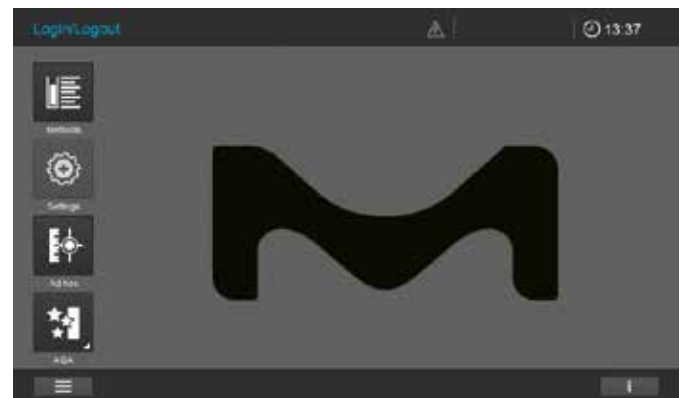
1. Remove all cells and close the cell compartment cover.
2. Start the self-test with the Start button **1**.
3. The spectrophotometer performs the self-test.

Self-test

The self-test covers:

- Checks on memory, processor, internal interfaces, filter and lamp
- A calibration of the wavelengths

When the self-test has ended, the display shows the main menu.



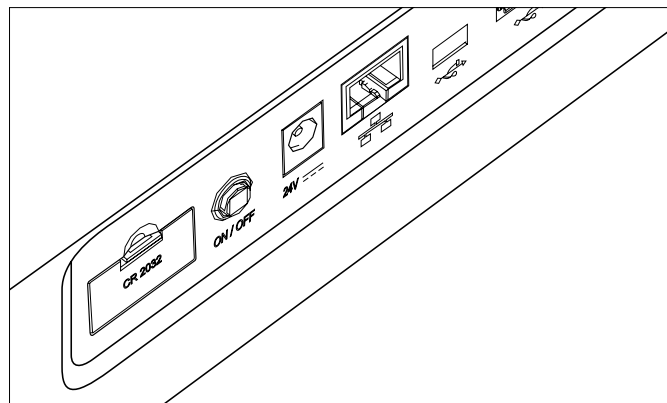
NOTE

The spectrophotometer also automatically runs a calibration of the wavelengths after every 100th measurement. A corresponding message pops up in the display as long as the calibration operation is in progress.



8.3 Connecting Optional Peripheral Devices

8.3.1 Communication Ports



You can connect the following peripheral devices to the spectrophotometer:

- Printer (see section 8.3.2)
- USB mass storage device (see section 8.3.3)
- Barcode reader (see section 8.3.4)

NOTE

If you want to connect several USB devices such as a USB PC keyboard and a USB memory device to the instrument, you can increase the number of USB-A sockets by attaching a commercially available USB-2 hub with separate power supply.

8.3.2 Printer

Printers can be connected to the spectrophotometer as follows:

Connecting the Spectroquant® Prove plus using a commercially available USB-A to USB Mini B cable enables its data to be printed out.

NOTE

All postscript printers can be used with Spectroquant® Prove plus.

8.3.3 USB Memory Device

Using a USB memory device (e.g. a USB mass storage device), you can

- Update the instrument firmware and method data (see section 9.2.8)
- Transfer data to the USB memory device (see section 9.13.7)

USB memory devices are connected to the USB-A port.

NOTE

Please follow the instructions on using USB memory devices (see section 9.13.7).

8.3.4 Barcode Reader

The barcode reader enables the simplified acquisition of alphanumerical character strings and can be used in all operating situations that require the entry of text or numerals. The barcode reader is connected to the USB-A port.

NOTE

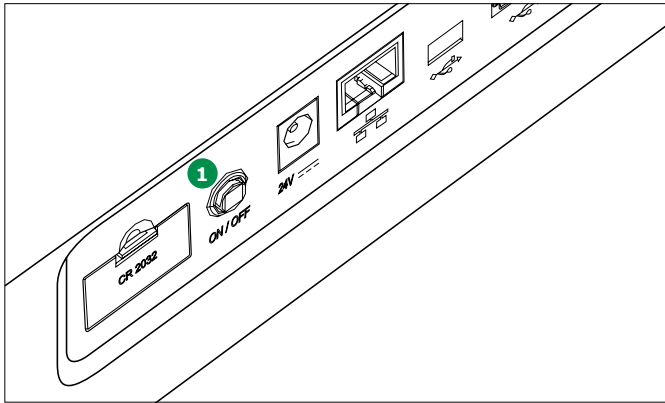
The barcode reader must support USB/HID.

1 9 Operation

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9.1 Switching the Spectrophotometer On or Off

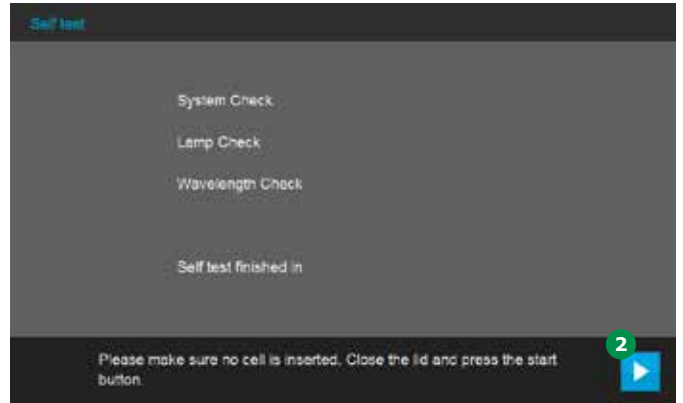
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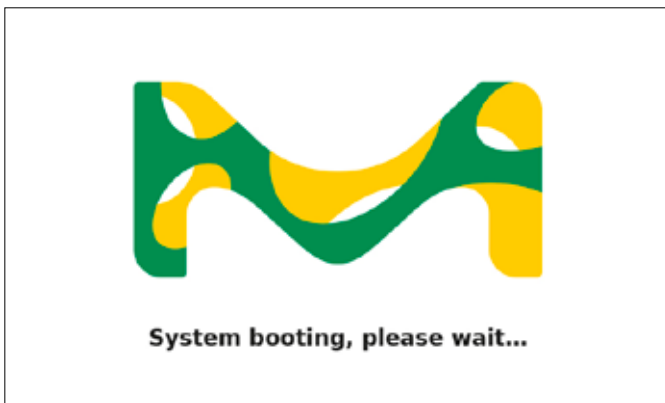


Switching on

1. Press the ON/OFF button (1). The spectrophotometer gives an audible signal (beep) and starts booting for approximately 2 minutes. You will see the following display:

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2. After the booting process the screen shows the self-test dialog.

Starting the self-test

3. Remove all cells and close the cell compartment cover.

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4. Start the self-test with the Start button (2).
5. The spectrophotometer performs the self-test.

Self-test

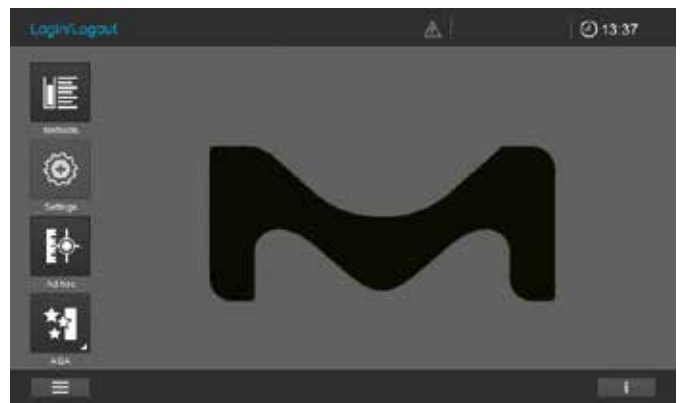
The self-test covers:

- Checks on memory, processor, internal interfaces, filter and lamp
- A calibration of the wavelengths

NOTE

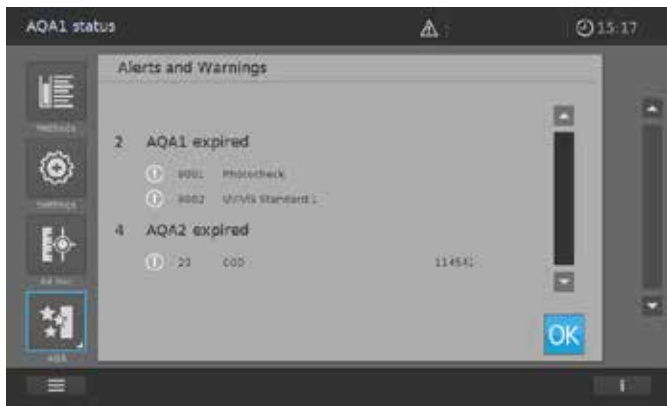
The spectrophotometer also automatically runs a calibration of the wavelengths after every 100th measurement. A corresponding message pops up in the display as long as the calibration operation is in progress (see section 8.2.5).

When the self-test has ended, the display shows the main menu.



NOTE

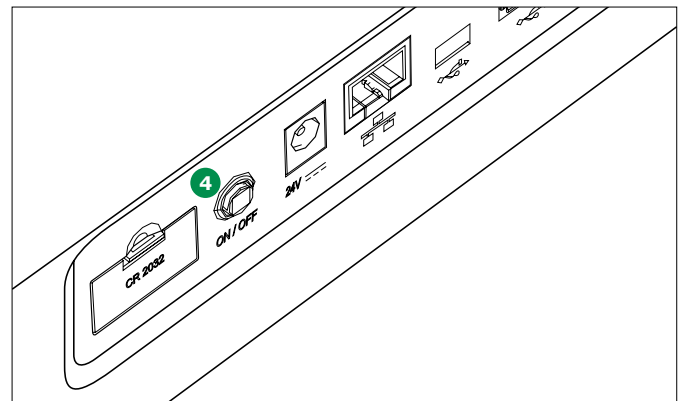
After the self-test, the system automatically checks the status of activated AQA tests. An overview of any failed and/or expired AQA tests automatically opens (see section 9.11).



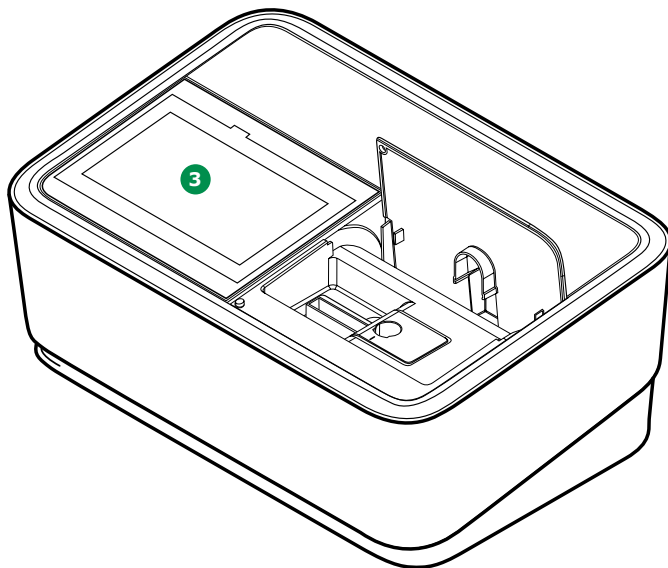
NOTE

You can set a user-defined time for this function (see section 9.2.5).

Switching off



Energy-saving mode – display



Press the ON/OFF button 4 to switch the spectrophotometer off.

NOTE

The instrument has an Auto-Power-Off function, which switches it automatically off after a user-defined time. This function is not active out of the box, but you can turn it on in "System (Instrument settings)".

The spectrophotometer automatically switches off the backlight of the display 3 when no button has been tapped within a period of 10 minutes. The backlight is switched on again with the next tap. The button functions are activated only following a further tap.



9.2 System Setup

General instrument setup is carried out in the "System" menu.



Buttons

Description

Information

This submenu displays the following information about the device:
Software/method versions, device class, lamp counter and serial number



Interface

This submenu displays the following settings options and standard settings:
Audible signals – ON, Backlight – 100%, Print to pdf – ON



Region

This submenu displays the following settings options and standard settings:
Language, date, time and country zone EU/US, decimal separator – "."/"," (dot or comma)



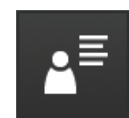
Quality

This submenu displays the following settings options and standard settings:
Quick zero – OFF, AQA1 and AQA2 lock – OFF, Zero Adjustment expiry – ON (interval: 7 days), Use expired reagents – OFF, Service reminder – ON



Automation (Setup 4)

This submenu displays the following settings options and standard settings:
Energy saving mode – ON (10 minutes), Auto Power off – OFF, Auto log off – OFF, Auto store – ON, Auto print – OFF, Sample ID popup – OFF



User management

This submenu displays the following settings options and standard settings:
Activation of user management and administrator settings, User login required – OFF





Service

This submenu displays the following settings options:
Various service functions such as backup, restore, export of log or system data and import of methods



Update

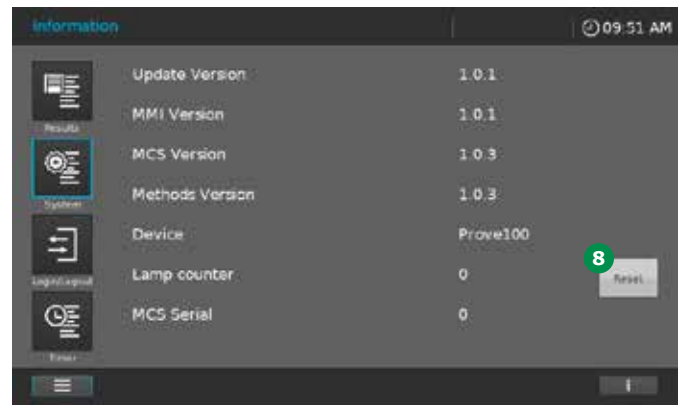
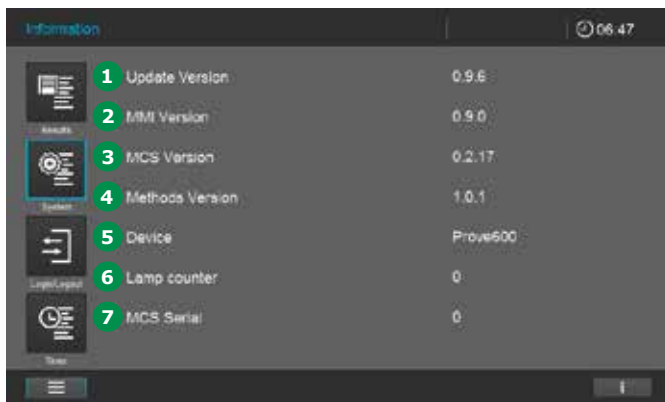
This submenu displays the option for performing software and method updates

Buttons	Description
	Network This submenu displays the setting options for connecting the Prove plus device with a network
	Prove Connect This submenu displays the settings options for connecting the Prove plus device with the Prove Connect software (the Prove Connect software is optionally available, order No. Prove Connect to LIMS Y110860001)



9.2.1 Information

This submenu displays the following information and settings options:



8 Reset button for lamp counter in Prove 100 plus

Press this button after the change of the halogen lamp to reset the lamp counter to zero.

1 Update Version

Instrument version number

2 MMI Version

Man-machine interfaces version number

3 MCS Version

Measurement and control software version number

4 Methods Version

Method version currently in use

5 Device

Class of device being used
(Prove 100 plus | 300 plus | 600 plus)

6 Lamp counter

Lifetime/service performance of the lamp

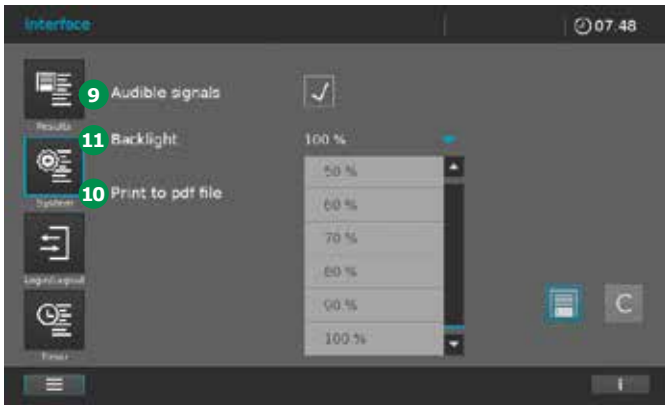
7 MCS Serial

Instrument serial number



9.2.2 Interface

This submenu displays the following information and settings options:



9 Audible signals

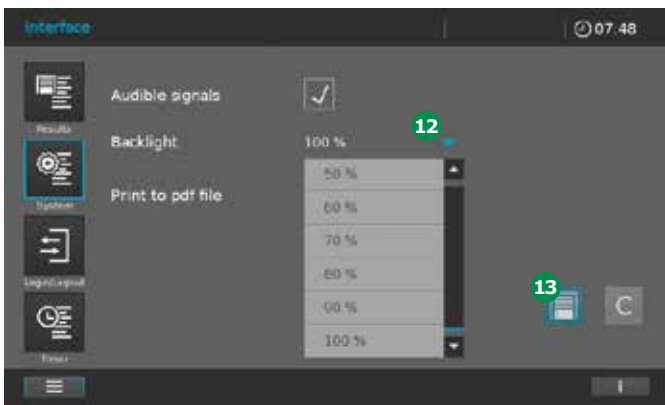
Ticking/unticking the box switches the audible alert on or off.

10 Print to pdf file

Activating the pdf printer transfers all print jobs to the external memory device (e.g. USB mass storage device) in pdf format.

11 Backlight

This setting enables you to adjust the backlight brightness to the ambient light conditions.

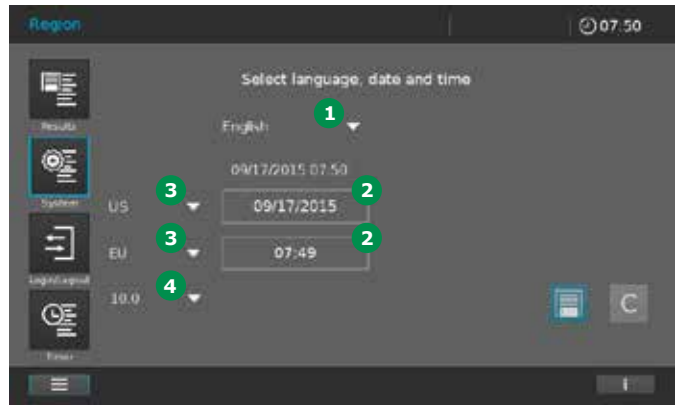


1. Select System.
2. Select Interface (Setup 1).
3. Set the backlight contrast 11 to the desired level using the drop-down menu 12.
4. Tap on the Save button 13 to store and close the settings.



9.2.3 Region

This submenu displays the following information and settings options.



1 Language

2 Date/time

3 Country zone EU/US

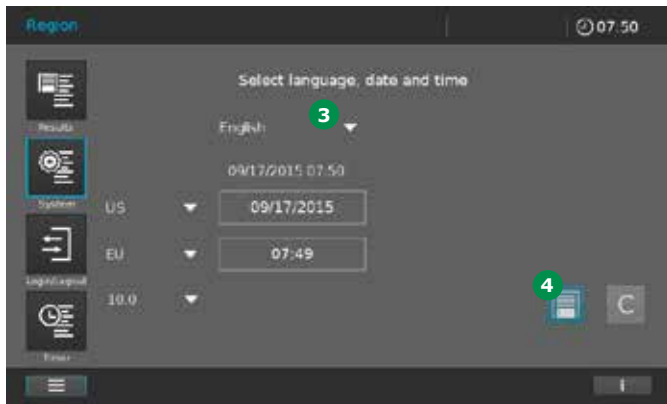
4 Decimal separator

Language

To change the user language, proceed as follows:



1. Select System 1.
2. Select Region (Setup 2) 2.



3. Select the desired language in the drop-down menu **3**.
4. Tap on the Save button **4** to store your changes and close the settings by touching the System button again.

Date/time

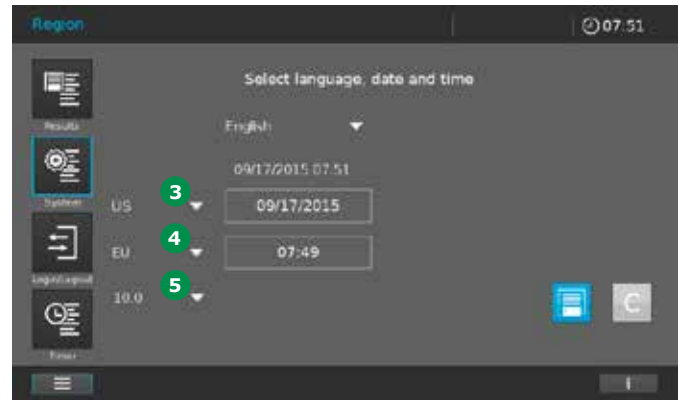
Depending on country, the date format is presented in the sequence e.g. Day.Month.Year (DD.MM.YY) or Month/Day/Year (MM/DD/YY or MM.DD.YY). To reset or change the figures, proceed as follows:



1. Select System **1**.
2. Select Region (Setup 2) **2**.

Country zone EU/US, decimal separator

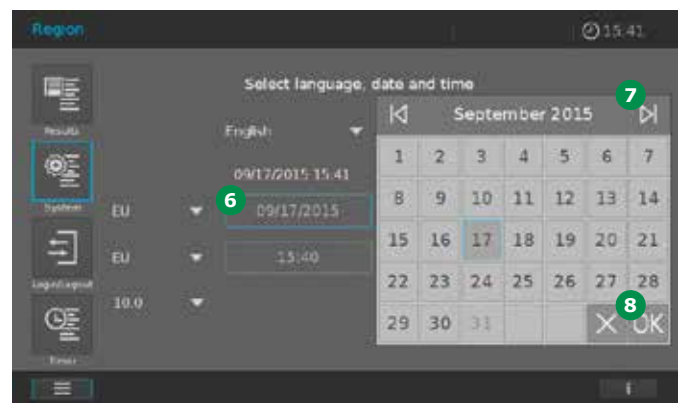
Opening the drop-down menu allows the country settings to be changed.



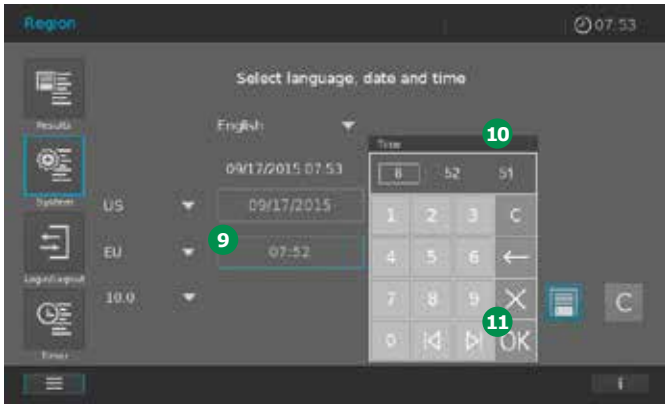
- Date display US/EU **3**
- Time display US/EU **4**
- Decimal separator "."/"," (dot or comma) **5**

NOTE

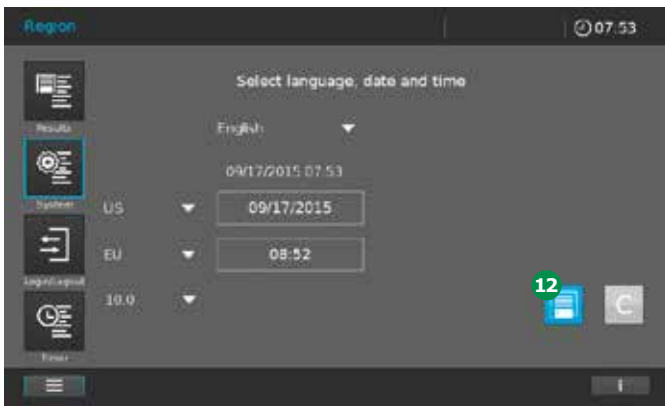
Make sure that the decimal separator used is the same which is used in your Excel software to avoid any problems with the format of your csv files.



3. Tapping on the Date field **6** pops up a calendar **7**. Here you can set the date and tap on OK **8** to confirm your selection.



4. Tapping on the Time field 9 pops up a selection field 10. Here you can set the time and tap on OK 11 to confirm your selection.

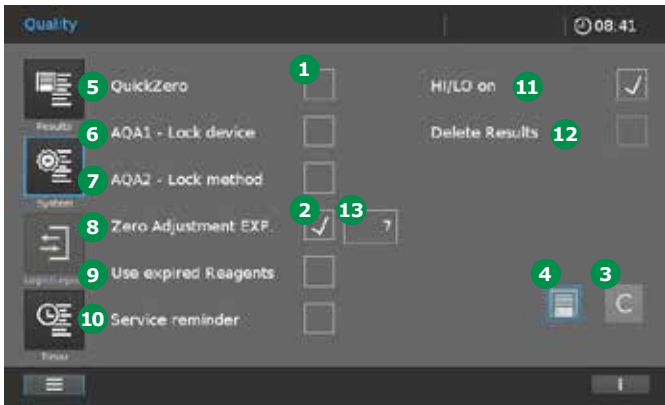


5. Tap on the Save button 12 to store all of the changed settings.



9.2.4 Quality

This submenu displays the following information and settings options:



To activate a function, tap on the input field **1**. A tick **2** appears when the setting option is activated. To cancel settings, tap on the C button **3**. This works only for changes that have been made but not yet stored. To accept the settings, tap on the Save button **4**.

Possible settings (items **5** to **12**):

Pos.	Name	Function – active	Function – inactive
5	QuickZero (Possible only for concentration methods)	Performance and direct saving of the zero adjustment for: <ul style="list-style-type: none"> all 12 wavelengths that are used for measuring Spectroquant® test kits the wavelength currently being used in the Concentration mode 	Performance and saving of the zero adjustment only for the currently selected concentration method.
6	AQA1 – Lock device	If an invalid AQA1 test is present, a warning message appears. The instrument is locked for all measurements except AQA1 tests.	If an invalid AQA1 test is present, a warning message appears. Measurements can still be performed. The instrument is not locked.
7	AQA2 – Lock method	If an invalid AQA2 test is present for a concentration method, a warning message appears when this method is selected. The performance of a concentration measurement using this method is locked.	If an invalid AQA2 test is present for a concentration method, a warning message appears when this method is selected. Measurements can still be performed. The instrument is not locked.
8	Zero adjustment EXP (Possible only for concentration methods)	When the pre-set expiry date in days 13 is reached, the zero adjustment must be repeated.	An already performed zero adjustment does not have to be repeated.
9	Use expired reagents	The use of Spectroquant® test kits beyond the date of expiry is allowed. A warning message appears when the barcoded Spectroquant® cell or the AutoSelector is inserted into the instrument; after the warning message is confirmed, however, the measurement is still carried out.	The use of Spectroquant® test kits beyond the date of expiry is not allowed. A warning message appears when the barcoded Spectroquant® cell or the AutoSelector is inserted into the instrument. No measurement can be made.
10	Service reminder	The instrument automatically signals the need to service the instrument.	The instrument does not signal the need to service the instrument.

1 9 Operation – 9.2 System Setup

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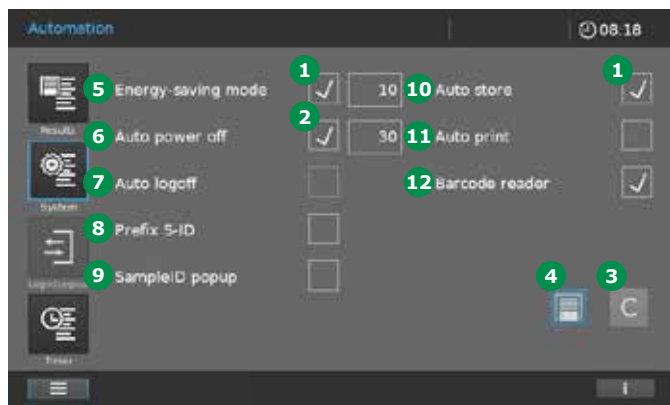
16

Pos.	Name	Function – active	Function – inactive
11	Deactivate message indicating results beyond measuring range	When results are higher than the measuring range of the selected method, the display of the device shows "HI". When results are lower than the measuring range of the selected method, the display of the device shows "LO".	Results beyond the measuring range of the selected method are also shown as a numerical value. Negative measurement results may also be shown here. (This function can be of help in calculating statistical parameters, e.g. in determining limits of detection.)
12	Allow deletion of results in the result list	When the user management is activated, results in the result list can be deleted. (This function can be activated only when the user management is activated by a user with administrator status.)	No results in the result list can be deleted.



9.2.5 Automation

This submenu displays the following information and settings options:



1 Energy-saving mode

To activate a function, tap on the input field 1. A tick 2 appears when the setting option is activated. To cancel settings, tap on the C button 3. This works only for changes that have been made but not yet stored. To accept the settings, tap on the Save button 4.

5 Energy-saving mode

After a user-defined time has elapsed, the backlight of the display switches off automatically. The backlight is switched on again with the next tap.

When the function is activated, a field pops up for setting the time. Here you can enter your individual time in minutes and confirm by tapping the OK button. Accept the time setting by tapping on the Save button.

6 Auto power off

After a user-defined time has elapsed, the instrument switches off automatically. When the function is activated, a field pops up for setting the time. Here you can enter your individual time in minutes and confirm by tapping the OK button. Accept the time setting by tapping on the Save button.

7 Auto logoff

The instrument logs the active user out after the user-defined time has elapsed and no entry has been made. The screen changes to the login/logout screen.

When the function is activated, a field pops up for setting the time. Here you can enter your individual time in minutes and confirm by tapping the OK button. Accept the time setting by tapping on the Save button.

8 Prefix S-ID

This function enables you to prefix a sample ID with a recurrent character string (e.g. Well), which is then saved together with the sample ID. When the function is activated, a field pops up to enter data. Here you can enter the individual string of characters or description, confirming your entry by tapping the OK button. Accept the entry by tapping on the Save button.

9 SampleID popup

After each measurement, an input window automatically pops up to enter the sampleID. The data can be entered via the virtual keyboard of the display, a keyboard connected via the USB port, or a hand-held scanner connected via the USB port.

2

3 **10 Auto store**

The instrument automatically saves the measurement results in the Concentration mode in the result list.

4

NOTE

The instrument is capable of storing 2,000 individual measurements of the measurement modes concentration, absorbance/transmission, and/or multiple wavelengths as well as 20 data sets with results of the spectrum or kinetics methods for each of these modes. It operates on the FIFO storage principle (first in – first out), meaning that when all storage locations are occupied, the next time a result is to be stored the oldest result on the list is automatically overwritten. Accordingly it is advisable to regularly back up stored data sets on external media (see section 9.13.7).

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The results of the measurement modi AQA1, AQA2, MatrixCheck, and PipeCheck are managed separately. A total of 500 results are stored. Results that determine a system or method status are not overwritten, even when all storage locations are already occupied.

10

11 Auto print

The instrument automatically starts a print operation after the measurement has been completed. Precondition: a USB memory device (print as pdf) or PostScript printer (print on paper) is connected.

11

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12 Barcode scanner

This function enables the barcode scanner for decoding round cells and AutoSelectors to be deactivated. When the barcode scanner is deactivated, the automatic method recognition of barcoded round cells and AutoSelectors is switched off and the method must be selected manually.

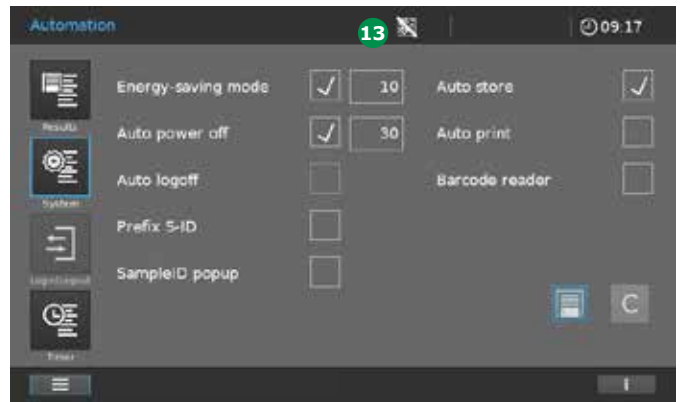
13

This function comes in handy when e.g. you wish to run your own methods in round cells.

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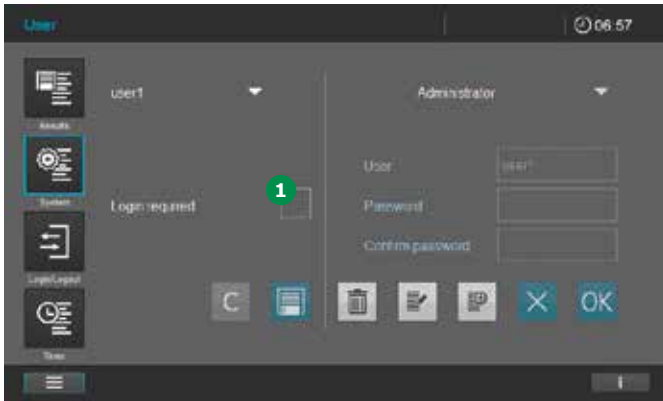


When the barcode scanner is deactivated, a corresponding symbol 13 is constantly shown in the upper status bar of the display.



9.2.6 User Management

This submenu offers the following setting options and is only accessible to administrators once "Login required" is active:

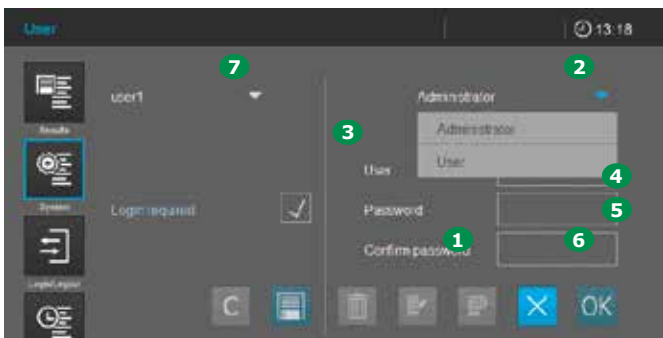


Activate user management:

When the "Login required" box **1** is ticked, users have to log in in the "Login/Logout" menu with their name and password to get certain access user rights (see section 9.14.1).

NOTE

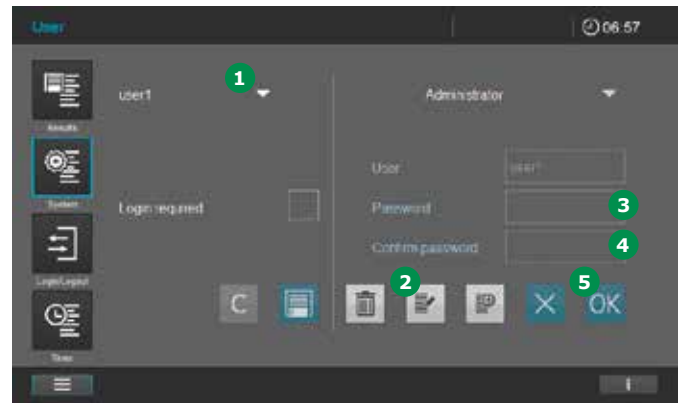
Once "Login required" is ticked, it can only be deactivated by an administrator.



Create user:

1. Tap on the Add new user field **1**.
2. Assign the user rights by tapping on the button **2**: full rights = administrator; restricted rights = user (see section 9.14).
3. Enter the user name **3**.

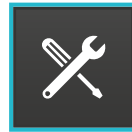
4. Enter the user password **4**.
5. Confirm the user password **5**.
6. Tap on OK to confirm **6**.
7. The newly created user appears in the pick-list **7**.



Edit user, e.g. change password:

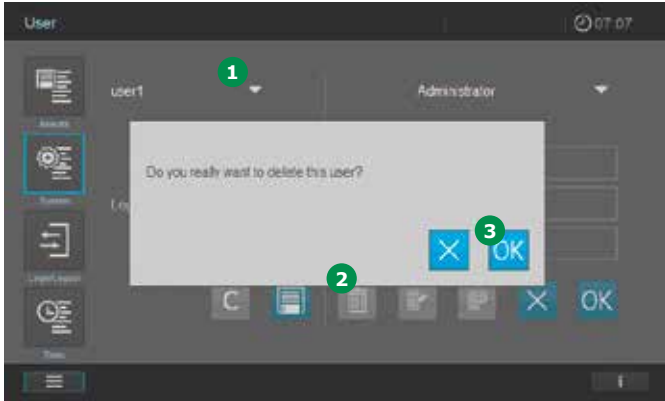
1. Select the user **1** whose password is to be changed.
2. Tap on edit **2** to edit the user.
3. Enter the new user password **3**.
4. Confirm the password **4**.
5. Tap on OK **5** to confirm.

9.2 System Setup



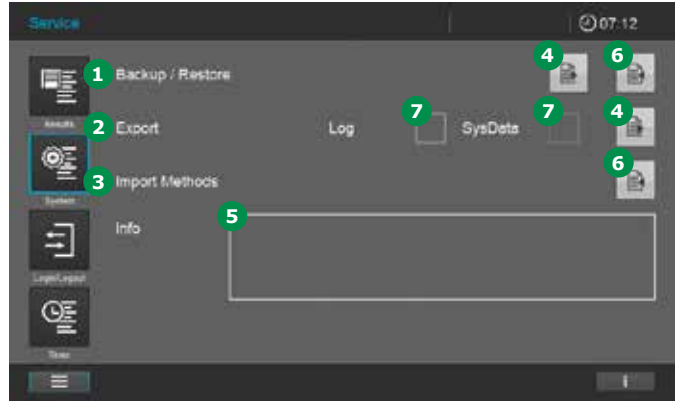
9.2.7 Service

This submenu offers the following setting options:



Delete user:

1. Select the user to be deleted **1**.
2. Tap on the Delete button **2**.
3. A window pops up asking "Do you really want to delete user?". Tap on OK **3** to confirm.
4. The user is deleted from the pick-list **1**.



To export or import data you need a commercially available USB mass storage device.

1 Backup/restore

Create a backup on the USB device.

1. Attach a blank (no data present) USB mass storage device to the spectrophotometer.
2. Tapping on the Export button **4** automatically stores the spectrophotometer data on the USB mass storage device.
3. A message appears in the info window **5** when the data have been successfully transferred.

Importing a backup from the memory device.

1. Attach the USB mass storage device containing the backed up data to the spectrophotometer.
2. Tapping on the Import button **6** automatically imports the spectrophotometer data to the instrument and stores them there.
3. A message appears in the info window **5** when the data have been successfully transferred.

2 Exporting log and/or system files

1. Tick the Log or SysData box **7**.
2. Attach a blank (no data present) USB mass storage device to the spectrophotometer. The memory capacity of USB mass storage device should be at least 512 MB.
3. Tapping on the Export button **4** automatically stores the spectrophotometer data on the USB mass storage device.
4. A message appears in the info window **5** when the data have been successfully transferred.

NOTE

When log files are exported, three separate log files are created and exported: an error log file, a user log file, and a service log file. The files are saved on the USB mass storage medium in the following folder structure:

Parent folder: PROVE

Subfolder: Log

Subfolder: Serial number of the device, underscore, "Date", underscore YYMMDD, underscore hhmm

Example: "PROVE\Log\SN1529610052_Date_201208_1001"

Folder/File	Created
apps	14.12.2020 07:56
data	14.12.2020 07:56
pc	14.12.2020 07:56
Error_1529610052_201208_1001	08.12.2020 10:01
Service_1529610052_201208_1001	08.12.2020 10:01
User_1529610052_201208_1001	08.12.2020 10:01

The error and service log files contain information that can be of use in dealing with service issues. The user log file contains information on activities carried out by the user, e.g. changes in the system settings. For further details on the contents of the log files and their interpretation please refer to [section 16](#).

3 Importing user-defined methods

1. Attach the USB mass storage device containing the method list with the user-defined methods to the spectrophotometer.
2. Tapping on the Import button **6** automatically imports the spectrophotometer data to the instrument and stores them there.
3. A message appears in the info window **5** when the data have been successfully transferred.

NOTE

Only users from the Administrator group have the right to perform the setting options in the Service submenu.



9.2.8 Updates

Firmware and method updates ensure your spectrophotometer is always up-to-date.

NOTE

Only users from the Administrator user group may perform firmware and method updates.

The update comprises:

- The latest firmware
- New or modified method data

NOTE

A firmware and method update does not alter user-defined data (such as settings, custom methods or measurement data).

The update is transferred to the spectrophotometer by using a USB mass storage device for temporary storage.

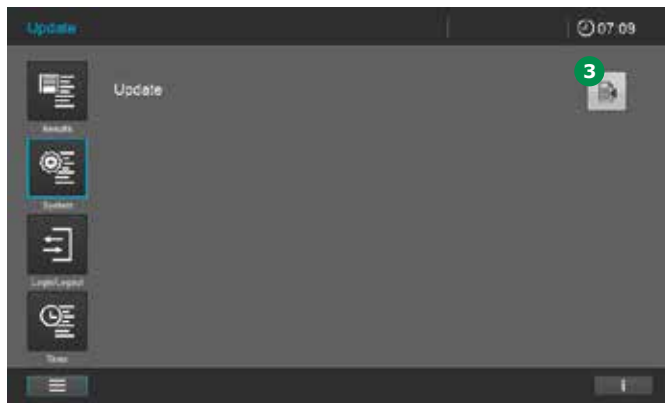
NOTE

To keep the instrument always up-to-date, we recommend always installing the latest update. The relevant updates are available on www.sigmaaldrich.com/photometer-service.

Firmware and method update spectrophotometer



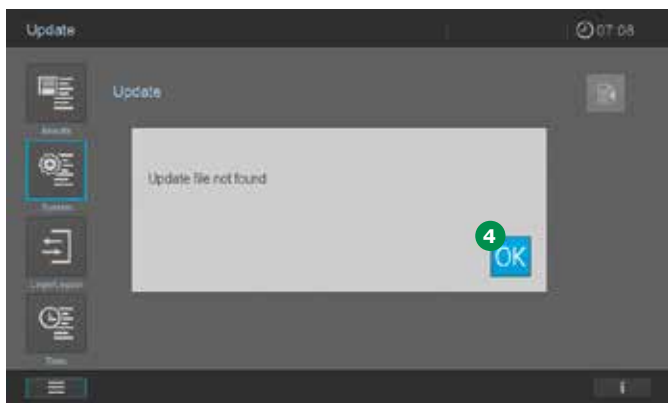
1. Download the update file from the website onto a **USB memory device**.
2. Unzip the file with the entire folder structure into the main directory of the **USB memory device**. After unzipping, a folder titled "PROVE" with a subfolder titled "Update" appears in the main directory of the USB memory device.
3. Select System **1**.
4. Tap on the Update button **2**.
5. Attach the **USB memory device** with the update to the spectrophotometer.



6. Tap on the Import field **3** starts the search for update files on USB device. Search needs some time (approx. 1 minute).
7. You will be asked whether you want to install the update version on the Prove plus. Confirm with OK.
8. The installation process is reported in the information window and confirmed by the final message that the data have been successfully transferred.
9. Confirm with OK.



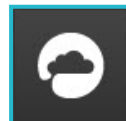
10. The instrument then shuts down and re-boots. The boot screen appears in the display. Depending on the data volume, this procedure may take several minutes.



11. If the import was unsuccessful, a corresponding message ④ appears. Try again. Before this, check whether the folder structure described above in item 2 is present on the USB memory device.



9.2.9 Network and Prove Connect



Connect the Prove plus spectrophotometer with a network and the Prove Connect software (optionally available, order No. Prove Connect to LIMS Y110860001)

The broad range of settings options are described in a separate manual.

9.3 Measurements

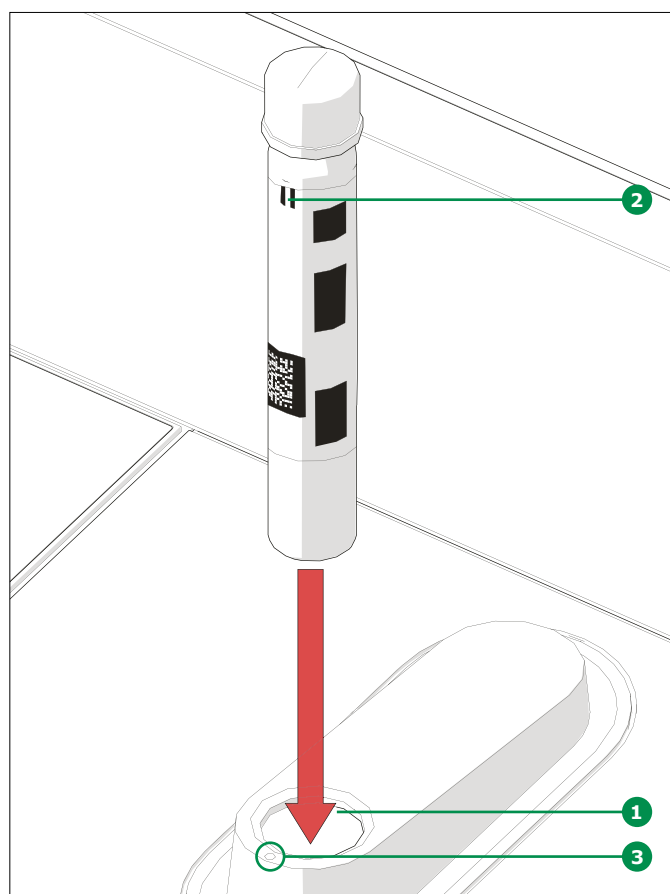
The spectrophotometer can be used to perform the measurements listed below.

Type of Measurement	Description
Concentration	<ul style="list-style-type: none"> Pre-programmed methods that can be executed using Spectroquant® test kits or self-prepared reagents User-programmed methods
Absorbance/transmission	<ul style="list-style-type: none"> Single-wavelength measurements for establishing the absorbance or transmission of solutions Multiple-wavelength measurements for establishing the absorbance or transmission of solutions
Spectrum	<ul style="list-style-type: none"> Programmed methods for establishing the absorbance or transmission of solutions over a defined wavelength range
Kinetics	<ul style="list-style-type: none"> Programmed methods for establishing the absorbance or transmission of solutions over a defined period
Quality checks	Instrument-supported analytical quality assurance: <ul style="list-style-type: none"> Instrument check (AQA1) Method-specific system check – pre-programmed for all Spectroquant® standards (AQA2) Pipette volume control (PipeCheck) Check interferences from foreign substances (MatrixCheck)

9.3.1 Performing a Measurement

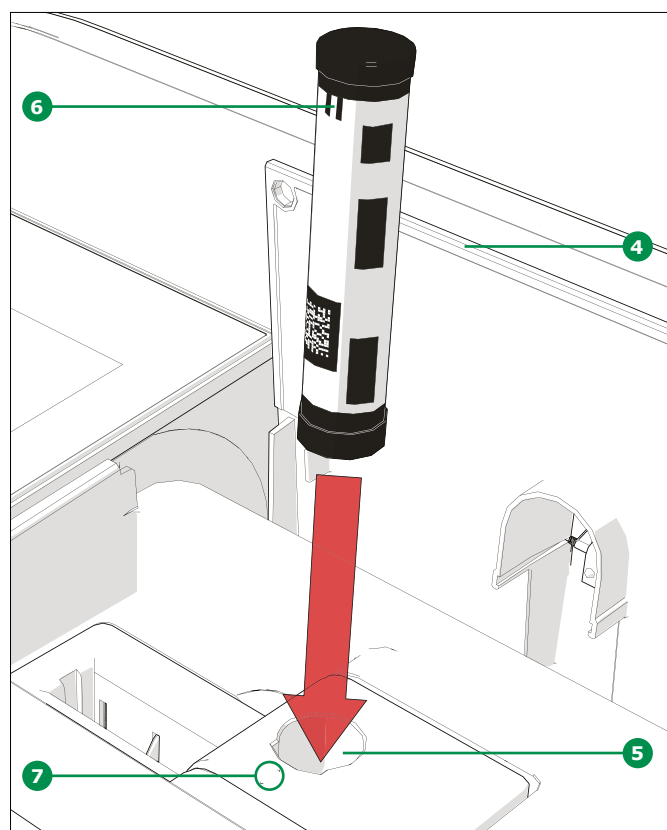
Measurements can be performed using rectangular cells of various path lengths (10, 20, 50 mm/100 mm Prove 600 plus) and Spectroquant® round cells. Insert cells as follows to start the measurement:

Measuring with a round cell with closed lid



- Insert the barcoded Spectroquant® round cell through the opening **1**, ensuring that the white position mark **2** on the cell is aligned with the positioning mark on the spectrophotometer **3**
- Measurement starts automatically, and the measurement result is displayed in the concentration measurement overview (see page 33)

Measuring with rectangular cells with open lid: insert AutoSelector



- Open the flip-up cover **4** by pushing it back with your fingers
- Insert the AutoSelector vertically into the cell compartment **5**, ensuring that the white position mark **6** on the AutoSelector is aligned with the positioning mark on the spectrophotometer **7**
- The photometer is ready to measure

NOTE

If the barcode cannot be read, please see section 9.7.1.

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Measuring with rectangular cells with open lid:
 Insert rectangular cells (10, 20, 50 mm)

4

Measuring with rectangular cells with open lid:
 Insert 100 mm rectangular cells (Prove 600 plus)

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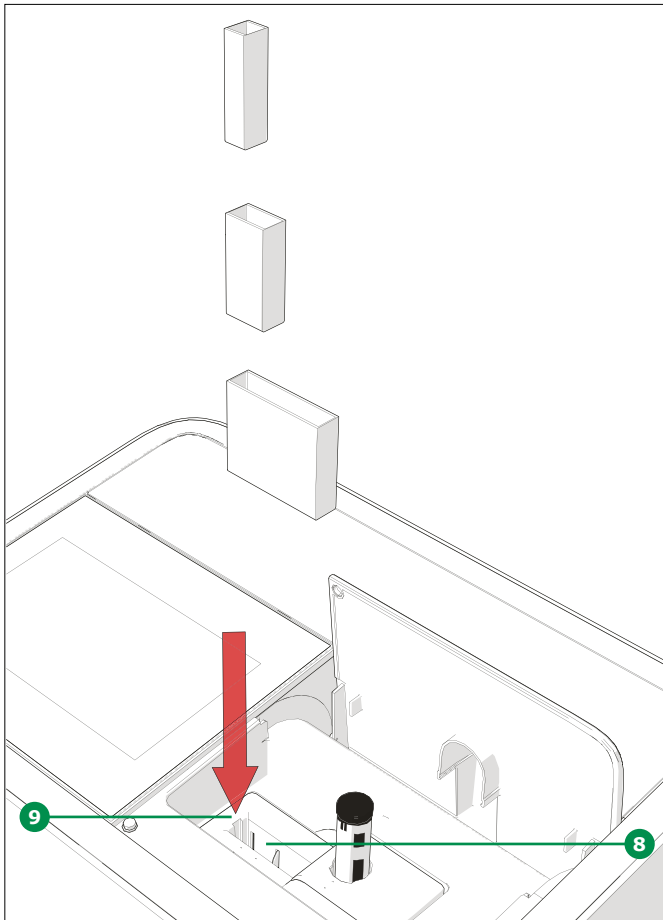
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- Insert the rectangular cell vertically into the cell compartment **8**, ensuring that the cell is flush against the left side of the cell holder **9** at all times
- Measurement starts automatically, and the measurement result is displayed in the concentration measurement overview (see page 33)

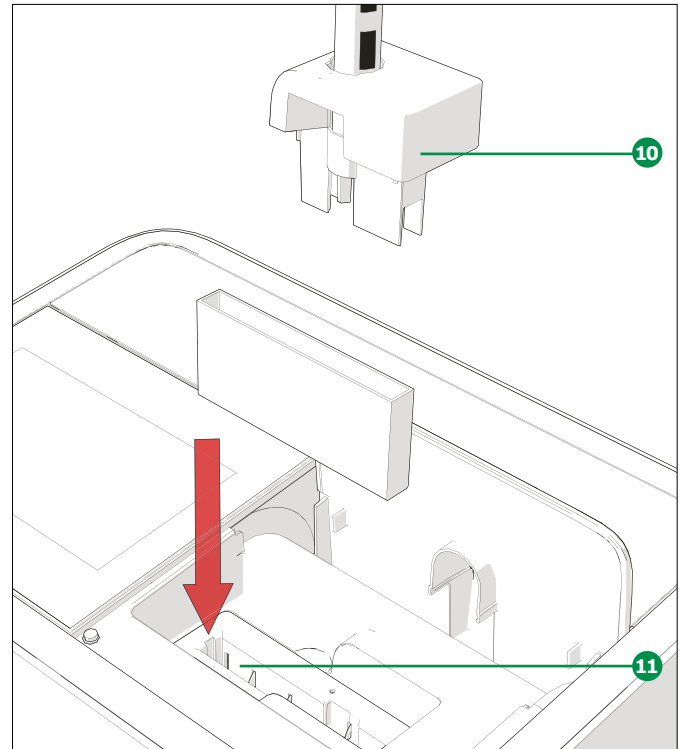
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- Remove the top of the round cell compartment including the AutoSelector **10**
- Insert the 100 mm rectangular cell vertically into the cell holder **11**. Make sure that you hold it with both hands on the small edges while inserting it carefully
- Measurement starts automatically, and the measurement result is displayed in the concentration measurement overview (see page 33)

NOTE

Please see Analytical Procedures and Appendices for detailed measurement procedures.

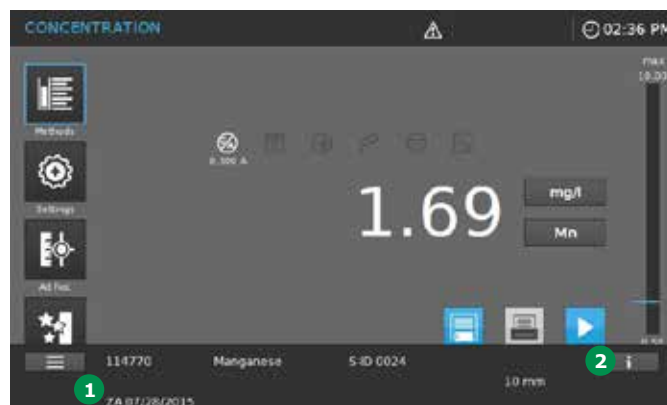
Minimum filling volumes for the cells used

Cell			Filling volume (minimum)
10 mm	Rectangular	Standard	2 ml
10 mm	Rectangular	Semimicro	1 ml
20 mm	Rectangular	Standard	4 ml
20 mm	Rectangular	Semimicro	2 ml
50 mm	Rectangular	Standard	8 ml
50 mm	Rectangular	Semimicro	4 ml
100 mm	Rectangular	Standard	16 ml
round			4 ml

9.4 Zero Adjustment

A valid zero adjustment is required for calculation of measurement values in Concentration, Absorbance/% Transmission, Special/Multi-wavelength and Kinetic modes. During zero adjustment, the absorbance of a cell filled with distilled water ("zero cell") is measured and stored.

A zero adjustment must be performed for each cell type. The zero adjustment for concentration methods is stored within the spectrophotometer separately for each cell type. The period of validity of the zero adjustment for concentration methods can be edited in the System settings (see section 9.2.4). When a zero adjustment has already been performed for the inserted cell type and the selected method, the date of the most recent zero adjustment ① is displayed in the info line ②.



9.4.1 Notes on Zero Adjustment

Zero adjustment with round cells

- Only use clean, scratch-free round cells and distilled water.
The minimum filling level is 20 mm. A ready zero cell is contained within the scope of delivery of the spectrophotometer
- A ready zero cell can, in principle, be used for an indefinite period of time. We recommend, however, that you regularly check the zero cell for visible contamination and scratches and refill or exchange it if necessary (at least every 24 months)
- Insert the round cell until it touches the bottom of the round cell compartment

Zero adjustment with rectangular cells

- With rectangular cells, zero adjustment must be carried out using the same cell type (manufacturer and cell material [e.g. optical glass, quartz glass, plastic]) as the one that will be used for measurement. This is important because cells of different manufacturers have different absorption characteristics. When changing the cell type, repeat the zero adjustment with the new type
- Prior to zero adjustment, clean the rectangular cell and fill it with distilled water. The minimum filling level is 20 mm
- Rectangular cells always have to be inserted in the cell compartment with the same orientation for measurement and zero adjustment (e.g. cell inscription always on the left side)
- Insert the rectangular cell until it touches the bottom and left edge of the holder. The opaque sides of the rectangular cell must point to the front and rear. The spectrophotometer detects stray light. If there is too much stray light, a message prompts you to close the cell compartment cover

NOTE

Ordering information for cells is provided in [section 13](#). The cells listed in [section 13](#) are specially intended for use with the Spectroquant® test kit system. Note that the spectral transparency of the cell must be suitable for the intended application (example, quartz cell for UV range).

9.4.2 When to Repeat the Zero Adjustment?

We recommend that you repeat the zero adjustment in the following cases:

- If the spectrophotometer was subject to mechanical stress such as strong shock or transport
- If the ambient temperature has changed by more than 5°C since the last zero adjustment
- At least once a week. The interval to repeat a zero adjustment is set in the instrument to 7 days. You can change this under "System (Instrument Settings)"
- If a new cell type (different manufacturer, different glass type) is used
- Basically, each time you want to measure with the highest possible accuracy

NOTE

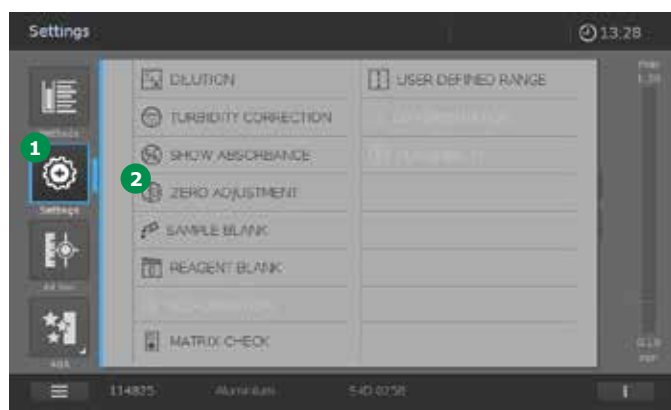
If an interval to repeat a zero adjustment is set you will be prompted to repeat it after the interval has passed. You can also repeat a zero adjustment by selecting a method, then touching the "Settings" icon. Choose "Zero adjustment" and insert a zero cell to start the measurement.

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9.4.3 Zero Adjustment for Concentration Measurement Methods

A concentration method must be selected to start the zero adjustment. There are two ways to select the concentration method:

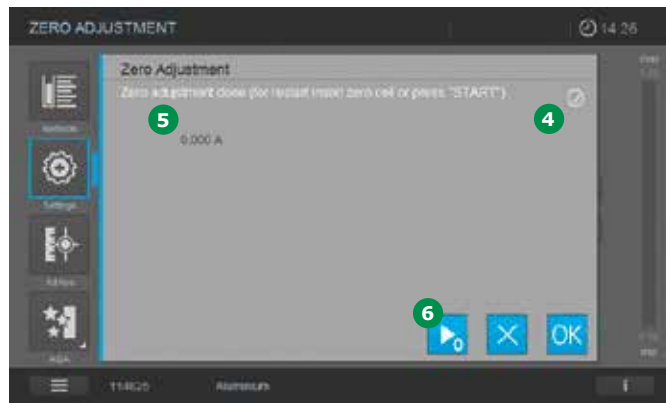
- By inserting a barcoded cell or the barcoded AutoSelector
- By manually selecting the concentration method via the method list (see section 9.5)



1. Once the concentration method is selected touch Settings 1.
2. Tap on the Zero adjustment button 2.



3. The Zero Adjustment screen opens. The status display field for the Zero adjustment is blank 3.



4. Insert the zero cell according to cell type. Zero adjustment starts automatically and, if the zero adjustment is passed, a tick 4 appears in the status display field for the Zero adjustment 3.
5. In the case of a method which only measures the sample at a single wavelength the absorbance of the Zero value 5 is also displayed.
6. With a cell inserted, the zero adjustment can be repeated manually by tapping on the Start zero button 6.
7. Tapping on the OK button accepts the zero adjustment value for the method.
8. The screen changes to show the concentration measurement screen.
9. The instrument is ready to start measuring the sample.

9.4.4 Zero Adjustment for Absorbance/Transmission Measurements (Ad hoc menu)

Zero adjustment must always be done before starting a measurement series and is automatically prompted by the instrument (see section 9.8.1).

NOTE

Cells must be absolutely clean and scratch-free. For zero adjustment, always use a cell of the same type to measure the sample.

9.4.5 Zero Adjustment for Spectrum Measurements

Zero adjustment must always be done before starting a measurement series and is automatically prompted by the instrument (see sections 9.8.2 and 9.9.2).

NOTE

Cells must be absolutely clean and scratch-free. For zero adjustment, always use a cell of the same type to measure the sample.

9.4.6 Zero Adjustment for Kinetic Measurements

Zero adjustment must always be done before starting a measurement series and is automatically prompted by the instrument (see sections 9.8.3 and 9.10.2).

NOTE

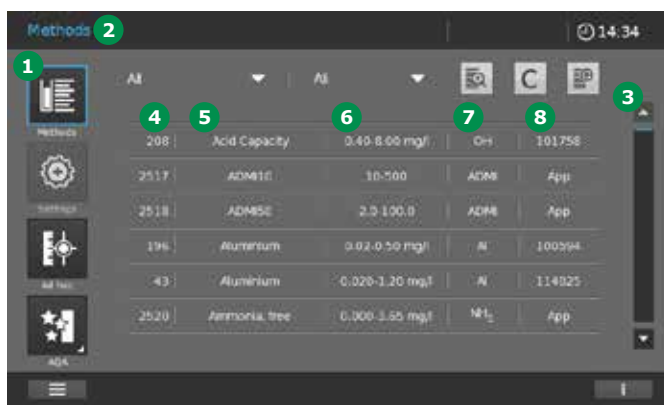
Cells must be absolutely clean and scratch-free. For zero adjustment, always use a cell of the same type to measure the sample.



9.5 Method List

9.5.1 Selecting a Method Manually

Select a method from the method list.



1. In the main menu tap on the Method button **1**.
2. The screen **2** changes and the list of all methods is displayed. The methods are listed alphabetically. The arrow bar **3** on the right edge indicates that the list contains more methods further up or down.
3. Select the required method.
4. The screen changes to show the method.
5. The instrument is ready to start measuring.

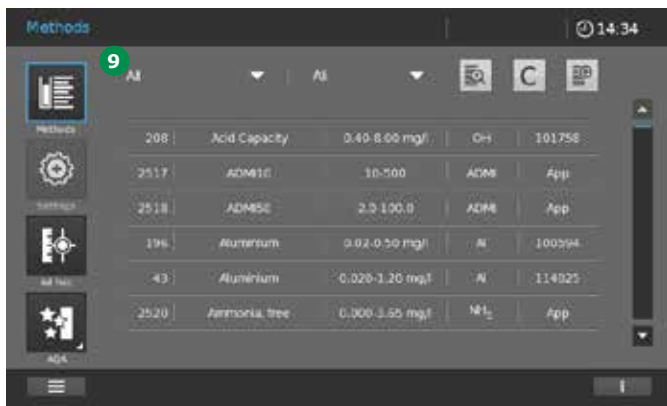
NOTE

The method designation contains the following information

- 4** Method number
- 5** Method name
- 6** Measuring range + unit (if the method is suited for several cell formats, the measuring range over all cell formats is displayed)
- 7** Citation (convertible)
- 8** Cat. No. (6 digits) or reference to application ("App" for test-kit-free methods)

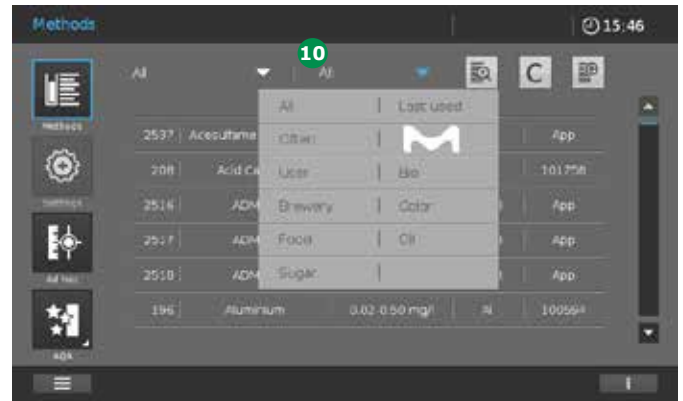
9.5.2 Searching and Filtering the Method List

You can search and filter the method list in order to make it easier to find the method you are looking for:



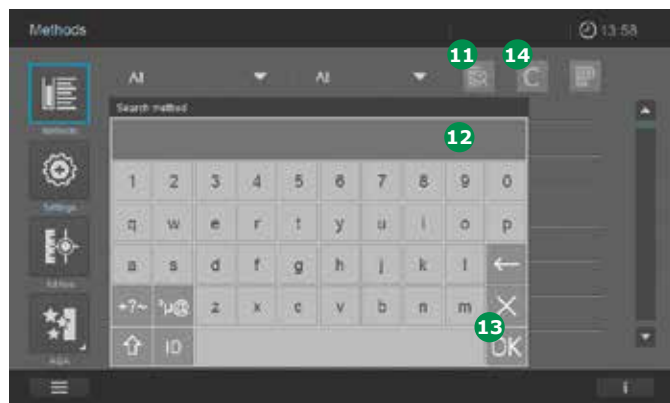
1. Filter by method type 9:

- All
- Concentration
- Kinetic
- Spectrum



2. Set filter by criteria 10:

- All methods
- Last used methods: last six used in alphabetic order
- Frequently used methods: six most frequently used in alphabetic order
- Factory pre-programmed methods only
- User-specific methods only
- Area of application (e.g. brewery, color, oils, sugar)



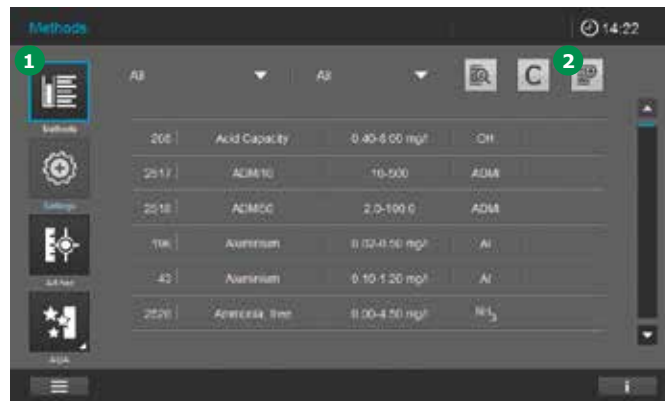
3. Search by character string 11. Proceed as follows:

1. Tap on the button 11.
2. The key pad 12 pops up.
3. Enter search criteria: method name, method number, item number (first six digits without any decimal point). If you type in fewer than three characters, the search runs only at the start of all search criteria (e. g. "ch" yields hits such as "Chlorine", "Chloride" etc.). Typing in three or more characters starts a search over the entire character string of the search criteria (e.g. "nitr" yields hits such as "Nitrate", "Nitrite", "Free amino nitrogen" etc.).
4. Tap on OK 13 to activate the search filter.
5. The method list shows all methods matching the search criteria.

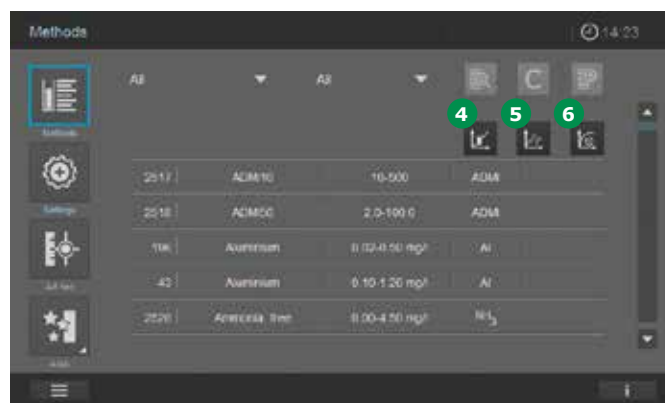
NOTE

Searching with subscripted characters is also possible. To search for a method with subscripted characters you need to place an underscore in front of the character to be subscripted. Tap on the C button 14 to deactivate the search filter.

9.6 Programming a User-defined Method



1. Select Methods 1 in the main menu.
2. Tap on Add New Method 2 in the method list.



3. The input window opens.
4. Select the type of method.
 - Concentration method 4
 - Spectrum method 5
 - Kinetic method 6
5. The screen changes.
6. To continue with the programming turn to the corresponding Sections 9.6.1 to 9.6.7.

9.6.1 User-defined Concentration Methods

Overview

For Concentration Mode you can develop and store your own user-defined methods under method numbers 1001 to 1100.

The spectrophotometer software supports you in creating the methods. Two different method types can be programmed.

- Single-wavelength methods
- Multi-wavelength methods (max. 5 wavelengths)

9.6.2 Calibration Data and Calibration Function for Single-wavelength Methods

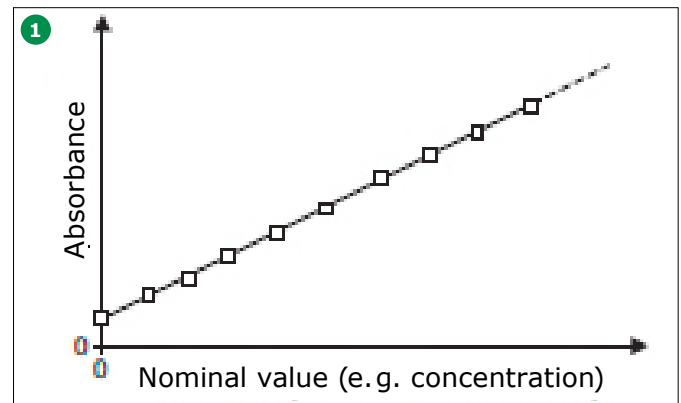
In photometry, the calibration function describes the dependency between the measured parameter (e.g. concentration) and the photometric measurement result (e.g. absorbance) of a sample.

The knowledge of this dependency is a prerequisite for the development of a photometric method. The calibration function is usually determined by means of a series of measurements with standard solutions of known concentrations (nominal value), e.g. as a 10-point calibration.

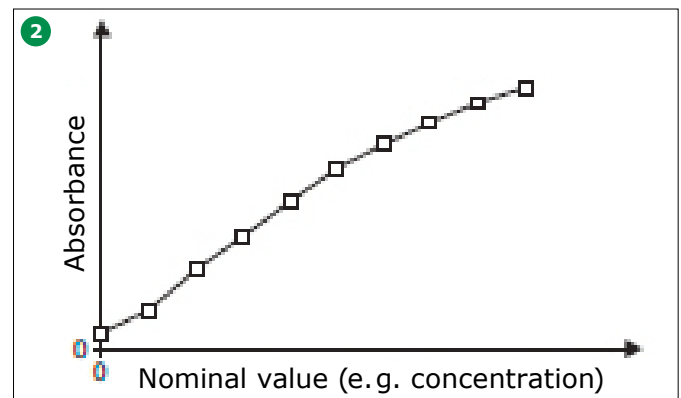
Line types

The dependency between the nominal value and absorbance is often linear in a wide range as shown in ① or non-linear as in ②.

- Example of a linear calibration function after a 10-point calibration ①. In the case of a linear dependency, the calibration function is determined by means of linear regression. The slope and axis intercept (E0) are the characteristics of the calibration line:



- Example of a non-linear calibration function after 10-point calibration ②. In the case of a non-linear dependency, the calibration function is calculated by a polynomial function:



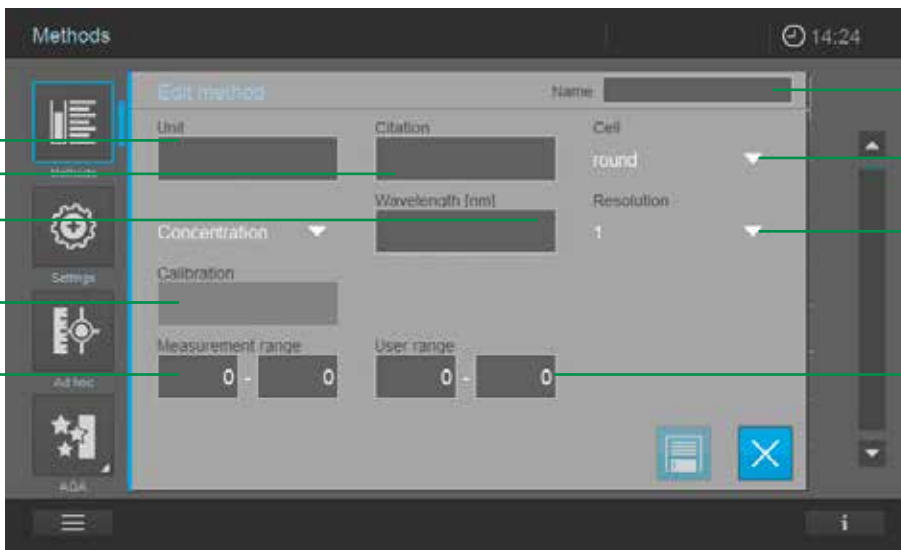
NOTE

In measuring operation, the reverse calibration function is used to output a measured absorbance as a concentration value.

3 9.6.3 Programming/Modifying User-defined Methods (Single Wavelength)

To program a user-defined single-wavelength method, proceed as follows:

1. Select the method type "Concentration" (see section 9.6).
2. The screen changes.



Item	Input field	Possible input
1	Name	Any name
2	Wavelength	Freely selectable (in nm)
3	Cell	16 (round), 10, 20, 50 or 100 mm
4	Citation form*	e.g. PO4-P
5	Unit*	e.g. mg/l
6	Resolution	0.001, 0.01, 0.1, 0.25, 0.5 or 1
7	Lower and upper limit of the measuring range	Any value between zero and the highest concentration of the standard solutions used
8	User-defined range*	Any value between zero and the highest concentration of the standard solutions used
9	Calibration function	(See examples on the following pages)

* Optional

3. Fill out input field items 1 – 8.

NOTE

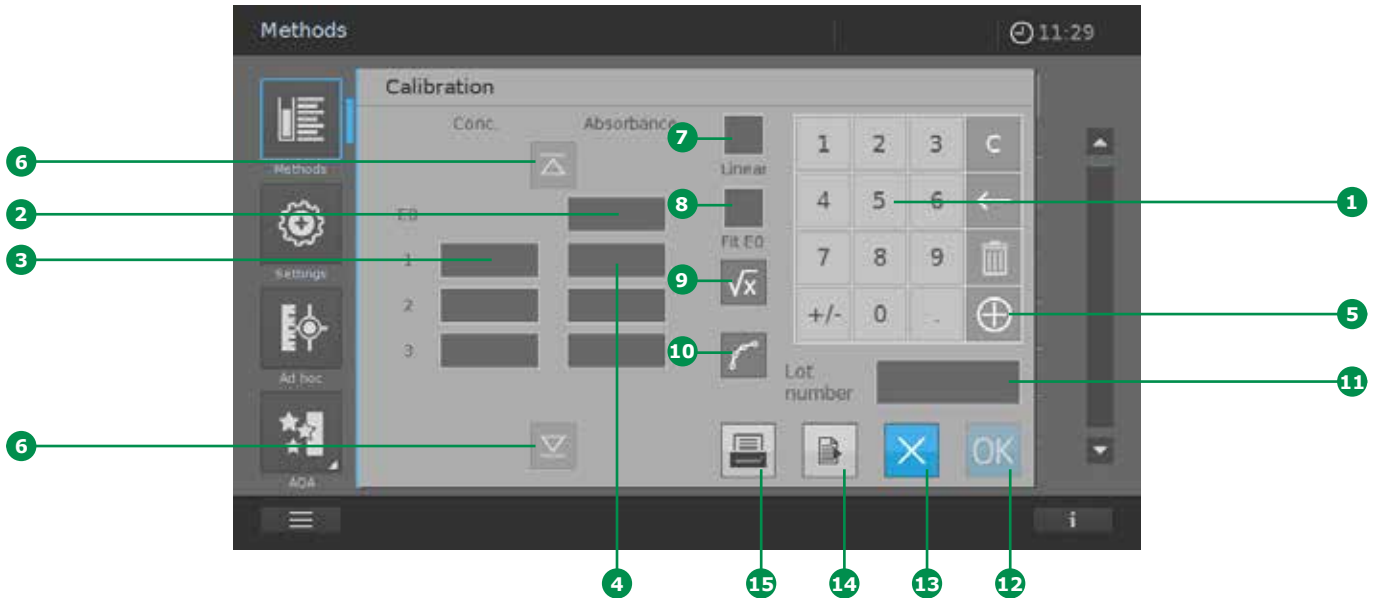
It is also possible to display characters in subscript and superscript. To put a character in subscript, an underscore "_" must be placed in front of the character in question (e.g. entry for H₂O = H_2O). To put a character in superscript, a circumflex "^" must be placed in front of the character in question (e.g. entry for m² = m^2).

4. Tapping on the calibration field 9 changes the screen.



5. You now have the following options for plotting a calibration curve:
- Entry or measurement of value pairs 10
 - Enter a function directly into the fields E0, A0 – A5 11

2
3 Enter value pairs



8 Enter the value pairs, nominal value (concentration)/measured absorbance einer of an already available test series with the following value pairs:

- E0 2 = reagent blank (see section 9.7.8)
- At least one, max. eleven value pairs in various concentrations

1. Enter E0 2, concentration of the standard solution 3 and associated absorbance 4 using the keypad 1. Tapping on the + button 5 allows further (up to eleven) value pairs to be entered. The UP&DOWN buttons 6 are activated if more than four value pairs are entered.
2. Activate the field "Linear" 7 to calculate a linear function. When "Linear" is not activated, a non-linear function of the second order is automatically calculated (square function).

10
11
12
13 NOTE

If you wish to calculate a linear function, you require at least the E0 value and 2 value pairs. If you wish to calculate a non-linear function, you require at least the E0 value and 3 value pairs.

3. "Fit E0" 5 can be activated as an additional option. With "Fit E0" activated, concentration 0 (= reagent blank value) intercepts the absorbance axis at the associated E0 value.
4. Once all values are available, tapping on the field "Function" 9 calls up an overview of the calculated coefficients. Tapping on the field "Graph" 10 shows the calibration curve.

14 NOTE

The calculated function maps the calculation of a result (e.g. concentration) via a measured absorbance in the form of a polynomial equation of the following type:

$$C = A0 + A1 \times (Abs - E0) + A2 \times (Abs - E0)^2$$

where:

- C = measurement result (e.g. concentration)
- A0, A1, A2 = coefficients (polynomial)
- Abs = measured absorbance
- E0 = absorbance of the reagent blank value

5. You can now enter an ID or a specific batch code for the calibration. Tapping on the field "Batch ID" 11 opens a virtual keyboard. Enter the code and confirm by tapping on the OK button.

6. To close the determination of the coefficients, confirm the data by tapping on the OK button **12**.
7. Tap on the Export button **14** to transfer the data in the CSV format to an external storage medium.
8. Tap on the Print button **15** to print out the data.
9. To close the operation without accepting the data, tap on the X button **13**. All entered data are deleted.



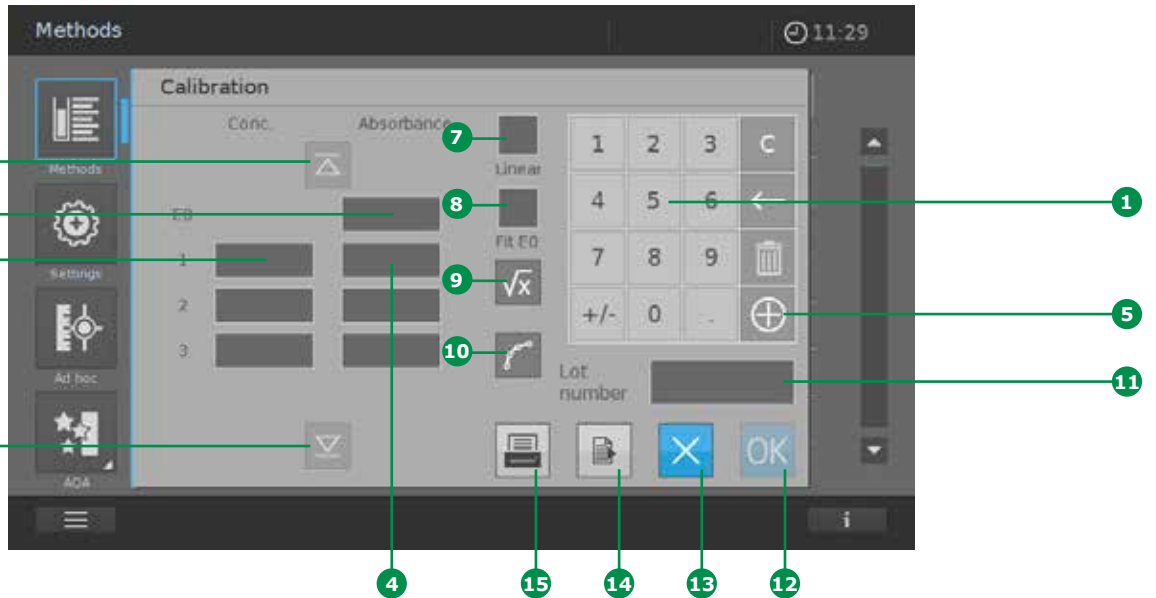
You now have the following options:

- Close the programming/processing of the method by tapping on the Save button **17**. All entered data are accepted. A method number appears **18**. Close the screen by tapping on the X button **19**. The screen changes to the method list.
- To call up coefficients, value pairs, or the graph again, tap on the field "Calibration" **16**.
- Cancel the programming/processing of the method by tapping on the X button **19**. All entered data are deleted. The screen changes to the method list.



10. Tapping on the OK button **12** confirms the entered data, and the screen changes to the method screen. A check appears in the field "Calibration" **16**.

Measure value pairs (see section 9.7.10)



1. Activate the Absorbance button E0 **2** (a blue frame appears).
2. Insert the cell with E0 (reagent blank value).

NOTE

If no zero adjustment has been made for the set measurement conditions (wavelength and optical path length), a zero adjustment is automatically prompted. Please follow the instructions that appear.



3. The screen changes. Measurement starts automatically. The measured absorbance is shown **16**. You have the option to perform multiple or repeated measurements. These can be performed by reinserting the cell or, if the cell has already been inserted, by tapping on the Start button **17**. The median value **18**, and also the number **19** of measurements that have already been performed are shown. Tapping on the arrow button **20** shows the individual results of the measurements that have been made. Tap on the OK button **21** to confirm the median value. Tapping on the X button **22** closes the operation. The screen changes.

4. Use the numerical keypad **1** to enter the next concentration **3** and activate the corresponding absorbance field **4** (a blue frame appears).
5. Insert the cell with the measurement solution of the corresponding concentration. Follow the procedure described above in step 3.
6. Perform steps 4 and 5 for all values that are required.
7. Activate the field "Linear" **7** to calculate a linear function. When "Linear" is not activated, a non-linear function of the second order is automatically calculated (square function).

NOTE

If you wish to calculate a linear function, you require at least the E0 value and 2 value pairs. If you wish to calculate a non-linear function, you require at least the E0 value and 3 value pairs.

8. „Fit E0" **8** can also be selected as a further option. With "Fit E0" activated, concentration 0 (= reagent blank value) intercepts the absorbance axis at the associated E0 value.
9. Once all values are available, tapping on the field "Function" **9** calls up an overview of the calculated coefficients. Tapping on the field "Graph" **10** shows the calibration curve.

NOTE

The calculated function maps the calculation of a result (e.g. concentration) via a measured absorbance in the form of a polynomial equation of the following type:

$$C = A0 + A1 \times (Abs - E0) + A2 \times (Abs - E0)^2$$

where:

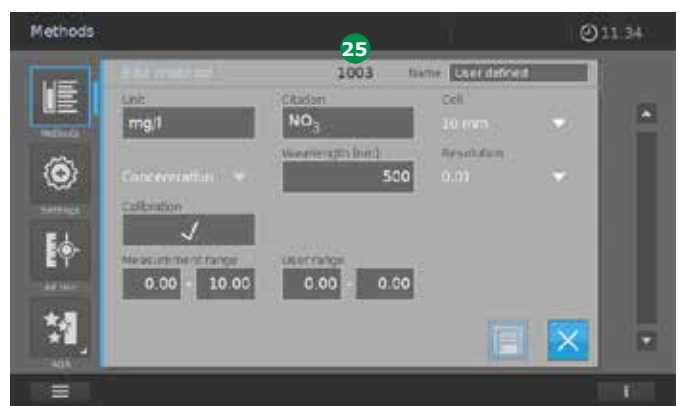
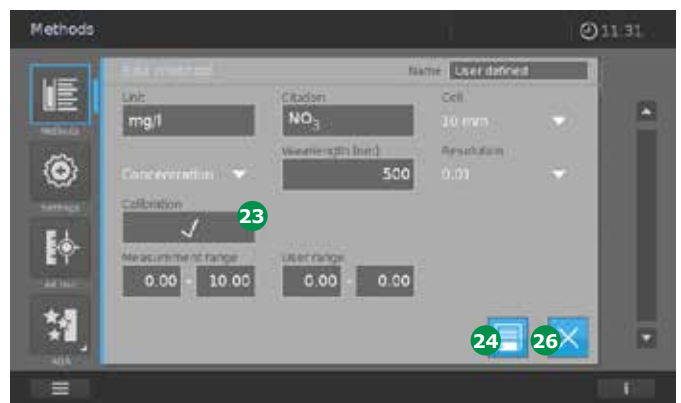
C = measurement result (e.g. concentration)

A0, A1, A2 = coefficients (polynomial)

Abs = measured absorbance

E0 = absorbance of the reagent blank value

10. You can now enter an ID or a specific batch code for the calibration. Tapping on the field "Batch ID" **11** opens a virtual keyboard. Enter the code and confirm by tapping on the OK button.
11. To close the determination of the coefficients, confirm the data by tapping on the OK button **12**.
12. Tap on the Export button **14** to transfer the data in the CSV format to an external storage medium.
13. Tap on the Print button **15** to print out the data.
14. To close the operation without accepting the data, tap on the X button **13**. All entered data are deleted.



Tapping on the OK button **12** confirms the entered data, and the screen changes to the method screen. A check appears in the field "Calibration" **23**.

You now have the following options:

- Close the programming/processing of the method by tapping on the Save button 24. All entered data are accepted. A method number appears 25.

Close the screen by tapping on the X button 26. The screen changes to the method list.

- To call up coefficients, value pairs, or the graph again, tap on the field "Calibration" 23.
- Cancel the programming/processing of the method by tapping on the X button 26. All entered data are deleted. The screen changes to the method list.

Enter a function:

This option can be used when an evaluation function is already available or has already been calculated previously by a calculation programme on the basis of available data.

Enter a function to calculate the concentration from the absorbance (reverse calibration function). You can enter on the spectrophotometer the coefficients of a polynomial equation of the following type:

$$C = A0 + A1 \times (Abs - E0) + A2 \times (Abs - E0)^2 + A3 \times (Abs - E0)^3 + A4 \times (Abs - E0)^4 + A5 \times (Abs - E0)^5$$

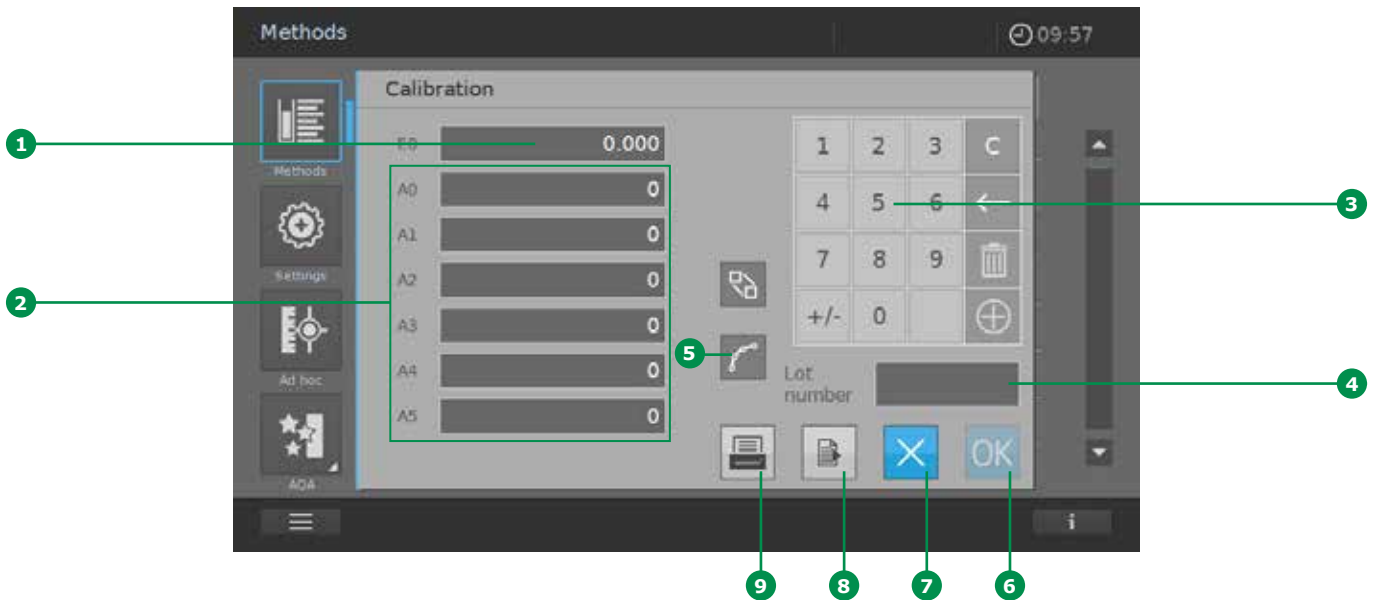
where:

C = measurement result (e.g. concentration)

A0, A1, A2, A3, A4, A5 = coefficients (polynomial)

Abs = measured absorbance

E0 = absorbance of the reagent blank value

Enter coefficients:

1. Enter E0 **1** and the required coefficients A0 – A5 **2** on the keypad **3**. At least one coefficient (A1) must be entered.
2. You can now enter an ID or a specific batch code for the calibration. Tapping on the field "Batch ID" **4** opens a virtual keyboard. Enter the code and confirm by tapping on the OK button.
3. Once all coefficients have been entered, tapping on the field "Graph" **5** shows the calibration curve.
4. To close the determination of the coefficients, confirm the data by tapping on the OK button **6**.
5. Tap on the Export button **8** to transfer the data in the CSV format to an external storage medium.
6. Tap on the Print button **9** to print out the data.
7. To close the operation without accepting the data, tap on the X button **7**. All entered data are deleted.



8. Tapping on the OK button **6** confirms the entered data, and the screen changes to the method screen. A check appears in the field "Calibration" **10**.

2

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You now have the following options:

4

- Close the programming/processing of the method by tapping on the Save button 11. All entered data are accepted. A method number appears 12.
- Close the screen by tapping on the X button 13. The screen changes to the method list.
- To call up coefficients, value pairs, or the graph again, tap on the field "Calibration" 11.
- Cancel the programming/processing of the method by tapping on the X button 13. All entered data are deleted. The screen changes to the method list.

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Example 1 (linear calibration function)

For entry as a formula, you can determine the coefficients of the reverse calibration function by linear regression. When doing so, the concentration has to be on the Y axis and the absorbance on the X axis. The absorbance of the individual value pairs must always be corrected by the reagent blank.

8

9

X value		Y value
Absorbance	Absorbance - RB*	Concentration
0.050	0.000	0.0 mg/l*
0.250	0.200	1.0 mg/l
0.451	0.401	2.0 mg/l
0.648	0.598	3.0 mg/l
0.850	0.800	4.0 mg/l
1.053	1.003	5.0 mg/l

* = reagent blank

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Calculated calibration function:

$$C = 0.0027 + 4.9914 \times A$$

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Example 2 (non-linear calibration function)

The coefficients of the reverse calibration function are determined by multiple regression. When doing so, the concentration has to be on the Y axis and the absorbance on the X axis. The absorbance of the individual value pairs must always be corrected by the reagent blank.

X value		Y value
Absorbance	Absorbance - RB*	Concentration
0.010	0.000	0.0 mg/l
0.020	0.010	0.1 mg/l
0.070	0.060	0.2 mg/l
0.150	0.140	1.0 mg/l
0.325	0.315	2.0 mg/l
0.490	0.480	3.0 mg/l
0.655	0.645	4.0 mg/l
0.825	0.815	5.0 mg/l

* = reagent blank

Calculated calibration function (third order polynomial):


$$C = -0.044983 + 7.4807 \times A - 4.5229 \times A^2 + 3.8305 \times A^3$$

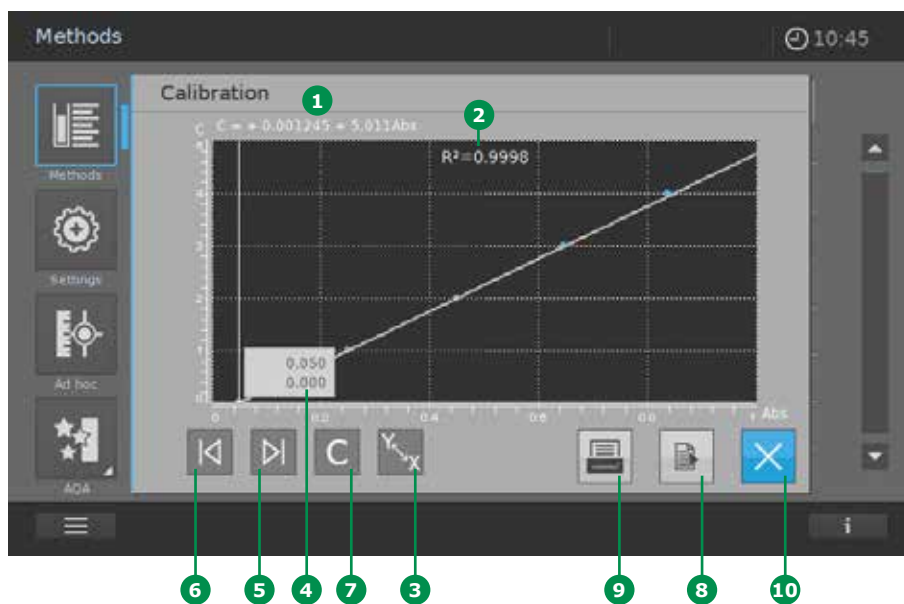
or

Calculated calibration function (fifth order polynomial):

$$C = -0.093083 + 9.9988 \times A - 27.549 \times A^2 + 78.315 \times A^3 - 99.226 \times A^4 + 46.604 \times A^5$$

Graphic presentation of the calibration function

As already described in the sections above, after entering/measuring value pairs or entering a function, the calibration curve can be graphically called up by tapping on the "Graph" button .



1. The calibration function **1** appears in the graph. When the function has been calculated using value pairs, the coefficient of determination "R2" **2** is also shown.

NOTE

The function determined in this way is used for calculating a result (e.g. concentration) via a measured absorbance in the form of a polynomial equation of the following type:

$$C = \text{Polynomial (Abs)}$$

where:

C = measurement result (e.g. concentration)

Abs = [measured absorbance of the sample or standard] **minus** [absorbance of the reagent blank value (E0)]

2. The X axis shows the absorbance values, the Y axis the corresponding results (e.g. concentration). Tapping on the X/Y button **3** changes the presentation of the axes around.

The formula of the calibration function **1** that is shown remains unchanged.

3. When the function has been calculated via value pairs, these pairs are shown in a separate field **4**. The forward and back keys **5**, **6** can be used to call up the next value pair. Tap on the C button **7** to reset the view.
4. Tap on the Export button **8** to transfer the data in the CSV format to an external storage medium.
5. Tap on the Print button **9** to print out the data.
6. Tap on the X button **10** to close the view of the graphic presentation. The screen changes.

3 9.6.4 Calibration Data and Calibration Function for Special Methods (e.g. Multi-wavelength)

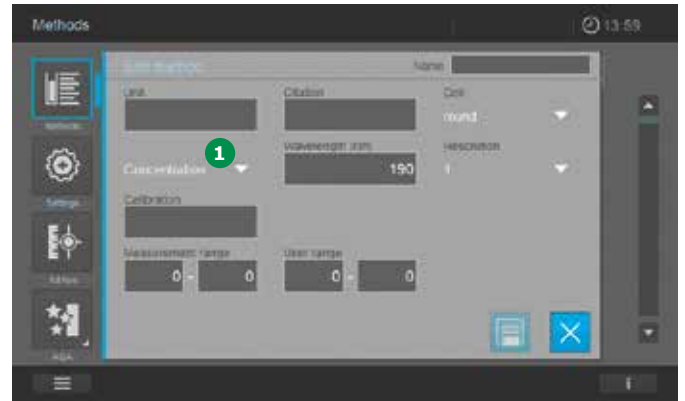
4 In this mode you can carry out measurements with special methods and functions. You can use the following functions for these methods:

- 5
- Measurements at different wavelengths
 - Multiple measurements at one wavelength (e.g. before and after adding a reagent)
 - Use of procedure variables. Procedure variables provide a value that has to be entered prior to each measurement on the spectrophotometer (e.g. volume, pH value or temperature)
 - Check whether a value meets a condition. With a condition you can check a value for validity (e.g. absorbance value, procedure variable or the result of a formula)

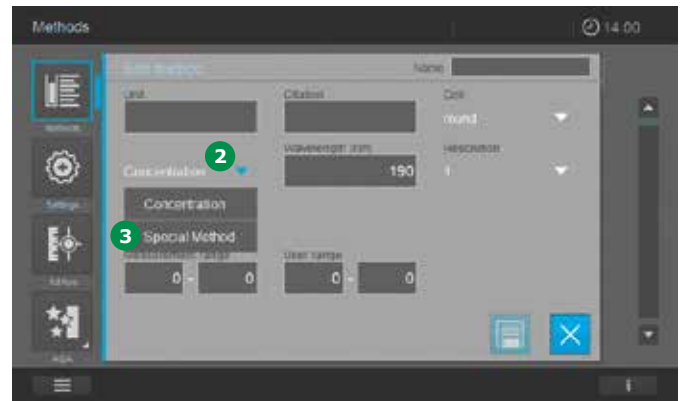
8 Formula editor for convenient programming of any user-defined methods (see section 9.6.5).

9.6.5 Programming/Modifying User-defined Special Methods (e.g. Multi-wavelength)

Proceed in the following manner to programme a special method:



1. Select the method type "Concentration" (see section 9.6).



2. Tapping on arrow opens the selection list.
3. Select Special Method from the displayed selection list.



4. The screen changes.

5. Fill out input field items 4 – 13. Tapping on the input fields 5, 11, 12, 13 changes the screen. These can be programmed as described in steps on the following pages.

NOTE

It is also possible to display characters in subscript and superscript. To put a character in subscript, an underscore "_" must be placed in front of the character in question (e.g. entry for $H_2O = H_2O$). To put a character in superscript, a circumflex "^" must be placed in front of the character in question (e.g. entry for $m^2 = m^2$).

Item	Input field	Possible input
4	Name	Any name
5	Wavelength	Up to 5 wavelengths definable
6	Cell	16 (round), 10, 20, 50 or 100 mm
7	Citation form*	e.g. PO4-P
8	Unit*	e.g. mg/l
9	Resolution	0.001, 0.01, 0.1, 0.25, 0.5 or 1
10	Lower and upper limit of the measuring range	Any value between zero and the highest concentration of the standard solutions used
11	Procedure variable*	Procedure variables provide a value that has to be entered prior to each measurement on the spectrophotometer (e.g. volume, pH value or temperature)
12	Formula function	Formula editor for convenient programming of any user-defined methods
13	Condition*	With a condition you can check a value for validity (e.g. absorbance value, procedure variable or the result of a formula).

* Optional

2

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4

5



6. Input field 5 – wavelength: Up to five wavelengths can be set. Add further entry fields for wavelengths 15 by tapping on the + button 14. Tapping the Delete button 16 removes the most recently programmed entry field 15. Tapping on the Save button 17 accepts the input. Tapping on the X button 18 closes the screen and opens the previous input mask.

Additional entry fields 19 are added by tapping on the + button 20. Tapping the Delete button 21 removes the most recently programmed input row 19. Tapping on the Save button 22 accepts the input. Tapping on the X button 23 closes the screen and opens the previous input mask.

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7. The number of wavelengths created appears in the display field 5.

8. Tapping on the Procedure variable button 11 changes the screen. Here you can program up to five different procedure variables 19. Define the following values.

- Name = name of the variable (e.g. temperature)
- Min = lower limit of the variable value
- Max = upper limit of the variable value
- RES = decimal places in the variable value (e.g. 0.1)
- Unit* (optional) = unit of the variable value (°C)

9. The number of variables created appears in the display field 11.

10. Tapping on the Formula button 24 changes the screen. Using the formula editor, you can now create a freely definable function from the variables and wavelengths you have defined.

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11. Tapping on the OK button **25** accepts the input. Tapping on the X button **26** closes the screen and opens the previous input mask.



13. Optional tapping on the Condition button **28** changes the screen. Here you can define a condition for valid measurements (e.g. absorbance wavelength $1 \leq 2.50$). Tapping on the Variable and/or wavelength button **29** accepts the selection and displays it in the pre-selected output field **30**.

NOTE

When methods are used that are subject to a condition, the measurement result is calculated only when the condition is met.



12. An excerpt of the formula you have defined appears in the display field **27**.

14. Tapping on the OK button **31** accepts the input. Tapping on the X button **32** closes the screen and opens the previous input mask.

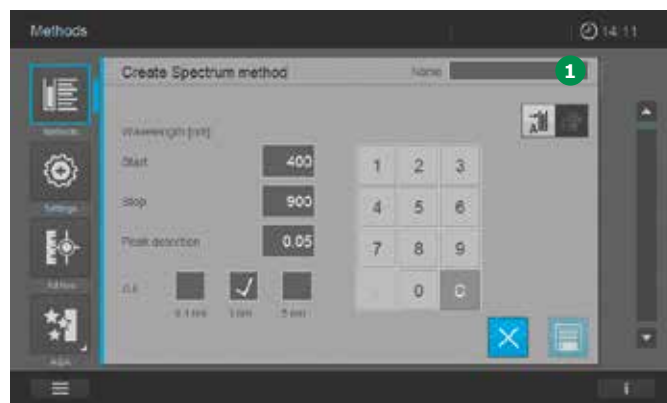
9.6.6 Programming a User-defined Spectrum Method

For Spectrum Mode you can develop and store your own userdefined methods under method numbers 1101 to 1120.

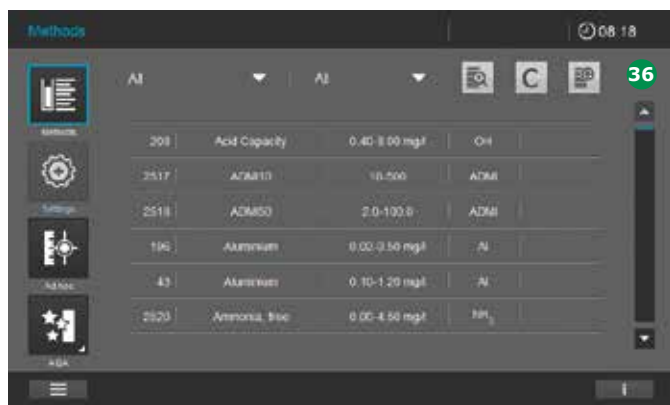
The spectrophotometer software supports you in creating the methods. To create a user-defined spectrum method, proceed as follows:



15. Tap on the Save button **33**. The method is automatically given a number generated by the system **34**. All values are stored.
16. Tap on the X button **35** to leave the edit method screen.



1. Define the method type (see section 9.6).
2. Enter a name for the method **1**. This name is displayed in the method list.

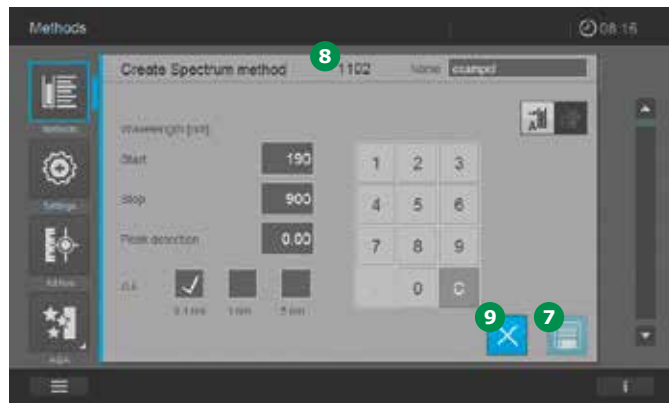
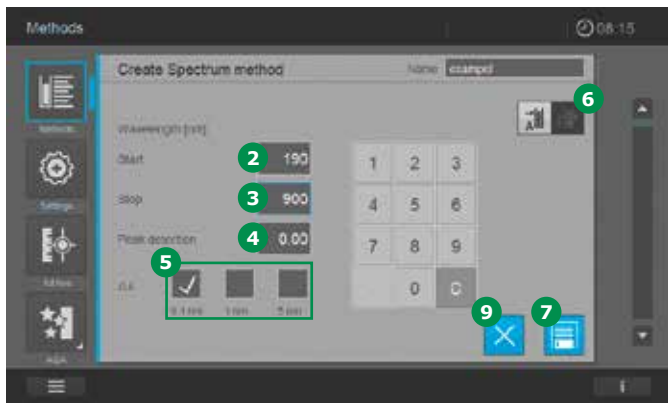


17. The screen changes to show the method list **36**.
18. The method is now created and stored in the instrument.

NOTE

To find the method more quickly, use the filter function (see section 9.5.2).

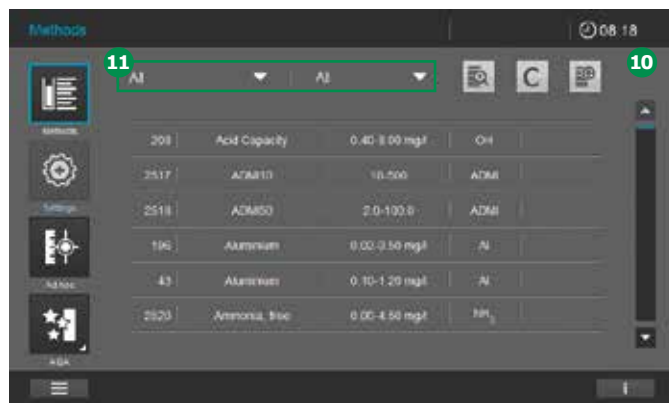
- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- 9
- 10
- 11
- 12
- 13
- 14
- 15
- 16



Item	Input field	Possible input
1	Name	Any name
2	Start & Stop	Wavelength range Prove 300 plus 600 plus: 190 – 1100 nm Wavelength range Prove 100 plus: 320 – 1100 nm
4	Peak detection	Threshold value for peak detection
5	Interval	Sampling rate for the wavelength range
6	Selection button	Choice between absorbance or transmission

3. Define the wavelength range for the method. Start (2) & Stop (3).
4. Determine the sensitivity (4) of the method.
5. Set the interval (5). Here you can choose between 0.1 nm, 1 nm, 5 nm.
6. Set the choice between absorbance or transmission (6).

7. Tap on the Save button (7). The method is automatically given a number generated by the system (8). All values are stored.
8. Tap on the X button (9) to leave the edit method screen.



9. The screen changes to show the method list (10).
10. The method is now created and stored in the instrument.

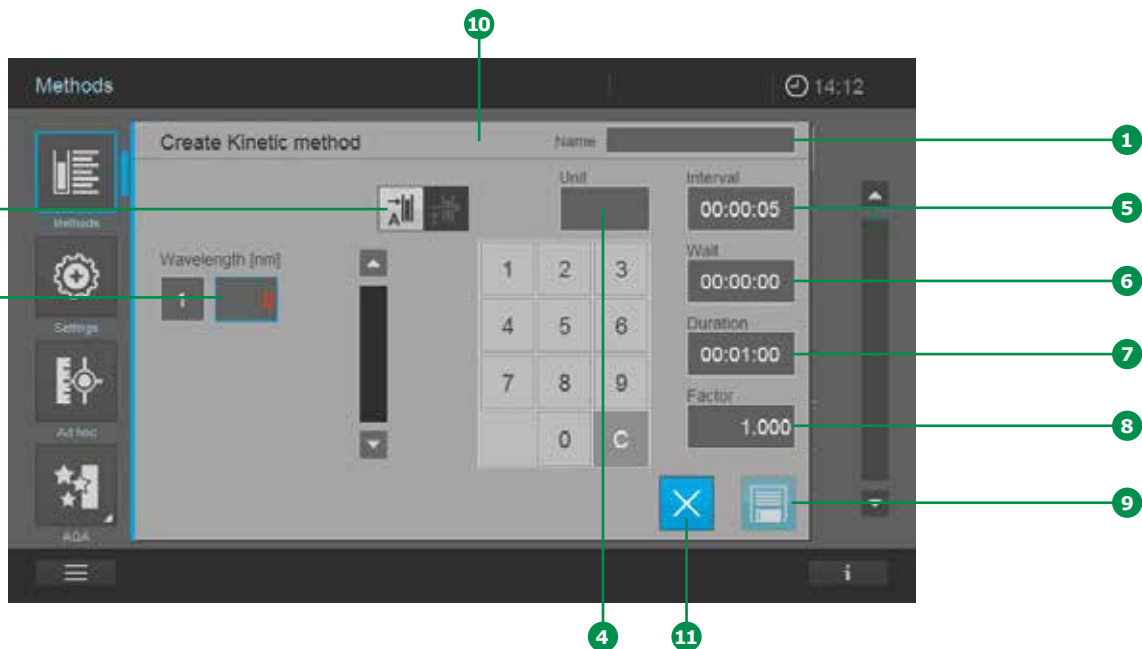
NOTE

To find the method more quickly, use the filter function (11) (see section 9.5.2).

NOTE

A spectrum can comprise up to a maximum of 1000 measurement points. If the entry is invalid, it is shown in red and cannot be accepted.

9.6.7 Programming a User-defined Kinetic Method



For Kinetic Mode you can develop and store your own user-defined methods under method numbers 1201 to 1220. The spectrophotometer software supports you in creating the methods. To create a user-defined kinetic method, proceed as follows:

1. Define the method type (see section 9.6).
2. Enter a name for the method **1**. This name is displayed in the method list.
3. Select type of measurement: absorbance or transmission measurement **2** by tapping on the button for the required measurement (the activated selection is light grey).

4. Create the user-defined parameters

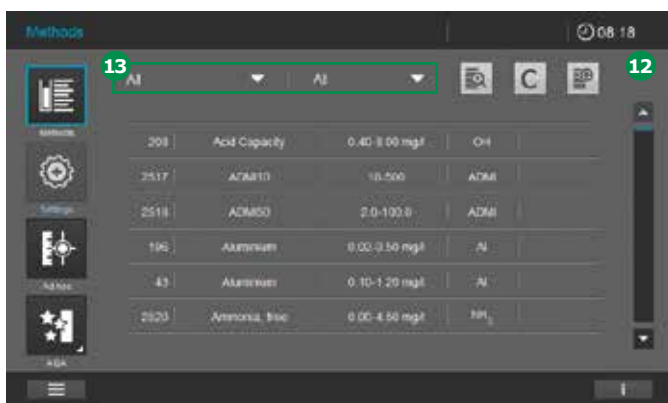
- Wavelength **3**
 - Unit **4**
 - Interval **5**
Prove 100 plus Minimum: 00:00:10 (hh:mm:ss)
Prove 300/600 plus Minimum: 00:00:05 (hh:mm:ss)
 - Delay **6**
 - Duration **7**
 - Slope factor **8**
5. Tap on the Save button **9**. The method is automatically given a number generated by the system **10**. All values are stored.
 6. Tap on the X button **11** to leave the edit method screen.

NOTE

Invalid entries are shown in red and cannot be accepted.

Item	Input field	Possible input
1	Name	Any name
2	Selection button	Choice between absorbance or transmission
3	Wavelength	Wavelength range Prove 300 plus 600 plus: 190 – 1100 nm Wavelength range Prove 100 plus: 320 – 1100 nm
4	Unit*	User-defined input when an end result is to be calculated (e.g. enzyme activity U/ml)
5	Interval	Time intervals between the measuring points (hh:mm:ss)
6	Wait	Lead time to start of the series of measurements (hh:mm:ss)
7	Duration	Difference in time between the first and last measuring point in the series of measurements (hh:mm:ss)
8	Slope factor*	User-defined input for calculating a result = "slope factor" × "Δ A/min" (instrument automatically calculates the difference in absorbance/minute = Δ A/min)

* = Optional (only useful for absorbance)



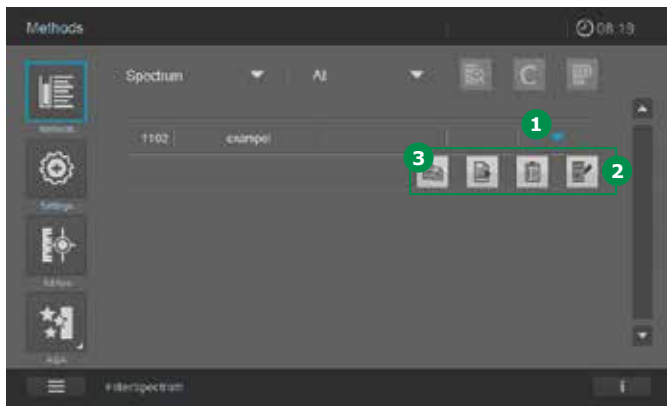
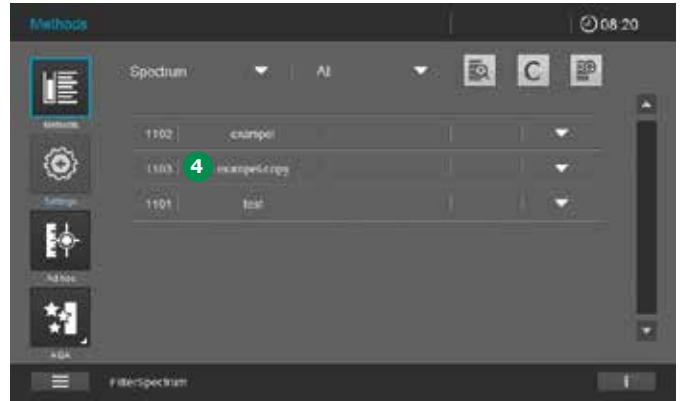
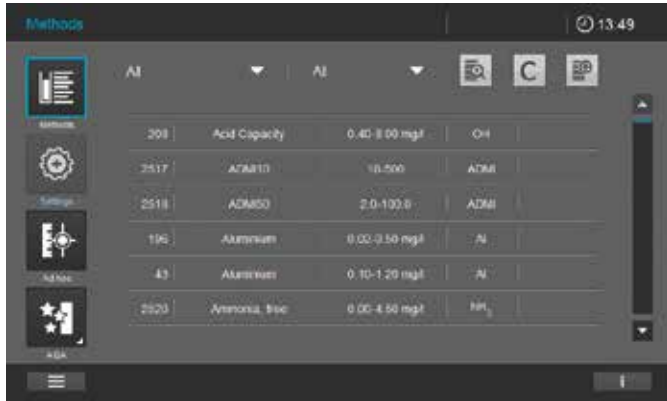
- The screen changes to show the method list 12.
- The kinetic method is now created and stored in the instrument.

NOTE

To find the method more quickly, use the filter function 13 (see section 9.5.2).

9.6.8 Copying/Duplicating a User-defined Method

1. Search and select the method (see section 9.5.2).

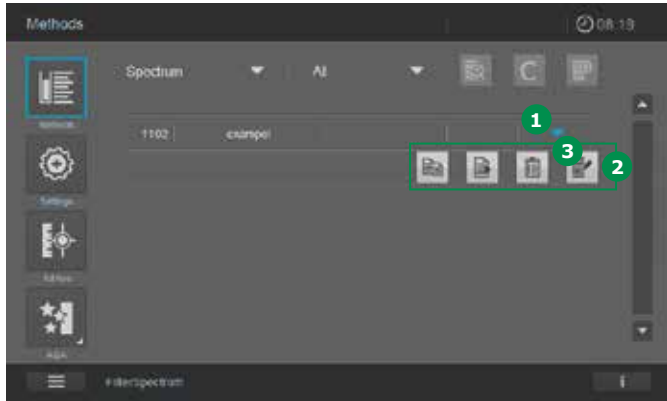


5. The method is created under the method name with the addition "name-copy" 4 and appears in the method list.
6. Modify the duplicated method as needed (see section 9.6.3).

2. Activate the method by tapping on the arrow in the right column of the method list 1.
3. A selection of various method editing possibilities shows up 2.
4. To copy the method, tap on the Copy button 3.

9.6.9 Modifying a User-defined Method from the Method List

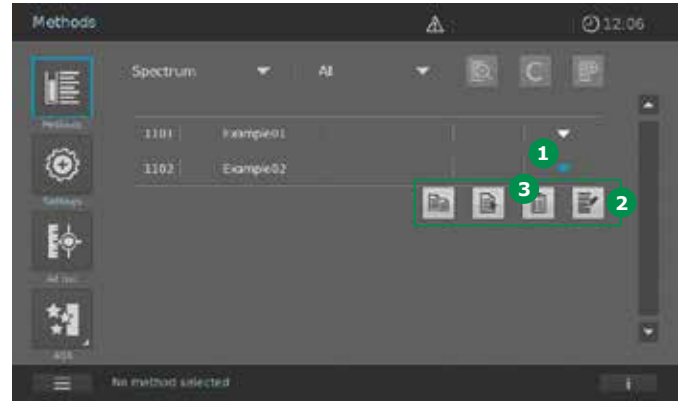
1. Search and select the method (see section 9.5.2).



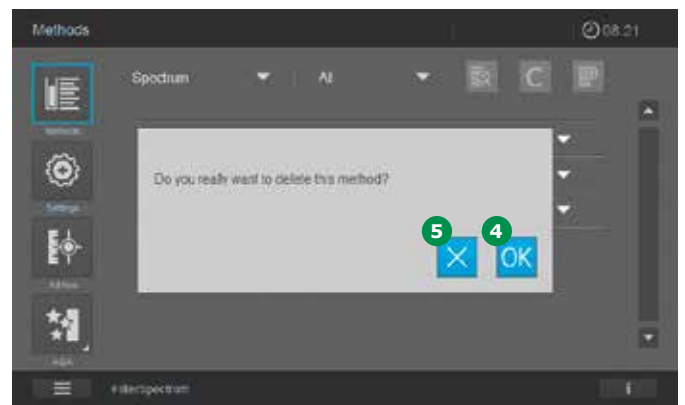
2. Activate the method by tapping on the arrow in the right column of the method list 1.
3. A selection of various method modification possibilities shows up 2.
4. To modify the method, tap on the Edit button 3.
5. Now follow the description in the sections on programming a:
 - User-defined concentration method (see section 9.6.1)
 - User-defined spectrum method (see section 9.6.6)
 - User-defined kinetic method (see section 9.6.7)

9.6.10 Deleting a User-defined Method from the Method List

1. Search and select the method (see section 9.5.2).



2. Activate the method by tapping on the arrow in the right column of the method list 1.
3. A selection of various method modification possibilities shows up 2.
4. To delete the method, tap on the Delete button 3.

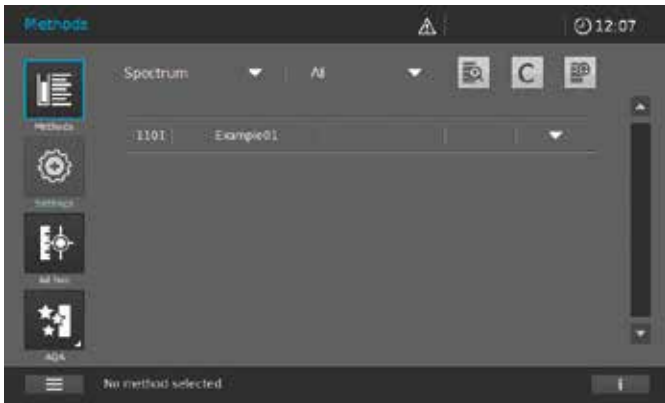


5. The confirmation box asking if you really want to delete the selected method pops up.
6. To delete the method, tap on the OK button 4 to confirm or on the X button 5 to cancel the deletion process.

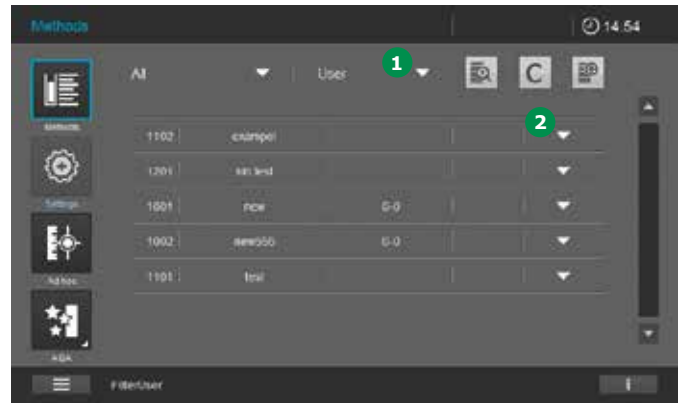
CAUTION

Following your confirmation the method is permanently deleted. Before deleting any method, we recommend you export a backup copy of it to an external memory device.

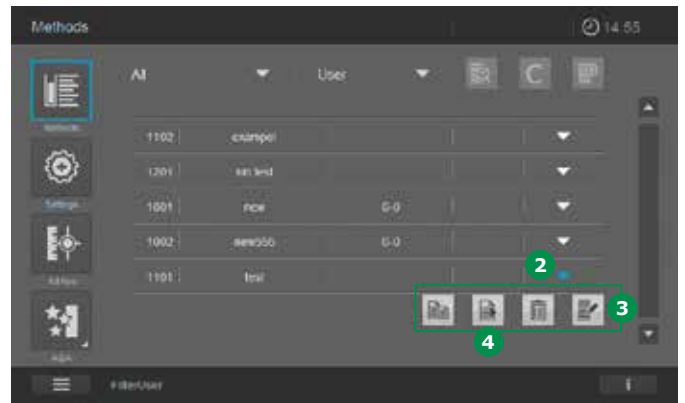
9.6.11 Export User-defined Methods to a USB Memory Device



7. After the OK button 4 has been pressed, the screen changes to Method List. The deleted method no longer appears in the method list.

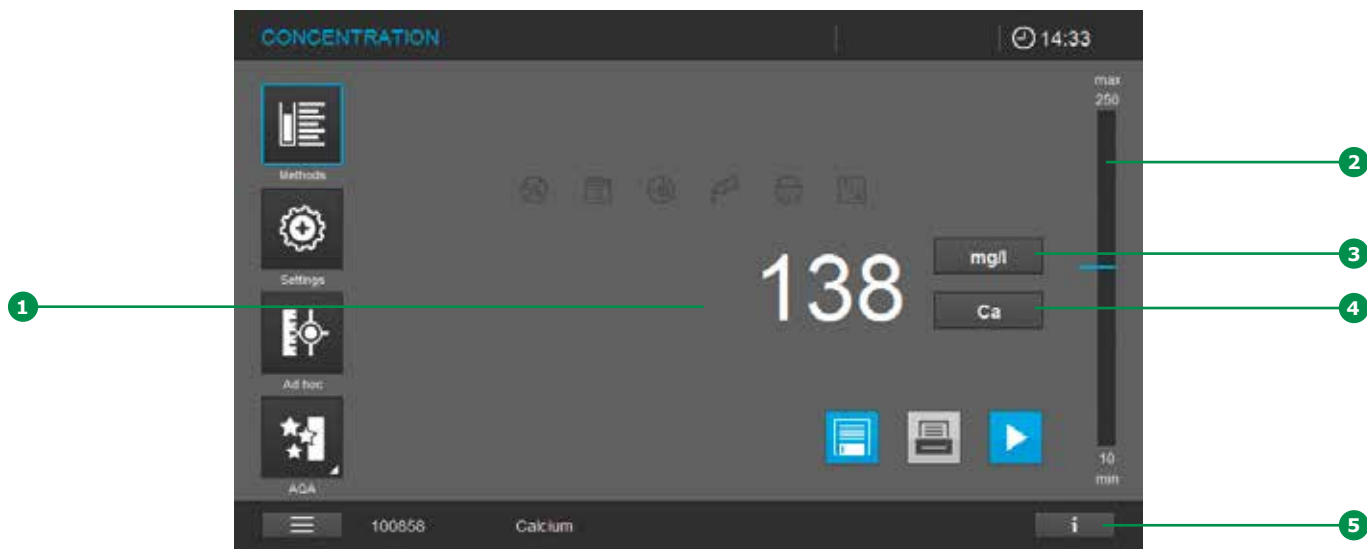


1. Filter the user-defined method in the method list, e.g. by using the search filter User 1.
2. Activate the method by tapping on the arrow 2.



3. A selection of various method modification possibilities shows up 3.
4. Make sure that an USB memory device is connected to the spectrophotometer.
5. To export the method, tap on the Export button 4.

9.7 Measuring in Concentration Mode



9.7.1 Measuring Cell Tests with a Barcode

Inserting a cell with a barcode starts a measurement (see section 9.3).

1. Insert the barcoded round cell through the opening in the cover. The white position line on the cell has to be aligned with the position mark on the spectrophotometer. Insert the cell until it touches the bottom of the round cell compartment. The spectrophotometer selects the method based on the barcode and automatically starts measuring.

NOTE

If the barcode cannot be read, a message appears. In this case you can make a new attempt by using the Spectroquant® round cell bearing the barcode or the AutoSelector as described. Care must be taken to ensure that the positioning mark on the round cell/ AutoSelector is aligned with the position mark on the spectrophotometer.

Alternatively, you can close the message and then select the required method manually from the method list.

2. The measurement result **1** is displayed. The position of the measurement result in the measuring range is shown on the measuring range display bar **2** with a blue line.

NOTE

Measurement results beyond the measuring range are marked separately in the display (see section 9.7.4).

3. Further options:

- Select a different citation form by tapping on the citation form display field **4** (e.g. $\text{NH}_4 \leftrightarrow \text{NH}_4\text{-N}$)
- Select a different measuring unit by tapping on the unit display field **3** (e.g. $\text{mg/l} \leftrightarrow \text{mmol/l}$)
- Make further settings such as dilution or blank value measurements with "Settings" (see section 9.7.5)

1 **9 Operation – 9.7 Measuring in Concentration Mode**

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4. Content of the information bar in the concentration mode:

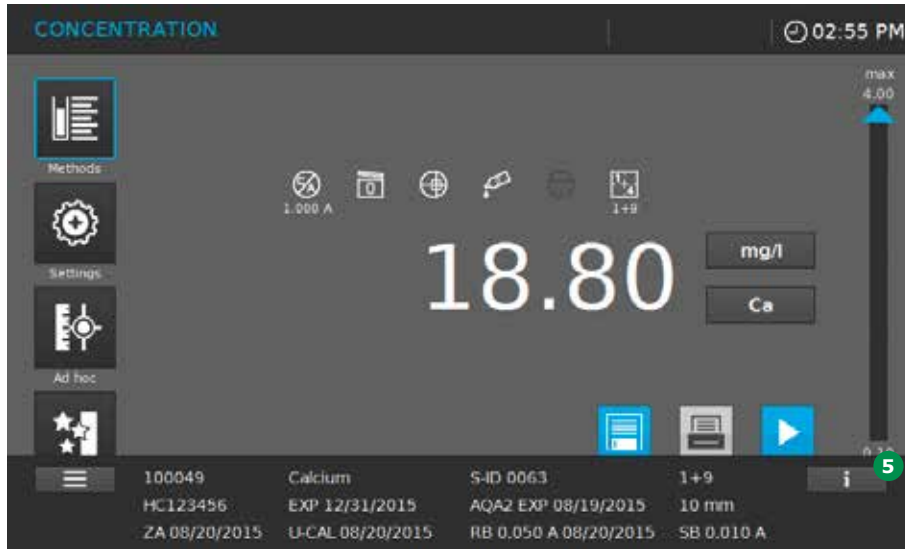
4

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Tapping on the Information bar button **5** opens the extended information bar. In the concentration mode the following information is displayed:

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100049	Calcium	S-ID 0063	1+9
Article number (first 6 digits of order no.)	Method Name	Sample ID with prefix "S-ID"	Sample Dilution
11 HC123456	12 EXP 12/31/2015	13 AQA2 EXP 08/19/2015	14 10 mm
Lot number test kit	Expiration date test kit with Prefix "EXP"	AQA2 status (valid until date/no. of measurements) with Prefix "AQA2 EXP"	Path length of inserted cell
12 ZA 08/20/2015	13 U-CAL 08/20/2015	14 RB 0,050 A 08/20/2015	15 SB 0,010 A
Date of Zero Adjustment with Prefix "ZA"	Date user calibration with Prefix "U-CAL"	Date + value user reagent blank with Prefix "RB"	Value sample blank with Prefix "SB"

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9.7.2 Measuring Reagent Tests with AutoSelector

Select the method by inserting the AutoSelector and the spectrophotometer is ready to start measuring.

1. Open the cell compartment cover.
2. Insert the AutoSelector in the cell compartment for round cell. The white position line has to be aligned with the position mark on the spectrophotometer. Insert the AutoSelector until it touches the bottom.

NOTE

If the barcode cannot be read, a message appears. In this case you can make a new attempt by using the Spectroquant® round cell bearing the barcode or the AutoSelector as described. Care must be taken to ensure that the positioning mark on the round cell/ AutoSelector is aligned with the position mark on the spectrophotometer.

Alternatively, you can close the message and then select the required method manually from the method list.

3. Insert the rectangular cell until it touches the bottom and left edge of the holder. The opaque sides of the rectangular cell must point to the front and rear. Inserting the rectangular cell (1, 2, 5, [10 cm Prove 600 plus only]) automatically selects the correct measuring range. The spectrophotometer starts measuring automatically. As the spectrophotometer has an inbuilt ambient light protection there is no need to close the cell compartment cover.

NOTE

Measurement results beyond the measuring range are marked separately in the display (see section 9.7.4).

4. Further options:

- Select a different citation form by tapping on the citation form display field ④ (e.g. $\text{NH}_4 \leftrightarrow \text{NH}_4\text{-N}$)
- Select a different measuring unit by tapping on the unit display field ③ (e.g. $\text{mg/l} \leftrightarrow \text{mmol/l}$)
- Perform further settings such as dilution or blank value measurements through Settings (see section 9.7.5)

9.7.3 Measuring Reagent-free Tests and User-defined Methods

User-defined methods and reagent-free methods generally have no barcode and hence no automatic method recognition. In such a case, select the method manually.

1. Select the method manually (see section 9.5.1).
2. The spectrophotometer is ready to start measuring.
3. Depending on the type, insert the cell as follows:

Round cell:

Insert the round cell in the cell compartment for round cells until it touches the bottom.

Rectangular cell:

Insert the rectangular cell vertically so it touches the bottom and left edge of the cell compartment. The opaque sides of the rectangular cell must point to the front and rear. As the spectrophotometer has an inbuilt ambient light protection there is no need to close the cell compartment cover.

NOTE

Measurement results beyond the measuring range are marked separately in the display (see section 9.7.4).

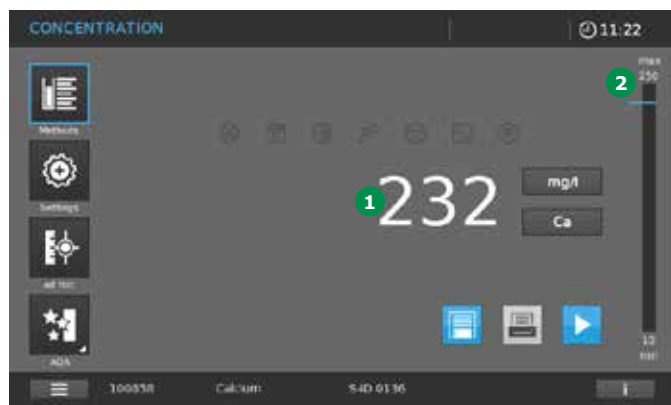
4. Further options:

- Select a different citation form by tapping on the citation form display field 4 (e.g. NH_4 <-> $\text{NH}_4\text{-N}$)
- Select a different measuring unit by tapping on the unit display field 3 (e.g. mg/l <-> mmol/l)
- Perform further settings such as dilution or blank value measurements through Settings (see section 9.7.5)
- Detailed information on the individual measurement is shown in the information bar 5 (see section 9.7.1)

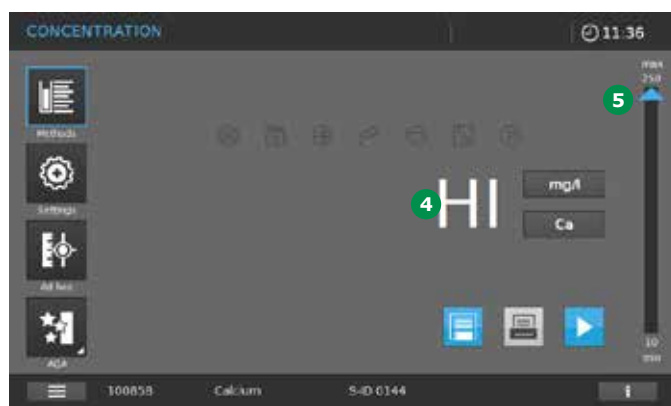
NOTE

For some methods, e.g. chlorophyll, the options listed under item 4 are not possible.

9.7.4 Exceeding the Upper or Lower Limits of the Measuring Range



Depending on the method, the measurement result is displayed (1) as long as it remains inside the measuring range between the upper and lower limit. The position of the measurement result in display bar (2).



Measurement results outside the measuring range are shown separately in the display. If a result is beneath the lower limit of the measuring range, a blue arrow (3) appears at the lower measuring range limit, while a result above the higher limit of the measuring range prompts a blue arrow at the higher measuring range limit (5).

A measurement result lying far outside the measuring range is not shown, and instead either the text "Lo" (for very low results) or respectively "Hi" (4) (for very high results) appears.

NOTE

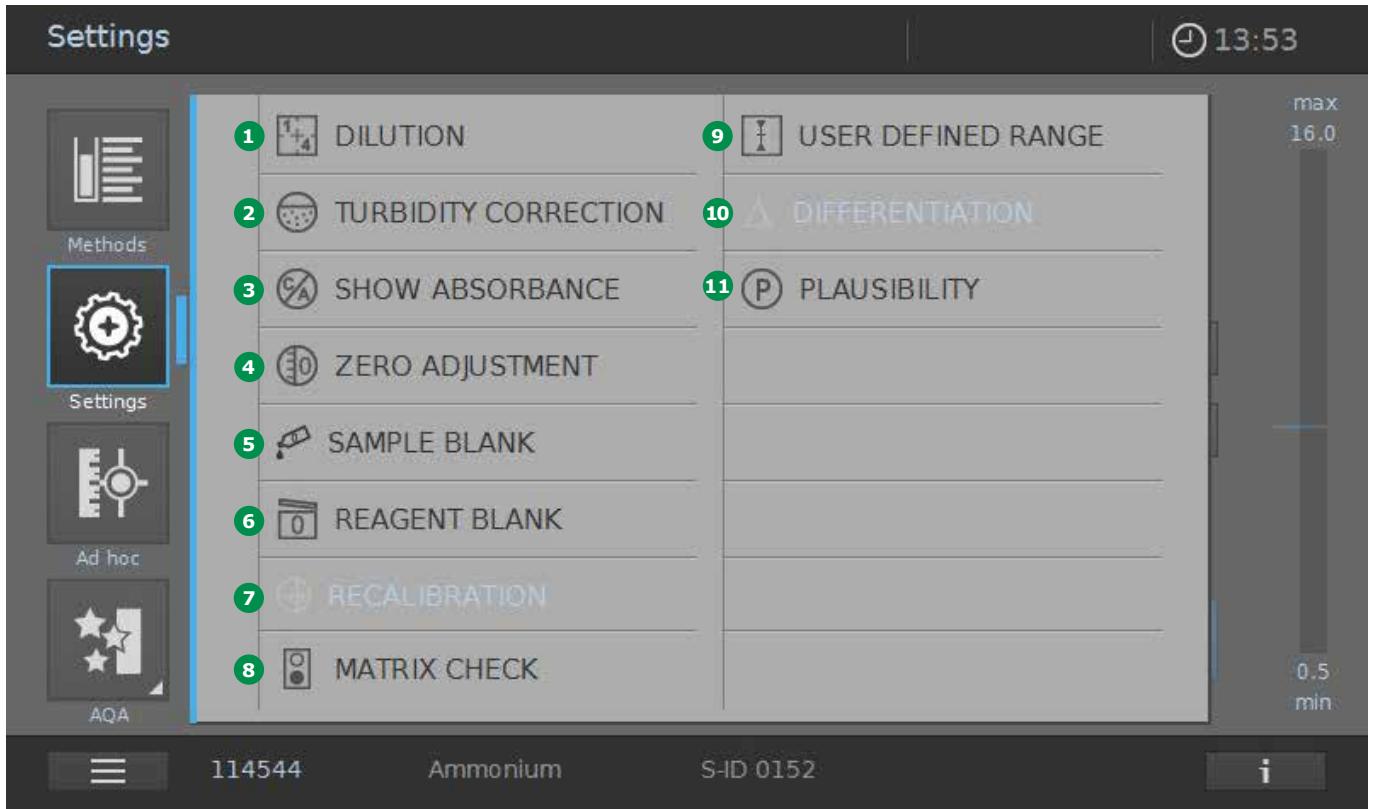
In the event that the display of "HI" or "LO" for results lying beyond the measurement range is deactivated in the "Quality" menu of the system settings (see section 9.2.4), under certain circumstances - e.g. the measurement of analyte-free samples - measurement results with a minus sign may also appear. This is entirely intentional and is not a defect of the Prove plus spectrophotometer. Experienced users know that every measurement result is subject to a so-called measurement uncertainty (actual result = displayed result ± measurement uncertainty). Many users also need to determine measurement results for analyte-free samples, e.g. in connection with method-validation operations. This is why the display of measurement results with a minus sign, which in certain conditions may be due to the measurement uncertainty of the measurement system, is allowed when the HI/LO display is deactivated.

NOTE

For methods involving a special measurement procedure, e.g. the chlorophyll analysis, results beyond the measuring range are shown by " --- ".



9.7.5 Method-specific Settings for Concentration Mode



When a method is selected, the Settings menu can be activated. Depending on the method selected, the settings available for the method are as follows:

- 1 Dilution
- 2 Turbidity correction (global setting)
- 3 Show absorbance (global setting)
- 4 Zero adjustment (see section 9.4)
- 5 Sample blank
- 6 Reagent blank
- 7 Recalibration
- 8 MatrixCheck
- 9 User-defined range
- 10 Differentiation
- 11 Plausibility (general setting)

NOTE

The individual settings are greyed out if they are not available for the selected method. Switching a global setting (turbidity correction, show absorbance) ON activates it for ALL methods where it is applicable.

9.7.6 Measuring Diluted Samples

If the concentration of a sample exceeds the measuring range of a method, you can specifically dilute the sample so that the concentration of the diluted sample is within the measuring range of the method. A valid measurement can be performed by this means. Once the factor for the dilution has been entered, the meter converts the concentration to that of the undiluted sample.

NOTE

Optimum measurement results are achieved if the concentration of the diluted sample is in the middle of the measuring range of the method after diluting.

Having selected the method, enter the dilution as follows:



1. Open the Settings menu 1.



2. Select Dilution 2 and confirm. The input screen 3 for Dilution appears.
3. Tap on the dilution value in the display fields 4, enter the factor on the keypad and tap on OK button 5.



4. The spectrophotometer is ready to start measuring. The display 6 changes to measuring mode.

The dilution that was just entered is used for the next measurement.

The value entered for the dilution is only valid for the selected method. The dilution factor is deleted:

- When the spectrophotometer is switched off
- When dilution value 0 (= no dilution) is entered in the Dilution screen.

NOTE

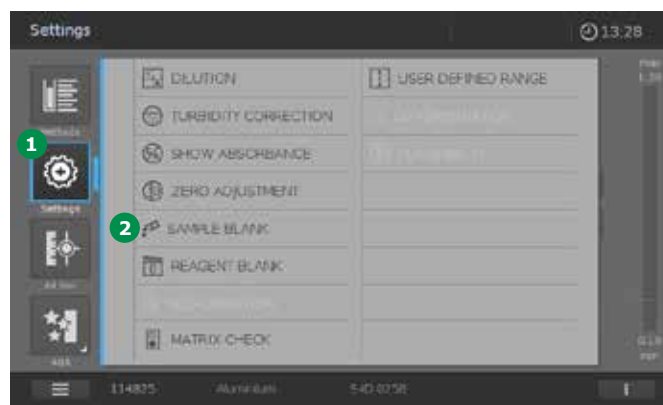
If a dilution factor is active, it is indicated on the display during measurement in the form [1 + x] 7. The dilution factor is also shown in the information bar at the bottom (see section 9.7.1). The maximum dilution is 1 + 999.

9.7.7 Sample Blank Value

By measuring and using a sample blank value, measurement errors due to coloring and turbidity of the sample matrix can be largely eliminated. The sample blank value is a characteristic of the sample (coloration) to be currently determined. The sample blank is diluted depending on the method being used, but does not contain any color reagents. The pH is the same as that of the test sample.

NOTE

Adding reagents dilutes the sample. This can change the pH of the sample. For this reason the sample blank also has to be diluted and the pH value adjusted accordingly. The sample blank value is valid for the next measurement only. The sample blank value can be determined by single or multiple determination. With multiple determination, the sample blank value is calculated as the median from the single measured values. Having selected the method, measure the sample blank value as follows:



1. Open the Settings menu 1.



NOTE

The use of the sample blank value is indicated by the symbol **8** in the display being lit. The sample blank value is also shown with prefix "SB" in the information bar at the bottom (see section 9.7.1).

2. Select Sample Blank Value **2**.
3. Insert the cell with a suitable sample blank. The sample blank measurement starts automatically. The value is used only for the next measurement.
4. The first single measurement for the sample blank value is performed. The following data is displayed as the result:
 - The measured absorbance from the (last) single measurement **4**
 - The median from all single measurements carried out so far **5**
5. If necessary, carry out further single measurements to calculate the median.



6. Tap on OK **6** to accept the measurement.
7. The screen changes to the measuring mode **7**.
8. The spectrophotometer is ready to start measuring.

9.7.8 Reagent Blank Value

The evaluation of the photometric measurement always refers to the comparison value of a test solution without the substance to be determined (reagent blank value). Thus the influence of the basic absorbance of the reagents on photometric measurement is compensated for. In practice, the reagent blank value is measured with the same amount of distilled or DI water instead of sample. With photometric concentration determination, the reagent blank value is a constant. The method data for all measurements with Spectroquant® test kits (Concentration Mode) include an exactly determined reagent blank value. This value is overwritten if you measure the reagent blank value yourself.

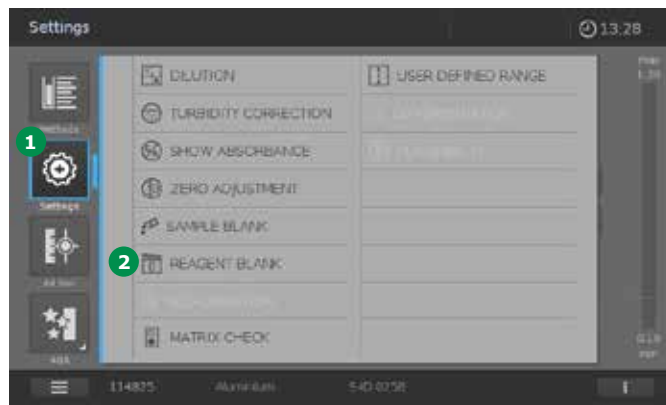
NOTE

You can increase precision if you determine the reagent blank value with a test from a new lot and use the reagent blank value for all further measurements with that lot. This is especially recommended for measurements in the vicinity of the lower limit of the measuring range. To enable the assignment in the result documentation at a later time, the batch code saved in the barcode of the inserted round cell or of the AutoSelector is also documented; alternatively, you can also enter the Lot Number on the reagent packaging (Lot ID) when determining the blank value.

The factory blank values always remain stored in the instrument and can be activated at any time. The reagent blank values you measured yourself also remain stored in the spectrophotometer until they are overwritten by a new blank value measurement.

The reagent blank value can be determined by single or multiple determination. With multiple determination, the reagent blank value is calculated as the median from the single measured values.

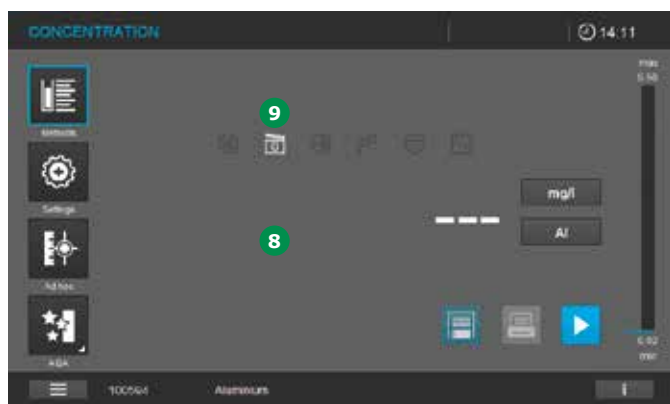
Having selected the method, measure the reagent blank value as follows:



1. Open the Settings menu ①.
2. Select Reagent Blank Value ②.



3. Insert the cell with a suitable reagent blank. The reagent blank measurement starts automatically.
4. The Lot ID ③ is read from the barcode. It can be edited manually, however.
5. The first single measurement for the reagent blank value is performed. The following data is displayed as the result:
 - The measured absorbance from the (last) single measurement ④
 - The median from all single measurements carried out so far ⑤
6. The function "User RB" is activated ⑥.
7. If necessary, carry out further single measurements to calculate the median.
8. Tap on OK ⑦ to accept the measurement.



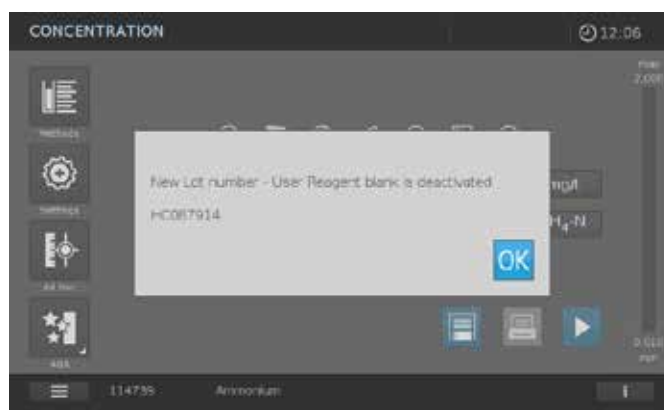
9. The screen changes to the measuring mode **8**.
10. The spectrophotometer is ready to start measuring.

NOTE

The use of the reagent blank value is indicated by the symbol **9** in the display being lit. The reagent blank value and its date of measurement are also shown with prefix "RB" in the information bar at the bottom (see section 9.7.1).

NOTE

In the event that a Lot ID different from the one used to measure the reagent blank value is used in a subsequent measurement, this is recognized by the barcode of the inserted round cell or of the AutoSelector. The activated user reagent blank value is then automatically deactivated and a corresponding message appears in the display. Tapping "OK" clears the message and the measurement is performed automatically without taking a user reagent blank value into account.



9.7.9 Automatic Turbidity Correction

The turbidity correction function activates the automatic recognition and compensation of the light absorption caused by turbid substances.

Following activation, the function remains permanently switched on. Measured values that were measured with turbidity correction are labeled with the turbidity correction button on the display **6** and in the documentation (printout and memory).

NOTE

The turbidity correction function is not active when the spectrophotometer leaves the factory. The setting for automatic turbidity correction is possible with all methods where the turbidity correction makes sense. Where a method does not permit turbidity correction, the button **2** is greyed out.

Having selected the method, activate the turbidity correction function as follows:



1. Open settings **1**.
2. Select turbidity correction **2**.



3. Select turbidity correction **3** with 0 = deactivated and 1 = activated (in light grey).
4. Accept the settings with OK **4**.



5. The screen changes to the measuring mode **5**.
6. The spectrophotometer is ready to start measuring.

NOTE

The use of the turbidity correction is indicated by the symbol **6** in the display.

9.7.10 User Recalibration (Standard Adjustment)

A few pre-programmed methods and the user-defined methods for concentration measurement provide the option to optimize the original calibration stored with the method by means of a user recalibration. When creating a user-defined method you can also allow a user recalibration (see section 9.6).

When a method is called up for which a user recalibration is required, measurement is only possible with a valid user calibration. The use of the user recalibration is documented along with the measured value and indicated in by the corresponding symbol in the display. Activation of user recalibration and its date are also shown with prefix "U-CAL" in the information bar at the bottom (see section 9.7.1).

NOTE

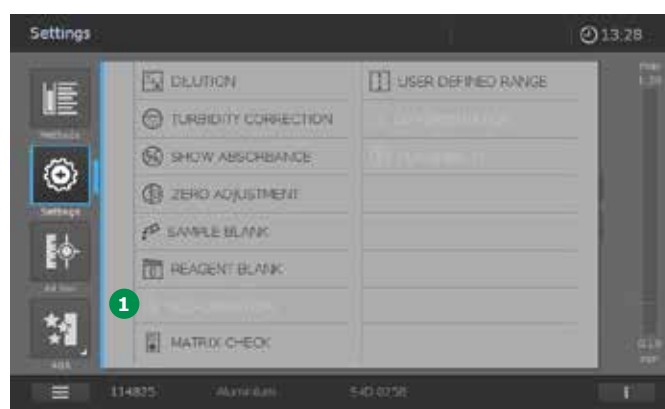
A user calibration is always stored for the method presently called up. A user calibration is erased only if a new user recalibration is carried out.

Calibration for user-defined methods

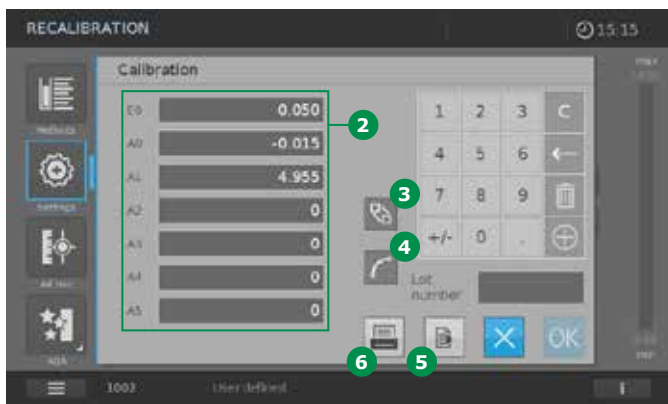
1. Select the method manually (see section 9.5.1).

NOTE

If a zero adjustment has not been performed, the spectrophotometer informs you that you need to perform a zero adjustment.



2. Tap on "Recalibration" ①.
3. The screen changes.



4. The data 2 of the current calibration are shown.
5. Tap on the "Value pair" button 3 to switch to the view of the value pairs.
6. Tap on the "Graph" button 4 to switch to the graphic presentation of the calibration curve.
7. Tap on the Export button 5 to transfer the data in the CSV format to an external storage medium.
8. Tap on the Print button 6 to print out the data.

A user recalibration can be performed by any of the means below. User recalibration by

- Entry of a function (see section 9.6.3)
- Entry as a value pair (see section 9.6.3)
- Measurement of value pairs (see section 9.6.3)

Calibration for Spectroquant® methods

NOTE

This option is applicable only for very few Spectroquant® methods.

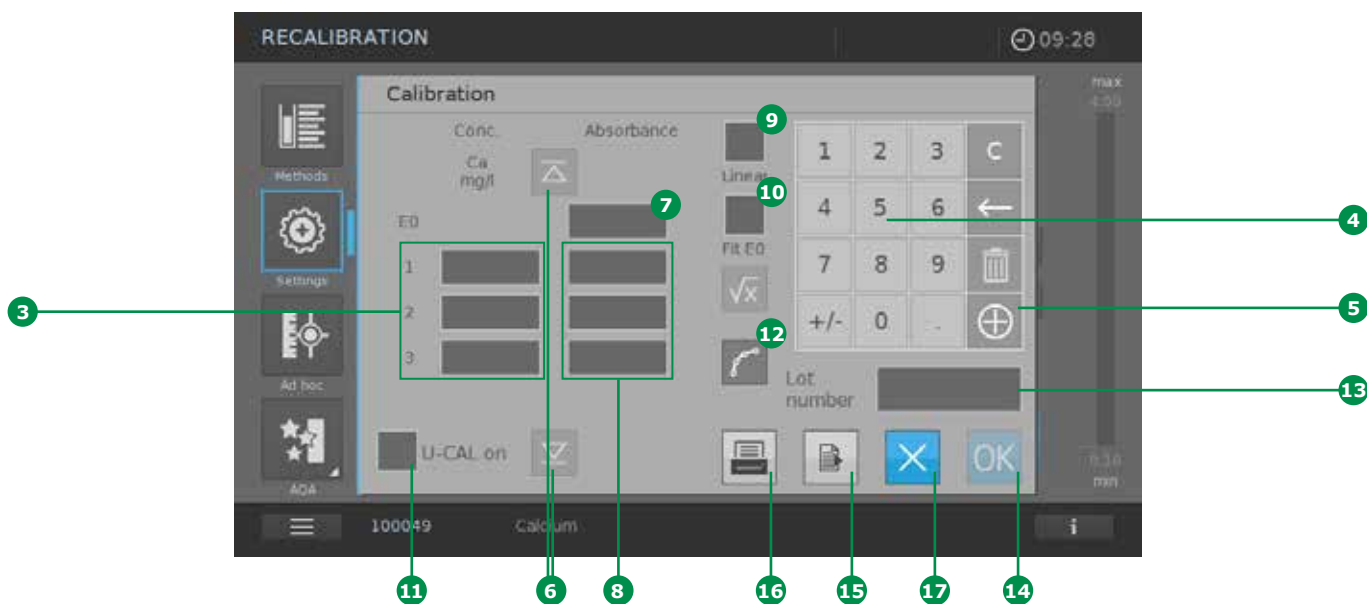
1. Select the method manually (see section 9.5.1), or by inserting a barcoded cell/ AutoSelector.

NOTE

If a zero adjustment has not been performed, the spectrophotometer informs you that you need to perform a zero adjustment.



2. Tap on the Settings button 1. The screen changes.
3. Tap on the Recalibration button 2. The screen changes.



4. Enter the user-defined nominal values (min 1/max 11) in the input fields provided **3** via the keyboard **4**. Tap on the "+" button **5** of the numerical keyboard to add lines for further value pairs. Use the cursor buttons **6** to navigate the screen up and down for the lines of the value pairs.
5. Activate the Absorbance button E0 **7** (a blue frame appears).
6. Insert the cell with E0 (reagent blank value). Measurement starts automatically.
7. The measurement result appears in the activated input field.
8. Activate the input field **8** of the absorbance of the next concentration.
9. Insert the cell with the measurement solution (= standard + reagents acc. to the method description of the selected method) of the activated concentration.
10. Insert cell with Standard 1 measuring solution. Measurement starts automatically.

NOTE

To calibrate further user-defined nominal values (max. 11), repeat steps 11 – 14 of the procedure. Be sure to activate each input field for the measurement values.

11. Activate the field "Linear" **9** to calculate a linear function. When "Linear" is not activated, a non-linear function of the second order is automatically calculated (square function).

NOTE

If you wish to calculate a linear function, you require at least the E0 value and 2 value pairs. If you wish to calculate a non-linear function, you require at least the E0 value and 3 value pairs.

12. "Fit E0" **10** can be activated as an additional option. With "Fit E0" activated, concentration 0 (= reagent blank value) intercepts the absorbance axis at the associated E0 value.

2

- 3 13. Activating the UserCalOn button **11** calculates the measurement results for the method based on the user-defined calibration that was performed. To restore the factory-set calibration for the method, deactivate the UserCalOn button **11**.
- 4 14. Once all values are available, you can tap on the field "Graph" **12** to view the calibration curve.

5

NOTE

The calculated function maps the calculation of a result (e.g. concentration) via a measured absorbance in the form of a polynomial equation of the following type:

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$$C = A0 + A1 \times (Abs - E0) + A2 \times (Abs - E0)^2$$

where:

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- C = measurement result (e.g. concentration)
- A0, A1, A2 = coefficients (polynomial)
- Abs = measured absorbance
- E0 = absorbance of the reagent blank value

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15. You can now enter an ID or a specific batch code for the calibration. Tapping on the field "Batch ID" **13** opens a virtual keyboard. Enter the code and confirm by tapping on the OK button **14**.

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16. To close the determination of the coefficients, confirm the data by tapping on the OK button **14**. If the field "U-CAL on" has been activated, an icon **18** pops up in the measurement display.
17. To call up the calibration data again, select Settings **1** and Recalibration **2** again.
18. Tap on the Export button **15** to transfer the data in the CSV format to an external storage medium.
19. Tap on the Print button **16** to print out the data.
20. To close the operation without accepting the data, tap on the X button **17**. All entered data are deleted.

9.7.11 MatrixCheck

The MatrixCheck function is used to check if the photometric determination is disturbed by other substances present in the sample (sample matrix). The MatrixCheck can be carried out by spiking or by diluting. The spectrophotometer enables a simplified MatrixCheck with the aid of the Spectroquant® CombiCheck R-2 addition solution or a pre-programmed ready-to-use standard. The MatrixCheck can be carried out immediately. The volumes required for the sample and standards are displayed on the screen. The MatrixCheck is then carried out with a single spiking. For the MatrixCheck with a standard of your own, however, you can enter the number of spikings or dilutions yourself (max. 3).

MatrixCheck by spiking

For the MatrixCheck by spiking, the photometric determination is repeated after a defined amount of analyte has been added to the test sample in the form of standard solutions. Recovery of the addition is automatically calculated as follows:

$$\text{Recovery of addition [\%]} = 100 \times \frac{\{\text{measurement value (sample + standard solution)} - \text{measurement value (sample)}\}}{\{\text{nominal value (sample + standard solution)} - \text{measurement value (sample)}\}}$$

A matrix disturbance is likely if recovery is less than 90% or more than 110%.

MatrixCheck by diluting

For the MatrixCheck by dilution, the photometric determination is repeated after the test sample has been diluted with distilled water.

The nominal value for the determination is calculated from the dilution, provided that there is no disturbance due to the sample matrix. After the photometric determination the measured value is compared with the nominal value and the recovery rate is calculated. A matrix disturbance is likely if recovery is less than 90% or more than 110%.

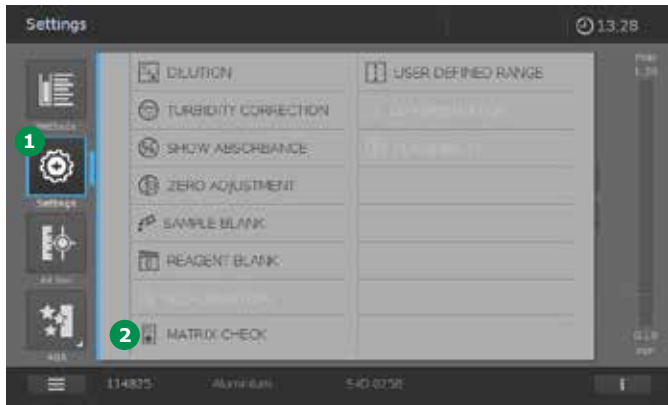
Practical instructions

- After evaluating the measured value of the sample, the spectrophotometer suggests for the MatrixCheck to spike or dilute the sample and standard with suitable volumes. For each spiking or dilution, the relevant nominal concentration value is displayed
- To be able to reliably recognize matrix effects by spiking, the increase in volume after spiking should be small
- To be able to reliably recognize matrix effects by diluting, the dilution factor should be high
- You can carry out the MatrixCheck as a series of measurements, consisting of up to three determinations with different spiking volumes or dilutions respectively
- Prepare all test sample solutions simultaneously at the beginning of the series of measurements

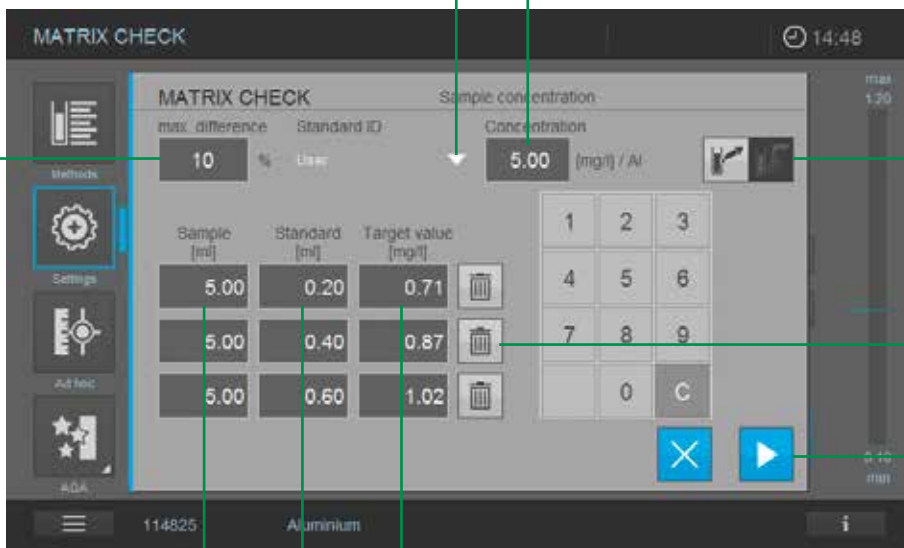
NOTE

The spectrophotometer suggests the optimal version for the MatrixCheck. Depending on the concentration of the sample in relation to the measuring range the spectrophotometer sets spiking or dilution. If both are possible you can make your own choice.

3 Performing the MatrixCheck

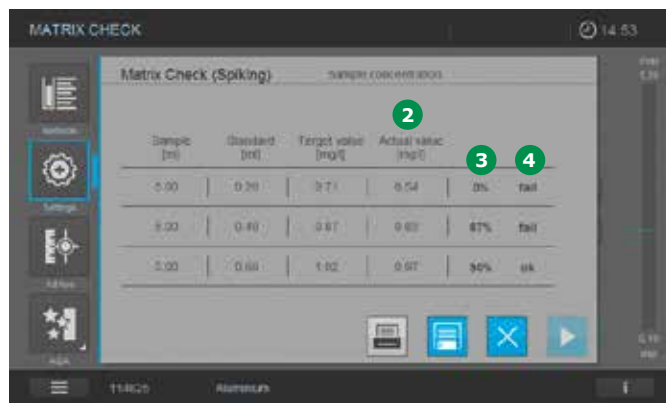
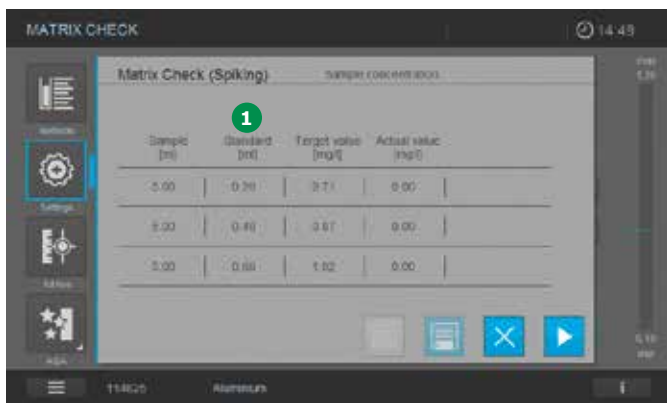


1. Measure the original sample without spiking or diluting it (see section 9.7).
2. The measured value is displayed.
3. Tap on the Settings button 1.
4. The screen changes.
5. Tap on MatrixCheck 2.
6. The screen changes. The following fields appear:
7. Perform the required settings if you wish to make your own choice 3, 4, 5, 9, 10.
8. Tap on the Start button 11.
9. The screen changes.



Item	Field name	Description
3	Toggle switch Dilution/Spiking	Dilution/Spiking option. (Acceptance of the instrument pre-sets is recommended. Switching the option is possible only as long as this does not cause values to be outside the measuring range.)
4	max. difference	Permitted deviation from the nominal value in%
5	Standard ID	Selection menu for factory-programmed standards or user-defined standard (concentration definable). This option is only active for spiking
6	Sample (ml)	Figure for the sample volume
7	Standard (ml)	Figure for the standard volume, in case of dilution the volume of distilled water is displayed
8	Target value (mg/l)	Expected measurement value
9	Concentration	Only active for user-defined standard (concentration definable).
10	Delete button	Remove rows that are not required

If Spiking is Active:



- Mix the sample with the defined standard 1 and perform the test procedure as described in the package insert.
- Insert the prepared cell.
- The instrument starts measuring automatically.
- Repeat this procedure for each standard addition.
- The display shows the actual value 2, recovery in% 3 and the assessment of the MatrixCheck 4 (ok/fail).

3 **If Diluting is Active:**



1. Dilute the sample as required **1** and perform the test procedure as described in the package insert.
2. Insert the prepared cell.
3. The instrument starts measuring automatically.
4. The display shows the actual value **5**, recovery in % **6** and the assessment of the MatrixCheck **7** (ok/fail).

7 **NOTE**

8 If the AutoStore function is active the results are stored automatically and can be recalled from the result list. If AutoStore is not active, the results are lost when the Close button **10** is touched. In this case touch Printer **8** or Save button **9** to store or print the results before closing the MatrixCheck.

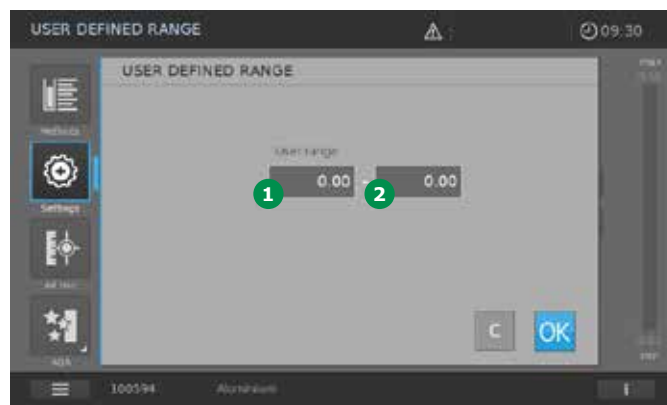
9.7.12 User-defined Range

The function "User-defined range" can be used to set acceptance ranges (limits) for measurement results. These acceptance ranges can be oriented to legal and/or other specifications.

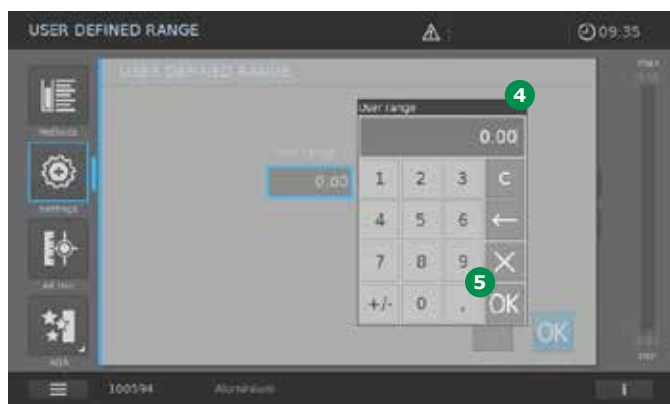
With the function activated and the lower and upper limits for measurement results set, the setting "User-defined range" is also shown in the measurement-range bar of the result screen. After the measurement has been made, the position of the measurement result on the measurement-range screen can be used to check whether it is within the defined limits. After selecting the method, the user-defined range can be activated as follows:



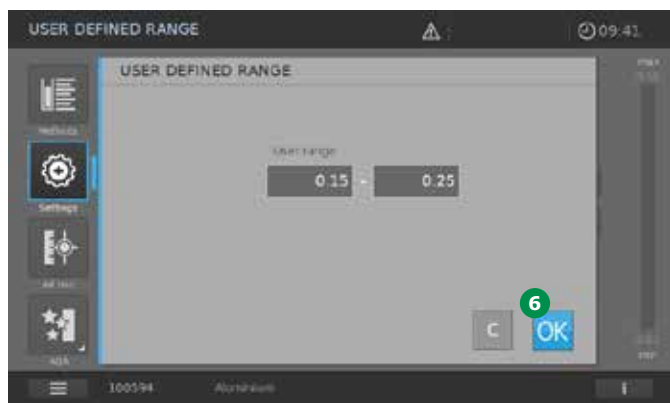
1. Open the menu "Method settings" **1**.
2. Select "User-defined range" **2**.



3. Activate the input field **3** for the lower limit.

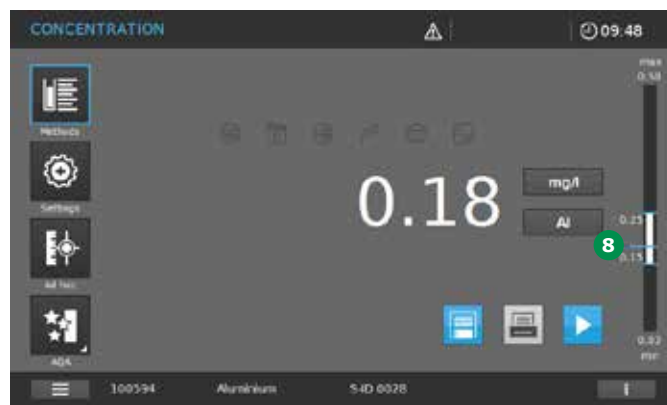


4. A virtual numerical keypad 4 pops up. Now enter the numerical value for the lower limit and tap the OK button 5 to confirm.
5. Repeat this procedure to enter the upper limit.

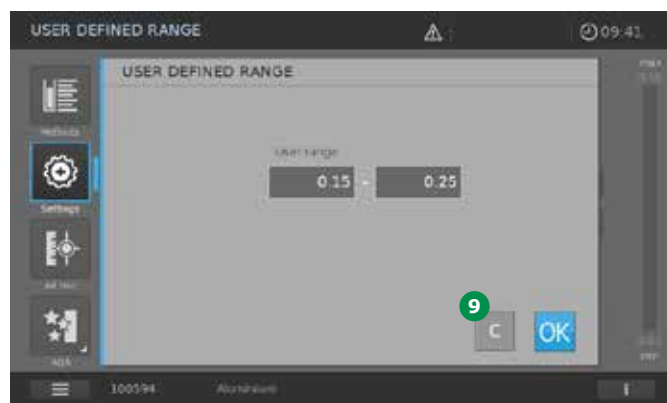


6. Tap the OK button 6 to accept the settings.
7. The screen changes to the Measurement mode.
8. The "User-defined range" setting is shown in the measurement-range bar 7 of the result screen.

9. The spectrophotometer is now ready to start the measurement.



10. After the measurement, the position of the measurement result is shown on the measurement-range screen 8.
11. To deactivate the user-defined range, open the "Settings" menu 1 and select "User-defined range" 2.



12. Tap on the "C" button 9. The user-defined range is reset. The upper and lower limits are shown as zero values.

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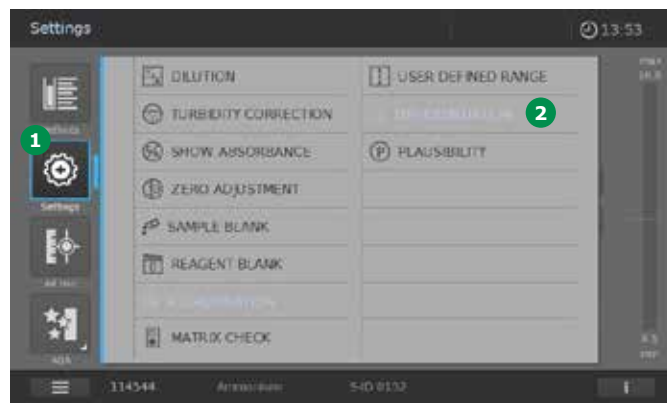
16



13. Accept settings by tapping on the OK button **10**.
14. The screen changes to the Measurement mode.
15. The spectrophotometer is now ready to start the measurement.

9.7.13 Differentiation

For certain methods there is a special "Differentiation" function that enables the user to differentiate between varying chemical formulas of the analyte when interpreting measurement results. In some methods for the determination of chlorine, for example, total chlorine can be distinguished from free chlorine and the proportion of bound chlorine can be automatically calculated and displayed. After selecting the method, you can activate the differentiation mode in the following manner:



1. Open the menu "Method settings" **1**.
2. Select "Differentiation" **2**.



3. Activate the differentiation function by tapping on the shift key **3**. The function is activated when "I" appears against a light gray background **3**.
4. Accept the settings by tapping on the OK button **4**.
5. The screen changes to the mode "Measurement with differentiation".
6. The spectrophotometer is now ready to start the measurement.

NOTE

For those methods for which the differentiation option is available, the procedures for activation and the measurement are individually described in detail in the manual section "Analytical Procedures and Appendices".



7. To deactivate the differentiation function, open the menu "Method settings" **5**. The submenu shows the available settings options.
8. Select "Differentiation" **6**.
9. Deactivate the differentiation function by tapping on the shift key **3**. The function is deactivated when "0" appears against a light gray background.
10. Accept the settings by tapping on the OK button **4**.
11. The screen changes to the Measurement mode.
12. The spectrophotometer is now ready to start the measurement.

9.7.14 Plausibility

The function "Plausibility" is available for the ammonium methods.

Once it has been activated, the function remains permanently switched on for all ammonium methods.

NOTE

In the practical environment it has emerged that when the sample contains very high ammonium concentrations a different color occurs and the measurement signal in the photometric measurement is no longer proportional to the ammonium concentration.

In these cases, the reaction solution is no longer yellow-green to green in color, the yellow component becomes diminished, and the solution turns turquoise to blue in color.

In this case a reliable statement on the ammonium content is no longer possible, in the worst case resulting in a substantial misinterpretation of the ammonium content with serious consequences for the environment. When the optional plausibility check in the Prove plus spectrophotometer is activated, the measurement is carried out at several wavelengths and the yellow component of the reaction solution is also measured. The Prove plus spectrophotometers are thus capable of recognizing this deviation in the color and giving a corresponding warning signal.

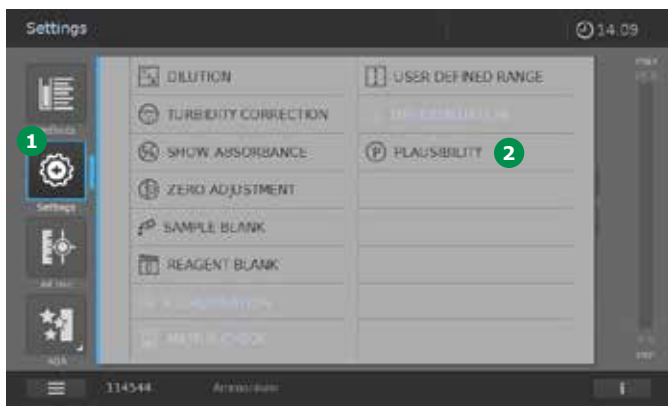
This plausibility check helps the user to avoid misinterpreting the results of the ammonium concentration.

1 9 Operation – 9.7 Measuring in Concentration Mode

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3 After selecting the method, you can activate the plausibility check in the following manner:

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NOTE

The active status of the plausibility check function is shown on the display by the symbol 5.

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1. Open the menu "Method settings" 1.
2. Select "Plausibility" 2.

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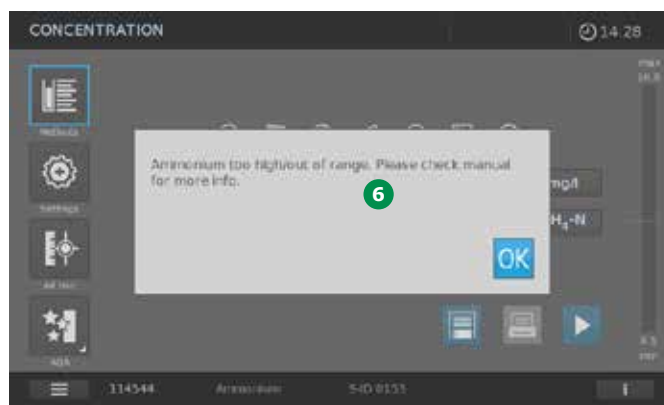
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3. Activate/deactivate 3 the plausibility check function with 0 = deactivated or 1 = activated (light gray).
4. Accept the settings by tapping on the OK button 4.
5. The screen changes.
6. The spectrophotometer is now ready to start the measurement.

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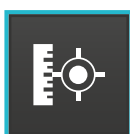


NOTE

If the plausibility check function is active and a very high ammonium concentration is present in the sample (concentration considerably beyond the measuring range of the selected method), a window with a warning message 6 pops up. After confirming by tapping on the OK button, the measurement result is shown as "---" 7.

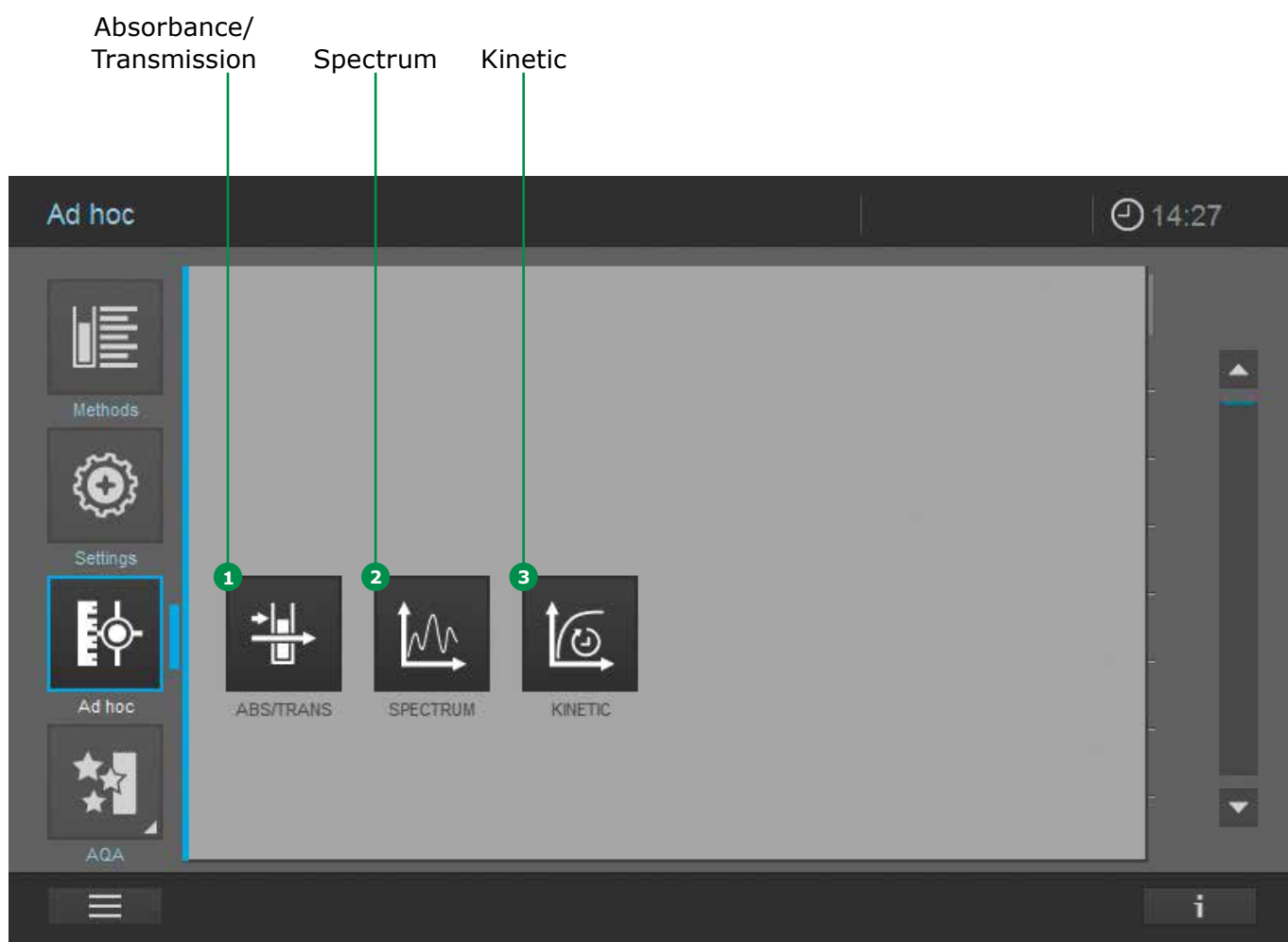
NOTE

If a zero cell (cell with distilled water) is measured as the sample when the plausibility check function is active, the warning message and the result “---” 7 also appear. The reason for this is that the zero cell does not show the yellow color described above.



9.8 Ad hoc Measurement (without selecting a specific method)

Tapping on the ad hoc button in the main menu changes the screen and the folder that allows the type of ad hoc measurement to be selected.





9.8.1 Ad hoc ABS/TRANS Measurement

Proceed as follows to perform an ad hoc ABS/TRANS measurement.



1. Select type of measurement: absorbance or transmission measurement by tapping on the button **1** for the required measurement (the activated selection is light grey).
2. Define the wavelength(s) for the measurement(s). Do this by tapping on the button **2**. A blue frame appears. Now enter the required wavelength by tapping on the keypad **3**.

NOTE

Tapping on the + button **4** brings up a new input field. Different wavelengths can be programmed for the measurement. The selection can be deleted by tapping on the Delete symbol **5**.

NOTE

Invalid entries are shown in red and cannot be accepted.

3. Confirm your input by tapping on the Start button **6**.
To cancel, tap on the X button **7**.

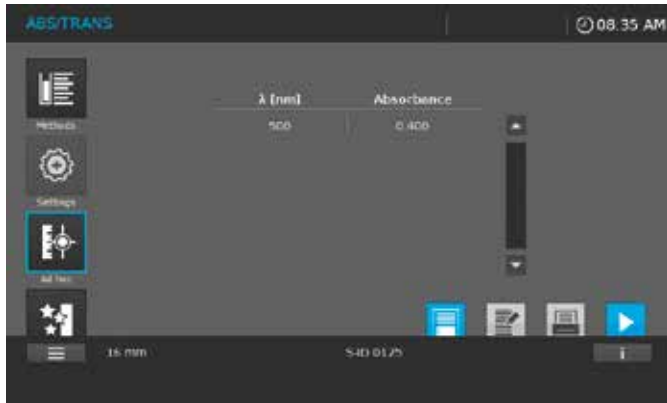


4. The screen changes **8**.
5. Perform zero adjustment by inserting a cell with distilled water or tapping on the Start zero button **9**.



6. The Start zero button changes to the Start button. The instrument is ready to start measuring.
7. Start the measurement by inserting a cell with sample or tapping on the Start button **11**. The measurement results are displayed in the absorbance column **10**.

Content of the information bar in ABS/TRANS measurements



16 mm

S-ID 0125

Path length of inserted cell Sample ID with prefix "S-ID"

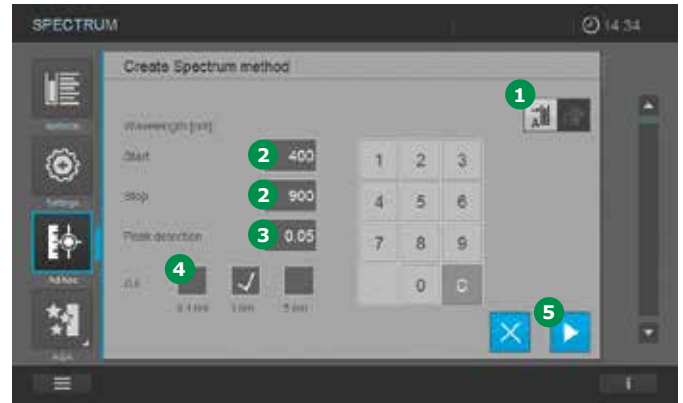
empty

empty



9.8.2 Ad hoc Spectrum Measurement

Proceed as follows to perform a spectrum measurement.



NOTE

A spectrum can comprise up to a maximum of 1000 measurement points. If the entry is invalid, it is shown in red and cannot be accepted.

1. Select type of measurement: absorbance or transmission measurement by tapping on the button ① for the required measurement (the activated selection is light grey).
2. Define the wavelength range for the method. Start & Stop ②.
3. Determine the sensitivity of the measurement ③.
4. Set the interval ④. Here you can choose between 0.1 nm, 1 nm, and 5 nm ④.

1 9 Operation – 9.8 Ad hoc Measurement (without selecting a specific method)

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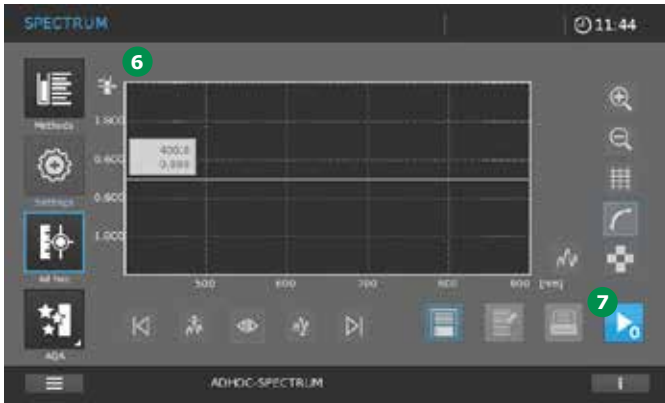
3

Content of the information bar for Ad hoc Spectrum Measurements

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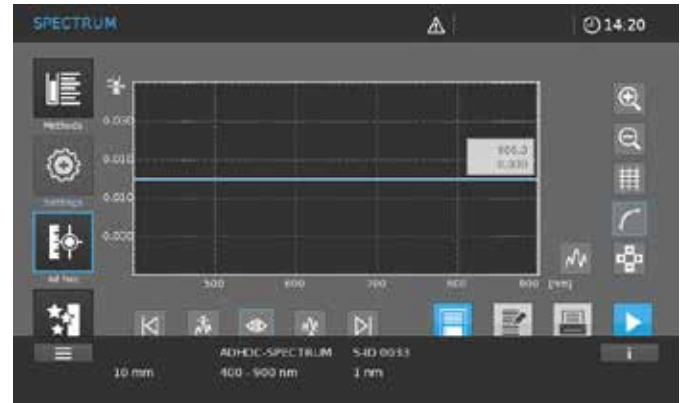
6



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5. Tap on the Start button 5.
6. The screen changes 6.
7. Perform zero adjustment by inserting a cell with distilled water or tapping on the Start zero button 7 (baseline determined).

8

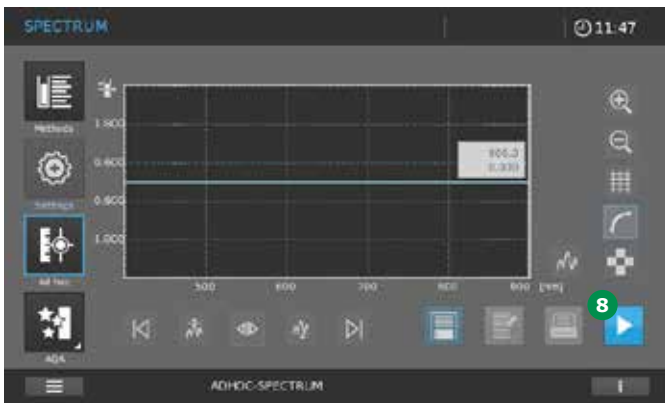


9

	ADHOC SPECTRUM	S-ID 0033
	Measurement mode	Sample ID with prefix "S-ID"
10 nm	400 - 900 nm	1 nm
Path length of inserted cell	Scan range	Scan interval
empty		

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8. Start the measurement by inserting a cell with sample or tapping on the Start button 8.
9. The screen changes, the instrument is ready to start measuring.

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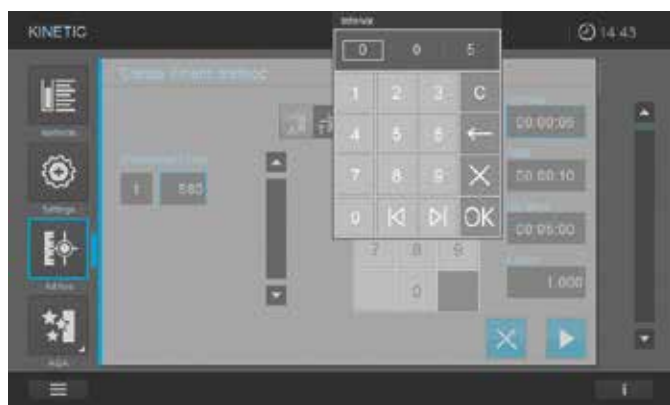
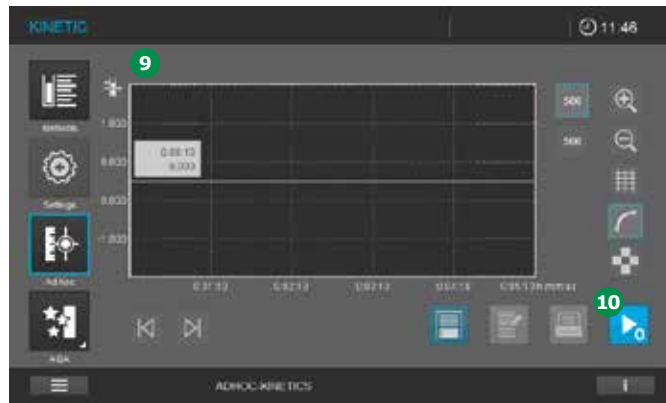
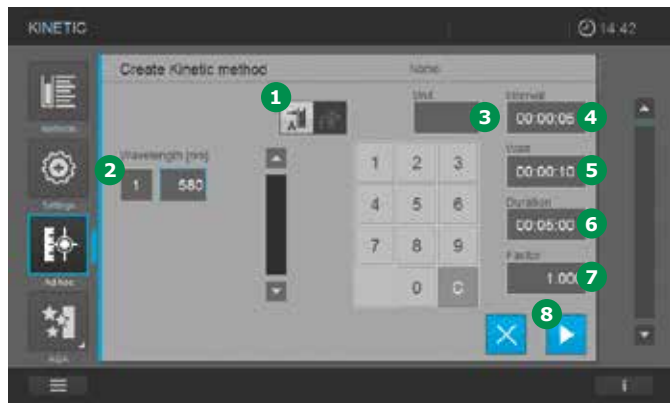
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9.8.3 Ad hoc Kinetic Measurement

Proceed as follows to perform a kinetic measurement.



- The screen changes (9).
- Perform zero adjustment by inserting a cell with distilled water or tapping on the Start zero button (10).



- Select type of measurement: absorbance or transmission measurement by tapping on the button (1) for the required measurement (the activated selection is light grey).
- Set the measuring range and the duration.
 - Wavelength (2)
 - Unit (3)
 - Interval (4)
 - Delay (5)
 - Duration (6)
 - Slope factor (7)

NOTE

Invalid entries are shown in red and cannot be accepted.

- Tap on the Start button (8).

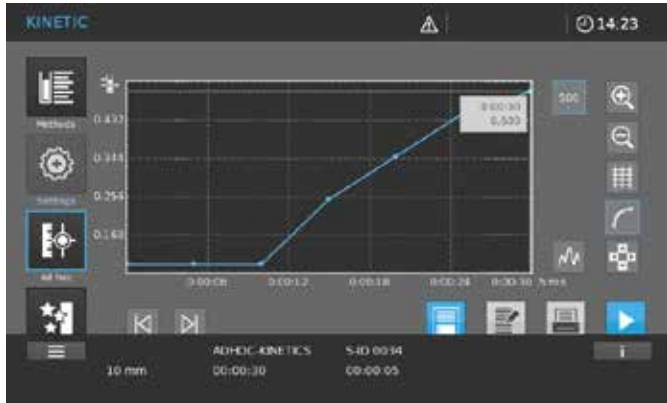
- Start the measurement by inserting a cell with sample or tapping on the Start button (11).
- The screen changes, the instrument is ready to start measuring.

9 Operation – 9.8 Ad hoc Measurement (without selecting a specific method)

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3 Content of the information bar for Ad hoc Kinetics Measurements

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ADHOC KINETIC S-ID 0034

Measurement mode Sample ID with prefix "S-ID"

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10 mm 00:00:30 00:00:05

Path length of inserted cell Duration Time interval

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empty

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9.9 Spectrum

9.9.1 General Information

With the Spectrum function, the absorbance or transmission in dependency on the wavelength is measured and recorded.

The wavelength range can be freely selected within the measuring range of the spectrophotometer. The interval is selectable (0.1 nm, 1 nm, 5 nm).

A spectrum can be recorded in ad hoc mode (see section 9.8), or loaded as a stored method (see section 9.6.6).

Baseline

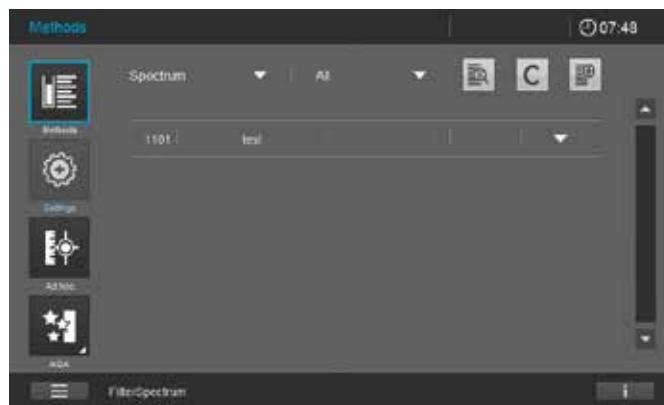
A baseline has to be recorded before a spectrum can be recorded. The baseline has to cover at least the wavelength range of the spectrum being recorded. Once the baseline is measured, it remains stored in the spectrophotometer until

- A new baseline is recorded
- Ad hoc Spectrum Mode is exited
- The loaded Spectrum method is exited
- The spectrophotometer is switched off

9.9.2 Recording the Spectrum

1. Select the method from the method list.

Record the baseline:



2. Zeroing against air: Tap on the Start zero button ①.
The spectrophotometer records the baseline.
- Or
- Zeroing against reference solution:
Insert cell with reference solution. The spectrophotometer records the baseline automatically.
3. Wait until the baseline has been fully recorded. Once the baseline has been recorded, the spectrophotometer is ready to start measuring.

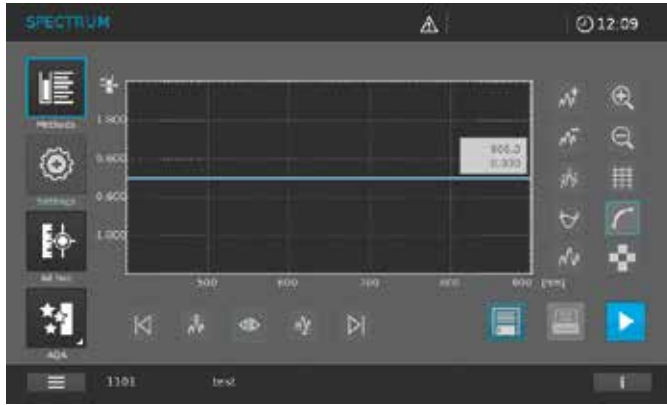
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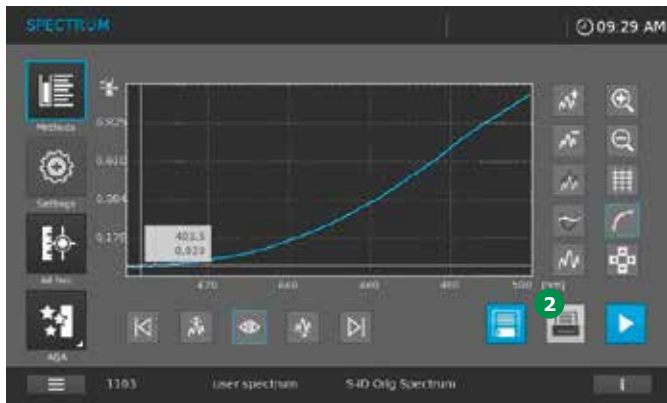
- Insert the cell with the sample vertically until it touches the bottom (rectangular cells should touch the left edge of the cell compartment; the opaque sides of the rectangular cell must point to the front and rear).

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- Recording of the spectrum starts automatically.
- Once the spectrum of your sample has been recorded you have the following options:
 - Evaluate the spectrum on the display immediately (see section 9.9.3)
 - Print the spectrum by tapping on the Printer button 2 either as a graph on a connected printer – or as a pdf file, if Print to pdf is activated and a USB device is connected
 - Save the spectrum to the result list. If AutoStore is on, this is done automatically

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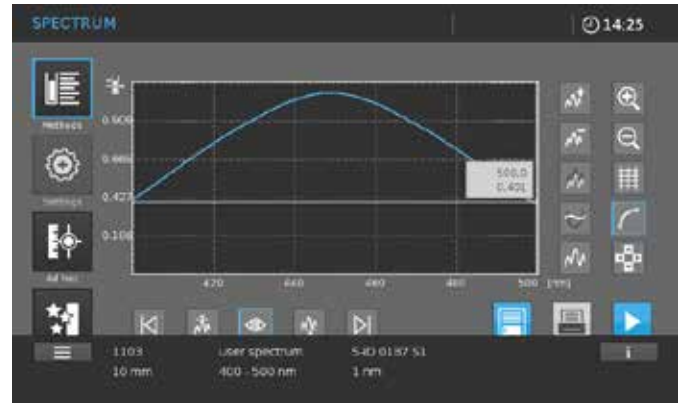
13

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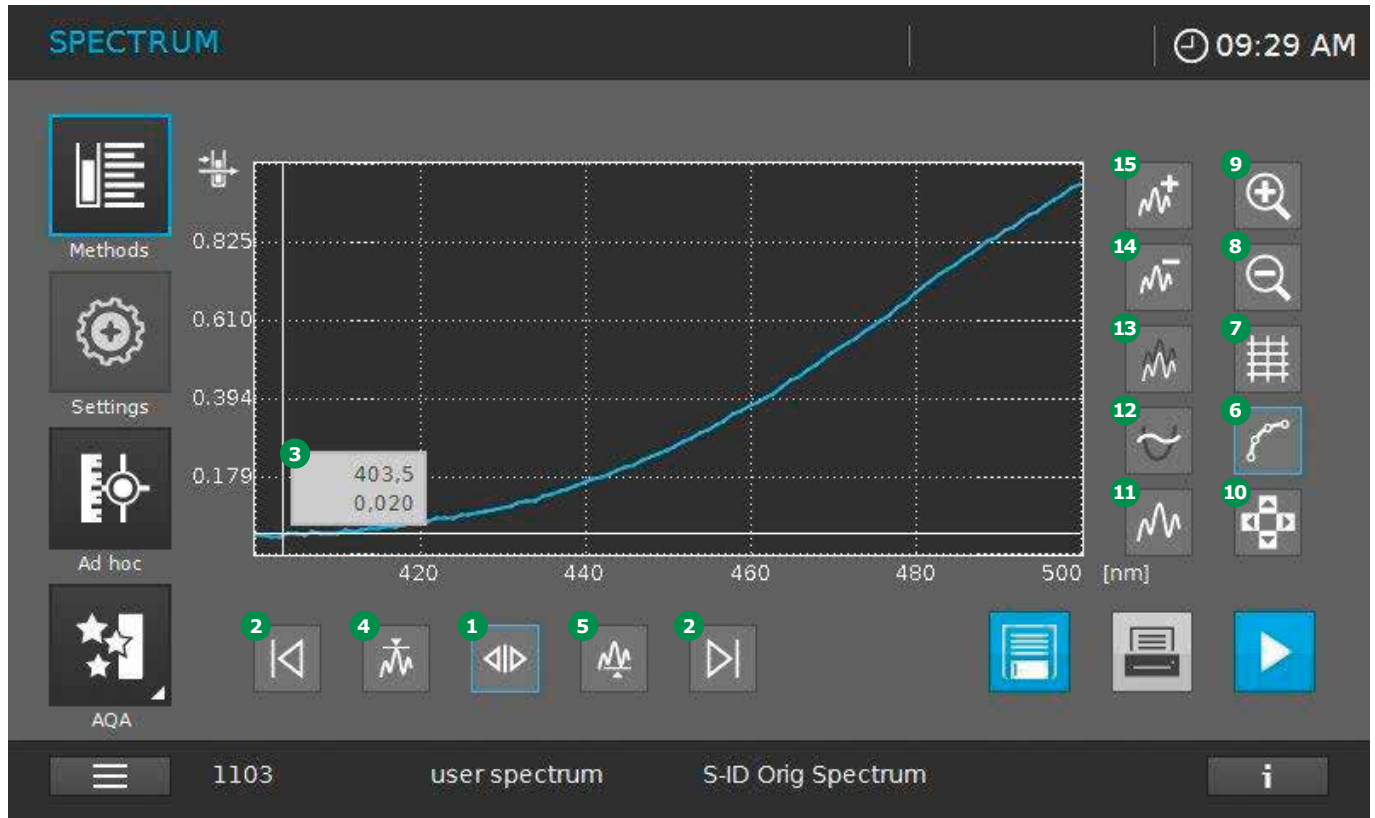
16

Content of the information bar in spectrum measurements



1103	user spectrum	S-ID 0187 S1
Method number	Method name	Sample ID with prefix "S-ID"
16 mm	400 – 500 nm	1 nm
Path length of inserted cell	Scan range	Scan interval
empty		

9.9.3 Evaluating a Spectrum



A spectrum can be evaluated immediately after measurement. Stored spectra can be loaded and evaluated from the results list as well. The following tools are available for editing:

- Moving to individual measurement points:
 - Activate action icon **1** and use the next left/next right icons **2** to move to all individual measurement points. The coordinates (wavelength and absorbance) of the respective measurement point appear in the Info box **3**
 - Activate icon **4** to move to maximum values and icon **5** to move to minimum values
- Switch between graph view **6** and table view **7**.
- In the graph view use icons **8** to zoom out and **9** to zoom in. Use navigation icon **10** to optimize the position of sections of the graph in the display.
- Tap icon **11** to return to the original spectrum.

- The following mathematical functions for various evaluating and calculating operations are available for selection:

- Derivate **12**: calculates the derivative of the total spectrum. To calculate the second and third derivative, the function can be carried out several times
- Compare spectrum **13**: loads a second spectrum into the same diagram for direct comparison
- Subtract spectrum **14**: subtracts a stored spectrum from the current spectrum
- Add spectrum **15**: adds a stored spectrum to the current spectrum

NOTE

The addition and subtraction of two spectra can be applied only to the common wavelength range of both spectra.

9.10 Kinetics

9.10.1 General Information

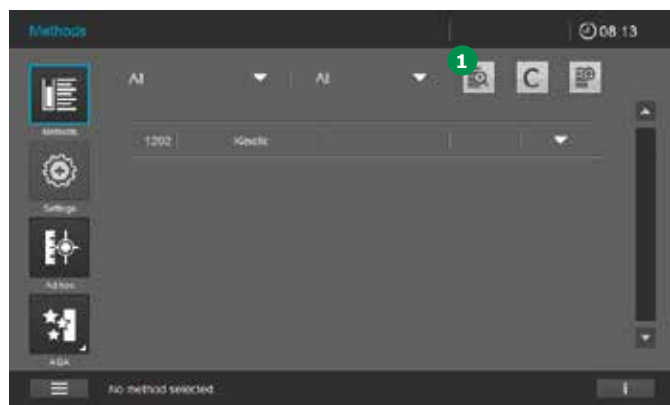
The kinetics function enables the temporal tracing of the absorbance or transmission of a sample at a certain wavelength.

The spectrophotometer automatically calculates the slope between two adjacent measuring points from the available measurement data.

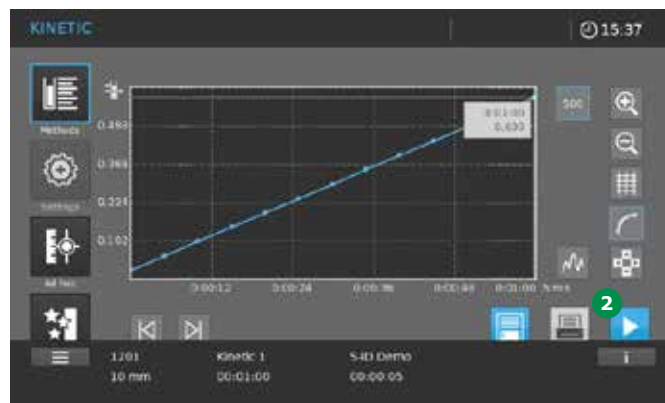
The catalytic activity can also be determined and displayed if required. To record the kinetics, the spectrophotometer carries out single measurements at regular intervals (measuring interval) and stores the measured values as a time function.

Kinetics can be recorded in ad hoc mode (see section 9.8), or loaded as a stored method (see section 9.6.7).

9.10.2 Recording Kinetics



1. Select the method from the method list by using the filter option **1**.

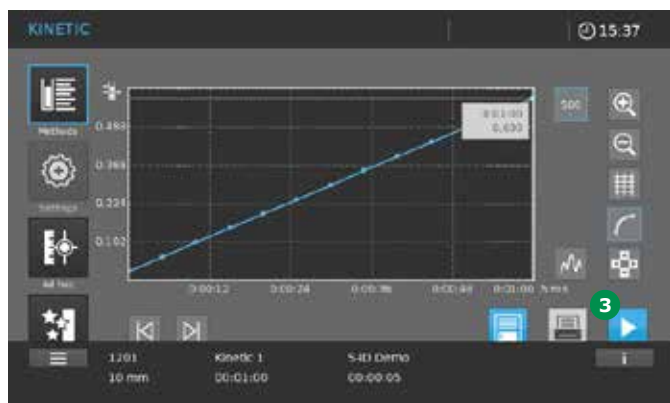


2. Once the kinetic method has been selected, the screen changes from the method list to the Kinetics screen. The Start zero button **2** is active.
3. Insert the zero cell according to cell type. Zero adjustment starts automatically.

NOTE

The zero adjustment can also be performed without a cell being inserted (measurement against air). Tap on the Start zero button to start the procedure.

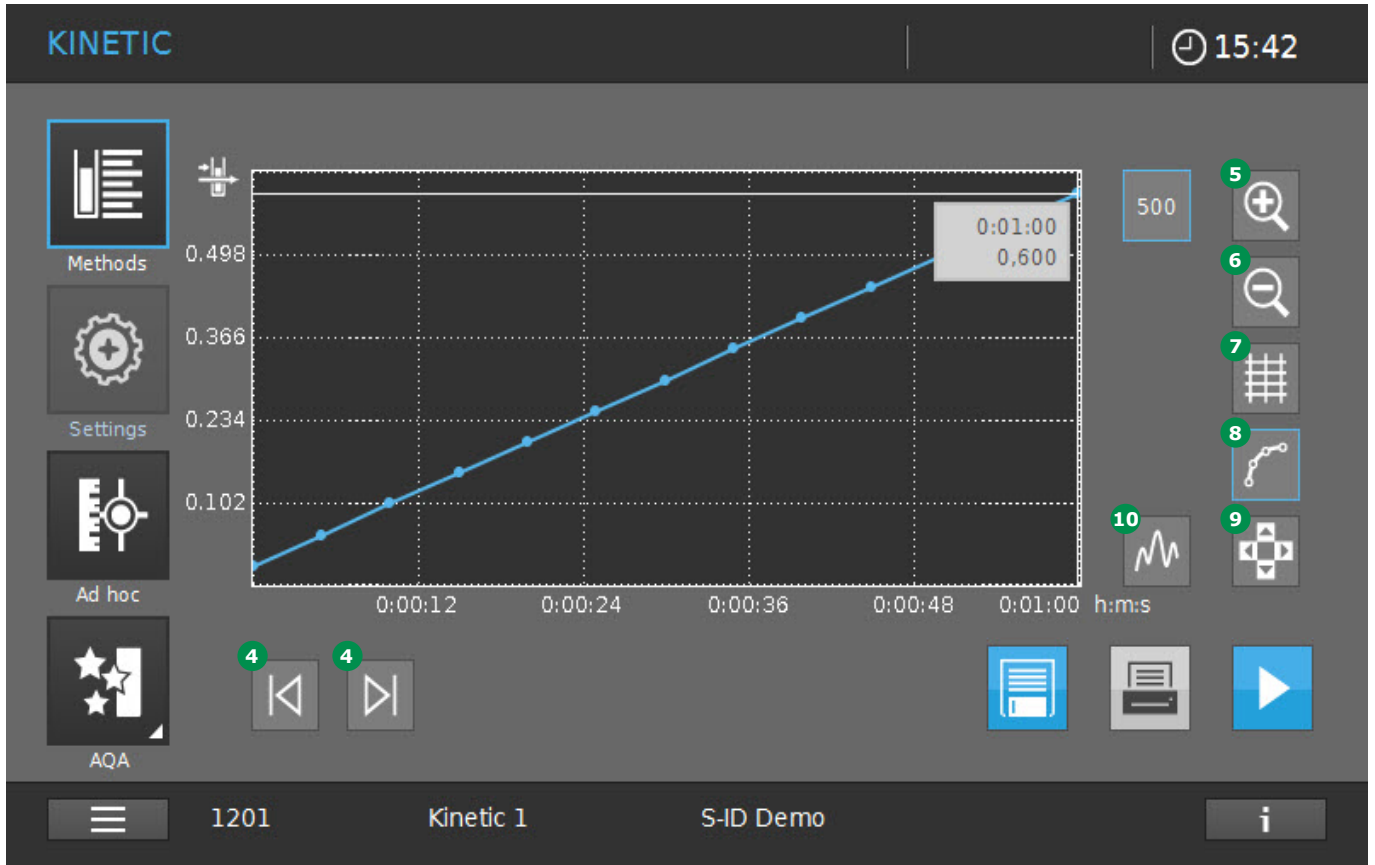
Content of the information bar in kinetics measurements



1201	Kinetic 1	S-ID Demo
Method number	Method name	Sample ID with prefix "S-ID"
10 mm	00:01:00	00:00:05
Path length of inserted cell	Duration	Time interval
empty		

- Following successful zero adjustment the Start zero button ② becomes the Start button ③.
- The instrument is ready to start measuring the sample.
- Insert the cell vertically until it touches the bottom (rectangular cells should touch the left edge of the cell compartment; the opaque sides of the rectangular cell must point to the front and rear).
- Recording of kinetics starts automatically.

9.10.3 Evaluating a Kinetic



A kinetic can be evaluated immediately after measurement. Stored kinetics can be loaded and evaluated from the results list as well. The following tools are available for editing:

- Left/Right tab function (4) to gradually scan the kinetics with the indication of x and y values
- Zoom function to scale a section up (5) or down (6)

- Change to tabular view (7)
- Change to graphic display (8)
- Cursor function (9) for incremental moves to ranges
- Call up original screen (10)



9.11 AQA (Analytical Quality Assurance)

General information

The objective of analytical quality assurance (AQA) is to secure correct and precise measurement results (see section 5).

NOTE

Only persons in the administrator user group have access to the settings for AQA checks. Every registered user can carry out the AQA check (see section 9.14).

Analytical quality assurance (AQA) can be carried out in two steps independent of each other:

- AQA1: Monitoring of the spectrophotometer
- AQA2: Total system monitoring.

AQA2 covers the spectrophotometer, the test that is used, the accessories and the user's way of working. Monitoring includes a check procedure that has to be successfully repeated by the user within a certain period (AQA interval).

NOTE

AQA monitoring is not active in the delivery state.

9.11.1 Spectrophotometer Monitoring (AQA1)

At least one set of test standards such as Spectroquant® PhotoCheck or Certipur® is required for spectrophotometer monitoring. The administrator specifies which test standard has to be used as the minimum requirement for AQA1 monitoring. The extent of the monitoring can be expanded with further test standards. The following can be tested:

- Photometric accuracy
- Wavelength accuracy
- Stray light test
- Spectral resolution (only Prove 600 plus)

NOTE

Only persons in the administrator user group have access to the settings for AQA checks. Every registered user can carry out the AQA check (see section 9.14).

Photometric accuracy

Normally test items of known absorbance values at defined wavelengths are used to monitor photometric accuracy. The instrument is pre-programmed with standard AQA1 tests that can be performed using Spectroquant® test items. Such test items are, for instance: Spectroquant® PhotoCheck, Certipur® UV/VIS-Standard 1A, Certipur® UV/VIS-Standard 1.

Each pack is provided with a lot-dependent test certificate with all nominal values (absorbances) and tolerances of the test standards. These nominal values and tolerances are already pre-programmed in the spectrophotometer. Compare them with the lot-dependent values and adjust them if needed (see section 9.11.8).

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NOTE

The value of the tolerance consists of the tolerance of the standard (listed in the lot-specific certificate) and the specified tolerance of the spectrophotometer (see [Technical Data Section 12](#)).

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NOTE

Pay attention to the stability of the test standard. A check on the values in the spectrophotometer is required whenever a new pack of test standards is used. The values must be adjusted if necessary.

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Wavelength accuracy

Normally test items of known absorbance maxima at defined wavelengths are used to monitor wavelength accuracy. The instrument is pre-programmed with standard AQA1 tests that can be performed using Spectroquant® test items. Such test items are, for instance: Certipur® UV/VIS-Standard 6.

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Each pack is provided with a lot-dependent test certificate with all nominal values (wavelengths with absorbance maxima) and tolerances of the test standards. These nominal values and tolerances are already pre-programmed in the spectrophotometer. Compare them with the lot-dependent values and adjust them if needed (see [section 9.11.8](#)).

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NOTE

The value of the tolerance consists of the tolerance of the standard (listed in the lot-specific certificate) and the specified tolerance of the spectrophotometer (see [section 12](#)).

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Stray light test

Normally test items with edge filter properties are used to monitor the effects of stray light. The instrument is pre-programmed with standard AQA1 tests that can be performed using Spectroquant® test items. Such test items are, for instance: Certipur® UV/VIS-Standard 2. Each pack is provided with a lot-dependent test certificate with all nominal values and tolerances of the test standards. These nominal values are already pre-programmed in the spectrophotometer. Compare them with the technical data of the spectrophotometer (see [section 12](#)).

NOTE

The value of the tolerance consists of the tolerance of the standard (listed in the lot-specific certificate) and the specified tolerance of the spectrophotometer (see [section 12](#)).

Spectral resolution

Spectral resolution can be monitored using the spectrum of a 0.02% solution of toluene in hexane. The minimum ratio between the absorbance in the maximum at 269 nm and the absorbance in the minimum at 266 nm is a measure for the spectral resolution. The instrument is pre-programmed with standard AQA1 tests that can be performed using Spectroquant® test items. The test item used here is: Certipur® UV/VIS-Standard 5.

9.11.2 Total System Monitoring (AQA2)

For total system monitoring, standard solutions with a defined analyte content are required.

NOTE

Only persons in the administrator user group have access to the settings for AQA checks. Any registered user can perform the AQA2 test. Spectroquant® CombiCheck standards are ready-to-use multiparameter standards, i.e. they can be used for several test kits (methods). Standard solutions are ready-to-use single-parameter standards, i.e. they can be used for single test kits (methods). In addition to the above solutions, single-parameter standard solutions (z.B. Certipur®) can also be used. They are adjusted by dilution to the respective end concentration. The end concentration should be approximately in the middle of the measuring range.

NOTE

Suitable CombiCheck standards and single-parameter standards are listed in the catalog "Water, Food and Environmental Analytics" or on the Internet.

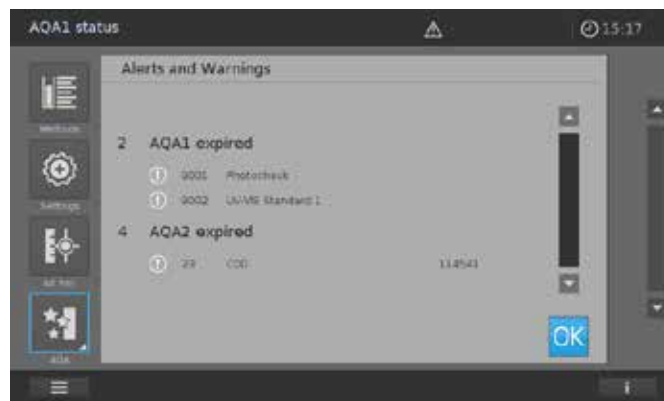


9.11.3 AQA Overview

This main menu offers the following submenus:



Item	Designation	Description
1	AQA1 status	Summary of the status of all activated AQA1 tests. (OK, fail, expired, next test in xx days)
2	AQA2 status	Summary of the status of all activated AQA2 tests. (OK, fail, expired, next test in xx days)
3	AQA1	Activate, edit, perform and create AQA1 tests
4	AQA2	Activate, edit, perform and create AQA2 tests
5	PipeCheck	Perform pipette check tests
6	Attention	Activated AQA1 test(s) and/or AQA2 test(s) are failed or expired. Tapping the symbol changes the display and opens an overview of the AQA tests involved.



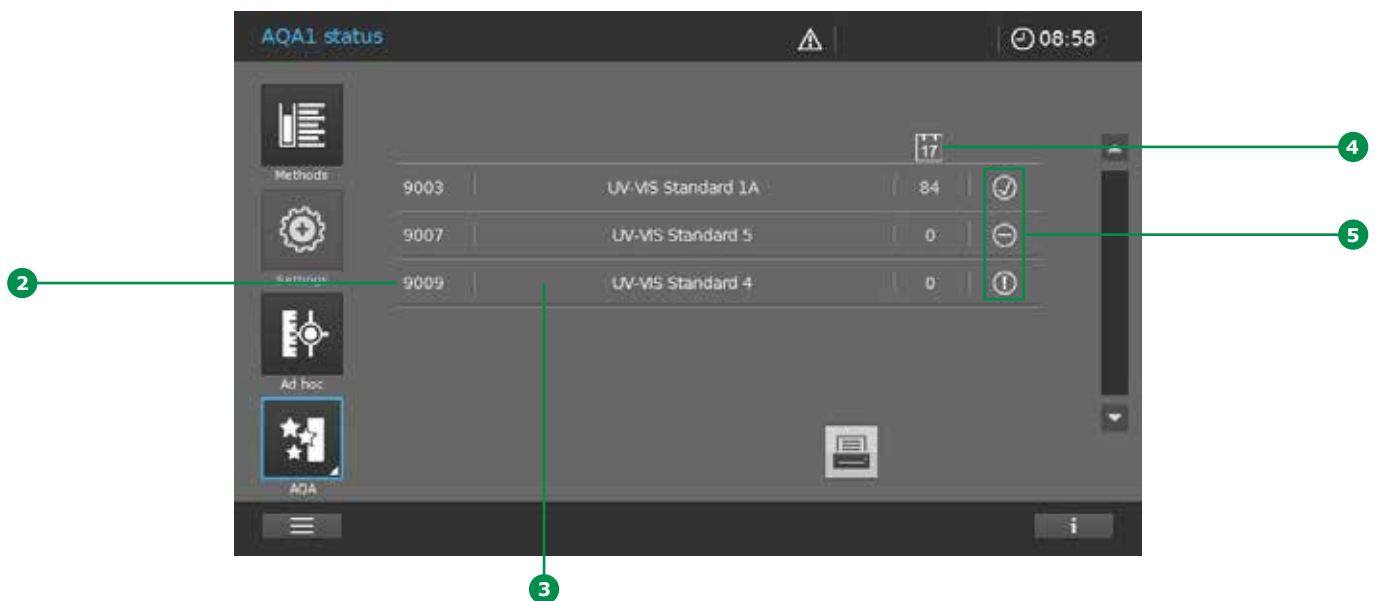


9.11.4 Perform AQA1 Status Check

To check the current AQA1 status of the instrument, proceed as follows.



1. Tap on the AQA1 status button 1.
2. The screen changes and a status overview of the activated AQA1 tests is shown.



3. The screen shows the following information:
 - AQA1 method number 2
 - Name of the AQA1 test 3
 - Number of days for which the AQA1 test is still valid before a new test has to be performed 4
 - Three different status symbols 5:
 - ⊙ = expired/invalid; ✓ = test OK; ⊖ = test failed
4. For quality or documentation purposes we recommend printing the list.

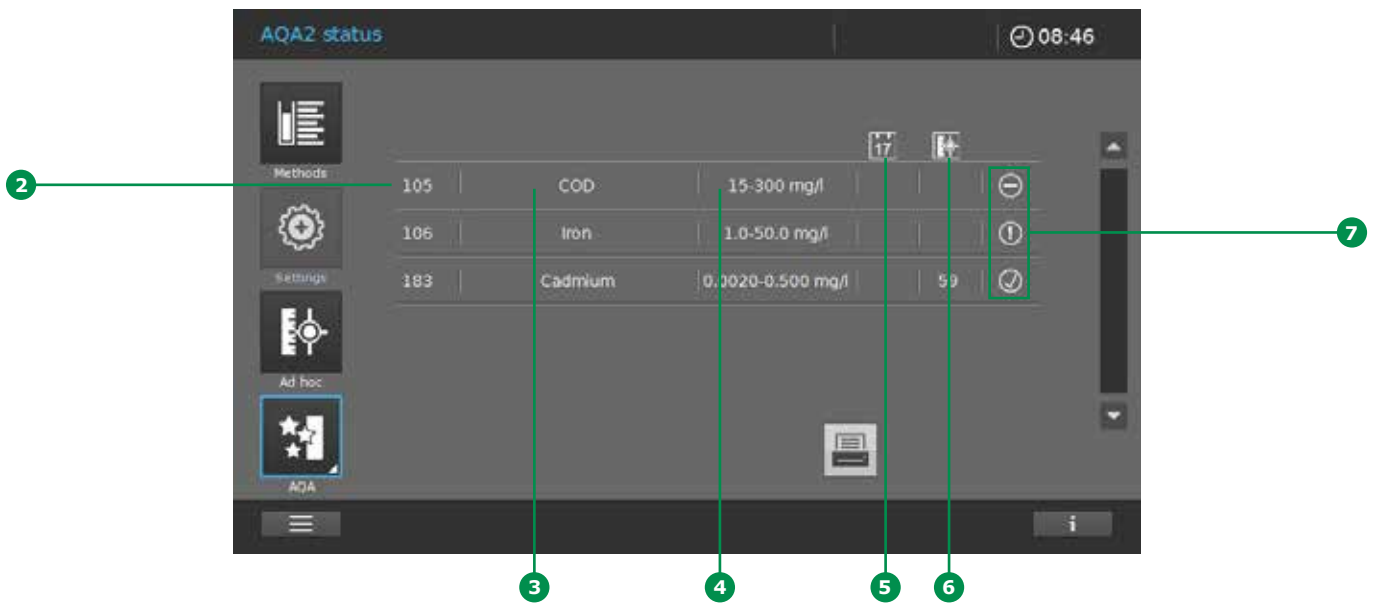


9.11.5 Perform AQA2 Status Check

To check the current AQA2 status of the instrument, proceed as follows.



1. Tap on the AQA2 status button 1.
2. The screen changes and a status overview of the activated AQA2 tests is shown.



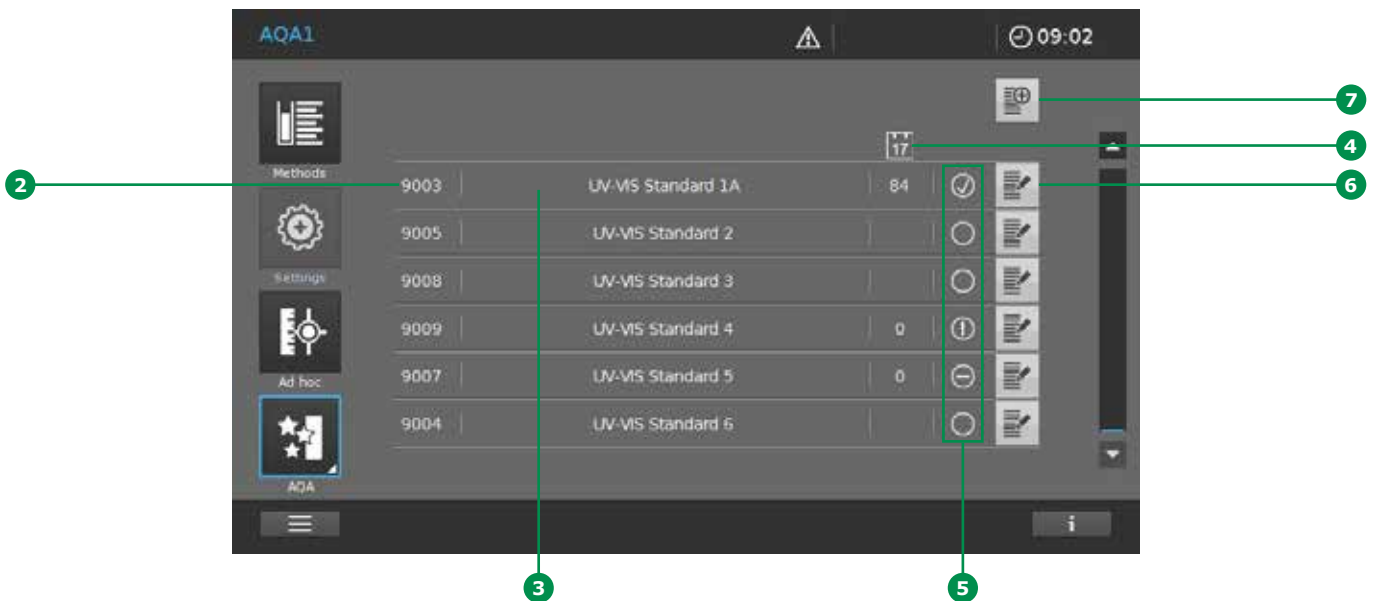
3. The screen shows the following information:
 - AQA2 method number 2
 - Name of the AQA2 test 3
 - Measuring range of the AQA2 check function 4
 - Number of days for which the AQA2 test is still valid before a new test has to be performed 5, or number of measurements before a new test has to be performed 6
 - Three different status symbols 7:
 - ⓘ = expired/invalid; ✓ = test OK; ⊖ = test failed
4. For quality or documentation purposes we recommend printing the list.



9.11.6 AQA1 Selection List



1. Tap on the AQA1 button ①.
2. The screen changes and a list of all AQA1 tests stored in the instrument is shown.

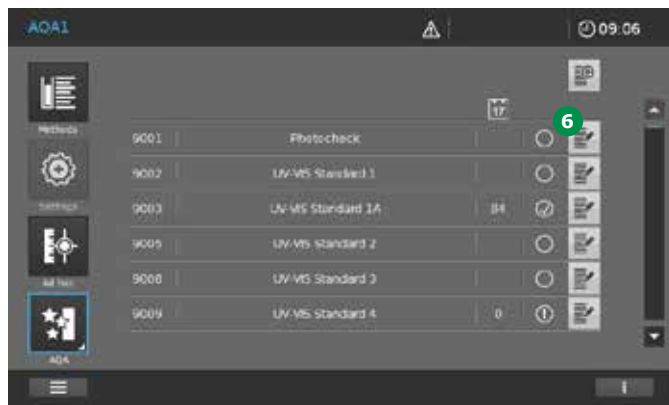


3. The screen shows the following information:

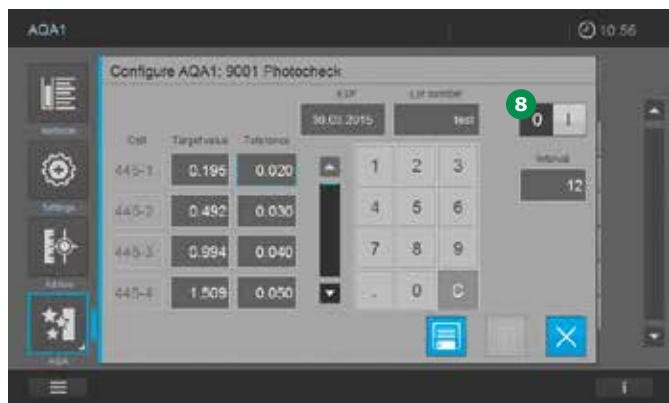
- AQA1 method number ②
- Name of the AQA1 test ③
- Number of days for which the AQA1 test is still valid before a new test has to be performed ④

- Three different status symbols ⑤ to remind you that a test is due. Ⓜ = expired/invalid; ✓ = test OK; ⊖ = test failed
- An empty circle ○ means that the AQA1 test is not activated
- Input buttons for editing ⑥ and creating ⑦ AQA1 tests

9.11.7 Activating and Deactivating an AQA1 Test



1. Tap on the Edit button **6**.



2. The screen changes.
3. Tapping on the ON/OFF button **8** activates/deactivates the AQA1 test. (I = on, 0= off, the light grey background shows which state is active).

NOTE

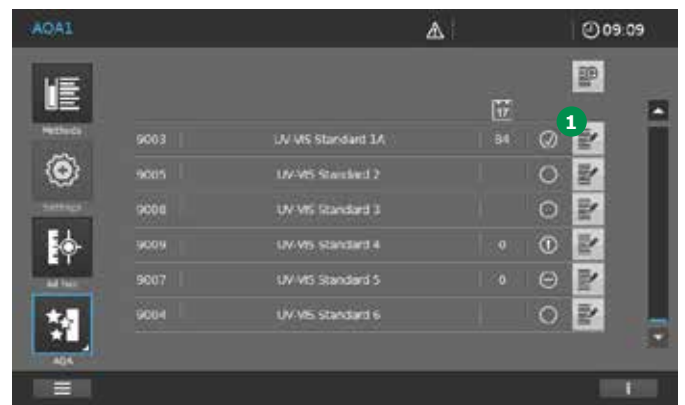
Before activating the lot-specific values for the current test item, compare with the existing entries for the input fields and make changes accordingly (see section 9.11.8).

9.11.8 Editing an AQA1 Test

Depending on the test type selected

- Photometric accuracy
- Wavelength accuracy
- Stray light test
- Spectral resolution (Prove 600 plus only)

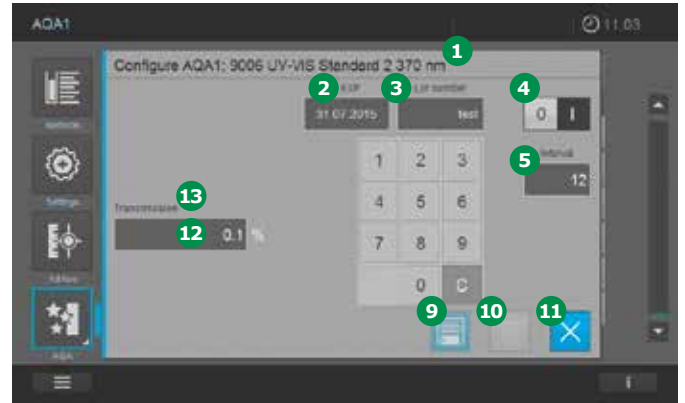
the particular display screen changes. The input values should be taken from the lot-specific certificates for the test items and adjusted to suit as follows:



1. Tap on the Edit button **1**.
2. The screen changes. Depending on the AQA1 test selected a type-specific screen appears. Make the AQA1 type specific changes in the corresponding screen (see following screens and table).

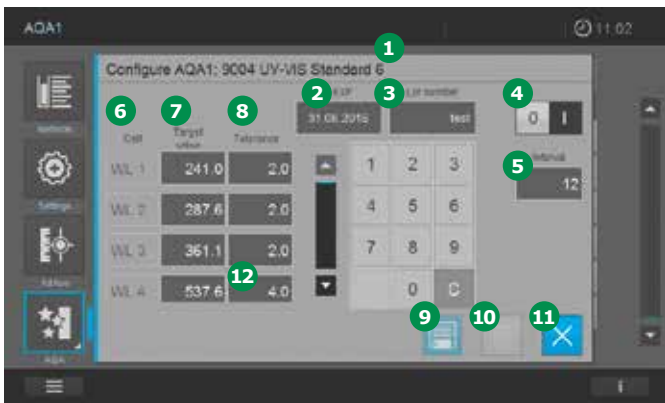
Photometric accuracy (P)

Stray light test (S)



Wavelength accuracy (W)

Spectral resolution (Prove 600 plus only) (R)



Item	Display field	Description	Test type
1	Name	Name of the test item	P, W, S, R
2	EXP	Expiry of the test item as shown in the certificate	P, W, S, R
3	Lot number	Lot number of the test item as shown in the certificate	P, W, S, R
4	"0"/"I" (OFF/ON)	Deactivate/activate the test	P, W, S, R
5	Interval	Test interval (input in weeks). For an active test the instrument reminds you when an AQA1 test is due.	P, W, S, R
6	Cell	Pre-set name of the cell	P, W
7	Target values	Lot-specific nominal values	P, W
8	Tolerance	Tolerance range for the measurement value. (Tolerance = measurement uncertainty of the test item + specification of the spectrophotometer)	P, W
9	Save	Adopt values into the instrument	P, W, S, R
10	Delete	Delete user-defined AQA1 tests	P, S
11	Close	Close display field	P, W, S, R
12	Numeric field	Touch the individual field to enter values	P, W, S, R
13	Transmission	Pre-set instrument-specific value (in% transmission)	S
14	Nominal (Amax/Amin)	Pre-set instrument-specific value (minimum ratio between absorbance in the maximum and absorbance in the minimum)	R

3. Make your individual changes in the type-specific screens and store them by the Save button 9. To close the editing screen touch the Close button 11.

NOTE

AQA1 tests pre-programmed by the manufacturer (e.g. PhotoCheck) cannot be deleted.

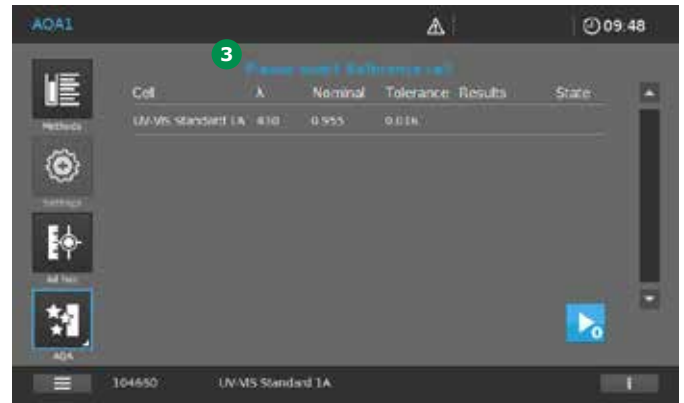
9.11.9 Performing an AQA1 Test



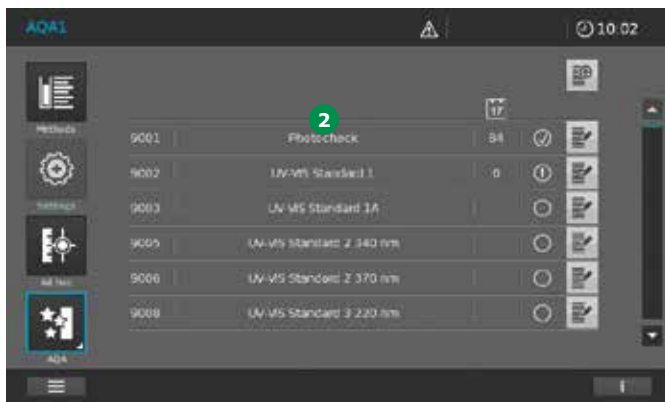
NOTE

In order to perform an AQA1 test it must be activated (see section 9.11.7).

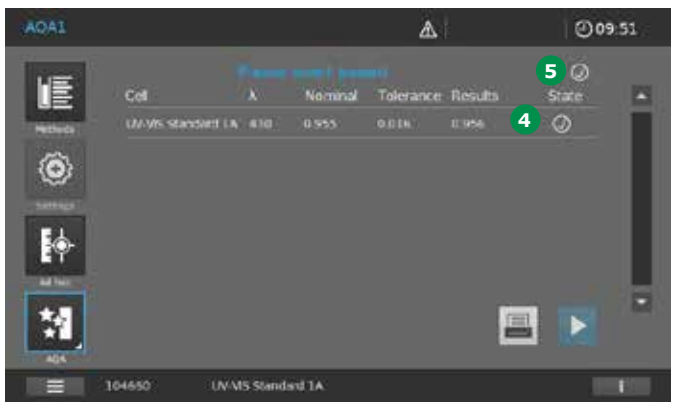
1. Tap on the AQA1 button ①.



4. The screen changes. A type-specific screen appears.
5. For further actions follow the on-screen commands ③.
6. Insert the corresponding reference cell (e.g. the zero cell as reference cell in the Photo-Check).
7. Insert following test cell as prompted in the command line.



2. The screen changes and you are presented with a list of all AQA1 tests stored in the instrument.
3. Select an AQA1 test by tapping on its name ②.

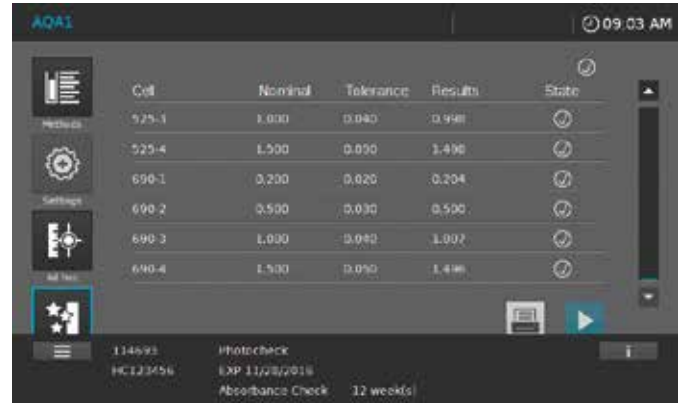


8. A tick appears following a successful test ④.
9. If all test steps are successful and the AQA1 test is passed, a tick appears in the command line ⑤.

NOTE

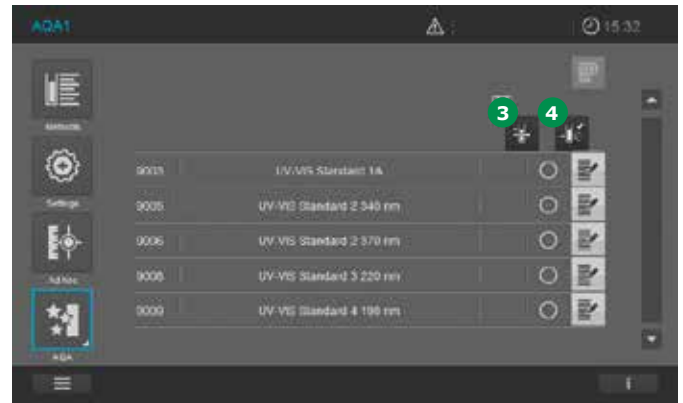
If the test has failed, a ⊖ symbol appears in the display instead of the tick ④ symbol for a successful test. If it is necessary to insert multiple cells in succession during the test and one of the individual test steps does not pass, check whether you have used the correct cell as prompted in the command line. Repeat the measurement with the correct cell. If one of the individual test steps in a multiple series is not passed, the AQA1 is not passed and the procedure is terminated.

Content of the information bar in AQA1 measurements



114693	PhotoCheck	
Article number (first 6 digits of order no.)	Method name	
HC123456	EXP 11/28/2016	12 week(s)
Lot number item	Expiration date item with Prefix "EXP"	Interval
	Absorbance check	12 week(s)
	Description of the checked function	Interval

9.11.10 Creating a User-defined AQA1 Test



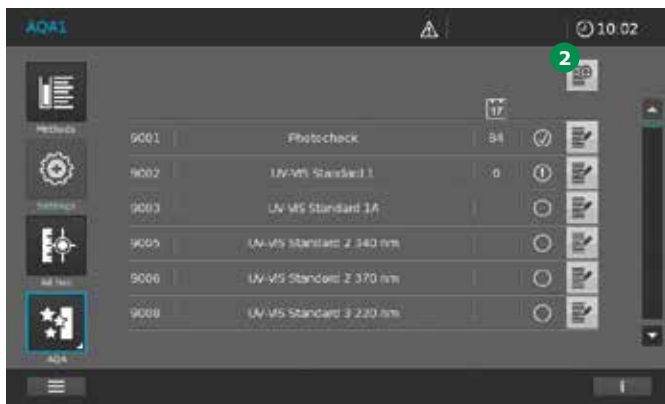
It is possible to create two different user-defined types of AQA1 tests.

- Photometric accuracy
- Stray light test

1. Tap on the AQA1 button ①.

4. The screen changes. In addition, selection options appear for the two types listed above (photometric accuracy ③; stray light test ④).

5. Tapping on the particular Option buttons ③ or ④ changes the screen. The entry mask for that type appears.



2. The screen changes and you are presented with a list of all AQA1 tests stored in the instrument.

3. Tap on the Add button ②.

6. For editing (see section 9.11.8).

NOTE

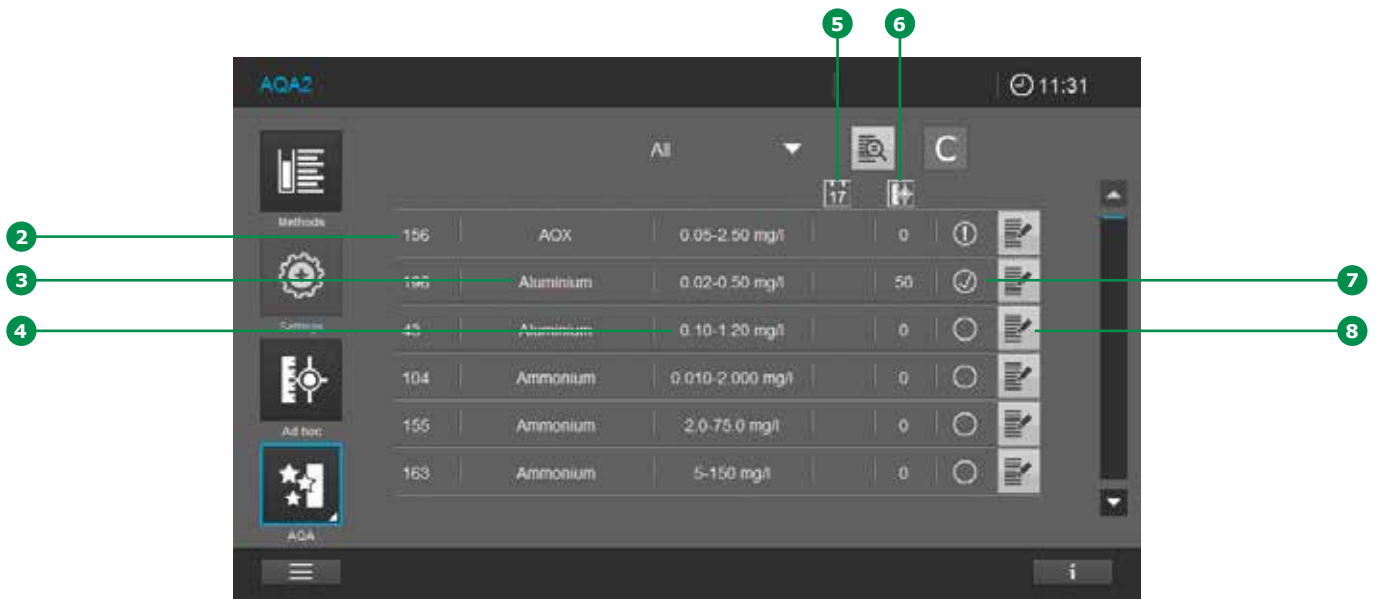
In the case of the user-defined AQA1 test for photometric accuracy the input fields for the test conditions (cell designation, testing wavelength, nominal values for absorbance and absorbance tolerance) are added to the screen by tapping on the + button ⑤.



9.11.11 AQA2 Selection List

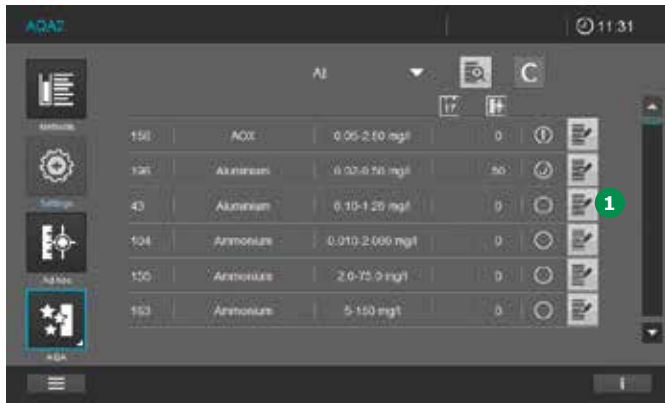


1. Tap on the AQA2 button 1.
2. The screen changes and a list of all AQA2 tests stored in the instrument is shown.



3. The screen shows the following information:
 - Number of the method being tested 2
 - Name of the method being tested 3
 - Display of the measuring range of the method being tested 4
 - Number of days for which the AQA2 test is still valid before a new test has to be performed 5
 - Number of measurements before a new AQA2 test has to be performed 6
 - Four different status symbols 7: ⓧ = test expired/invalid; ⓪ = test OK; ⓧ = test failed; ⓪ = not activated
 - Buttons to edit 8 AQA2 tests

9.11.12 Activating and Deactivating an AQA2 Test



1. Tap on the Edit button ①.
2. The screen changes.
3. Tapping on the ON/OFF button ② activates/deactivates the AQA2 test. (I = on, 0 = off, the light grey background shows which state is active).

NOTE

Before activating the lot-specific values for the current test item, compare with the existing entries for the input fields and make changes accordingly (see section 9.11.13).

9.11.13 Editing an AQA2 Test



The input values should be taken from the lot-specific certificates for the AQA2 test items and adjusted to suit as follows.

1. Tap on the Edit button ①.
2. The screen changes. A method-specific screen appears. See example screen on the next page.
3. This submenu offers the following setting options: See description in the table below the example screens on the next page.
4. Make your individual changes in the type-specific screens and store them by the Save button ③.
5. To close the editing screen touch the Close button ④.

1 9 Operation – 9.11 AQA (Analytical Quality Assurance)

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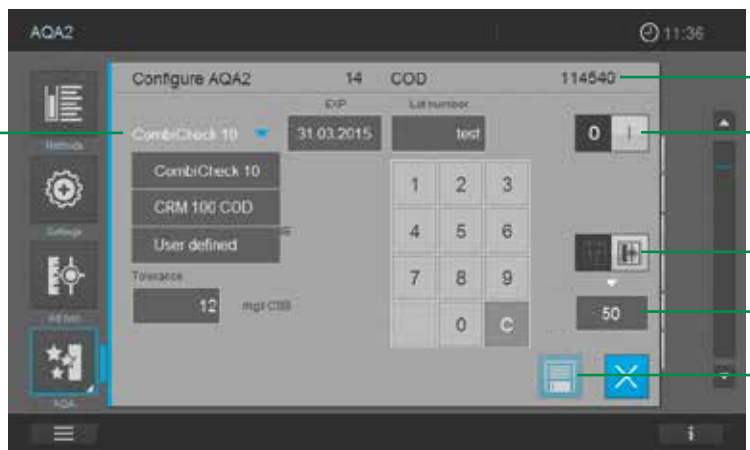
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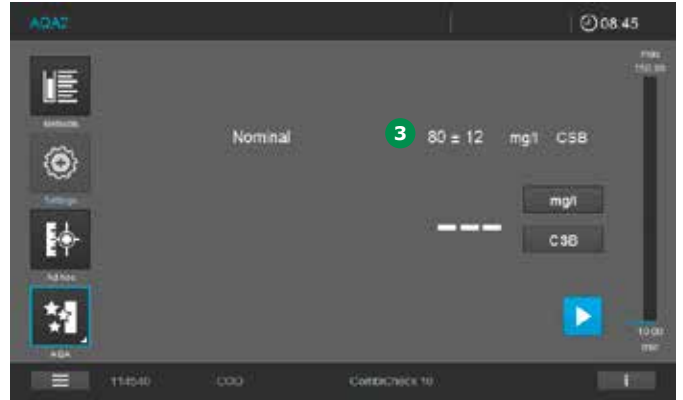


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Item	Display field	Description
1	Name	Name of the method being tested
2	Selection of standards	Selection of the AQA2 standard (a choice can be made between Spectroquant® pre-programmed standards such as CombiCheck and a freely definable standard)
3	EXP	Expiry of the standard as shown in the certificate for the standard
4	Lot number	Lot number of the standard as shown in the certificate for the standard
5	"0"/"I" (ON/OFF)	Deactivate/activate the test
6	Interval mode	Test interval choice between weeks and and number of measurements
7	Interval (values)	Enter test interval. For an active test the instrument reminds you when an AQA2 test is due.
8	Target value	Lot-specific nominal value
9	Tolerance	Tolerance range for the nominal value*
10	Save	Adopt values into the instrument
11	Close	Close display field
12	Numeric field	Touch the individual field to enter values
13	Article number	First 6 digits of the order number of the pre-programmed test kit corresponding to the selected method

* The user must edit the tolerance range according to his/her requirements. The tolerance range should include typical errors (measurement uncertainty) of the test medium used and of the method being checked. The typical error of the test medium used can be taken from the batch-specific certificate of the test medium. The typical error of the method being checked must be calculated by the user under his/her conditions.

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9.11.14 Performing an AQA2 Test

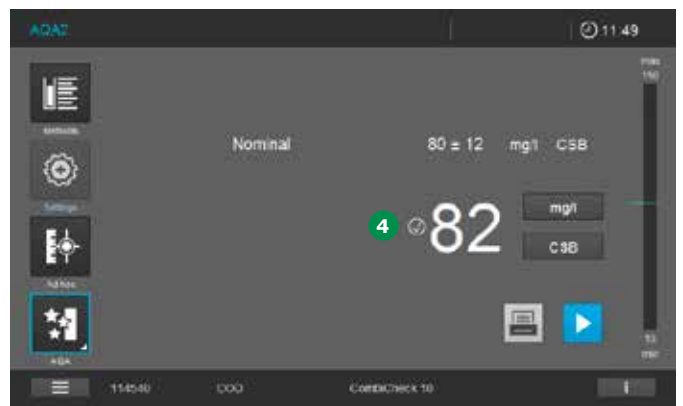
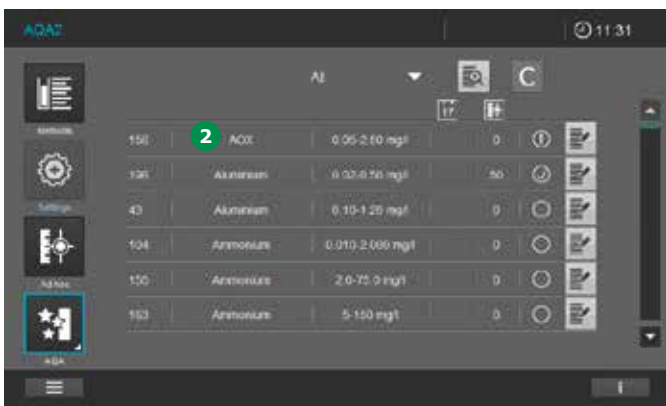


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NOTE

In order to perform an AQA2 test it must be activated (see section 9.11.12).

1. Tap on the AQA2 button ①.

5. Perform an analysis as per the method description using the selected AQA2 standard as sample and insert the cell.
6. Measurement starts automatically.
7. The measurement result appears in the display.
8. A tick appears following a successful test ④.



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2. The screen changes and a list of all AQA2 tests stored in the instrument is shown.
3. Select an AQA2 test by tapping on its name ②.
4. The screen changes and shows the nominal values and the tolerances ③ for the measurement with the selected AQA2 standard.

NOTE

If the test has failed, a ⊖ symbol appears in the display instead of the tick ④ symbol for a successful test.

Content of the information bar in AQA2 measurements



114942	Nitrate	CombiCheck 20	
Article number (first 6 digits of order no.)	Method name	AQA2 Standard Name	
HC123456	EXP 12/31/2015	AQA2 EXP 08/28/2015	10 mm
Lot number test kit	Expiration date test kit with Prefix "EXP"	Interval	Path length of inserted cell
ZA 08/21/2015		RB 0,100 A 08/21/2015	
Date of Zero Adjust- ment with Prefix "ZA"		Date + value user reagent blank with Prefix "RB"	

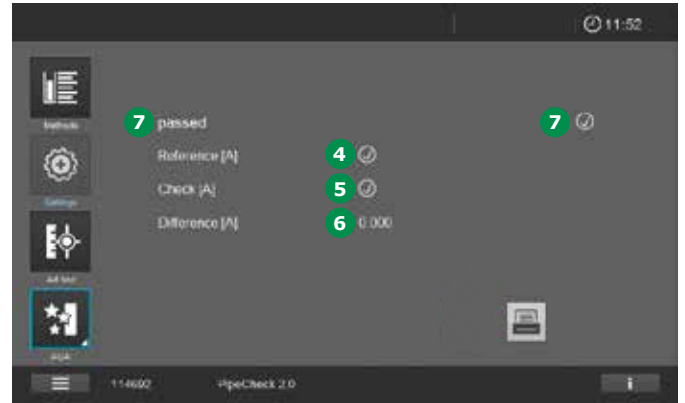


9.11.15 Perform PipeCheck

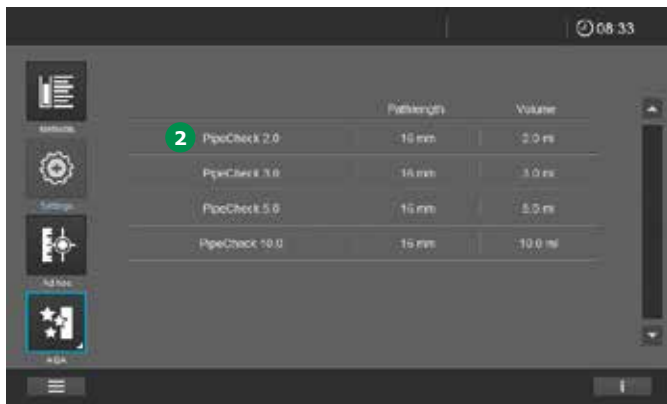


1. Tap on the PipeCheck button 1.
2. The screen changes and a list of all PipeCheck tests stored in the instrument is shown.

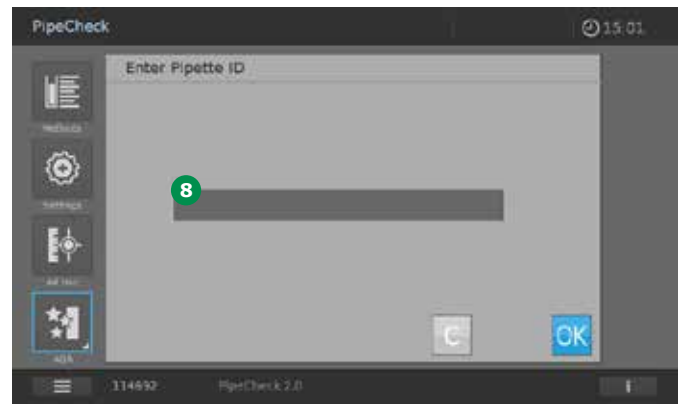
4. The screen changes 3.



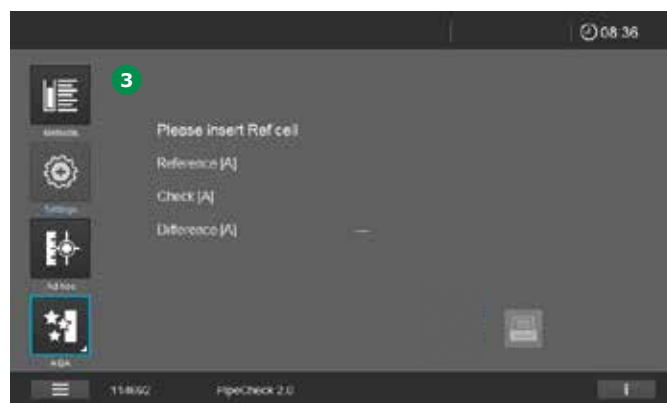
5. Insert the reference cell.
6. After the reference cell has been successfully measured, tick 4 appears on the display.



3. Select a PipeCheck by tapping on the name 2.

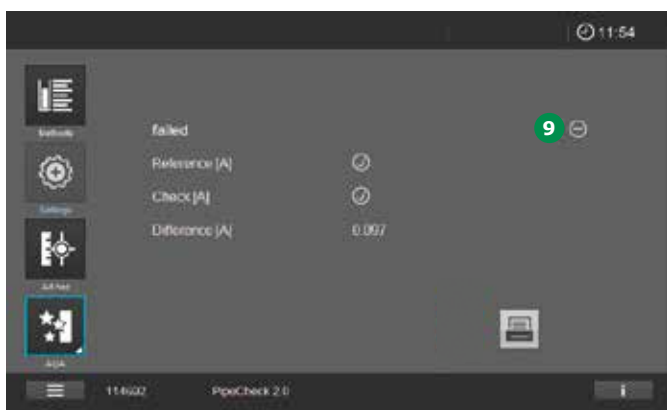


7. A window pops up in which a name or code can be entered for the pipet being tested (e.g. manufacturer, serial number or similar). Tap on the input field 8 and enter the name or code. Tap the OK button to accept the entry.



8. The screen changes.

9. Insert the "Check" cell.
10. After the "Check" cell has been successfully measured, tick **5** appears on the display.
11. The difference between reference and Check cell is calculated automatically. If this value **6** is within the pre-programmed tolerance, the PipeCheck is passed shown by text and tick **7**.



NOTE

If this value of the difference is outside the tolerance, the test has failed and a **9** appears.

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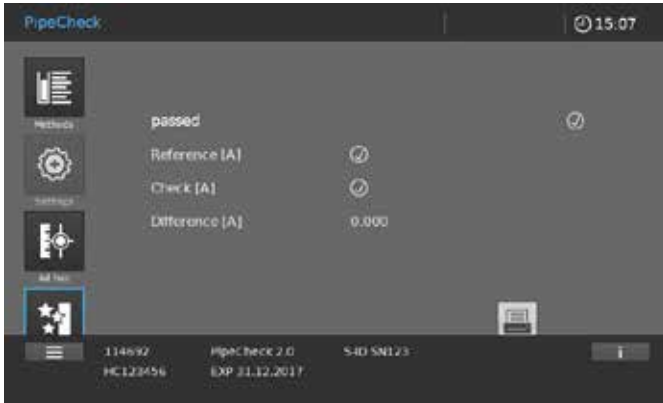
2

3 Content of the information bar in PipeCheck measurements

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114692	PipeCheck 2.0	S-ID SN123
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Article number (first 6 digits of order no.)	Method name (incl. pipette volume)	Pipet designation/ identification
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HC123456	EXP 31.12.2017
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Lot number item	Expiration date item with Prefix "EXP"
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9.12 Timer

You can use the timers to remind you by an acoustic signal of a time interval that has expired.

The spectrophotometer has two types of timers:

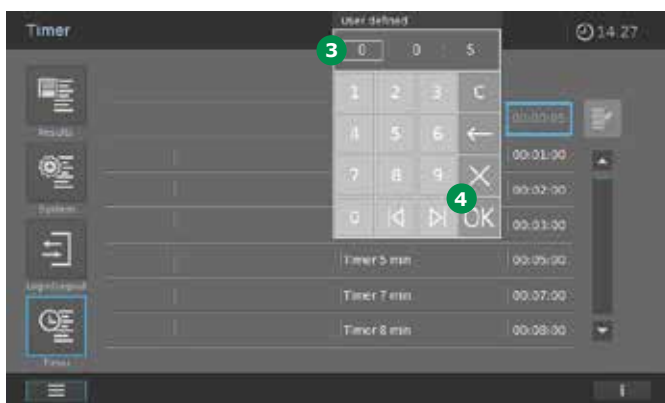
- The user-defined timer is a timer that can be freely assigned
- Pre-programmed timer is a timer which offers preset reaction times (≤ 15 min) for pre-programmed factory methods



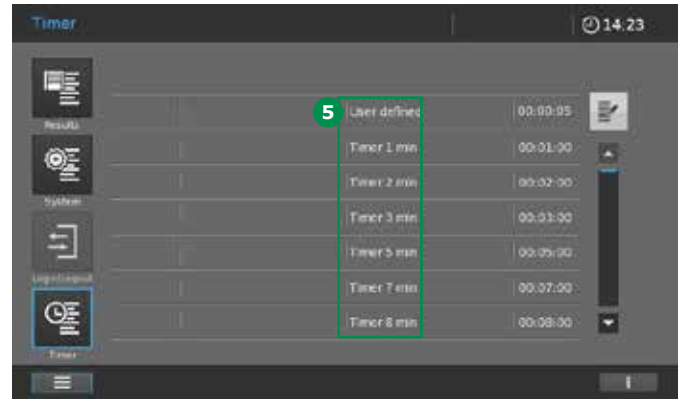
The spectrophotometer manages all timers in the timer list. The timer list is opened with the Timer list button 1.

If you want to manually enter time intervals, use the user-defined timer function.

1. Tap on the Edit button 2.

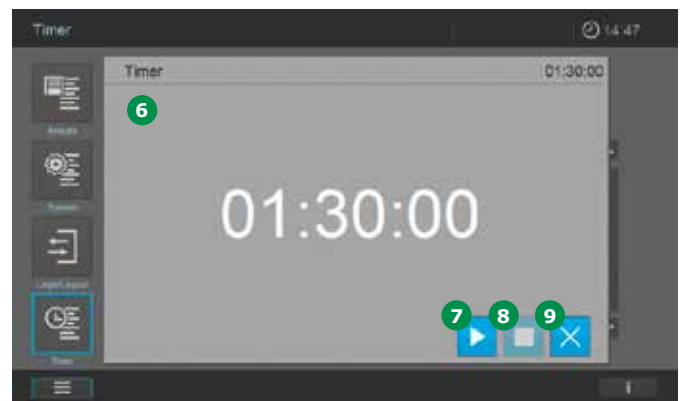


2. The input window 3 opens.
3. Enter the required time by tapping on the corresponding field and confirm with OK 4.



4. The screen changes back to the timer overview.

5. Tap on the timer name 5 and the screen changes 6.



6. Tap on the Start button 7 to start the timer. Tap on the Stop button 8 to stop the timer. The count down is interrupted. Tap on Start button 7 again will continue the count down. When the count down is finished an acoustic signal sounds. The insertion of a barcoded round cell enables a measurement to be started immediately. The insertion of an AutoSelector enables a method to be selected immediately. Tapping on the Start button 7 is active again and the timer can be started once more.
7. Tap on the X button 9 to close the timer. The display changes to timer list.

9.13 Results and Measurement Datasets

All results and measurement datasets in all measurement modes are stored automatically in the result list, as the instruments are delivered with a factory pre-set AutoStore function (see section 9.2.5).

All stored results and measurement datasets can be retrieved, exported and printed out.

NOTE

The instrument is capable of storing 2000 individual measurements of the measurement modes concentration, absorbance/transmission, and/or multiple wavelengths as well as 20 data sets with results of the spectrum or kinetics methods for each of these modes. It operates on the FIFO storage principle (first in – first out), meaning that when all storage locations are occupied, the next time a result is to be stored the oldest result on the list is automatically overwritten. Accordingly it is advisable to regularly back up stored data sets on external media (see section 9.13.7).

The results of the measurement modi AQA1, AQA2, MatrixCheck, and PipeCheck are managed separately. A total of 500 results are stored. Results that determine a system or method status are not overwritten, even when all storage locations are already occupied.



If the AutoStore function is deactivated, results and datasets have to be stored manually after each measurement.

1. Tap on the Save button ①.
2. The system suggests a sample ID ②.
3. Tapping on Save ① again stores the result under the suggested sample ID.



4. To replace the sample ID by an individual one, tap on the sample ID field ②.
5. Enter a new sample ID with the key pad ③.
6. Confirm with the OK button ④.

9.13.1 Displaying the Results

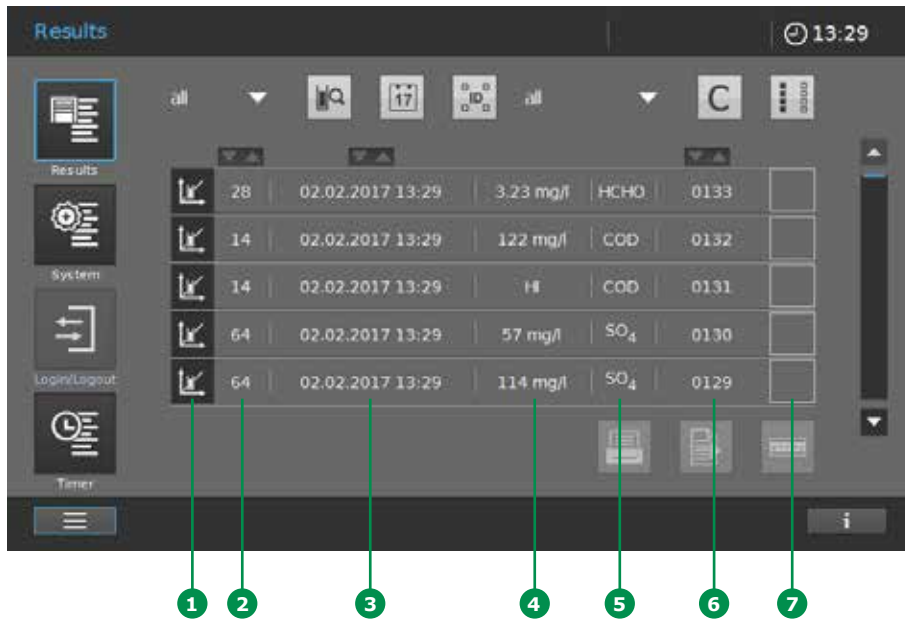


ID	Date/Time	Concentration	Method	Selection
28	02.02.2017 13:29	3.23 mg/l	HCHO	0133
14	02.02.2017 13:29	122 mg/l	COD	0132
14	02.02.2017 13:29	HI	COD	0131
64	02.02.2017 13:29	57 mg/l	SO ₄	0130
64	02.02.2017 13:29	114 mg/l	SO ₄	0129

By tapping on the Results button **1** you can access the result list via the main menu.

The menu offers you the following choices:

- Sort ascending/descending **2**
- Filter result list **3** – (see section 9.13.3)
- Clear filter **4**
- Select/deselect all results **5**.
- Results are selected by ticking the box **10**. Remove the selection by tapping on the tick symbol and the box will be emptied
- Export selected results **6**. To export results they have to be selected by ticking the box **10**
- Print selected results **7**. To print results they have to be selected by ticking the box **10**
- Scrollbar **8**. Scroll through the result list by tapping on the arrows of the scrollbar
- Panoramic view of selected results from one specific method **9** (see section 9.13.4)

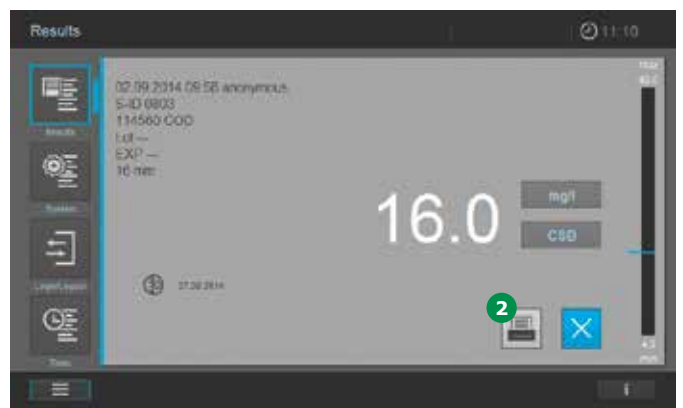
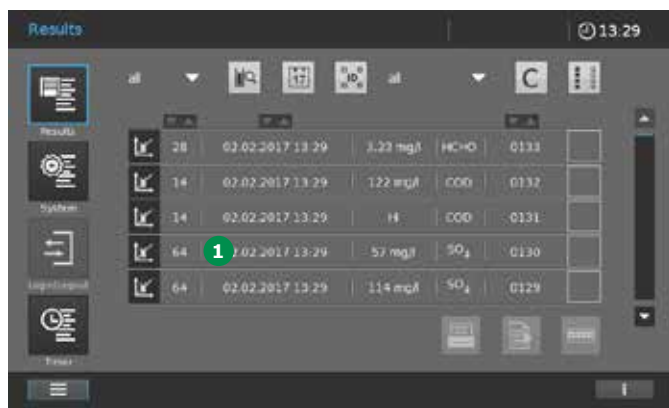


The individual result line shows the following information:

- Measurement mode (e.g. concentration, spectrum, kinetic, AQA) 1
- Method number 2
- Date and time of measurement 3

- Result (e.g. in units or passed/failed, depending on measurement mode) 4
- Analyte tested 5
- Sample ID 6
- Tick box to select a result line to print or export the results 7

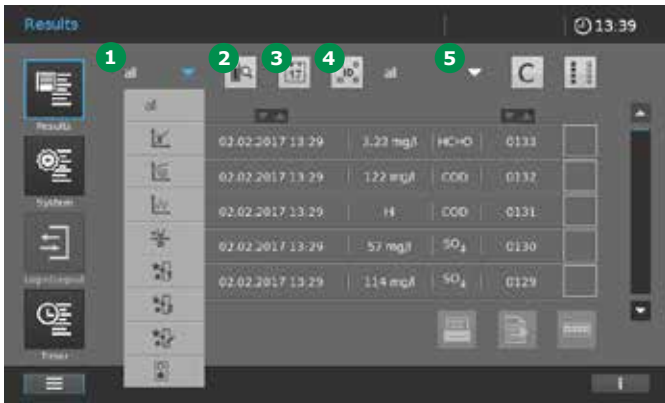
9.13.2 Show Details of One Result



1. Tap on an individual result line 1

2. A screen showing all details of one result or dataset opens.
3. Tap on the print button 2 to print the individual dataset on a printer or as a pdf.

9.13.3 Filtering Results to Further Process Measurement Datasets



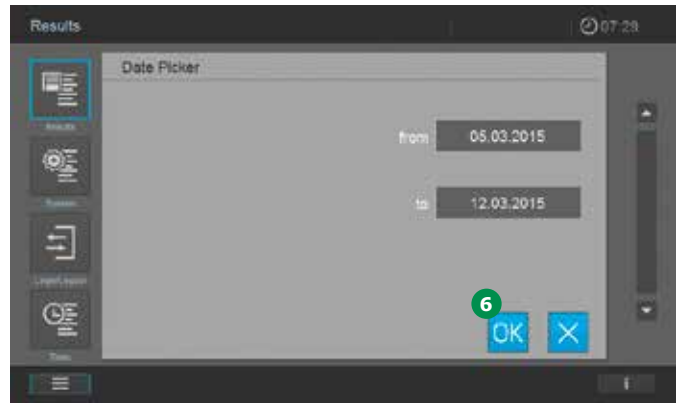
Specified filter criteria can be set to select certain results and datasets to be exported, printed, displayed or deleted.

The following criteria can be set:

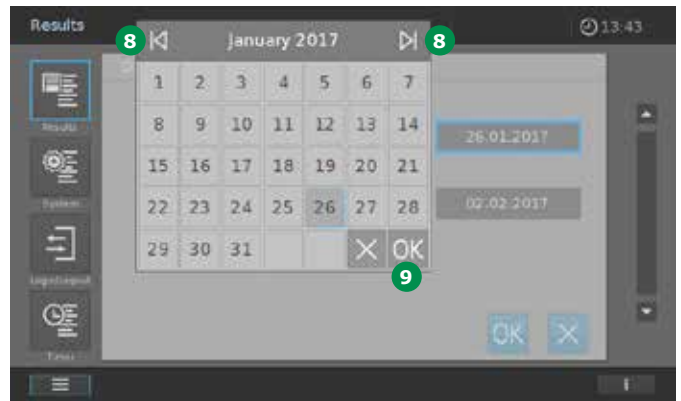
- **Filter using the individual measuring mode 1.** The list shows the following modes: concentration, kinetic, spectrum, ad hoc, AQA1, AQA2, PipeCheck and MatrixCheck



- **Filter using character strings.** Tapping on the Search icon 2 brings up the keypad display field. Enter search criteria such as method name, method number or article number (first six digits of order number) no decimal point. Tap on OK to activate the search filter



- **Filter by date.** Tapping on the Date button 3 brings up an input mask for the date range from ... to ...
A calendar screen pops up.



- Use the forward and back buttons 8 to scroll through the calendar. Select the required date and confirm by tapping on the OK button 9. The calendar closes.
- Tap on the OK button 6 to adopt the selected period for filtering.

NOTE

Keeping your finger on the "Forward" and "Back" buttons 8 scrolls through the calendar forwards and backwards year by year.

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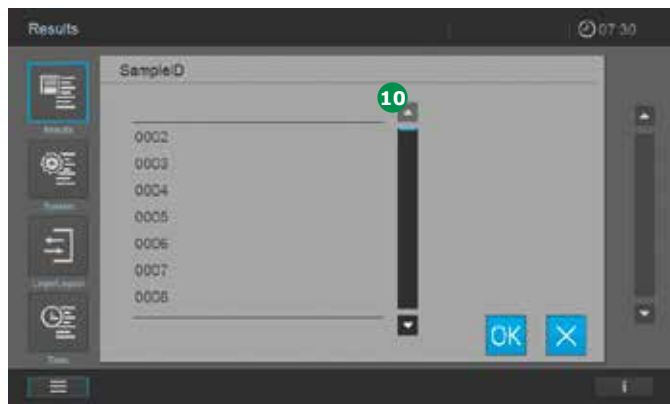
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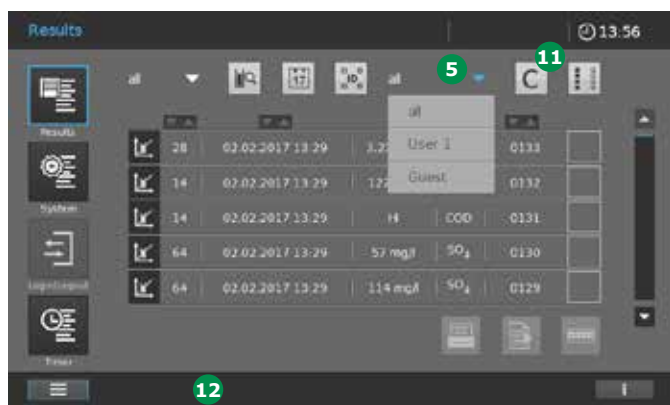
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16



- Filter by sample ID (4). Tapping on the button brings up a selection bar (10) which you can use to filter according to sample ID



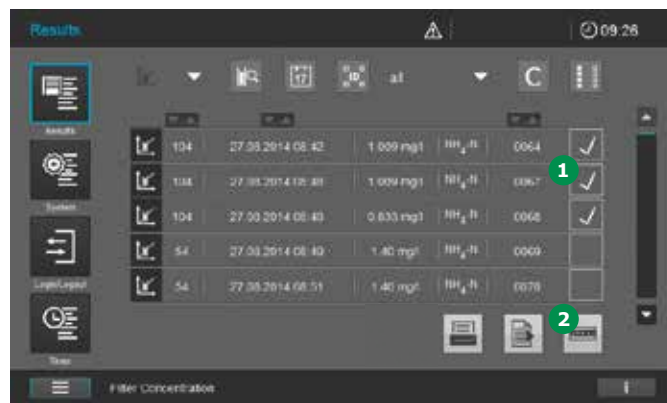
- Filter by user name (5). Tapping on the button brings up a selection bar showing you the users created for the instrument. When you select a user, the measurement data list displays all measured results for that user

NOTE

Tapping on the C button (11) cancels all of the filters and the complete measurement data list appears. You can also search in filtered lists or set more filters, the filter status is shown in the Infobar (12).

9.13.4 Panorama – Value Control Card

The panorama function allows you to get a graphical view of selected results from one single method (e.g. ammonium). The graphical view corresponds to a value control card.



1. Use the filter option to create a result list for one single method (see section 9.13.3).
2. Select the results to be included into the panorama value control card by ticking the boxes (1).
3. The Panorama button is activated (2).



4. Tapping on the Panorama button (2) opens the graphical view of the panorama value control card for the selected values.
5. Tap on the Forward/Backward buttons (4) to get the individual datasets (5) for each value displayed.

9.13.5 Print Results and Measurement Datasets

If a postscript printer is connected to the spectrophotometer, results and measurement datasets can be printed on paper by touching the Print button (see section 8.3.2).

In addition, you can print the results and measurement datasets as a pdf. Connect an USB memory device and activate "Print to pdf" in the submenu "Interface" in the "System" menu (see section 9.2.2). To print to pdf touch the Print button.

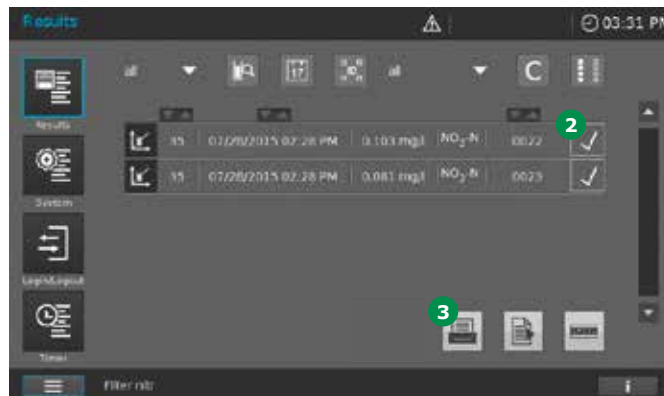
Print to pdf will create the folder PROVE on your USB memory device. This folder has several subfolders. You will find the pdf print files in the folder "Print".

NOTE

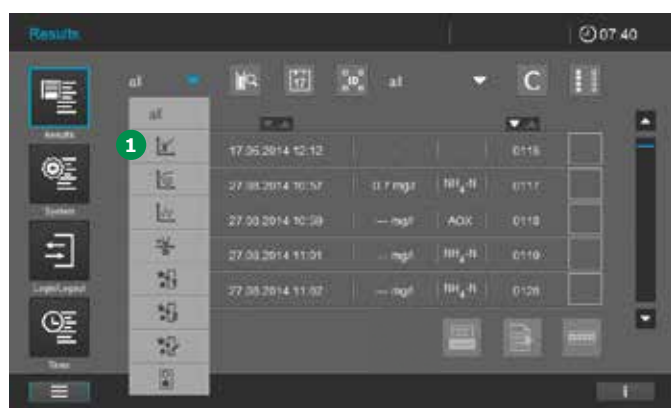
While printing more than one result, only results from a single measuring mode can be printed at one time as each measuring mode has a different printing format.

NOTE

In the Spectrum and Kinetics measurement modes the results must be selected and printed out separately.



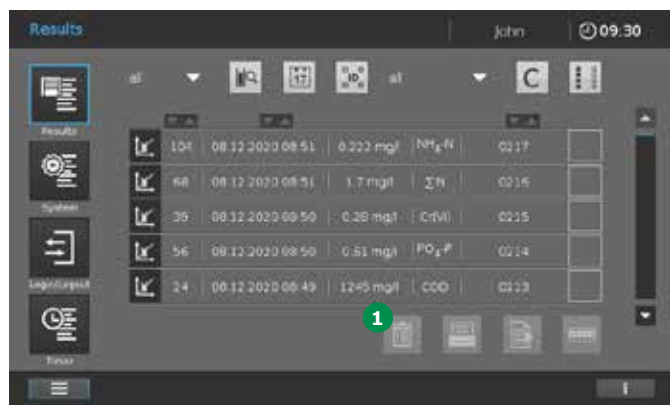
2. Select the results to be included into the printout by ticking the boxes 2.
3. Tap on the Print button 3 to print the results.
4. The in-progress icon appears during the data-export procedure.
5. If you print as pdf to the USB memory device, wait for some more time before removing the USB device to make sure all data are transferred.



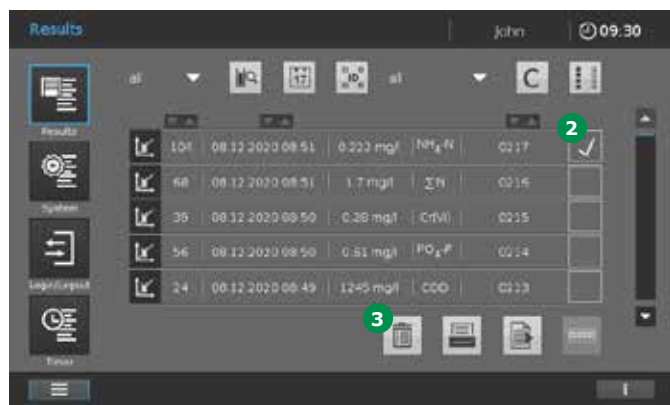
1. Select the measuring mode for the results you want to print, e.g. concentration 1.

9.13.6 Deleting Results

The function "Delete Results" is available only when the user administration is activated (see section 9.2.6) and the function "Delete Results" is activated in the "Quality" menu of the system settings (see section 9.2.4).



When the function is activated, the symbol for the function "Delete" 1 is shown in the screen of the results list.



1. Click on the results that you wish to delete 2.
2. Tap "Delete" 3 to delete these results.

NOTE

The deletion of results is documented in the user log file (for further details on log files please see section 9.2.7 and section 16).

9.13.7 Export Results and Measurement Datasets

In many cases it is advisable to export results and measurement data sets, e.g. to archive them or to analyze them in greater detail using a suitable software tool. Besides offering data transmission to a suitable memory device via the USB port, the Spectroquant® Prove plus spectrophotometer also supports the automatic transfer of measurement data via a local network (Spectroquant® Prove Connect to LIMS, Y11086). Spectroquant® Prove Connect is optionally available at www.sigmaaldrich.com/spectroquant-prove-connect.

Data Transfer from Spectroquant® Prove plus with USB Memory Device

NOTE

The reliability of data stored on USB memory devices depends on the quality of the memory device and the data transmission.

Data are stored partly or not at all if for example:

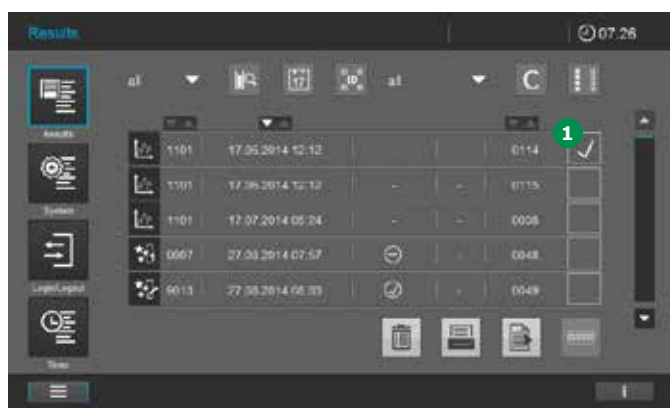
- The power supply of the external memory device is interrupted during the write process, or
- The external memory device is prematurely disconnected from the spectrophotometer during the data backup

To prevent a data loss we recommend the following:

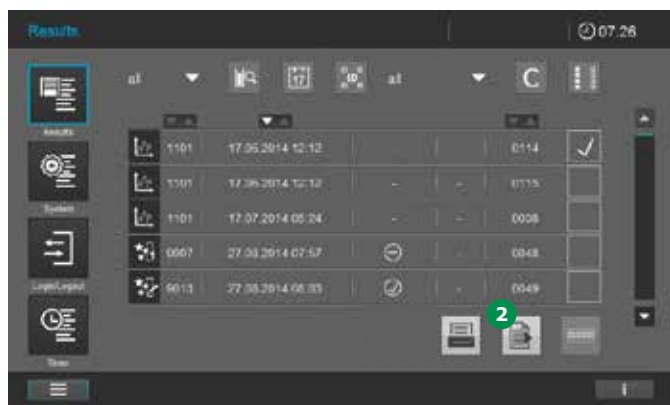
- Store all data internally in the spectrophotometer first
- After performing a backup leave the USB memory device connected to the spectrophotometer for some time
- Check whether the stored data is complete, e.g. on a PC
- Use the USB memory device for data transport but not for permanent data storage

NOTE

The data are exported as CSV files. To open them in a spreadsheet make sure that your PC calculation program is set to the same decimal separator as the spectrophotometer (see section 8.2.4).



1. Select the results you want to export by ticking the box **1**.



2. Export the selected results by tapping on the Export button **2**.
3. The in-progress icon appears during the data-export procedure.
4. When the in-progress icon disappears, wait for some more time before removing the USB device to make sure all data are transferred.

9.14 User Management

The Spectroquant® Prove plus allows the management of up to 100 users. Every user is member of a user group with defined user rights.

Administrators and users log in to the spectrophotometer with their user name and password. Thus, documented measured values can later be assigned to the user.

User groups

There are two hierarchical user groups:

- Administrator (top level)
- User (user account registered by the administrator)

NOTE

The user management function is not active in the Spectroquant® Prove plus when it leaves the factory. Every user can carry out all functions. Activating the user management creates an administrator user account.

User rights in detail

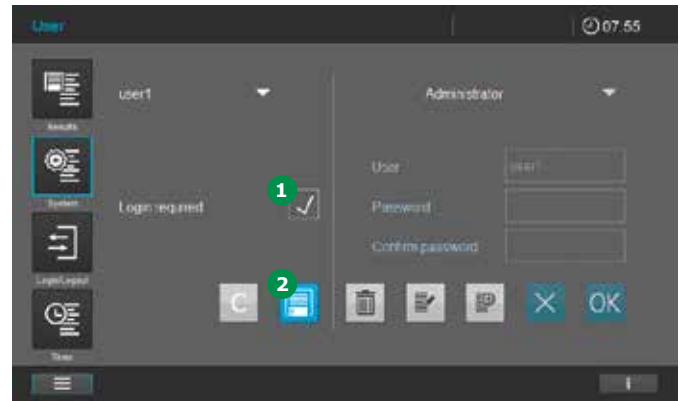
Action	Administrator	User
Change system date/time	X	
Change GUI language	X	X
Firmware update	X	
Language update	X	
Method update	X	
Export error log	X	X
Run AQA1/AQA2	X	X
Create/edit AQA1/AQA2	X	
Display AQA status	X	X
Display AQA results	X	X
User management On/Off	X	
Run measurements	X	X
Evaluate measurements	X	X
Export results and measurement datasets	X	X
Handle user-defined methods	X	X
Recalibrate factory pre-programmed methods	X	X
Backup/restore	X	

9.14.1 Activating/Deactivating the User Management Function

If the user management function is activated by ticking **1**, each user has to log in to the spectrophotometer. After the login, the user has certain rights depending on the user group. Only an administrator can deactivate the user management function. If the function is deactivated, every user has full instrument rights.

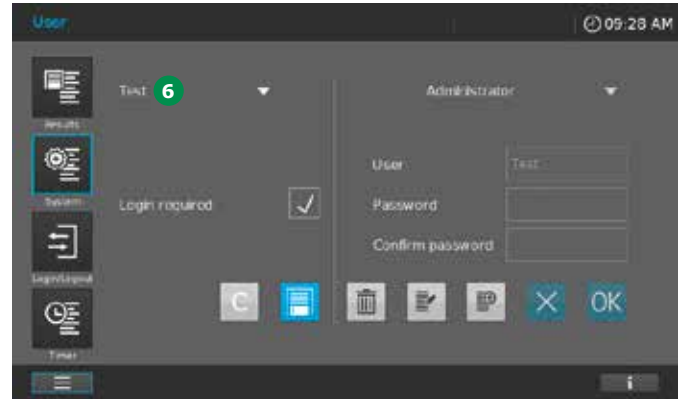
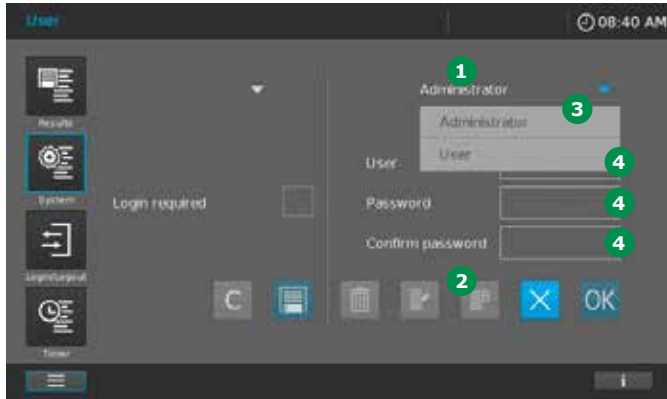


1. Tapping on "System" and "User" opens the screen to activate the user management.



2. Tap on the box **1**. A tick appears.
3. Tap on the Save button **2** and the user management is active.
4. An administrator can deactivate the User management function by tapping on the box **1** to remove the tick.
5. Tap on the Save button **2** to store the changes. The User management is deactivated.

9.14.2 Create an Administrator/ User Account



On the right part 1 of the screen "User Management" administrators or users can be created.

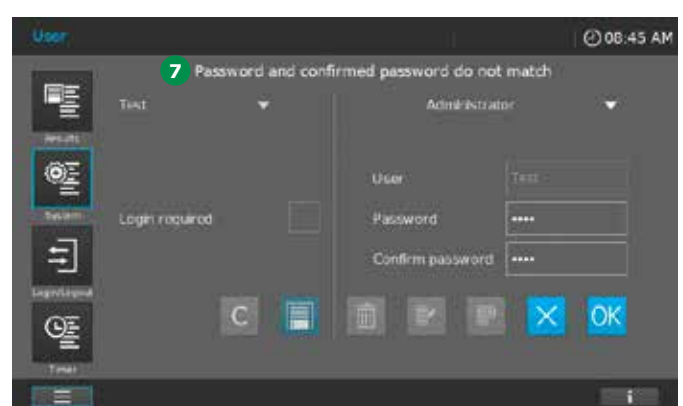
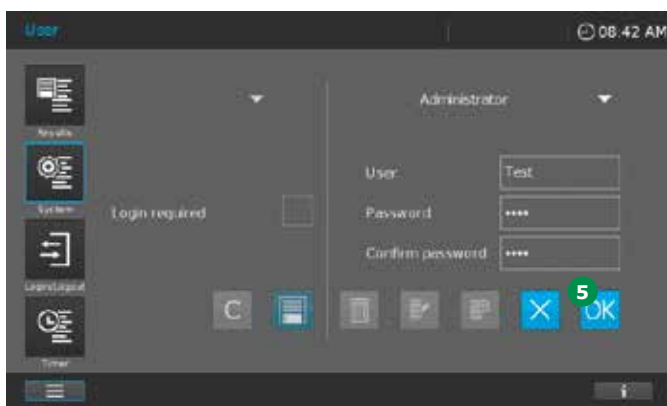
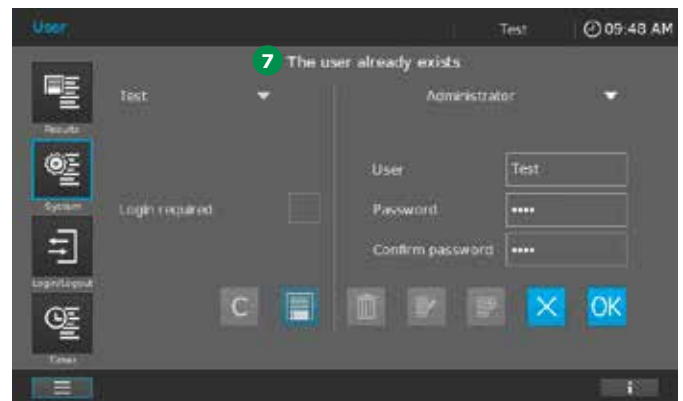
1. Tap on the Add button 2 to start to create an administrator/user.
2. Select whether you want to create an administrator or user by tapping on field 3.

NOTE

The first person who is created is automatically assigned administrator rights. Here it is not possible to select "Administrator" or "User".

3. Enter name, password and confirm password in the following fields 4.

5. If the new user has been created successfully, the user name appears on the left 6.



4. The administrator resp. user is created by tapping on the OK button 5.

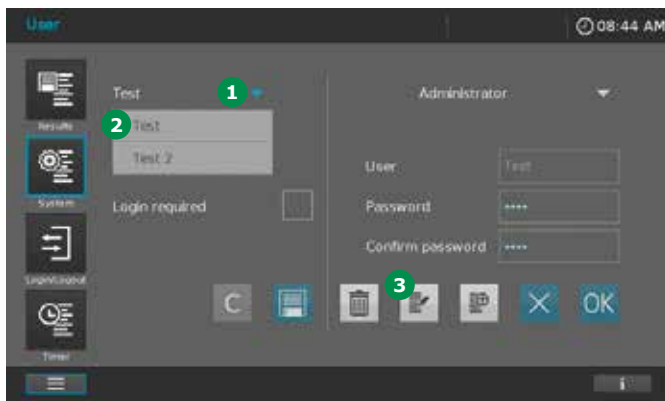
NOTE

Error messages 7 appear if the user name already exists or the password is not confirmed correctly.

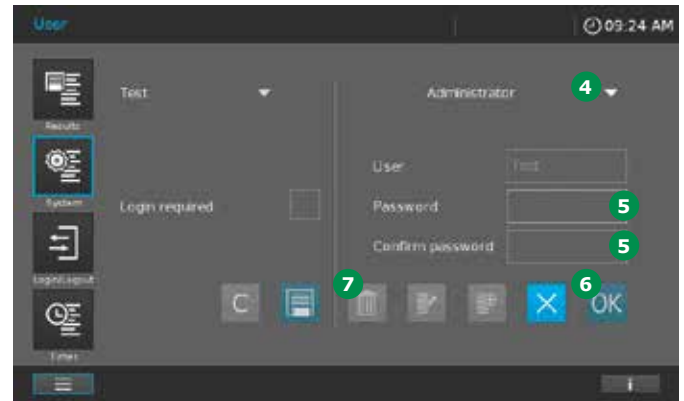
9.14.3 Edit or Delete a User

NOTE

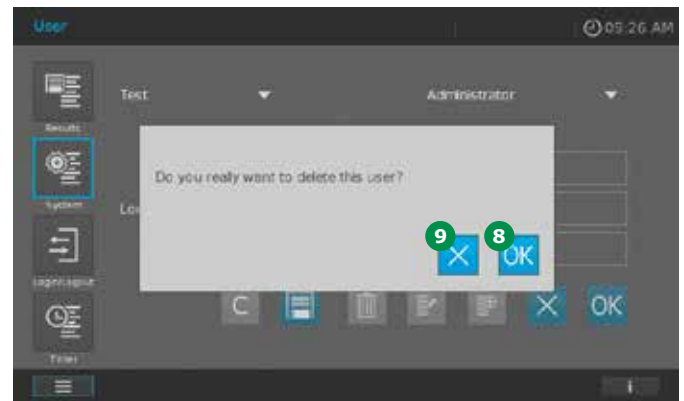
Edit or delete a user is possible only for administrators. A regular user cannot access the User management submenu and can change the password in the Login/Logout menu only (see section 9.15.1).



1. Tap on the System menu button and select the submenu User.
2. Select the user from the list on the left 1 by tapping on the corresponding name 2.



3. Tap on the Edit button 3.
4. You can edit the access rights (Administrator or User) 4 and change the password 5.
5. Confirm your changes with the OK button 6.
6. To delete a user proceed as before and tap on the Delete button 7.



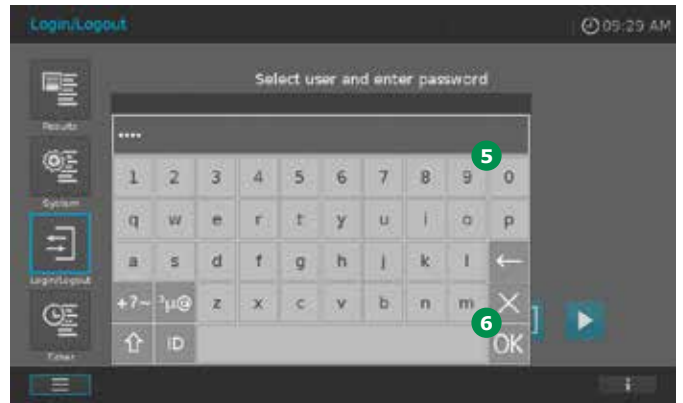
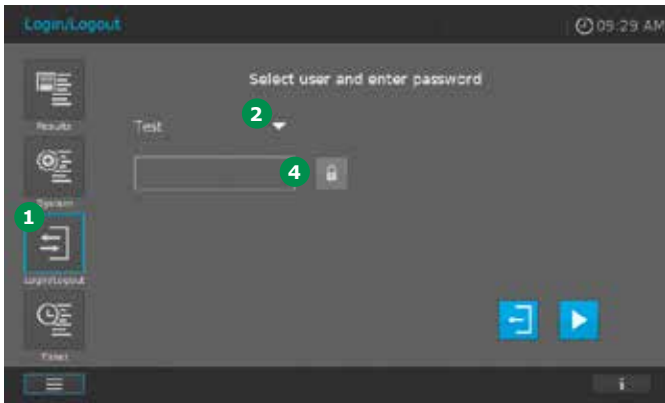
7. Confirm your changes with the OK button 8. You can quit your decision with the X button 9.



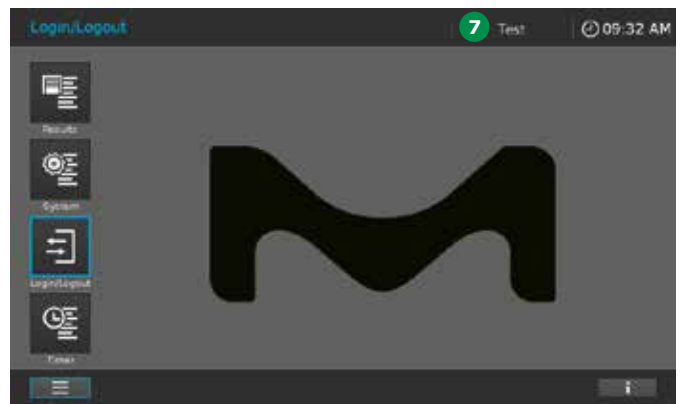
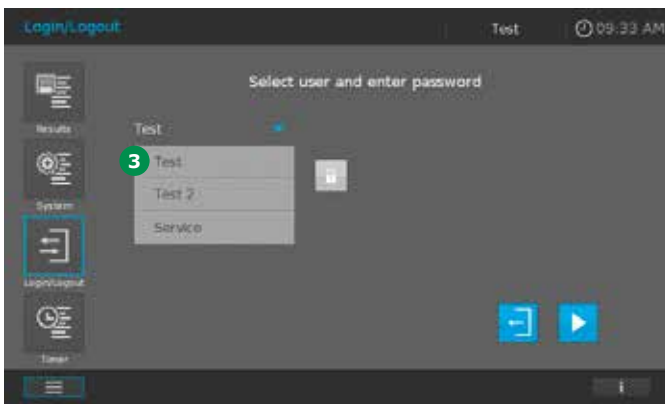
9.15 Login/Logout

If the user management is activated (see section 9.14.1), login is mandatory to receive user or administrator rights.

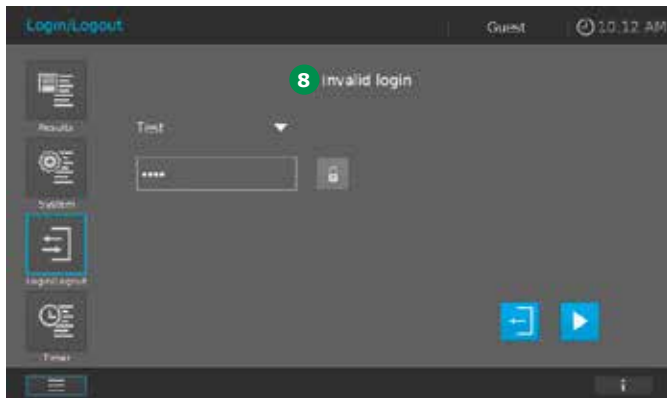
To login into the spectrophotometer proceed as follows:



1. Select Login/Logout **1** from the main menu.
2. Tap on the arrow to open the user list **2**.
5. Enter the user password by using the key pad **5** and confirm it with OK **6**.

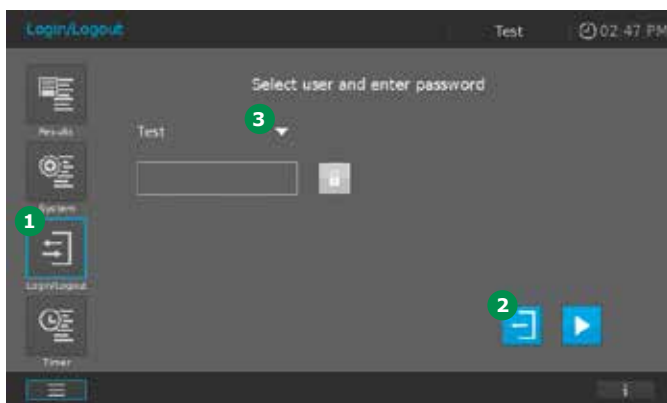


3. Select the user name from the user list **3**.
4. Tap on the entry field **4**.
6. The screen changes to the start screen. The user name of the logged in user appears in the upper status bar **7**.



- Wrong entry of the password creates the warning "Invalid login" (8). Repeat the procedure above with the correct password.

To Logout as user or administrator



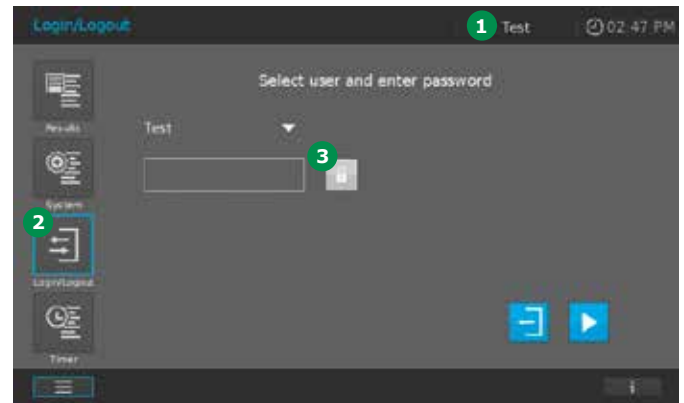
- Select Login/Logout (1) from the main menu.
- Tap on the Logout button (2).

NOTE

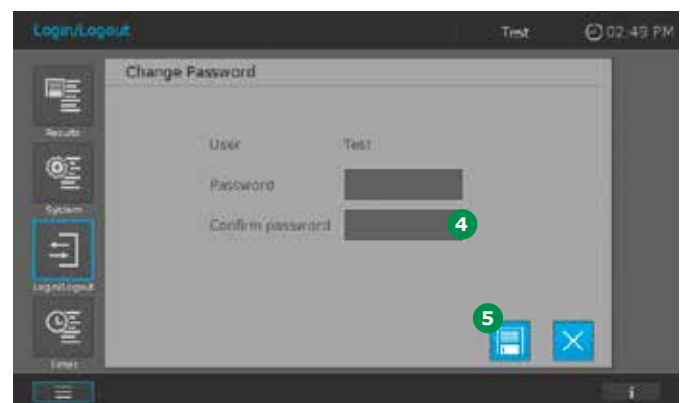
To continue as a different administrator or user, open the user list by tapping on the arrow (3) and select the user from the list. Enter the corresponding password as described above.

9.15.1 Change Password with User Rights Only

If you are registered with user rights only, you have to change your password in the Login/Logout mode.



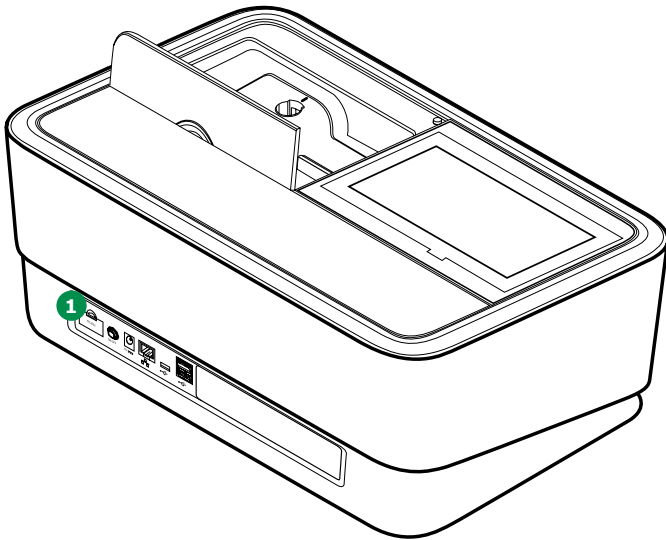
- To change your password you have to be logged in (see section 9.15). After successful login your user name appears in the upper status bar (1).



- Select Login/Logout (2) from the main menu.
- Tap on the lock icon (3).
- Enter the new password and confirm it in the entry fields (4).
- Store your changes with the Save button (5).
- Login with your new password (see section 9.15).
- The screen changes back to the Login/Logout mode.
- Press Start again to continue.

10 Maintenance and Cleaning

10.1 Exchanging the Buffer Battery



Battery service life

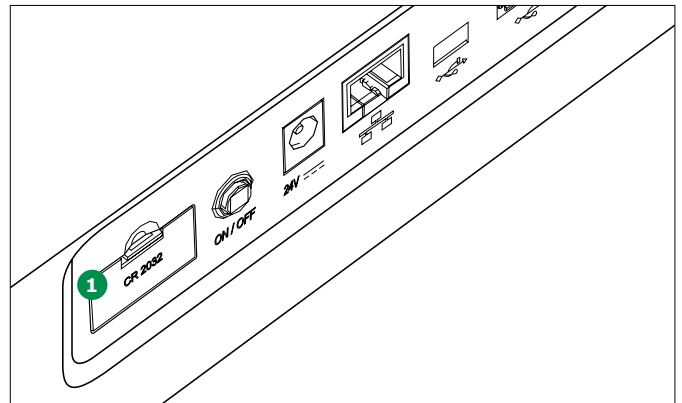
The power consumption of the clock is very low. The service life of high-quality batteries is at least five years.

Disposal of batteries

Dispose of the batteries at a suitable facility according to local legal requirements. Please do not dispose of the batteries with household refuse.

Within the European Union, the batteries are removed at specialized treatment centers at the end of the instrument's life. Instruments are taken to one of these specialized treatment centers via the recycling system set up for this purpose.

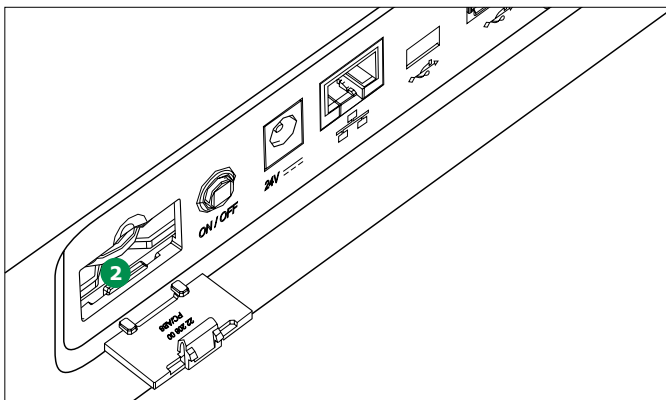
3. Insert the new batteries in the battery compartment, making sure the polarity is correct. Use only lithium ion batteries of the type CR 2032. Insert the battery with the writing facing upwards. The \pm signs on the batteries must match the \pm signs in the battery compartment.



4. Close the battery compartment cover **1**.

NOTE

If you leave the spectrophotometer switched on during the exchange or insert the new batteries within a minute after taking out the old ones, the date and time are retained in the spectrophotometer.



1. Open the battery compartment cover **1**.
2. Remove the old batteries **2** from the battery compartment using a pair of tweezers.

10.2 Exchanging the Halogen Lamp (Prove 100 plus)

⚠ WARNING

Before exchanging the lamp, switch the instrument off and disconnect the power plug from the power supply! If the lamp has snapped off or is broken, it must be exchanged by the Customer Service Department, as there is a risk of significant injury!

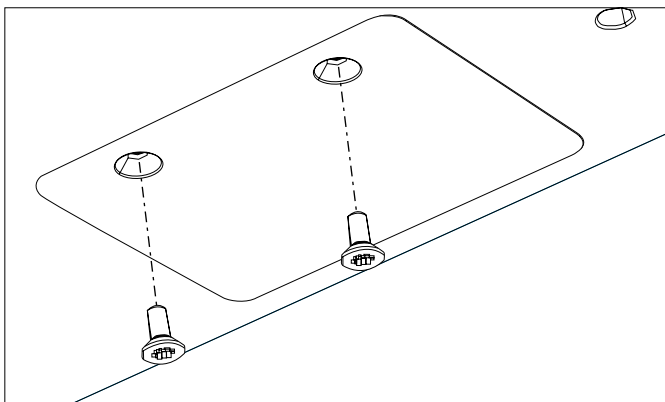
⚠ CAUTION

There is a risk of explosion if unsuitable lamps are used.
Use only the lamp that is intended for use with your instrument.

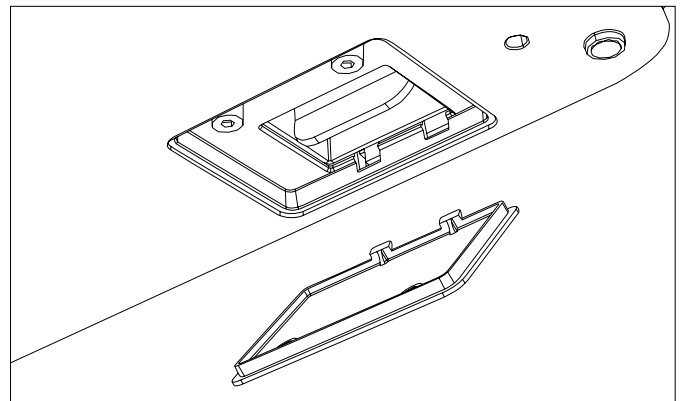
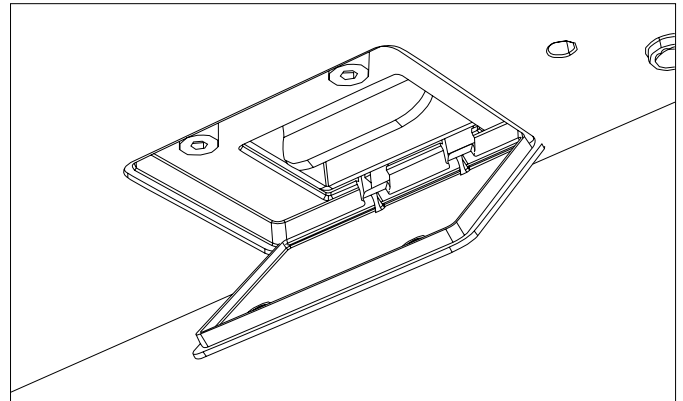
Disposal of the lamp

Dispose of the lamp at a suitable facility according to local legal requirements. Please do not dispose of the lamp along with household refuse. Within the European Union, the lamp is removed at specialized treatment centers at the end of the instrument's life. Instruments are taken to one of these specialized treatment centers via the recycling system set up for this purpose.

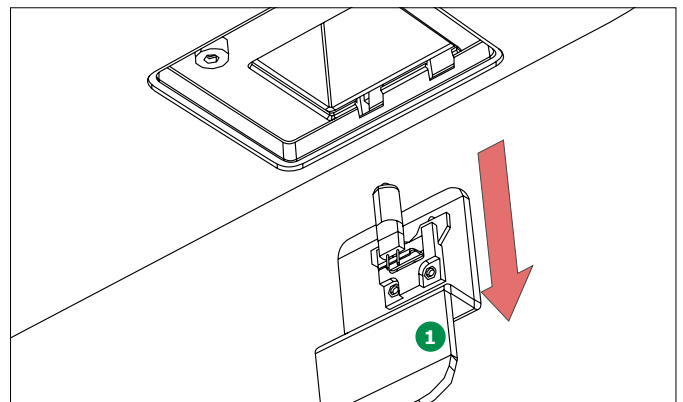
Procedure



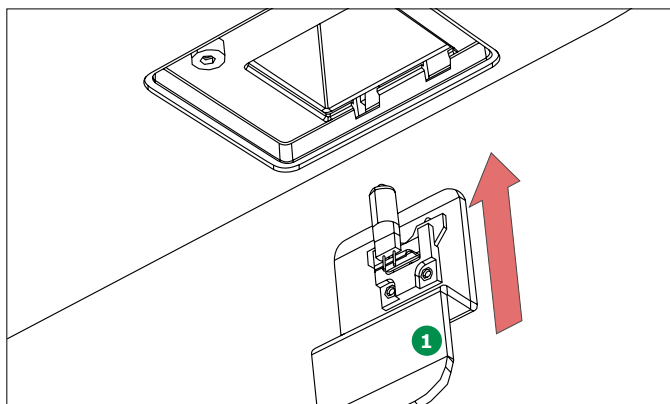
1. Place the spectrophotometer bottom-side up on a soft surface.
2. Remove the screws of the lamp compartment cover with an appropriate screw driver.



3. Open the lamp compartment cover and remove it.



4. Carefully remove the lamp module from the lamp compartment. Do not touch the lamp. Use the mount **1** to take it off.



5. Install the new lamp module in the lamp compartment. Use the mount **1** to insert the lamp module.
Do not touch the lamp to ensure that the service life of the lamp is not affected!
6. Close the lamp compartment cover with an appropriate screw driver.

NOTE

Upon renewed use of the spectrophotometer, reboot the instrument and reset the lamp counter to zero (see section 9.2.1). If the self-test is passed the instrument is ready for further measurements.

10.3 Cleaning

If a cell has broken or in the event of a reagent accident, the spectrophotometer must be cleaned immediately.

⚠ WARNING

Cells can contain dangerous substances. If the contents are released, follow the safety instructions of the Material Safety Data Sheet (MSDS). If necessary, apply appropriate protective measures (protective goggles, protective gloves etc.).

⚠ CAUTION

Do not turn the spectrophotometer upside down to remove the liquid. Doing so can cause the liquid could come into contact with electronic components and damage the spectrophotometer.

⚠ CAUTION

The spectrophotometer has two drains at the bottom through which the contents of broken cells or spilled liquid can drain off without causing any damage to the instrument.

10.3.1 Cleaning the Housing and Display

⚠ CAUTION

The housing components are made of synthetic materials. Avoid any contact with acetone, similar solvents and detergents containing such solvents. Wipe off any splashes immediately.
Displays: Avoid contact with concentrated mineral acids, concentrated caustic solutions, benzyl alcohol and methylene chloride. Wipe off any splashes immediately.

Clean the spectrophotometer housing as follows:

- If the housing surface is dirty, wipe it with a soft cloth and mild soapy water
- Remove any chemicals splashes as soon as possible
- For disinfection, brief use of isopropanol is permitted

Clean the displays with a soft cloth, if needed moistened with clean water and a mild detergent.

10.3.2 Cleaning the Cell Compartment

⚠ CAUTION

The cell compartment components are made of synthetic materials. Avoid any contact with acetone, similar solvents and detergents containing such solvents. Wipe off any splashes immediately.

Routine cleaning of the cell compartment is normally unnecessary. Remove dust and slight contamination with a moist, lint-free cloth. In case of spilled reagents switch the instrument off and take the cell compartment out. Rinse it with clean water.

Use isopropanol briefly to remove persistent contamination (e.g. reagent residues).

⚠ CAUTION

Clean the cell compartment only while wearing proper gloves to protect your hands!

Make sure that you wear appropriate gloves and clean the cell compartment as follows:

1. Open the cover **1**.

Prove 100 plus and 300 plus:

2. Take the cell compartment **2** with both hands, put the left forefinger against the left side of the interior of the compartment and take the round cell holder with your right hand.
3. Remove the cell compartment by pulling evenly with both hands and hold it in a horizontal position.

Prove 600 plus:

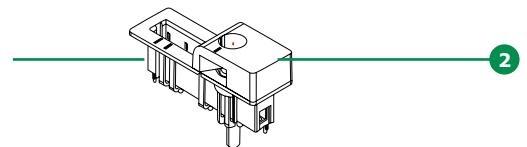
2. Take the round cell holder **3** out. Take the cell compartment **4** with both hands, put the left and right forefingers against the interior left and right of the compartment.
3. Remove the cell compartment by pulling evenly with both hands and hold it in a horizontal position.

NOTE

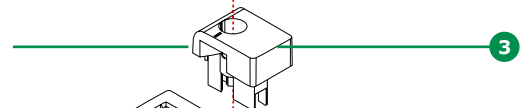
Put the cell compartment back in place by the same procedure.

It is important that the compartment is completely pushed down to avoid false measurement results.

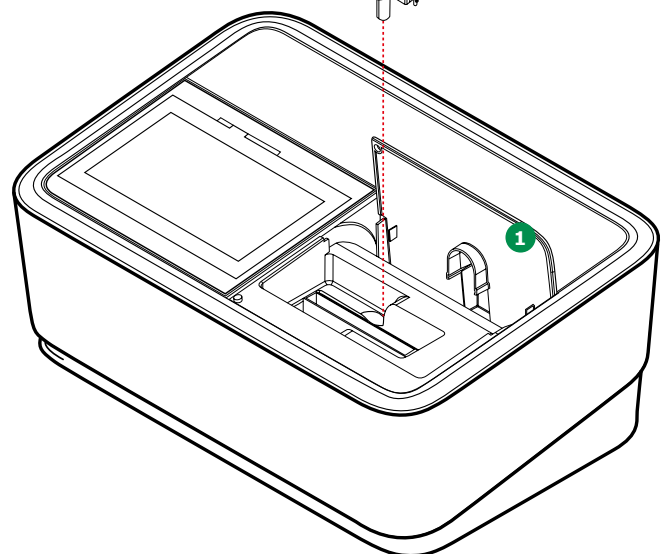
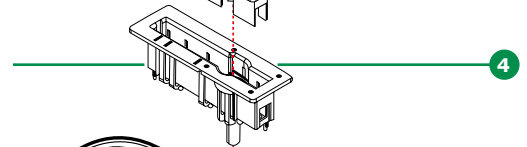
Prove
100 plus
Prove
300 plus



Prove
600 plus

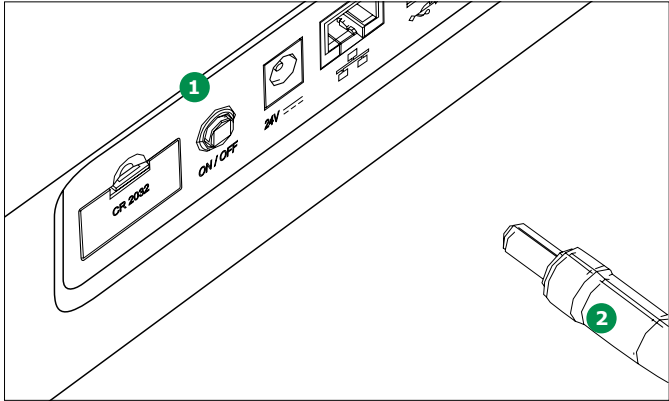


Prove
600 plus



3 In case a cell is broken in the cell compartment proceed as follows:

- 4 1. Switch off the spectrophotometer ① and disconnect the power plug ②.
- 5 2. Liquid might have drained onto the lab bench through the drains on the bottom of the instrument. Remove the instrument and clean the bench.
- 6 3. Wipe the bottom of the instrument clean without turning it upside down.
- 7 4. Remove the cell compartment as described above.
- 8 5. Carefully remove all broken glass, e.g. with a pair of tweezers.
- 9 6. Rinse the cell compartment thoroughly with clean water. Dry it with a lint-free cloth. Use isopropanol briefly to remove persistent contamination.
- 10 7. In case the non-removable part of the compartment is dirty clean it with a clean cloth.
- 11 8. Insert the cell compartment as described above.



9 NOTE

Upon renewed use of the spectrophotometer, reboot the instrument. If the self-test is passed the instrument is ready for further measurements. If the self-test fails, check whether the detector lens is dirty and clean it (see section 10.3.4).

10.3.3 Cleaning the Cell Compartment Cover and the Rear Cavity

⚠ CAUTION

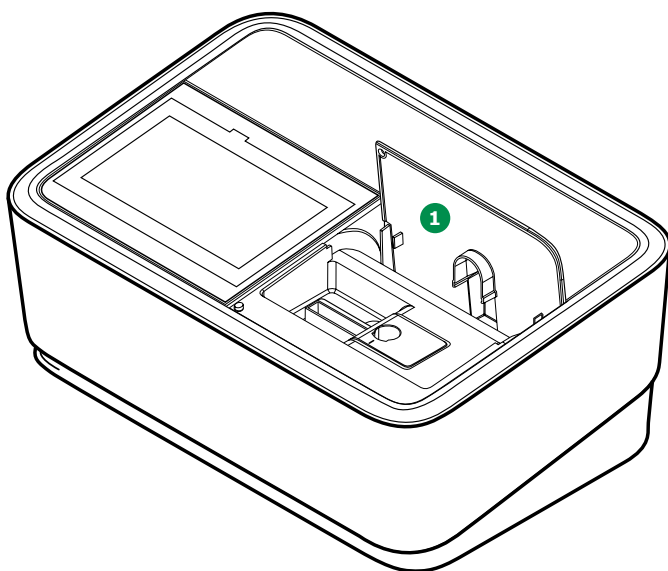
The cell compartment cover is made of synthetic materials.

Avoid any contact with acetone, similar solvents and detergents containing such solvents. Wipe off any splashes immediately.

Clean the cell compartment cover as follows:

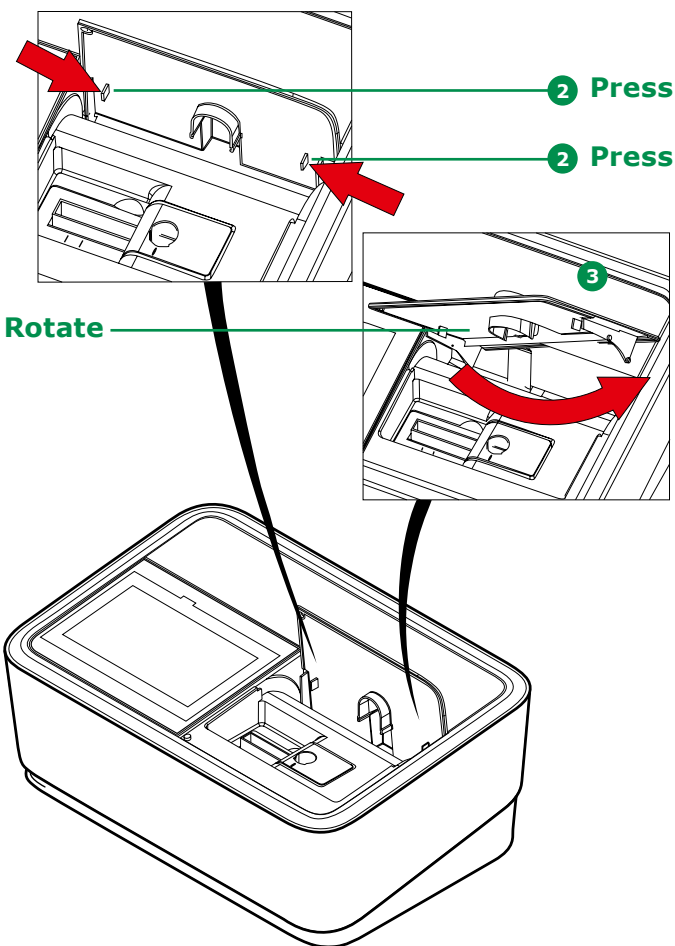
- If the surface of the cell compartment cover is dirty, wipe it with a soft cloth and mild soapy water
- Remove any chemicals splashes as soon as possible
- For disinfection, brief use of isopropanol is permitted

You can remove the cell compartment cover in case anything is spilled or fallen into the rear cavity. Proceed as follows:



1. Open the cell compartment cover **1**.
2. Press the two fittings inside of the cover **2** and rotate the cover slightly. It will turn and you can take it out.

3. Clean the cover and the rear cavity with clean water and dry it with a soft lint-free cloth.
4. Insert the cover: Put the round fittings at both sides **3** into the sliding cavities left and right by pressing the fittings **2** again and moving it slowly and carefully back and forth until the round fittings sit and the cover slides perfectly again.



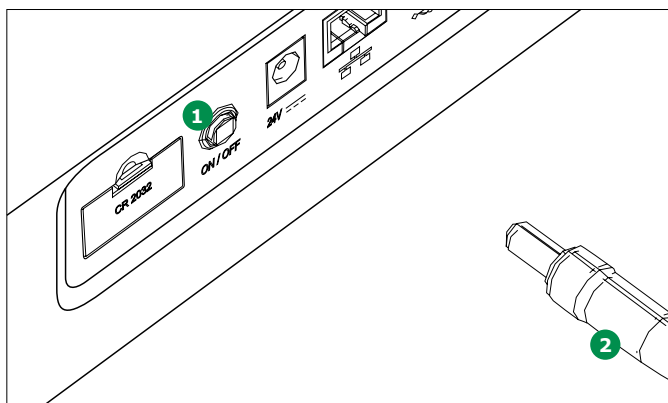
10.3.4 Cleaning the Detector Lens

Routine cleaning of the detector lens is normally unnecessary. Cleaning the detector lens can be necessary in the following cases:

- If the lens is visibly smudged, e.g. after a cell has broken or after a reagent accident (see section 10.3.2)
- If the self-tests fails

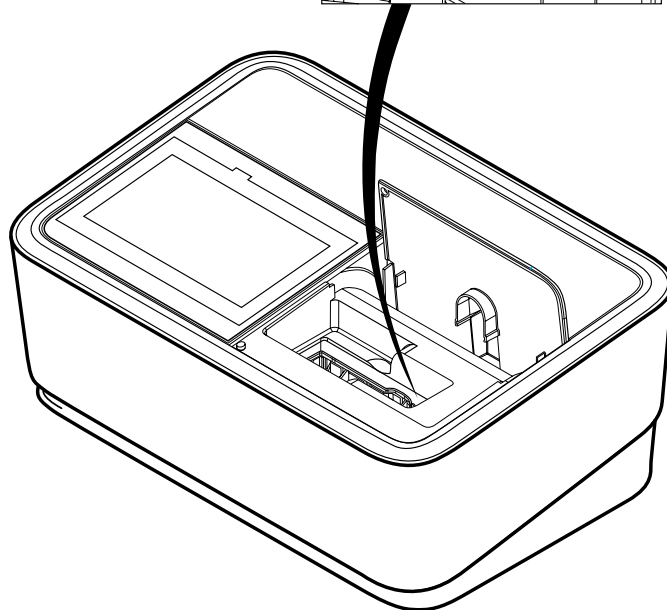
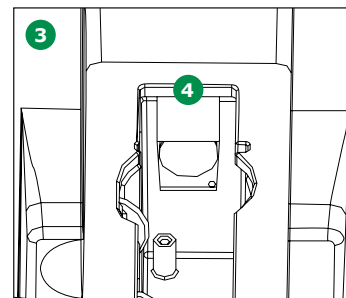
NOTE

If the lens is often smudged make sure to protect the instrument from dirt, dust and evaporates of chemicals. Check operation conditions of temperature and humidity. They have to be in accordance with the values specified in the technical data sheet (see section 12).



Proceed as follows to clean the detector lens: The detector lens is situated on the front left side of the rectangular cell compartment 3.

1. Switch off the spectrophotometer 1 and disconnect the power plug 2.



2. Cut off the end (approx. 2 cm) of a Dacron® swab, e.g. HY-LiTE® sampling pen, Cat. No. 1.30102.0021.
3. Grasp the cut-off end with the tip of a pair of tweezers or small pliers. Clean the lens 4 with the dry head of the swab. To do so, move the head from the center of the lens outward in circles. If there is persistent contamination, moisten the swab with a little deionized water or isopropanol.

NOTE

Upon renewed use of the spectrophotometer, reboot the instrument. If the self-test is passed the instrument is ready for further measurements.

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11 Error Causes and Trouble-shooting

Error	Cause	Remedy
Self-test does not start. Start button is inactive	<ul style="list-style-type: none"> • A cell is inserted in one of the cell compartments • A foreign object is inserted in one of the two cell compartment • The cell compartment is dirty • Instrument defective 	<ul style="list-style-type: none"> • Remove the cell • Then tap on the Start button • Remove the foreign object • Then tap on the Start button • Clean the cell compartment (see section 10.3.2) • Restart the instrument ✓ Contact service department
Self-test failed	<ul style="list-style-type: none"> • System check: Instrument defective • Lamp check: Lamp defective • Wavelength check: <ul style="list-style-type: none"> • Foreign bodies in the cell compartment • Lens dirty • Instrument defective 	<ul style="list-style-type: none"> • Contact service department • Prove 100 plus: Change the lamp • Prove 300 plus 600 plus: Contact service department • Remove the foreign object • Clean the lens (see section 10.3.4) • If this happens repeatedly, check the operating conditions (see section 8.1) • Contact service department
The message "system error" shows up	<ul style="list-style-type: none"> • System has frozen 	<ul style="list-style-type: none"> • Switch the instrument off, wait 1 minute and turn it on again. If error message remains contact service department
Instrument does not react to touchscreen operation	<ul style="list-style-type: none"> • Operating condition undefined or EMC load unallowed 	<ul style="list-style-type: none"> • Disconnect instrument from the electricity supply, wait 1 minute and re-connect
Measuring range under-cut or exceeded	<ul style="list-style-type: none"> • Selected method's measuring range not suitable to sample concentration 	<ul style="list-style-type: none"> • Select method with suitable measuring range • Dilute the sample
Obviously incorrect measured values	<ul style="list-style-type: none"> • Cell dirty • Dilution set incorrectly • Selected method not suitable • Zero measurement incorrect • Blank value incorrect 	<ul style="list-style-type: none"> • Clean the cell • Set the dilution • Select different method • Perform zero measurement • Re-measure the blank value

Error	Cause	Remedy
Data transfer to USB not working	<ul style="list-style-type: none"> Power supply of USB is interrupted USB has been disconnected while data transfer was still running 	<ul style="list-style-type: none"> Connect power supply Wait for one more minute before disconnecting the USB device from the instrument
Connected printer does not print	<ul style="list-style-type: none"> Print to pdf is activated Printer is not a PostScript printer 	<ul style="list-style-type: none"> Deactivate print to pdf Connect a printer that can interpret Post-Script
Data format in PC calculation program not correct	<ul style="list-style-type: none"> Decimal separator not adjusted to PC calculation program 	<ul style="list-style-type: none"> Use the same decimal separator in the instrument which is used in the PC (see section 8.2.4)

12 Technical Data

The serial number of the spectrophotometer is printed on the type plate at the rear of the instrument starting with "SN". The serial number is also stored in the instrument and can be looked up under "System" and submenu "Information", the last line MCS serial contains the serial number of the instrument (see section 9.2.1).

12.1 Spectroquant® Prove 100 plus

Spectroquant® Prove 100 plus	
Measuring technology	Spectrophotometer with reference beam technology
Wavelength range	320 – 1,100 nm
Lamp type	Tungsten halogen lamp
Measuring modes	Concentration, absorbance, transmission, multi wavelengths, spectra and kinetics in absorbance and transmission mode
Spectral bandwidth	4 nm
Wavelength resolution	1 nm (scan 0.1 nm)
Wavelength reproducibility	± 0.2 nm
Wavelength accuracy	± 1 nm
Stray light	≤ 0.1% transmission at 340 nm
Photometric range	± 3.0 Abs
Absorbance resolution	0.001 Abs
Absorbance reproducibility	± 0.003 absorbance at 1 absorbance between 320 nm and 900 nm
Absorbance accuracy	at 340 – 900 nm 1 absorbance: ± 0.005 absorbance 2 absorbance: ± 0.005 absorbance 2.5 absorbance: ± 0.010 absorbance
Scan	Limits freely selectable within the wavelength range Increment: 0.1/1/5 nm Scan speed: up to 170 nm/min (depending on the increment)
Smart Screen Display	Display p-cap glass touch screen
Live ID barcode	Automatic 2-D barcode reading system for all Spectroquant® cell and reagent tests Barcode contains lot, expiry, and calibration data. Data stored with each measurement
Cell size	16 mm round cells, 10, 20 and 50 mm rectangular cells with automatic recognition
Minimum filling volumes	16-mm round cells: 4 ml 10-mm rectangular cells (Standard): 2 ml (Semimicro): 1 ml 20-mm rectangular cells (Standard): 4 ml (Semimicro): 2 ml 50-mm rectangular cells (Standard): 8 ml (Semimicro): 4 ml
Cell holder	Removable for easy cleaning
Methods	Programmed methods of all Spectroquant® cell and reagent tests, additional user-defined methods: 99 concentration mode, 20 kinetic mode, 20 wavelength scans

Spectroquant® Prove 100 plus	
Applications	Free pre-programmed applications: bromate, brewery packages (MEBAK/EBC methods), sugar (ICUMSA), oil (DOBI, olive oil), color, and food
Ambient light protection	Measurement with open shaft possible due to proprietary solution (patent pending)
AQA prime	Individual settings for all methods in AQA1 mode: instrument check using PhotoCheck and/or Certipur® standards AQA2 mode: system check using CombiCheck or standard solutions
Monitoring functions	Instrument-supported pipette check and sample matrix check
Ad hoc measurement	Direct access to absorbance/transmission, kinetic and spectrum measurement
Software and method update	Free updates on our website (www.sigmaaldrich.com/photometer-service) via internet and USB stick
Communication interfaces	USB: 2 × USB-A (for printer, USB memory devices, keyboard or bar code reader), 1 × USB-mini-B Ethernet: LAN connection
Data storage	7,000 single measured values from the measuring modes concentration, absorbance/% transmission and multi wavelengths. 500 measurement result records of spectra, kinetics, AQA1, and AQA2 methods each
Languages	English, German, Spanish, French, Italian, Brazilian-Portuguese, Chinese (simplified and traditional), Japanese, Russian, Bulgarian, Czech, Danish, Dutch, Greek, Hungarian, Indonesian, Malay, Macedonian, Norwegian, Polish, Romanian, Serbian, Slovene, Swedish, Thai, Turkish, Vietnamese, Korean
Protection class	IP 31 for optics and electronics
Power supply	Power supply with 4 cables (1.2 m long) fitting US, EU, UK, and China plugs Total cable length 3 m (1.8 and 1.2 m)
Power requirements	100 V – 230 V, 50 – 60 Hz
Power consumption	Standard working condition: 12 W; power save mode: 8.8 W In regular measurement state: 55.2 W
Temperature	Operation: 10 – 35 °C; storage: -20 °C to +60 °C for 24 hours
Allowable relative humidity	Operation: 20 – 80% rH, storage in ambient relative humidity conditions of 20% to 95% Non-condensing
Dimensions	418 × 278 × 169 mm (width × depth × height)
Weight	approx. 6.8 kg
Warranty	24 months
EMC	Directive 2014/30/EU, EN IEC 61326-1:2021, IEC 61326-1:2020
Instrument safety	Directive 2014/35/EU, IEC 61010-1:2010/AMD1:2016, EN 61010-1:2010/A1:2019, UL 61010-1:2012/R:2019-07, CSA C22.2 No. 61010-1:2012/A1:2018-11

12.2 Spectroquant® Prove 300 plus

Spectroquant® Prove 300 plus

Measuring technology	Spectrophotometer with reference beam technology	
Wavelength range	190 – 1,100 nm	
Lamp type	Xenon flash lamp	
Measuring modes	Concentration, absorbance, transmission, multi wavelengths, spectra and kinetics in absorbance and transmission mode	
Spectral bandwidth	4 nm	
Wavelength resolution	1 nm (scan 0.1 nm)	
Wavelength reproducibility	± 0.2 nm	
Wavelength accuracy	± 1 nm	
Stray light	≤ 0.1% transmission at 340 nm; ≤ 1% transmission at 198 nm	
Photometric range	± 3.0 Abs	
Absorbance resolution	0.001 Abs	
Absorbance reproducibility	± 0.003 absorbance at 1 absorbance between 200 nm and 900 nm	
Absorbance accuracy	at 300 – 900 nm 1 absorbance: ± 0.005 absorbance 2 absorbance: ± 0.005 absorbance 2.5 absorbance: ± 0.008 absorbance	
Scan	Limits freely selectable within the wavelength range Increment: 0.1/1/5 nm Scan speed: up to 750 nm/min (depending on the increment)	
Smart Screen Display	Display p-cap glass touch screen	
Live ID barcode	Automatic 2-D barcode reading system for all Spectroquant® cell and reagent tests Barcode contains lot, expiry, and calibration data. Data stored with each measurement	
Cell size	16 mm round cells, 10, 20 and 50 mm rectangular cells with automatic recognition	
Minimum filling volumes	16-mm round cells: 4 ml 10-mm rectangular cells (Standard): 2 ml (Semimicro): 1 ml 20-mm rectangular cells (Standard): 4 ml (Semimicro): 2 ml 50-mm rectangular cells (Standard): 8 ml (Semimicro): 4 ml	
Cell holder	Removable for easy cleaning	
Methods	Programmed methods of all Spectroquant® cell and reagent tests, additional user-defined methods: 99 concentration mode, 20 kinetic mode, 20 wavelength scans	

Spectroquant® Prove 300 plus

Applications	Free pre-programmed applications: bromate, brewery packages (MEBAK/EBC methods), sugar (ICUMSA), oil (DOBI, olive oil), color, and food
Ambient light protection	Measurement with open shaft possible due to proprietary solution (patent pending)
AQA prime	Individual settings for all methods in AQA1 mode: instrument check using PhotoCheck and/or Certipur® standards AQA2 mode: system check using CombiCheck or standard solutions
Monitoring functions	Instrument-supported pipette check and sample matrix check
Ad hoc measurement	Direct access to absorbance/transmission, kinetic and spectrum measurement
Software and method update	Free updates on our website (www.sigmaldrich.com/photometer-service) via internet and USB stick
Communication interfaces	USB: 2 × USB-A (for printer, USB memory devices, keyboard or bar code reader), 1 × USB-mini-B Ethernet: LAN connection
Data storage	7,000 single measured values from the measuring modes concentration, absorbance/% transmission and multi wavelengths. 500 measurement result records of spectra, kinetics, AQA1, and AQA2 methods each
Languages	English, German, Spanish, French, Italian, Brazilian-Portuguese, Chinese (simplified and traditional), Japanese, Russian, Bulgarian, Czech, Danish, Dutch, Greek, Hungarian, Indonesian, Malay, Macedonian, Norwegian, Polish, Romanian, Serbian, Slovene, Swedish, Thai, Turkish, Vietnamese, Korean
Protection class	IP 31 for optics and electronics
Power supply	Power supply with 4 cables (1.2 m long) fitting US, EU, UK, and China plugs Total cable length 3 m (1.8 and 1.2 m)
Power requirements	100 V – 230 V, 50 – 60 Hz
Power consumption	Standard working condition: 12 W; power save mode: 8.6 W In regular measurement state: 46.5 W
Temperature	Operation: 10 – 35 °C; storage: -20 °C to +60 °C for 24 hours
Allowable relative humidity	Operation: 20 – 80% rH, storage in ambient relative humidity conditions of 20% to 95% Non-condensing
Dimensions	418 × 278 × 169 mm (width × depth × height)
Weight	approx. 6.8 kg
Warranty	24 months
EMC	Directive 2014/30/EU, EN IEC 61326-1:2021, IEC 61326-1:2020
Instrument safety	Directive 2014/35/EU, IEC 61010-1:2010/AMD1:2016, EN 61010-1:2010/A1:2019, UL 61010-1:2012/R:2019-07, CSA C22.2 No. 61010-1:2012/A1:2018-11

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12.3 Spectroquant® Prove 600 plus

Spectroquant® Prove 600 plus	
Measuring technology	Spectrophotometer with reference beam technology
Wavelength range	190 – 1,100 nm
Lamp type	Xenon flash lamp
Measuring modes	Concentration, absorbance, transmission, multi wavelengths, spectra and kinetics in absorbance and transmission mode
Spectral bandwidth	1.8 nm
Toluene/hexane ratio	> 1.4 – the correlation of spectral bandwidth to resolution for a toluene in hexane solution standard measured at ambient temperature 25 °C
Wavelength resolution	1 nm (scan 0.1 nm)
Wavelength reproducibility	± 0.1 nm
Wavelength accuracy	± 1 nm
Stray light	≤ 0.1% transmission at 340 nm; ≤ 1% transmission at 198 nm
Photometric range	± 3.3 Abs
Absorbance resolution	0.001 Abs
Absorbance reproducibility	± 0.003 absorbance at 1 absorbance between 200 nm and 900 nm
Absorbance accuracy	at 230 – 900 nm 1 absorbance: ± 0.004 absorbance 2 absorbance: ± 0.004 absorbance 2.5 absorbance: ± 0.006 absorbance
Scan	Limits freely selectable within the wavelength range Increment: 0.1/1/5 nm Scan speed: up to 750 nm/min (depending on the increment)
Smart Screen Display	Display p-cap glass touch screen
Live ID barcode	Automatic 2-D barcode reading system for all Spectroquant® cell and reagent tests Barcode contains lot, expiry, and calibration data. Data stored with each measurement
Cell size	16 mm round cells, 10, 20, 50 and 100 mm rectangular cells with automatic recognition
Minimum filling volumes	16-mm round cells: 4 ml 10-mm rectangular cells (Standard): 2 ml (Semimicro): 1 ml 20-mm rectangular cells (Standard): 4 ml (Semimicro): 2 ml 50-mm rectangular cells (Standard): 8 ml (Semimicro): 4 ml 100-mm rectangular cells (Standard): 16 ml
Cell holder	Removable for easy cleaning
Methods	Programmed methods of all Spectroquant® cell and reagent tests, additional user-defined methods: 99 concentration mode, 20 kinetic mode, 20 wavelength scans

Spectroquant® Prove 600 plus

Applications Free pre-programmed applications: bromate, brewery packages (MEBAK/EBC methods), sugar (ICUMSA), oil (DOBI, olive oil), color, and food

Ambient light protection Measurement with open shaft possible due to proprietary solution (patent pending)

AQA prime Individual settings for all methods in
AQA1 mode: instrument check using PhotoCheck and/or Certipur® standards
AQA2 mode: system check using CombiCheck or standard solutions

Monitoring functions Instrument-supported pipette check and sample matrix check

Ad hoc measurement Direct access to absorbance/transmission, kinetic and spectrum measurement

Software and method update Free updates on our website (www.sigmaaldrich.com/photometer-service) via internet and USB stick

Communication interfaces USB: 2 × USB-A (for printer, USB memory devices, keyboard or bar code reader),
1 × USB-mini-B
Ethernet: LAN connection

Data storage 7,000 single measured values from the measuring modes concentration, absorbance/% transmission and multi wavelengths. 500 measurement result records of spectra, kinetics, AQA1, and AQA2 methods each

Languages English, German, Spanish, French, Italian, Brazilian-Portuguese, Chinese (simplified and traditional), Japanese, Russian, Bulgarian, Czech, Danish, Dutch, Greek, Hungarian, Indonesian, Malay, Macedonian, Norwegian, Polish, Romanian, Serbian, Slovene, Swedish, Thai, Turkish, Vietnamese, Korean

Protection class IP 31 for optics and electronics

Power supply Power supply with 4 cables (1.2 m long) fitting US, EU, UK, and China plugs
Total cable length 3 m (1.8 and 1.2 m)

Power requirements 100 V – 230 V, 50 – 60 Hz

Power consumption Standard working condition: 12 W; power save mode: 8.6 W
In regular measurement state: 46.5 W

Temperature Operation: 10 – 35 °C; storage: -20 °C to +60 °C for 24 hours

Allowable relative humidity Operation: 20 – 80% rH, storage in ambient relative humidity conditions of 20% to 95%
Non-condensing

Dimensions 418 × 278 × 169 mm (width × depth × height)

Weight approx. 6.8 kg

Warranty 24 months

EMC Directive 2014/30/EU, EN IEC 61326-1:2021, IEC 61326-1:2020

Instrument safety Directive 2014/35/EU, IEC 61010-1:2010/AMD1:2016, EN 61010-1:2010/A1:2019,
UL 61010-1:2012/R:2019-07, CSA C22.2 No. 61010-1:2012/A1:2018-11

13 Accessories and Test Media

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13.1 Accessories

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Description	Order No.
Halogen lamp module for Spectroquant® Prove 100 plus	1.74010.0001
Case for Spectroquant® spectrophotometer Prove 100 plus 300 plus 600 plus	1.73020.0001
Rectangular cells 10 mm (1 pack = 2 pcs)	1.14946.0001
Rectangular cells 20 mm (1 pack = 2 pcs)	1.14947.0001
Rectangular cells 50 mm (1 pack = 2 pcs)	1.14944.0001
Semi-microcells 50 mm (1 pack = 2 pcs)	1.73502.0001
Rectangular cells quartz 10 mm (1 pack = 2 pcs)	1.00784.0001
Empty cells 16 mm Ø (1 pack = 25 pcs) with screw cap	1.14724.0001
Zero Cell (1 pack = 1 pc)	1.73503.0001
Rectangular cell 100 mm	1.74011.0001
Prove Connect to LIMS	Y110860001

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13.2 Optional Equipment/Connection Cables

Optional equipment	Description	Order No.
	USB barcode reader (hand-held scanner)	Trade
	USB PC keyboard	Trade
Connection cables	Cable with USB-mini-B and USB-A plug	Trade

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13.3 Test Media

	Description	Order No.
Test media for instrument check (AQA1)	Spectroquant® PhotoCheck	1.14693.0001
	Certipur® UV/VIS Standard 1 potassium dichromate solution to check absorbance according to DAB and Ph.Eur.	1.08160.0001
	Certipur® UV/VIS Standard 1A potassium dichromate solution to check absorbance at 430 nm according to DAB and Ph.Eur.	1.04660.0001
	Certipur® UV/VIS Standard 2 – sodium nitrite solution to check scattered light according to DAB and Ph.Eur.	1.08161.0001
	Certipur® UV/VIS Standard 3 – sodium iodide solution to check scattered light according to DAB and Ph.Eur.	1.08163.0001
	Certipur® UV/VIS Standard 5 – toluene solution in n-hexane to check resolution power according to Ph.Eur.	1.08165.0001
	Certipur® UV/VIS Standard 6 – holmium oxide solution reference material for wavelength according to DAB and Ph.Eur.	1.08166.0001
Test media for system check (AQA2) and MatrixCheck (AQA3)	Spectroquant® CombiCheck, standard solutions, and Certipur® standard solutions are listed in the catalog "Water, Food and Environmental Analytics" and on the Internet under www.sigmaaldrich.com	
Test equipment for pipet volume	Spectroquant® PipeCheck	1.14962.0001

1 14 Appendix

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Absorbance Logarithmic dimension for the absorption of the sample; negative decadal logarithm of the transmission.

Analysis instructions The exact workflow for carrying out the detection procedure is described in the analysis instructions.

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AQA Analytical Quality Assurance.

AQA1 1st step of analytical quality assurance: monitoring of the instrument.

AQA2 2nd step of analytical quality assurance: monitoring of the total system.

5

AQA2 labeling In the documentation, measured values are given an AQA2 labeling if the measurement was carried out with AQA2.

AutoSelector Plastic cylinder with barcode. It transmits the code for a reagent test kit to the spectrophotometer. To insert it into the spectrophotometer open the lid and place it into the round cell compartment.

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Barcode 2-D barcode containing information on method number, expiry and lot number. If needed, it also contains data for a calibration update. Barcode is read by the inbuilt barcode reader.

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Baseline Reference value for the spectrum of reference absorbances or reference transmissions.

Cell Vessel to take a liquid sample for measurement in a spectrophotometer. The cell material (mostly glass) must have certain optical features to be suitable for photometry.

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Citation forms Different forms of representing a measured concentration value that can be derived from each other. The method for the determination of phosphate, for example, provides a measured value for phosphorus P. This measured value can alternatively be given in the citation forms PO_4 , PO_4 -P or P_2O_5 .

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CombiCheck Multiparameter standards used to check the total system for a method and for the Matrix-Check.

Concentration Mass or amount of a dissolved substance per volume, e.g. in g/l or mol/l.

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Detection procedure The detection procedure designates the general principle of how a sample is brought into a form suitable for measurement. Different methods can be based on the same detection procedure.

Kinetics Measurement over a period of time.

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Log files These contain the automatically recorded log of all or specific actions of processes in the device.

MatrixCheck Check on whether the photometric determination is disturbed by other sample ingredients (sample matrix). The MatrixCheck can be carried out by spiking or diluting.

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Measuring solution Name for the sample ready to be measured. A measurement sample is obtained from the analytical sample (primary sample), usually through work-up. Measuring solution and analytical sample are identical when there has been no work-up.

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Measured value The measured value is the special value of a measured parameter to be determined. It is expressed as a combination of the numerical value and unit (e.g. 3 m; 0.5 s; 5.2 A; 373.15 K).

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Method A method comprises a chemical detection procedure and special method data (calibration line) that is required to evaluate the measurement results. How to carry out the method up to measuring with the spectrophotometer is described in the analysis instructions. All Spectroquant® Prove plus spectrophotometers contain a database with methods. Furthermore, user-defined methods can be entered in the database as well.

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PhotoCheck standard Stable color solution with defined absorbance values for the check of AQA1 on the spectrophotometer.

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Reagent blank	The evaluation of the photometric measurement always refers to the comparison value of a test solution without the substance to be determined (reagent blank value). Thus the influence of the basic absorbance of the reagents on photometric measurement is compensated for. For all measurements with Spectroquant® test kits (concentration mode) there is an exactly determined reagent blank value stored in the spectrophotometer. This value can, however, be overwritten by a reagent blank value measured by yourself. If needed the 2-D barcode on the cell tests and the AutoSelector may also contain an updated reagent blank which overwrites the pre-programmed reagent blank in the instrument.
Recovery	Recovery is the found measured value divided by the default value (percentage). Example: Default value 20 mg/l; Found 19.7 mg/l => recovery 98.5%.
Recovery in MatrixCheck	Recovery in MatrixCheck means recovery of the addition. Example of calculation: value without addition = 100; addition of 20 = 120 theoretical value. Measured value = 115, only 15 from the addition of 20 were found, recovery = $(115-100)/(120-100) = 75\%$
Sample blank	The sample blank value is a characteristic of the sample (coloration) to be currently determined. The blank is diluted depending on the method being used, but does not contain any color reagents. The pH is the same as that of the test sample.
Spectrum	Distribution of the intensity, transmission or absorbance depending on the wavelength.
Standard	Sample with a defined concentration of the analyte to be determined.
Test kit (test)	A test kit contains all reagents that are required for the photometric determination of the sample according to the analysis instructions.
Transmission	Part of the light that passes through the sample.
Turbidity	Light attenuation caused by diffuse scattering at undissolved substances.
Zero adjustment	Adjusting a spectrophotometer with a water-filled cell.

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15 List of Smart Icons on Display

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Main menu Buttons

Description



Method list

List of all methods, irrespective of mode

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Settings

This button is used to activate method-specific settings (e.g. sample dilution, turbidity correction, zero adjustment, sample blank, reagent blank)

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Ad hoc

For performing measurements (absorbance/transmission, spectrum, kinetics)
Allows measurements to be performed without the need to create methods

6



AQA

Overview and list of all Analytical Quality Assurance (AQA) modes

7



Results list

List of all stored results

8



System – instrument setup

This button is for optional instrument settings (e.g. date, time, updates etc)

9



Login/logout

Check on users in and out

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Timer list

List of stopwatch functions

Info Buttons

Description



Methods information



Main menu selection button – switches between 2 main menu overviews

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Switch between different citations (NH₄, NH₃ etc)



Switch between different units (mg/l, ppm etc)

12

Sub-menu Buttons

Description



Absorbance/Transmission Mode

Ad hoc submenu: perform absorbance or transmission measurements
Result list: filter concentration mode

13



Concentration

Method list: create methods -> Concentration Mode
Result list: filter Ad Hoc ABS/Trans measurements

14



Spectrum Mode

Ad hoc submenu: record spectrum
Method list: create methods -> Spectrum Mode
Result list: filter spectrum mode

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Sub-menu Buttons	Description
	Kinetic Mode Ad hoc submenu: perform kinetic measurement Method list: create methods -> Kinetic Mode Result list: filter kinetic mode
	AQA Status 1&2 AQA submenus: Status display of the period of validity and the outcome (passed / failed)
	AQA1 AQA submenu: List of AQA1 methods
	AQA2 AQA submenu: List of AQA2 methods
	Pipette check AQA submenu: List of pipette checking methods
	Information System submenu displays the following information about the device: Software/method versions, device class, lamp counter and serial number
	Interface System submenu displays the following settings options – and standard settings: Audible signals – ON, Backlight – 100%, Print to pdf – ON
	Region System submenu displays the following settings options – and standard settings: Language, date, time and country zone EU/US, decimal separator – "." (dot)
	Quality System submenu displays the following settings options – and standard settings: Quick zero – OFF, AQA1 and AQA2 lock – OFF, Zero Adjustment expiry – ON (interval: 7 days), Use expired reagents – OFF, Service reminder – ON
	Automation System submenu displays the following settings options – and standard settings: Energy saving mode – ON (10 minutes), Auto Power off – OFF, Auto log off – OFF, Auto store – ON, Auto print – OFF, Sample ID popup – OFF
	User management System submenu displays the following settings options – and standard settings: Activation of user management and administrator settings, User login required – OFF
	Service System submenu displays the following settings options: Various service functions such as backup, restore, export of log or system data and import of methods
	Update System submenu displays the option for performing software and method updates

1 15 List of Smart Icons on Display

2

Sub-menu Buttons

Description



Network

This submenu of the "Instrument settings" menu displays the setting options for connecting the Prove plus device with a network



Prove Connect

This submenu of the "Instrument settings" menu displays the setting options for connecting the Prove plus device with Prove Connect

Selection & Action Icons

Description



Start



Start zero

Start zero adjustment for a method



Apply



Save



Stop



Close



Logout

User logout



Search method



Reset resp. clear filter options



Edit

For editing parameters



Create method



Duplicate/copy

The selected method is duplicated/copied



Print

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Selection & Action Icons**Description****Export button**

All selected methods are exported to an external memory device

**Import button**

Updates/methods are imported from an external memory device into the instrument

**Delete**

The selected items are deleted

Notification Icons in Menu "Settings"**Description****Dilution**

Activate and notify predilution

**Turbidity on**

Activate and notify the turbidity correction

**Show absorbance**

Activate and notify display of absorbance value in the result screen

**Zero adjustment**

Perform zero adjustment

**Sample blank value**

Activate and notify Sample blank value

**Reagent blank**

Activate and notify user-defined Reagent blank

**Recalibrate**

Activate and notify user-defined recalibration

**MatrixCheck**

Activate MatrixCheck

**User defined measurement range**

Activate user-defined lower and upper limit of the measuring range

1 15 List of Smart Icons on Display

Toggle Button

Description



OFF/ON Button

0 = Off, I = On – the part displayed in light grey is active – here: 0 = OFF



Date/measurement

Switch between date or measurement interval (AQA2); active here: measurement interval



Absorbance/transmission

Switch between absorbance or transmission mode; active here: transmission mode



Spiking/dilution

Switch between spiking and dilution (MatrixCheck); active here: dilution

Action Icons on Datepicker/Keyboard/Calculator

Description



Back



Close



Clear



Delete



Apply



Add

Radio Buttons/ Checkboxes

Description



Warning

Warnig symbol check info box



Barcode scanner deactivated

The barcode scanner for reading out the Live ID barcode on round cells and AutoSelectors has been deactivated










Locked

Change password



Chosen

Check mark

Selection & Action Icons, e.g. Result List	Description
	Search list Search function, search criterion: method number, method name or article number (first 6 digits)
	Set date/date filter
	Sample ID Search/results list. Search function, search criterion: sample ID
	Select all/select none
	Panorama view Graphic representation of measurement series (control card, control chart, for trend analyses)
Selection & Action Icons e.g. User-defined Methods	Description
	Set value pair(s) for method calibration
	Set formula for method calibration
	Show graphic view
Selection & Action Icons e.g. Spectrum Kinetic	Description
	Table view of values
	Return to the recorded spectrum
	Next left/Step/next right
	Zoom out
	Zoom in
	View of peak max of a spectrum

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1 15 List of Smart Icons on Display

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Selection & Action Icons e.g. Spectrum Kinetic



View of peak min of a spectrum

4



Calculate and show sum of spectra

5



Calculate and show difference of spectra

6



Overlay of spectra

7



First-order derivative of a spectrum

8



Navigation in graphic view

9

Status Icons

Description



Attention
Warning symbol check info box

10



Time
Time Stamp

11



Passed
Status of a check; ✓ = passed

12



Off
Status of a check; ○ = inactive

13



Failed
Status of a check; ⊖ = failed

14



Expired
Status of a check; ⊕ = overdue

15



Progress
The instrument is in progress

16



Progress
The instrument is in progress

16 Contents of log files

As already mentioned in [section 9.2.7](#), the procedure for the export of log files involves the creation and export of three separate files.

16.1 Error log file

The error log file contains the documented collection of error messages generated by the operating system. These error messages are presented in a coded format.

Each entry contains details on the date and time of the error, the error type, the process and the components involved, and the severity of the error.

The content of the error log file supports the processing of service issues and remote diagnoses.

16.2 User log file

The user log file contains the documented collection of relevant operations and changes in the settings initiated by the user.

The operations are saved in a coded format. Each entry contains details on the date and time, the user, and the action.

The information documented in the user log file are coded in the following way:

Group	Action code	Additional information
0 = General	1 = Power On	-
	2 = Power Off (by User)	-
	3 = Auto Power Off	-
	10 = Self-Test passed	-
	11 = Self-Test failed	1 = System-, 2 = Lamp-, 3 = WLCheck
	20 = Login	-
	21 = Logoff (by User)	-
1 = AQA1 Management	0 = AQA1 Locking switched Off	-
	1 = AQA1 Locking Switched On	-
	10 = De-Activated AQA1 Check	Check ID No
	11 = Activated AQA1 Check	Check ID No; Interval
	12 = Changed AQA1 Interval	Check ID No; Interval
	20 = AQA1 Check failed	Check ID No
	22 = AQA1 Check passed	Check ID No
2 = AQA2 Management	0 = AQA2 Locking switched Off	-
	1 = AQA2 Locking Switched On	-
	10 = De-Activated AQA2 Check	Method No;
	11 = Activated AQA2 Check	Method No; Interval; Mode
	12 = Changed AQA2 Interval	Method No; Interval
	13 = Changed AQA2 Mode (M/D)	Method No; Mode
	20 = AQA2 Check failed	Method No
	22 = AQA2 Check passed	Method No
3 = General AQA	0 = Allow expired reagents	-
	1 = Prohibit expired reagents	-
	10 = Override AQA2 overdue	Method No
	11 = Override pass on reagents	Method No
	20 = Result deleted	Method No
4 = Zero Management	1 = Zero Adjustment	Wavelength; Pathlength

1 16 Contents of log files

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Group	Action code	Additional information
5 = General Settings	0 = User Management Off	-
	1 = User Management On	-
	10 = Change Date	New Date (Format?)
	11 = Change Time	New Time (Format?)
	12 = Change Language	New Language (Enumeration)
	13 = Change Zero Expiration	New Interval (Days)
6 = System	1 = Instrument Software Up-date	Version (n;m;r)
	10 = Backup	
	11 = Restore	

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Example of entries in a user log file:

Devicename;Prove 600 plus
Serialnumber;1529610052
Software Version;ISW 1.5.0
Timestamp;UserId;Actiongroup;Actioncode;Info1
;Info2;Info3;Info4
201208_0959;logout;0;10;0;0;0;0
201208_0959;anonymous;0;20;0;0;0;0
201208_1000;pm;0;20;0;0;0;0
201208_1000;pm;1;0;0;0;0;0
201208_1000;pm;2;0;0;0;0;0
201208_1000;pm;3;0;0;0;0;0
201208_1000;pm;3;20;9001;0;0;0
201208_1001;pm;3;20;9002;0;0;0

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Explanation of an example:

201208_1001;pm;3;20;9002;0;0;0

Timestamp = 201208_1001

UserId = pm

Actiongroup = 3 = General AQA

Actioncode = 20 = Result deleted

Info1 = 9002 = Method No

Info2 = 0 = no further details

Info3 = 0 = no further details

Info4 = 0 = no further details

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Interpretation = on 8 Dec 2020 at 10:01am, user "pm" made a change in the group "Quality (General AQA)". A result of method 9002 was deleted. No further details.

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16.3 Service log file

The service log file contains the documented collection of operations carried out in the course of service operations by service engineers. The error messages are presented in a coded format.

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Merck Life Science KGaA, 64271 Darmstadt, Germany, Tel. +49(0)6151 72-2440

www.sigmaaldrich.com