FlavourSpec® with PAL RSI

User Manual

G.A.S. Gesellschaft für analytische Sensorsysteme mbH

FlavourSpec®– User Manual

Version 4.00, October 2020

Valid from FlavourSpec® Firmware Version 4.00 in combination with Autosampler PAL3-RSI Series II

G.A.S. reserves the right to realize technical changes to the product without explicitly mentioning them**.**

CE-Marking according to:

International Standard EN ISO 17050-1:2004
Directive 2014/35/EU (Low voltage directive);
Directive 2014/30/EU (Electromagnetic compatibility);
Directive 2011/65/EU (RoHS);
Directive 2012/19/EU on waste disposal (Waste Electrical and Electronic Equipment – WEEE)

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1 General Information

1.1 Information about the Manual

This manual describes a safe and adequate handling of the device. Following the instructions of the indicated safety aspects and instructions as well as the national and/or local rules and general safety regulations concerning the prevention of accidents are absolutely imperative.

Before starting the work with the device read the manual completely and thoroughly particularly the chapter security and respective safety references. Assure that you/the operator comprehend the terms described.

The manual is part of the device. It must be stored together with and next to the device at any time.

INFORMATION!

The graphics in this user manual are schematic and may differ from the actual conditions. The firmware and PC software screenshots in this user manual may differ from the actual conditions.

1.2 Explanation of Symbols

Important and safety-relevant references in this manual are characterized by symbols. These indications which are in-line with industrial safety must be respected and followed at any time.

INFORMATION

This symbol calls information, which are to be considered for efficient and perfect handling of the equipment.

WARNING

This symbol indicates references, which can lead to damages, malfunctioning and/or loss of the device.

DANGER

This symbol marks references, which can lead to health impairments, injuries, lasting body damages or to death due to electric current.

DANGER

This Symbol marks paragraphs, which describe potential dangers and damage due to exposure to radioactive radiation.

1.3 Notation for dialogs, elements and references

Example Dialog:

System › Connections › LAN File Transfer › Settings... › Test Connection

Example Elements:

Gas Out, Sample gas in

Example: References

Advanced User Manual, Chapter 5.1 Installation Reguirements

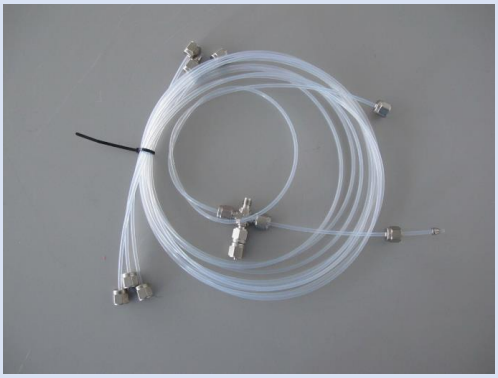
Example: Information

keep the transport box

1.4 Scope of Supply

Assure that you have received the full scope of supply. If there is any part missing, please contact the GAS-hotline immediately.

FlavourSpec Scope of Supply	
	**FlavourSpec Device coupled Autosampler PAL3 Series II**

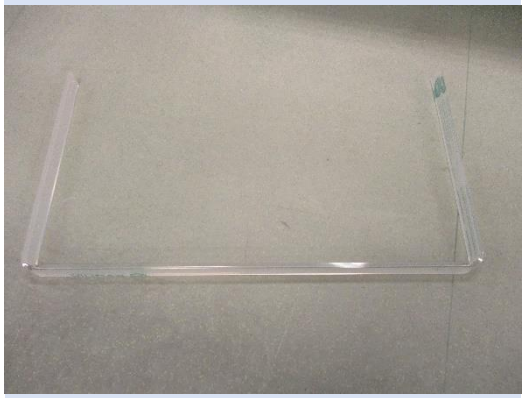
	FlavourSpec Power supply with cable (1 piece)
	**FlavourSpec Gas tube Kit** • Driftgas/Carriergas (1 piece) • 2 m 3mm PFA Tubes with 3 mm Swagelok-Connector (2 Pieces) • 0,65 m 3mm PFA Tubes with 3 mm Swagelok-Connector (1 Pieces)
	Molecular sieve 200 ml with 1/8” connections (1 piece)
	LAN Cable (1 piece)

	FlavourSpec-PAL3 Connection Cable
	**FlavourSpec Blind plug Set** (4 pieces) (Swagelok 3mm Blind plug with red cap installed on device connectors)
	**FlavourSpec Torx Tool Kit** • Torx Srewdriver 8 mm (1 piece) • Torx Srewdriver 10 mm (1 piece)
	Document Map with Documents and Device User Manuals

	USB-Stick Box with Software und Documents (1 piece)
Autosampler PAL3 Series II Scope of Supply	
	Autosampler Power supply with cable (1 piece)
	Terminal with Connection Cable (1 piece)
	Agitator Connection Cable (installed) (1piece)

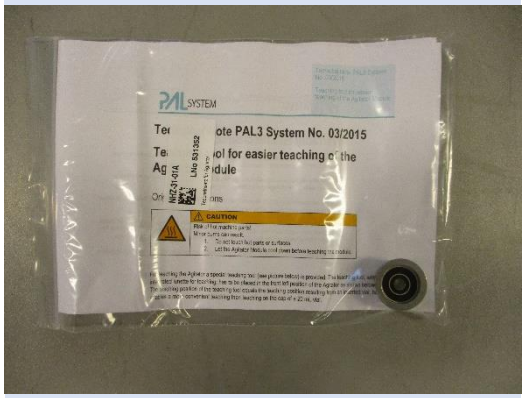
PAL3 Torx Tool Kit

- Torx Screwdriver 8 mm (1 piece)
- Torx Screwdriver 10 mm (1 piece)
- Torx Screwdriver 20 mm (1 piece)
- Torx Screwdriver 25 mm (1 piece)

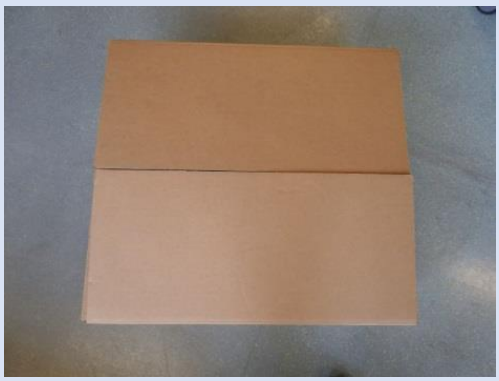


Safety Guard including screws (1 piece)

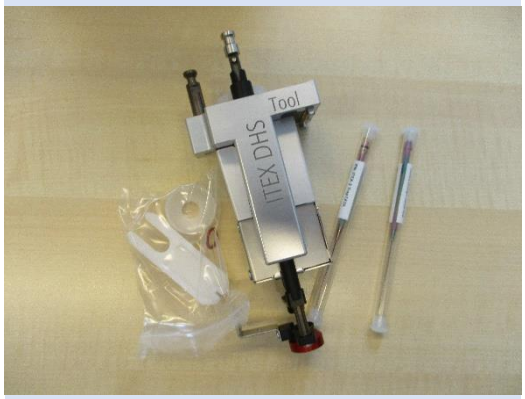
Syringe Kit (2 pieces)



PAL3 Teaching Tool

	**Starter Kit** (100 x 20 ml Headspace Vials, 100 magnetic caps, 3 Septa for Injector
	Transport box (1 piece)
	FlavourSpec Transport palett (120 x 80 cm)

Optional Scope of Supply (only available if ordered)

	Nitrogen Generator with accessories (example picture)
	Laptop Computer (different design) including software for control and evaluation
	PAL ITEX-Kit
	Crimper for H 20 ml Headspace Vials

1.5 Liability and Guarantee

This user manual describes the safe and proper handling of the device.

All data and reference within this manual are compiled under the valid regulations, the state-of-the-art as well as G.A.S. experiences of several years.

This user manual must be stored together with and close to the device at any time and accessible to all persons, who operate or handle the device at any time.

This user manual must be read carefully before starting to work with the device. G.A.S. does not assume any liability for damage and disturbances, resulting from disregard of the instructions contained in this user manual. All claims of any kind related to damage from a not intended use of the device will be rejected.

G.A.S. reserves the right to realize technical changes of the product due to improvements without explicitly mentioning them.

1.6 Copyright

The manual is confidential. It is beyond doubt exclusively made and also meant for the personnel directly dealing with the equipment. All data, texts, designs, pictures and other representations within this manual are protected in the sense of the copyright law and are subject to further commercial patent rights. Each abusive is punishable by law.

Passing it on to third persons as well as duplications in any kind and form - also in part - as well as the use and/or report of contents are not permitted without written agreement of the manufacturer. Offences lead to payment of damages. We reserve ourselves all rights of the practice of commercial patent rights.

1.7 Return and Disposal

For an adequate disposal, the device or/and its equipment must be returned to the G.A.S. or to a third party authorized by the G.A.S.! For questions please contact G.A.S.

1.8 Software Updates

If there are any software updates customers will be contacted by G.A.S. Gesellschaft für analytische Sensorsysteme mbH as soon as the updates are available. The updates are free of charge within the first 12 month after delivery. Users will be

provided with information about the changes and instructions for executing the updates.

1.9 Customer Service

For questions concerning G.A.S. products a customer service is available:

G.A.S. Gesellschaft für analytische Sensorsysteme mbH
Otto-Hahn-Straße 15
44227 Dortmund
Germany
Phone: +49 (0) 231 / 97 42 - 65 50
Fax: +49 (0) 231 / 97 42 - 65 55
support@gas-dortmund.de

The telephone hotline is available from monday to friday from 9:00 to 16:00 hours. In urgent cases or if you use fax or email please provide a telephone number for callbacks.

2 Safety

2.1 Intended Use Only

WARNING!

Usage other than described in this manual may damage the device and/or harm persons involved.

Do not use the device for other purposes. Damages due to misuse are not covered by the guarantee. Such damage claims will be rejected.

The device and its equipment are not certified for the employment in areas with explosive gas air mixtures.

All claims or requirements of any kind against the manufacturer and/or its authorized persons that arise due to damages from a not intended use of the device will be rejected. All damages that arise from a not intended use are of the operator's responsibility.

The intended use of the equipment and its correct handling according are described in the operating instructions of this manual. Other parts than the parts belonging to the scope of supply, may only be used after G.A.S. approval.

2.2 Responsibility of Operator

The device may only be operated in a perfect technical condition. Before putting the device into operation the condition of the device and its equipment must be checked. The information and instructions provided in this manual have to be followed at any time.

Besides the instructions provided in this manual the local rules for the prevention of accidents, general safety regulations - valid for the area of application of the device - as well as the valid environmental-protection regulations must be considered and respected.

The responsible technicians and operators have to make sure a failure-free use of the device. Responsibilities among the involved persons regarding installation, operation, maintenance and cleaning must be made clear.

2.3 Requirements of Personnel

Only authorized and trained technical personnel may work with the instruments. The operator must have received an instruction over existing and all possible dangers and should be regularly instructed in safety procedures and environmental protection and that the personnel is fully aware of the complete operating instructions and particularly the safety notes. Personnel that might be under the influence of drugs or alcohol are to be kept off the device at any time.

Technical personnel in this context are defined as skilled employees who are knowledgeable due to their educational background. In case the foreseen personnel do not have the necessary qualifications to operate the instrument, it must be trained. Further to that non-authorized personnel should not operate the device.

The competencies for the work on and with the device must be specified and kept undoubtedly at any time so that with respect to security issues no unclear situation might come up.

Any changes of the equipment, which impair security of the personnel, must immediately be reported to the operator and every person dealing with it.

2.4 Dangers

The device and its equipment is subject to an endangerment analysis. The construction and execution of the device corresponds to the today's state-of-the-art. The device is reliable in service when operated according to its intended use.

INFORMATION!

If the housing of the device is damaged, the device must not be used anymore and must be returned to the G.A.S. by using the original transportation case.

DANGER

The FlavourSpec® device contains a radioactive radiation Tritium source of 75 MBq which in all EURATOM countries is below the exemption limit. However, do not open the device! Do not try to recover malfunctions of the device! Malfunction recovery, repairs and any maintenance work may only be performed by G.A.S. or by qualified personnel authorized by G.A.S.

DANGER

The FlavourSpec® and its equipment is not certified for the employment in areas with explosive gas air mixtures (Zone 0).

DANGER

Exercise great care in handling current-carrying parts like the power supply cord. Do not get directly in touch with current-carrying parts. Do not open the housing. Do not use damaged parts.

DANGER

When Nitrogen is used as drift gas and helium as carrier gas, ignition of a helium plasma may occur due to the high voltage present in conjunction with a radiation source. This can damage the IMS.

3 Transport, Packing and Storage

3.1 Inspection after Transport

Check the supply immediately after delivery concerning its completeness and/or transport damages. If you detect externally visible transport damage, do not receive the supply, or only under reservation. State the extent of the damage on the provided delivery note and/or the transportation documents of the feeder. Generate a complaint. Lodge a complaint of covered defect immediately after recognizing, as claims due to transport damages can only be made valid within the complaint periods (usually 7 days).

3.2 Packing

If no return agreement regarding the packing was agreed upon dispose the packaging material always in an environmentally friendly way and according to valid local regulations. If additional information is required please ask a recycling company.

INFORMATION!

It is recommended to **keep the transport box** for a safe return transport.

3.3 Storage and Transport

Store the device only under the following conditions:

- **When not in use store the equipment in the supplied casing**
- **Prevent unauthorized access**
- **Do not store outside**
- **Protect the equipment from moisture and dust**
- **Put protective caps on all gas sockets**
- **Avoid mechanical vibrations**
- **Do not expose the equipment to aggressive substances**
- **Protect the equipment from direct sun light**

- **Storage temperature: 5 to 40 °C**
- **Relative Air Humidity: 0- 90%Rh, prevent condensation**
- **Instrument's position: Horizontal**

The equipment should be moved only packaged into the provided transport case. By these means, transport damages can be avoided. The above-mentioned values are considered for an instrument transported in its original new packing.

WARNING!

Protective caps should be put on gas sockets in case the device is stored or transported.

4 Cleaning and Maintenance

Natural aging and the wear of certain components of the equipment require a regular cleaning and maintenance.

4.1 Cleaning

Clean the device only with a dry or easily damp cloth.

WARNING!

Do not use cleaning agents, which contain solvents, acids, or bases.

4.2 Maintenance

INFORMATION!

Maintenance of the device should only be carried out at G.A.S. or through specially trained and by G.A.S. authorized personnel.

The recommended **maintenance interval is 24 months.**

5 Introduction

5.1 Working principle of IMS technologie

Ion Mobility Spectrometry (IMS) is an analytical technology to separately detect gaseous compounds in a mixture of analytes. The separation is based on the specific drift times, that ionized compounds need to pass a fixed distance (drift tube) in a defined electric field.

Drift velocity: $v_d = KE$ Mobility: $K = \frac{L^2}{t_D U}$

$$K = \frac{3}{16}\sqrt{\frac{2\pi}{\mu kT}}\frac{Q}{n\sigma}$$

Q	*ion charge*
n	*drift gas number density*
μ	*reduced mass of the ion and the drift gas molecules*
k	*Boltzmann constant*
T	*drift gas temperatures*
σ	*ion's collision cross section with the drift gas*

Figure 1: Ion Mobility Spectrometer - Basic Relations

Compared to other techniques e.g. TOF-MS, ions travel at atmospheric pressure versus a flow of inert drift gas. The drift time of each substance is determined by its ion mass and geometric structure, as slowing collisions with the drift gas molecules are more frequent for sterically demanding structures. Therefore, IMS can even differentiate isomeric molecules. For detection, the resulting ion current is measured by an electrometer as a function of time.

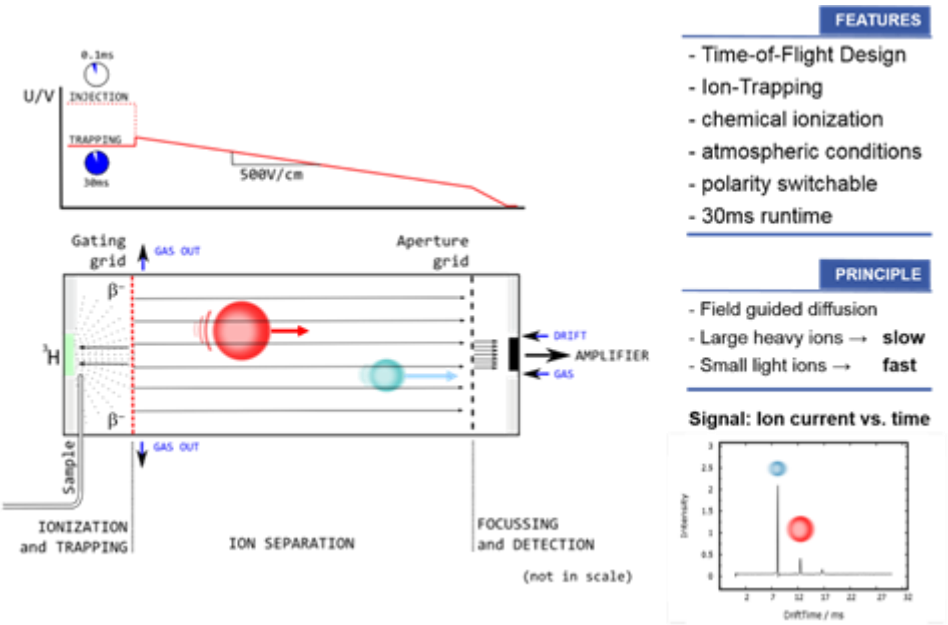


Figure 2: Ion Mobility Spectrometer -Working Principle

Atmospheric Ionization of molecules can be obtained by several techniques. G.A.S. uses photoionization with a 10.6eV UV-lamp or soft chemical-ionization initiated by a low-radiation tritium (H3) source (below exemption limits of EURATOM). While the first directly produces positive ions, the latter generates *reactant ions* with the gas atmosphere by a cascade of reactions following the collision of a fast electron emitted from the *β*-radiator H3. The so-called Reaction Ion Peak (RIP) representing the total of all ions available is formed as a first step. In nitrogen and air, resp., the *reactant ions* can be described as $H^+(H_2O)_n$ and $O_2^-(H_2O)_n$. Chemical ionization of analytes by *reactant ions* then result in the formation of specific analyte ions, when the affinity of the analyte towards the reactant ion is higher in case compared to water (using the positive ionization mode). The proton affinity of water is 691kJ/mol, so all molecules with a higher proton affinity will be ionized by a proton transfer, which is typically given for all heteroatom-organic compounds. The ionization takes place at ambient pressure, so that the analyte concentration is not diluted as compared to other analytical methods where a vacuum must be applied. Therefore, IMS is extremely sensitive. The detection limits typically are in the low ppb-range for *volatile organic compounds* (VOC).

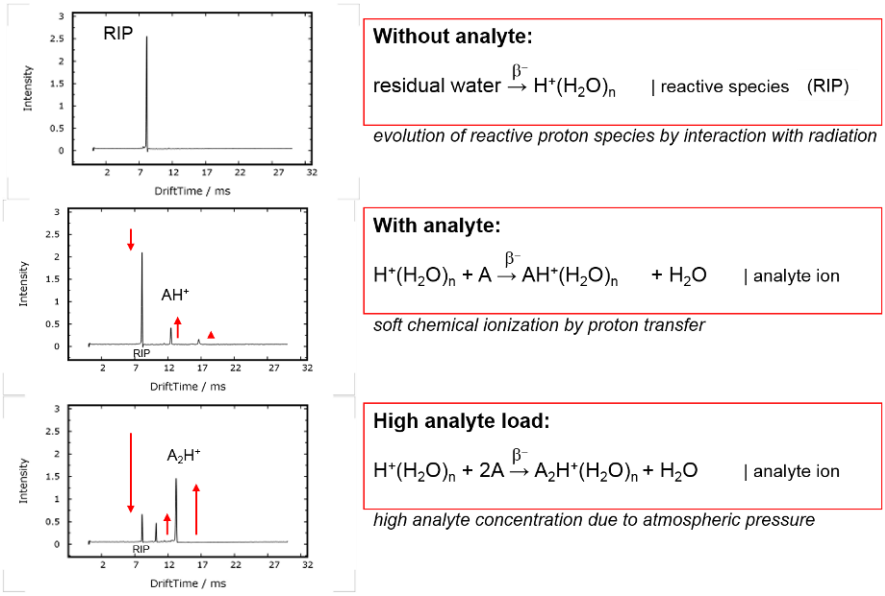


Figure 3: IMS Predominant Ionization (positive polarization)

The above figure exemplarily shows typical IMS spectra without analyte and with analyte. The RIP is formed as a sharp signal proving the cleanliness of the system and at a specific position that is used as internal standard. The spectrum containing analytes shows a decreased RIP, while new (analyte) peaks are correspondingly formed. The drift time is specific to each ion, therefore analyte identification is possible. The peak height and area correlate with the analyte concentration, so that a quantification is also possible.

Protone Affinities

Aromatic Amines	930.0 KJ/mol	Pyridine
Amines	899.0 KJ/mol	Methyl Amine
Phosphorous Compounds	890.6 KJ/mol	Trimethylphosphate
Sulfoxides	884.4 KJ/mol	Dimethyl Sulfoxide
	853.6 KJ/mol	Ammonia
Ketones	832.7 KJ/mol	2-Pentanone
Esters	821.6 KJ/mol	Methyl Acetate
Alkenes	805.2 KJ/mol	1-Hexene
Alcohols	789.2 KJ/mol	Butanol
Aromatics	750.4 KJ/mol	Benzene
	691.0 KJ/mol	**Water**
Alkanes	543.5 KJ/mol	Methane

Source: Gary Eiceman & Zeev Karpas, *Ion Mobility Spectrometry*, CRC Press, 2005, ISBN 0-8493-2247-2

Protone affinities of various VOCs can be found at the NIST chemistry webbook
http://webbook.nist.gov/chemistry/

Figure 4: Protone Affinities of VOC's

Complex analyte mixtures, like e.g. food flavours, often demand a second and independent separation step to separately analyse the multiplicity of compounds at low concentrations. Therefore G.A.S. -according to application- equips its IMS systems with gas chromatographic (GC) columns. The volatile compounds of samples under testing are pre-separated in time by a GC column. The discrete compounds are consecutively fed into the IMS ionization chamber, so that analyte and/or ion interactions are avoided.

Furthermore, a competition of analytes on the reactant ions is excluded, enhancing the sensitivity of the system for individual compounds.

The GC-IMS setup enables a twofold separation of analyte mixtures and the detection by the IMS electrometer. Since the IMS measurements are extremely fast (30ms / spectrum) a continuous and high-resolution recording of analyte signals is provided.

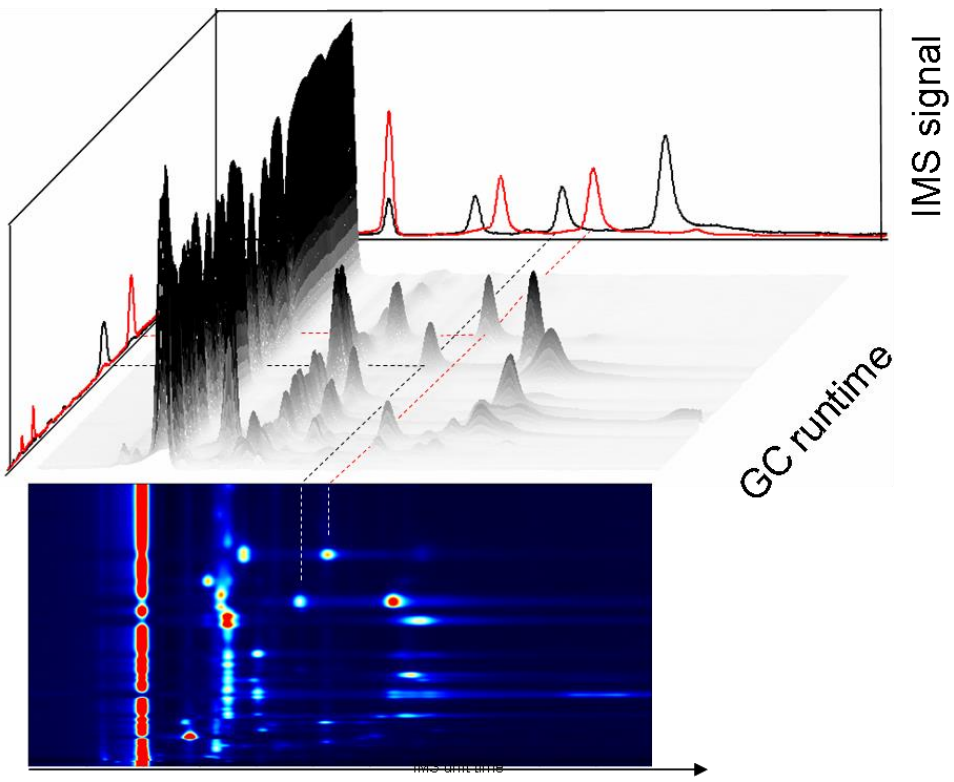


Figure 5: GC-IMS measurement 3D

The above figure sketches the GC-IMS measurement‘s 3D-dataset and the corresponding heatmap visualization.

5.2 Purpose of the device

The FlavourSpec® represents the synergies of a fast gas chromatograph and the outstanding sensitivity of an IMS. Thus traces of Volatile Organic Compounds (VOCs) become detectable without any special sample preparation.

The purpose of the FlavourSpec® is the headspace-measurement of traces of volatile organic compounds (VOCs) of solid or liquid samples.

Results are available within a few minutes and compounds are typically detectable even at ppbv-/pptv-levels. The technical configuration, its menu as well as its extremely easy. The headspace samples are introduced into the FlavourSpec® system by injecting them with a gastight syringe into the sample injection port at the top of the housing.

WARNING!

The FlavourSpec® device must not be operated by introducing aggressive gases or any kind of liquids or solids. The operational reliability is only ensured when the equipment is applied for this intended purpose.

INFORMATION!

Any use of the device, that differs from the intended purpose will be regarded as “out of purpose”. Any claims of any kind against G.A.S. or her associates that are related to damages from an use not covered by the aforesaid will be rejected.

The FlavourSpec® contains several parameterized components that can be modified for optimizing measurement data in terms of separability of substances and clarity of resulting peaks.

The FlavourSpec® can be operated in negative or positive drift voltage mode. The reactant ion peaks (RIPs) and analyte ion peaks (AIPs) in the positive drift voltage mode will be displayed as maxima in the spectra. In the negative drift voltage mode both will be shown as minima. One of these modes may be more suitable for specific substances.

The FlavourSpec® can be operated together with an automatic sampling system (auto-sampler) for batch processing. Measurements can be initiated by the connected auto-sampler as the auto-sampler and instrument have a master/slave configuration. To do so the instrument has to be in the trigger mode. The syringe of the auto-sampler will transport the headspace sample from the vial to the injector port where it injects a defined volume.

When no auto-sampler device is connected, the injection of headspace gas can be done manually using a gas-tight headspace syringe.

Measurement data can be acquired by employing user-defined measurement programs. In these programs the operational parameters of various components of the FlavourSpec® can modified at defined sequences of the measurement run.

Alternatively measurement data can acquired in a manual way using the “Monitoring” mode.

Acquired measurement data are stored in measurement files either on the internal storage volume of the FlavourSpec® or – when activated – in a shared net-work folder. Stored measurement files can further be copied to a connected USB volume.

For using a shared network folder the FlavourSpec® can be integrated into a local area network (LAN) by using the Ethernet socket at the rear side of the device.

5.3 Principle setup and internal gasflow

The schematic drawing shows the principle structure of the gas flow system of the FlavourSpec® is shown. The system consists of the IMS coupled to a gas chromatographic column.

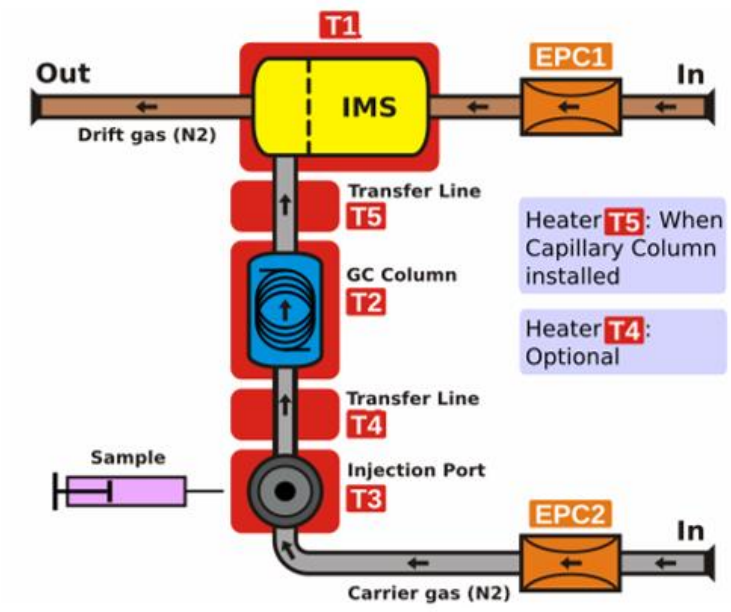


Figure 6: GC-IMS device plan (exemplary)

The drift gas for the IMS is supplied using an electronic pressure control unit (EPC1). The carrier gas for the column is supplied using a second electronic pressure control unit (EPC2). Both gases (carrier and drift gas) leave the device at the gas out, which should be connected to an exhaust system.

INFORMATION!

To ensure correct measurements it is absolutely necessary to **connect the supplied exhaust tubes** (Gas out and Sample gas out).

The exhaust tubes (Gas out and Sample gas out) **must be led separately into the exhaust system and must not be connected.**

The exhaust system must **not generate any negative pressure**.

IMS (T1), GC-Column (T2), Injector-Unit (T3) and Transferline (T4 andT5) are heated.

The headspace sample is introduced into the FlavourSpec® system by injecting with a gastight syringe into the sample injection port at the top of the housing.

The carrier gas stream now transports the sample gas to the GC-column, where the substances in the sample gas are separated by time. The eluting substances are introduced into the ionization region of the IMS and leave the system via the Gas Out socket.

5.4 Housing Device Versions

5.4.1 FlavourSpec

5.4.1.1 Front

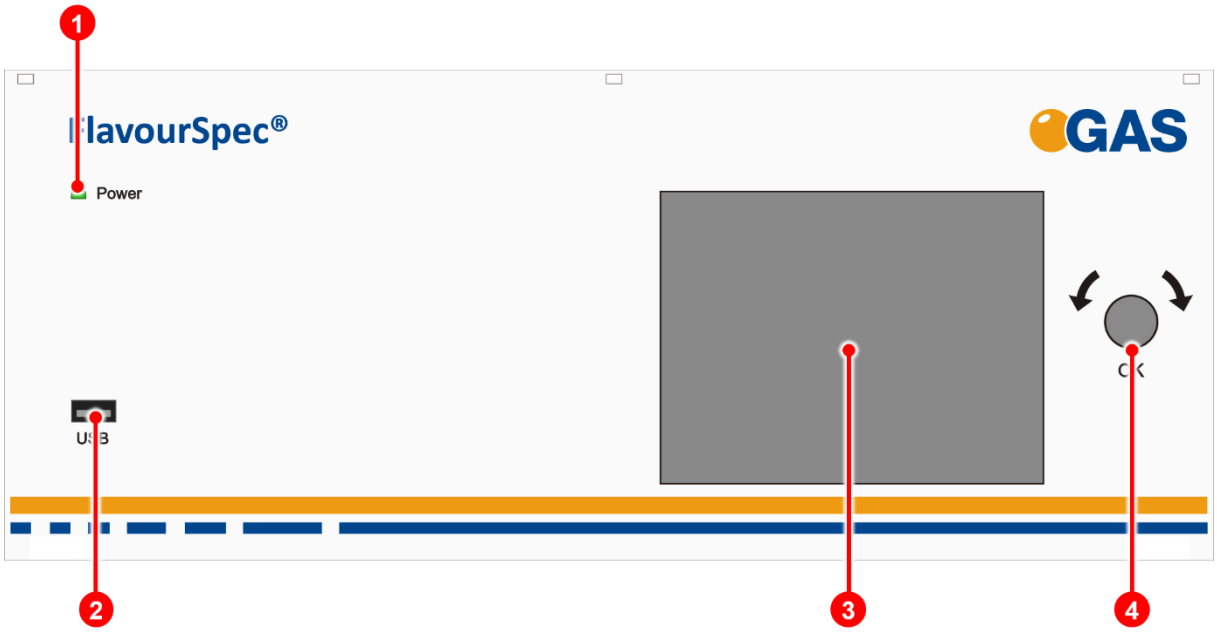


Figure 7: FlavourSpec - Housing of device - Front

1	**Power LED**	• Indicates whether or not the device is connected to a power supply and is switched on • Indicates an internal system error.
2	**USB Socket**	USB socket for connecting external USB storage volumes. These volumes can be used for: • exporting measurement files • importing sample name lists • upgrading the device's firmware • saving/loading system settings.
3	**Touch screen Display**	Displays the graphical user interface and allows the control of the device by touch screen.

4	**Pushable Rotary Knob**	Input control for cycling through and activating the control elements of the graphical user interface.

5.4.1.2 Rear

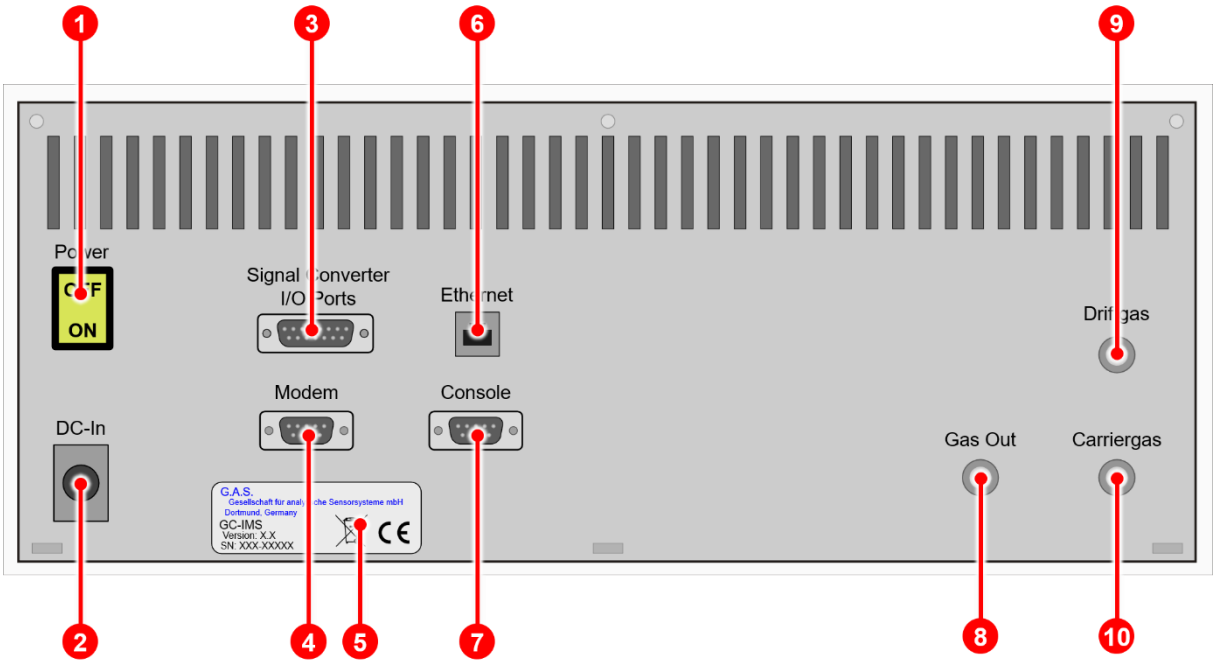


Figure 8: FlavourSpec - Housing of device - Rear

1	**Power Switch**	Switches the device on or off.
2	**DC-In Socket**	24V XLR-Connector for connecting the power supply.
3	**Signal Converter –I/O Socket**	Socket for connecting a PLC (Programmable Logic Controller) or other devices.
4	**Modem Socket**	Socket for connecting an external modem. **For service purpose only**.
5	**Device Type/Serial Number Plate**	Displays manufacturer identification, device type, serial number and version.

6	**Ethernet Socket**	Socket for connecting the device to a local area network (LAN) or directly to a computer.
7	**Console Socket**	Console interface socket. **For service purpose only.**
8	**Gas Out Socket**	3 mm Swagelok plug for connecting the device to an adequate laboratory waste gas ventilation system/fume hood.
9	**Drift Gas In Socket**	3 mm Swagelok inlet plug for connecting the device to a drift gas source.
10	**Carrier Gas In Socket**	3 mm Swagelok inlet plug for connecting the device to a drift gas source.

5.5 Device Type / Serial Number Plate

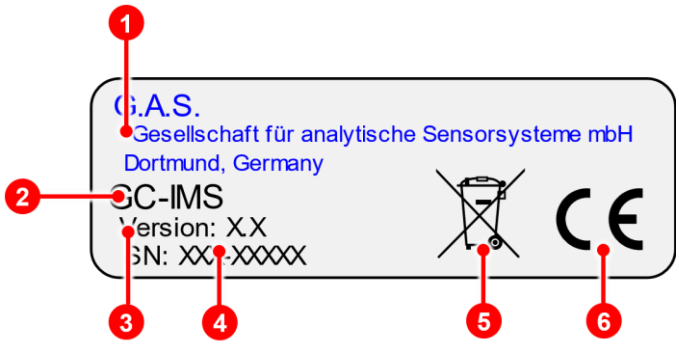


Figure 9: Device Type / Serial Number Plate

1	**Manufacturer**
2	**Type Name**
3	**Version Number**
4	**Serial Number**
5	**Disposal Instructions** This marking on the instrument indicates that they must not be disposed of in domestic waste. The disposal is carried out by return to the manufacturer or by the corresponding municipal authorities (see EU directive 2012/19/EU)
6	**CE Marking** **CE, Communauté Européenne** Instruments bearing this mark comply with the relevant European directives

6 Operating Interface

The graphical user interface of the device can be controlled by using the touchscreen in combination with the pushable rotary knob at the front of the device.

The selected control (button, input field etc.) element is marked blue. To activate it the knob can be pressed.

INFORMATION!

As the product is under continuously development, the screen shots in this user manual may differ from the actual conditions.

6.1 Overview

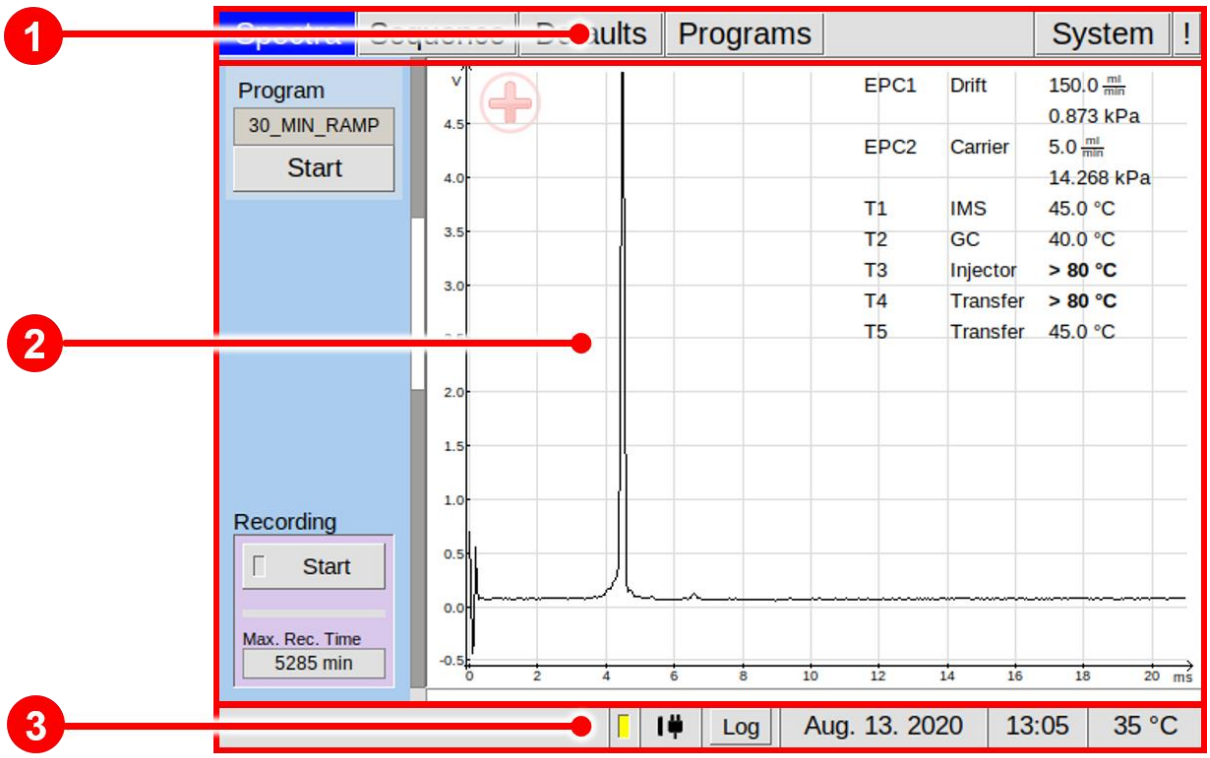


Figure 10: Operating Interface - Overview

1	**Window Selection Bar**	The main windows can be selected.
2	**Window Display Area**	The content of the selected main window will be displayed.

3	**Status Bar**	Status messages and system information are displayed.

6.1.1 Windows Selection Bar

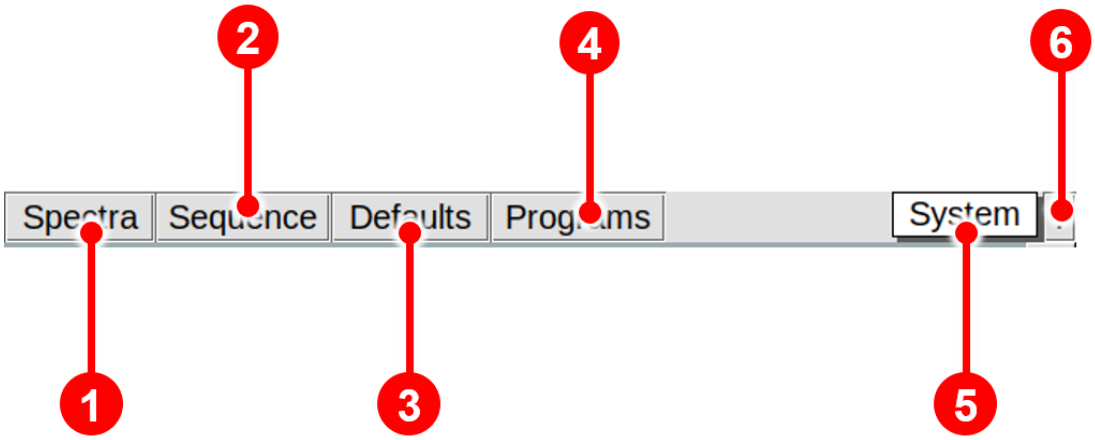


Figure 11: Operating Interface - Windows Selection Bar

1	**Spectra Window Tab**	In Spectra Window the data acquisition process is controlled.
2	**Sequence Window Tab**	In Sequence Window user created sequence files using the Sequence Designer software can be imported.
3	**Defaults Window Tab**	In Defaults Window the default settings can be set.
4	**Programs Window Tab**	In Programs Window user-defined measurement programs can be set.
5	**System Window Tab**	In System Window system specific information are displayed system specific settings and can be set.
6	**Errors Information Window Tab**	In Error Information Window current error information are displayed.

6.1.2 Windows Display Area

In Window Display Area the content of the following main windows is displayed:

- **Spectra Window**
- **Sequence Window**
- **Defaults Window**
- **Programs Window**
- **System Window**
- **Error Information Window**

6.1.3 Status Bar

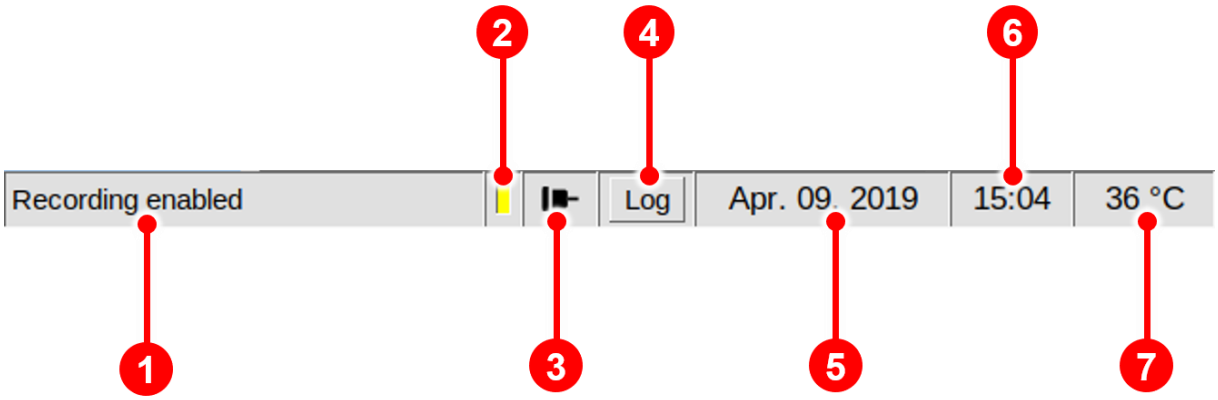


Figure 12: Operating Interface - Status Bar

1	**Status Message Section**	Device events information will be displayed.
2	**Export Message Section**	Displays the current connection status. Export on: Export of
3	**LAN Connection Section**	Displays the current connection status: Connected: Disconnected:
4	**Log Section**	Displays the current log status. New entry: Log No modification: Log Selecting this button will open the Log Section Window with a chronical list of system events
5	**Date Section**	Displays the current date of the device clock. It can be set in System Window.

6	**Time Section**	Displays the current time of the device clock. It can be set in System Window.
7	**Temperature Section**	Displays the current inner housing temperature of the device.

6.1.4 View Control Bar

The view control bar function is available in the Spectra window and in the Defaults window. By touching the screen, the control bar is displayed underneath the displayed spectra.

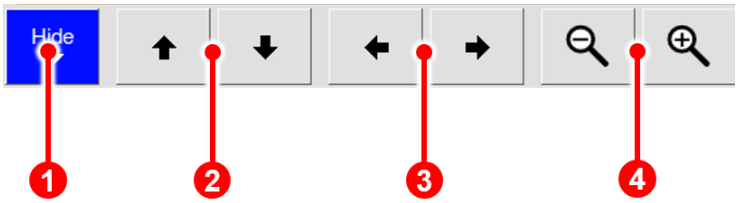


Figure 13: Operating Interface – View Control Bar

1	**Hide Button**	The control bar can be hidden manually. After 3 seconds of inactivity it is hidden automatically.
2	**Vertical Control Buttons**	Moves the vertical position of the display area on the screen up or down.
3	**Horizontal Control buttons**	Moves the horizontal position of the display area on the screen left or right.
4	**Zoom Control buttons**	Reduces or enlarges the view of the display area on the screen

6.1.5 Low/High Pressure Control

The device pressure is monitored. Two types of error are defined:

6.1.5.1 Low Pressure Error

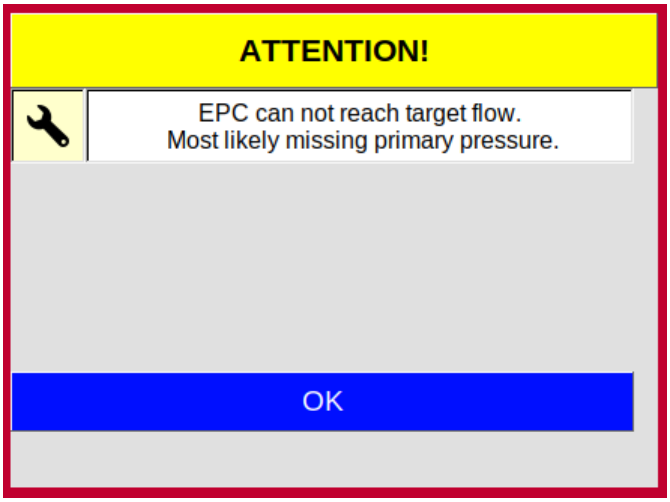


Figure 14: Operating Interface - Low Pressure Alarm Box

1. After 10 seconds a dialogue box is displayed and an acoustic alarm sounds.
2. After 5 minutes all temperature controllers are switched off.
3. When the pressure is reached again the alarm is switched off and all temperature controllers switch themselves on automatically

6.1.5.2 High Pressure Error

WARNING!

High pressure can destroy the device.

Figure 15: Operating Interface - High Pressure Alarm Box

1. If overpressure is detected, a visual and audible alarm is triggered immediately. At the same time all temperature controllers and flow controllers are switched off.
2. Before continuing to operate the unit, the cause of the spotlight must be eliminated.
3. By confirming the dialogue box or restarting the system, all temperatures and flows are reset to their normal values.
4. Verify if the drift-gas out connection is done as described.

6.2 Spectra Window

6.2.1 Overview

After switching on the device and the system start is completed the Spectra Window is displayed. In the Spectra Window the data acquisition can be controlled.

The current spectrum is displayed. The Recording Mode can be activated. The selected measurement program can be started.

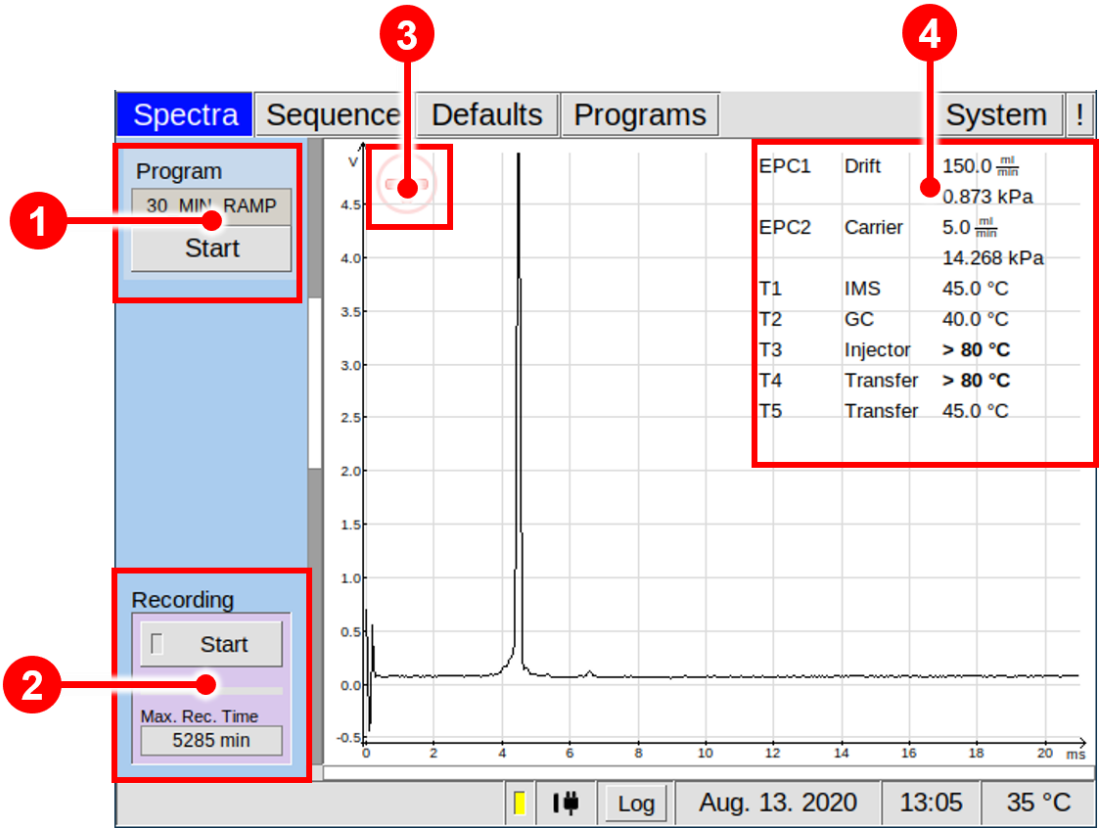


Figure 16: Operating Interface - Spectra Window

1	**Program Start Button**	By selecting this button the displayed program is started.
2	**Recording Check Box**	The live monitoring of measurements can be recorded manually. The available storage capacity in minutes is displayed.
3	**Drift Voltage Mode**	Displays the current selected Drift Voltage state (positive / negative).

4	**Device Parameter**	Displays the current temperature, flow and pressure values.

6.2.2 Measurement modes

Three measurement modes are available:

- Measurement with user defined programs
- Manually operated measurement (Recording)
- Automatic operated measurement with coupled Autosampler (Trigger Mode)

6.2.2.1 Measurement with user defined programs

In this mode data acquisition with user-defined measurement programs can be started. The executable measurement program can be created and selected in the Programs Window. The name of the current selected program is displayed in the upper left of the Spectra Window. The selected measurement program can be started by activating the Program button in the upper left of the Spectra Window.

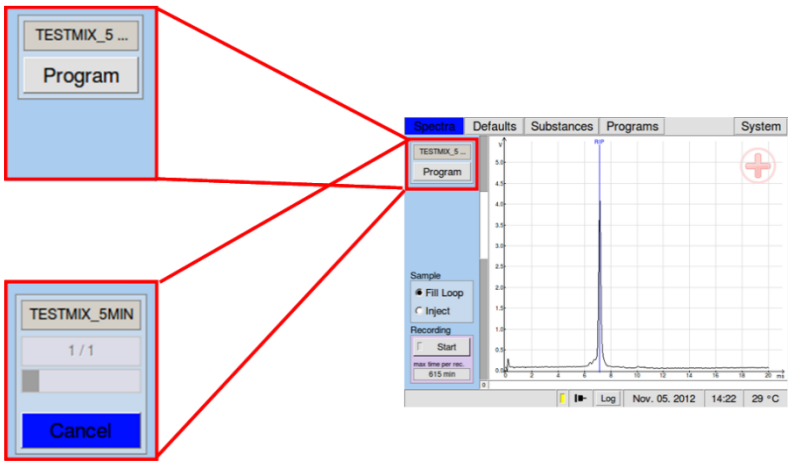


Figure 17: Start Program

6.2.2.2 Manually operated measurement (Recording)

To record a measurement manually the Recording button can be switched on. If recording is not active the button is set to START and the checkbox is grey. If recording is active the button is set to STOP and the checkbox is yellow.

In this case a measurement file is generated from the recorded data and saved to the internal flashcard. The remaining time for data storage to the internal flashcard is shown. It depends on the number of measurement data that were released for export but were not yet exported and their file size depends on the value of spectra averages that are used.

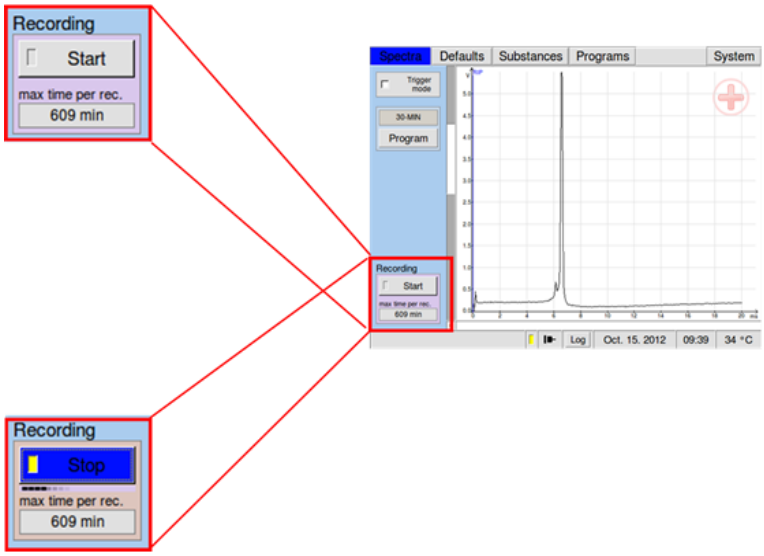


Figure 18: Recording Check Box

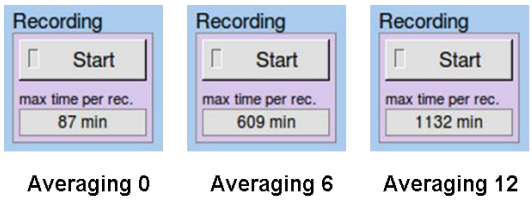


Figure 19: Recording Check Box

6.2.2.3 Automatic operated measurement with coupled Autosampler (Trigger Mode)

In the Trigger Mode the FlavourSpec® device is remotely controlled by a connected autosampler that operates as master device to it. When the Trigger Mode is active the Acquisition Control Area on the left side of the window displays a different set of controls.

Instead of the Recording Mode the Sample Names List and the Import Names button are displayed. The Program Start button is inactive because in this mode the currently selected program is started by an external trigger sent from the connected

autosampler. The measurement program that will be executed can be selected in the Programs Window.

The Sample Names List displays the currently loaded ordered list of sample. The sample names are consecutively assigned to measurements triggered by the connected autosampler. The list must therefore match the order and kind of the autosampler samples batch. The Sample Names List can be imported by activating the Import Names button.

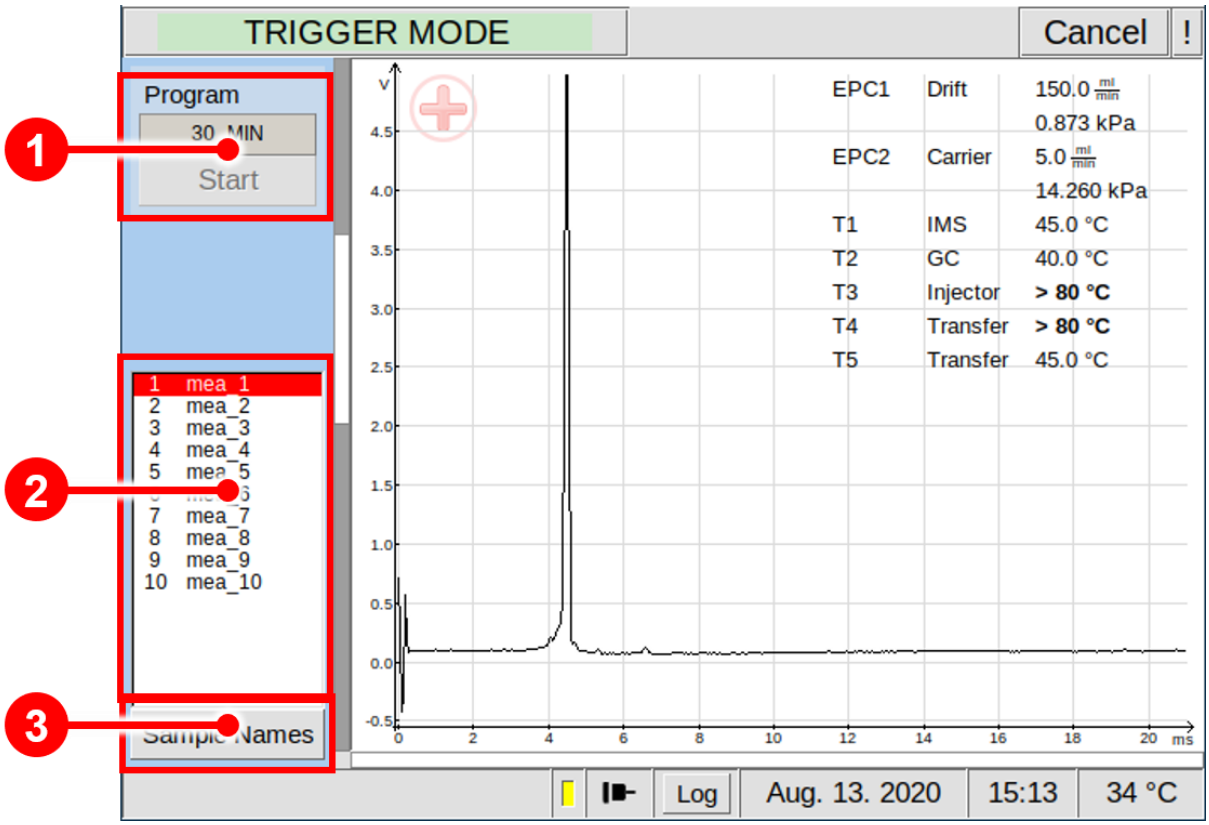


Figure 20: Trigger Mode Window

1	**Trigger Mode View**	Shows the activated trigger mode
2	**Sample Names List**	Displays the currently loaded sample names list. The current sample name is highlighted red.
3	**Sample Names Button**	With this button the sample names list file **SampleNames.txt** can be (re)loaded.

6.2.2.4 Create and Import Sample Names Lists

The FlavourSpec® can hold a list of sample names which are assigned to specific measurements during an autosampler batch measurement process. A list of sample names can be imported by the FlavourSpec®. The sample names in this list are consecutively assigned to measurement data recordings triggered by the connected autosampler device and written into the resulting measurement files. The list must therefore match the order and kind of the autosampler samples batch. Usually these names should correspond to the content of the sample vials on the autosampler tray. The sample name list can be generated as follows:

- Autogenerate function of the device
- Manual editing with an editor application

The sample name list can be loaded from a file located in a folder in the shared network folder of the device or on a connected USB volume.
When both a USB device and a shared folder are connected the USB device will be chosen.

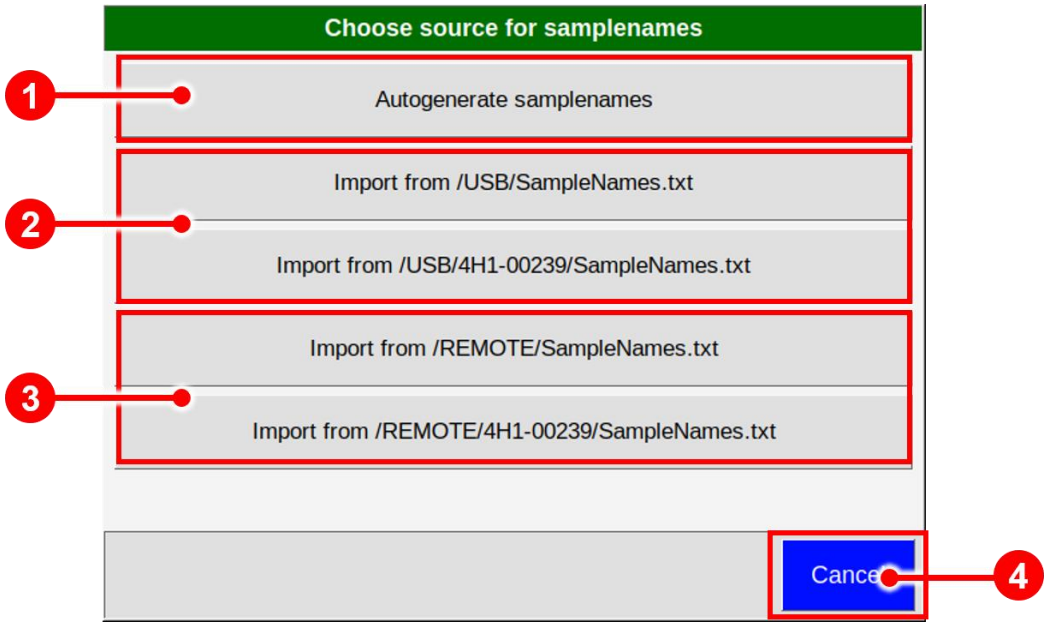


Figure 21: Choose source for samplenames

1	**Autogenerate samplenames**	Autogenerates a Sample names list named mea_1 – mea_999 (max)
2	**Import from USB**	Imports a sample names list file **SampleNames.txt** from a connected USB device.
3	**Import from REMOTE**	Imports a sample names list file **SampleNames.txt** from a connected shared network folder.

INFORMATION!

The sample names list file must be named **SampleNames.txt**. Any other file in the respective folder is ignored by the FlavourSpec® sample names import.

Creating a Samplename file

The file must be a plain text file which can be created or edited with a simple text editor application such as the Microsoft® Windows® Notepad. The content of each text line in this file will be regarded as one sample name. The order of the sample names in the file corresponds to the order of the sample names after the import.

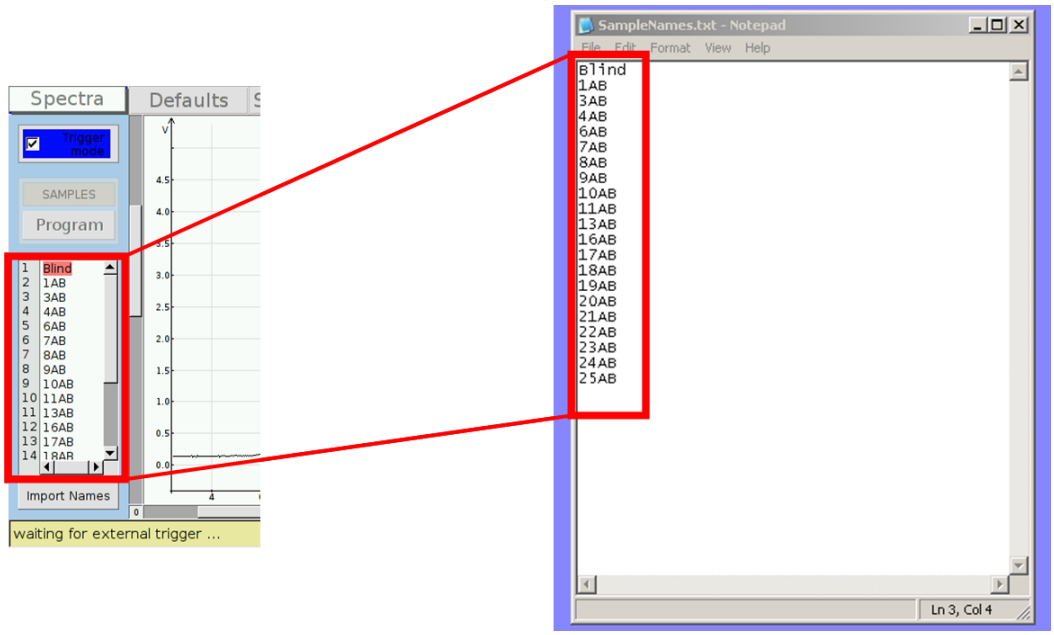


Figure 22: Sample Names List

INFORMATION!

The sample names list file must be named **SampleNames.txt**. Any other file in the respective folder is ignored by the FlavourSpec® sample names import.

By entering of tags (so-called XML-tags) in front and behind the samplename-string the samplename can be appended to the default filename which is created from the day and time information when the measurement is started:

The default (autogenerated) Filename format is defined as follows:

YYYYMMDD_hhmmss.mea

Use the tags in front and after the samplename string as shown below:

<FILENAME>samplename</FILENAME>

This produces the user-defined Filename as follows

YYYYMMDD_hhmmss_samplename.mea

The XML tags must be entered in all capital letters. The samplename can contain upper and lower case letters as well as numbers. Special characters are not allowed, except the underscore character. If a special characters is used it will be automatically converted to underscore.

6.3 Sequence Window

In Sequence Window Sequence files can be imported and started by clicking on the Start Button. The processing status of a user created sequence file can be watched:

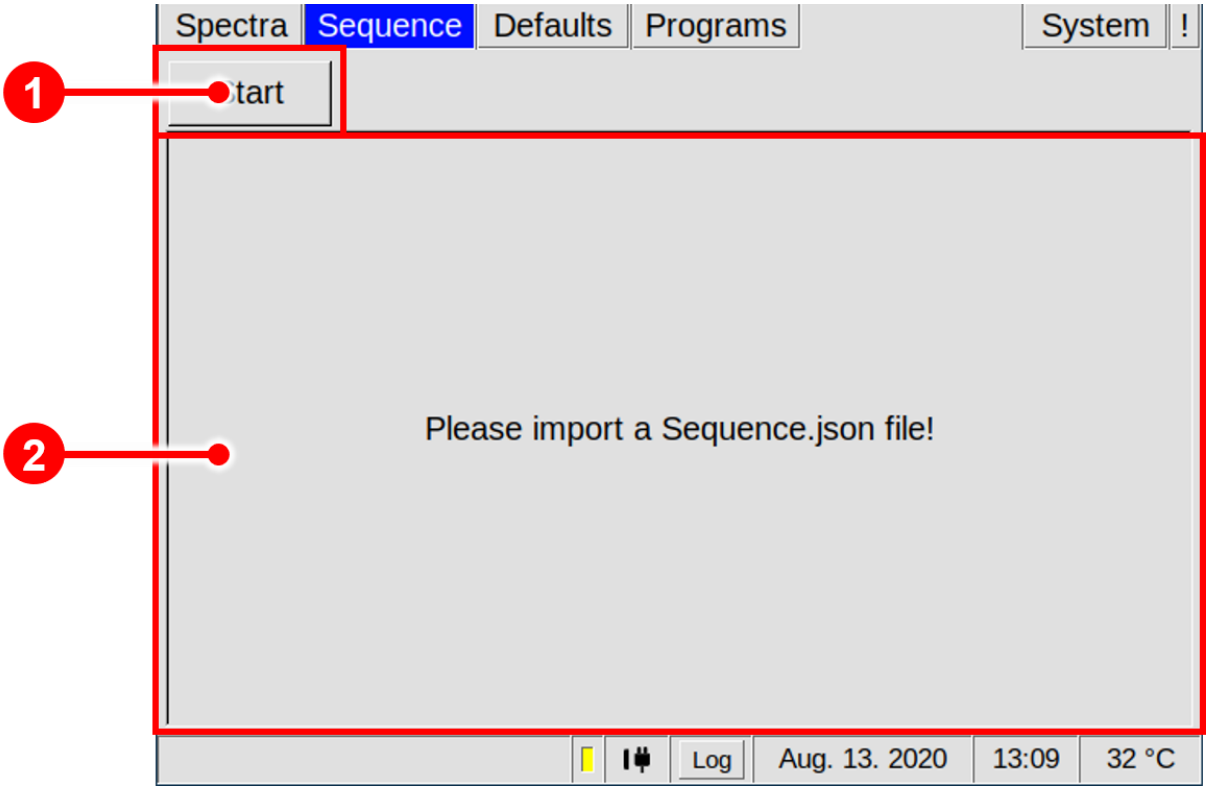


Figure 23: Operating Interface - Sequence Window

1	**Start Button**	A user created sequence files, created by **G.A.S.Sequence Designer Software**, can be imported.
2	**Information Window**	The live monitoring of measurements can be recorded manually. Displays the available storage capacity in minutes.

INFORMATION!

The sequence file must be named as **sequence.json**.

After selection, the software will try to import and analyse the sequence file. If the file could be imported and the analysis showed no errors, the sequence will be executed. The following figure shows the execution of a sequence:

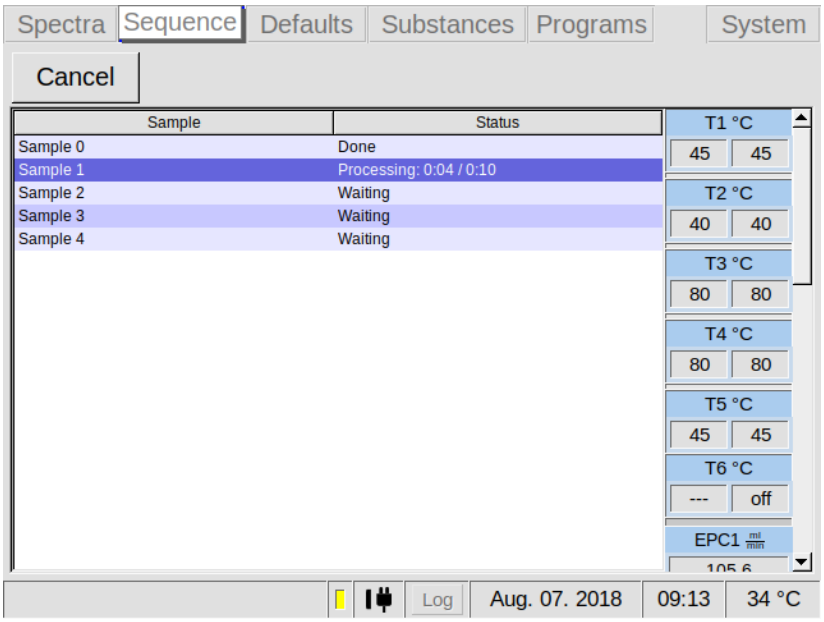


Figure 24: Operating Interface - Sequence Window - Processing

You will see the sequence being processed, one Sample after another. The time passed and the total time for each Sample are displayed, showing you the progress. The scrollable area on the right displays the current and the target device parameters for temperatures and flows, as well as some IMS specific values such as voltages and the trigger duration. Clicking on the cancel button will stop the Sequence, but still apply all the After Run Settings. Once the Sequence has finished, all Samples will be marked as done, the last After Run Settings are applied and the software will display the message Execution finished. The system is now ready for further sequences or manual operation.

INFORMATION!

The sequence file must be created with the **G.A.S. Sequence Designer Software**. For detailed Information refer to the **G.A.S. Sequence Designer Software Manual.**

6.4 Defaults Window

6.4.1 Overview

The Defaults window allows the monitoring and modification of various device component parameters. The electronic pressure controllers (EPC 1 and EPC 2) and the heating modules of the device can be controlled (T1 – T6). Further, the sample pump performance, averaging and drift voltage polarity can be switched manually.

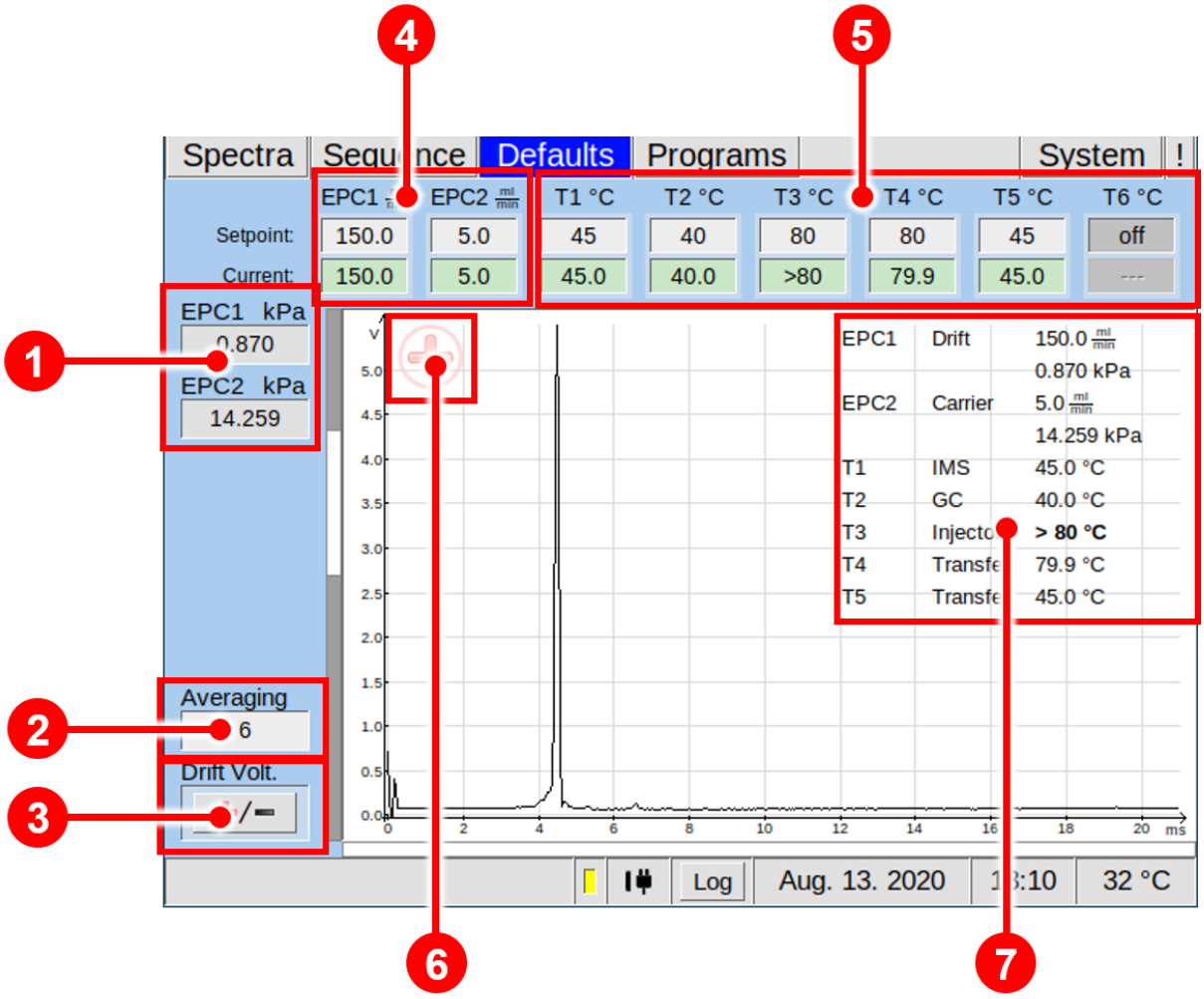


Figure 25: Operating Interface - Defaults Window

1	**Pressure display**	Displays the relative overpressure of the gas flow. EPC1 displays the current the overpressure of the drift gas flow. EPC2 displays the overpressure of the carrier gas flow.
2	**Averaging display**	Displays the current average value. The averaging value determines how many

		raw spectra are averaged to generate one single spectrum as result in the stored measurement file. Modifying the averaging parameter affects the number of recorded spectra per time period. A typical average value is 6. The maximum is set to 99. A value of 0 (Off) disables averaging.
3	**Drift-Voltage Button**	Drift Voltage polarity can be selected and switched (positive/negative).
4	**Flow display**	In Input Field Setpoint the flowrate of Drift gas (EPC1) and Carrier gas (EPC2) can be set. The current flowrates for Drift gas (EPC1) and Carrier gas (EPC2) are displayed. The maximum value for EPC1 is 500 ml/min. The maximum value for EPC2 is 150 ml/min. The working value for EPC1 is 150 ml/min. The working value of EPC2 depends of the application measurement and is influenced by the build-in GC-Column (length, inner diameter).
5	**Temperature display**	In Input Field Setpoint the temperature values of the heating modules **IMS (T1)**, **Column (T2)**, **Injector (T3)**, **internal Transferline (T5)** and **optional external Transferline (T4)** can be set. The current Temperatures (T1–T5) are displayed. Temperature module T6 is currently not available. The maximum setable value is 80 °C.
6	**Drift Voltage mode**	Displays the current selected Drift Voltage state (positive / negative).
7	**Device Parameter**	Displays the current temperature, flow and pressure values.

6.4.2 Drift Voltage

The Drift Voltage can be switched between positive and negative drift voltage mode. One of these two modes may be more suitable for specific substances.

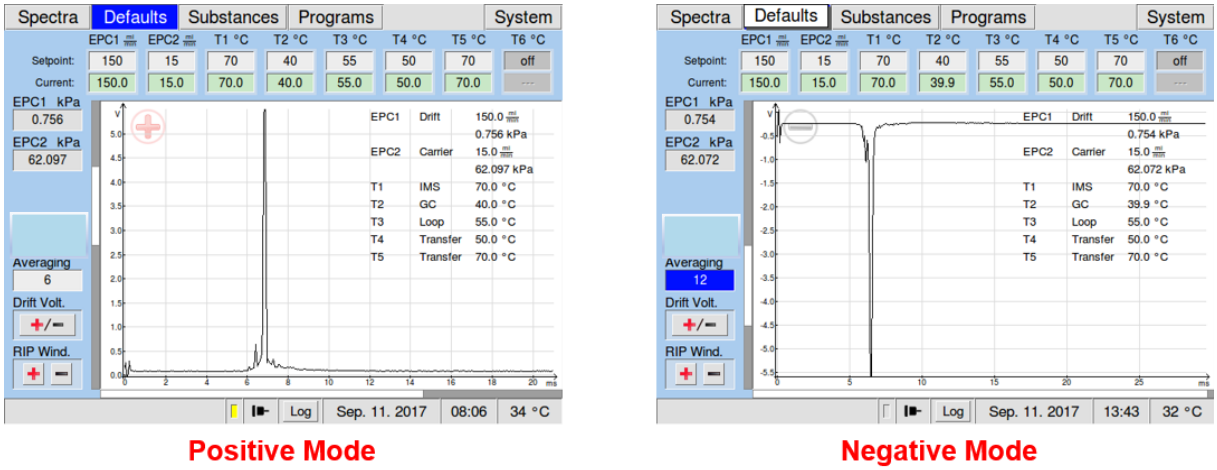


Figure 26: Drift Voltage Windows - positive and negative Mode

6.4.3 Flow Controls and Heating Modules

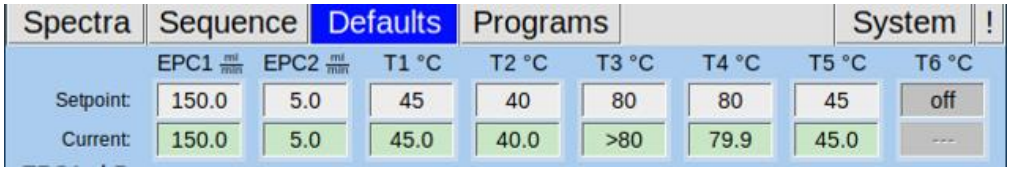


Figure 27: Flow and Temperature Control (Example)

The component parameters are displayed and can be modified in the upper section of the window and in the left section of the window.

Above the spectra chart the flow rates of the drift and carrier gas controlled by the two electric pressure controllers (EPC 1 and EPC 2) and the temperatures of the heating elements of the device are managed. Unused elements are greyed out. The current flow rates and set-points for EPC 1 (drift gas) and EPC 2 (carrier gas) are displayed. The maximum value for EPC 1 is 500 ml/min. The maximum value for EPC 2 is 150 ml/min (Depending on the column used). The current temperatures and the set points of the IMS (T1), the column (T2), the injector (T3) and the inner heated transferlines (T4 and T5) are displayed. The set points can be set using these controllers. The maximum adjustable temperature value is 80 °C. During the cleaning process the heating modules can reach temperatures up to 100 °C. These will be displayed as “> 80 °C”. Heating modules can be turned off by decreasing the respective value to “off”.

6.5 Programs Window

6.5.1 Overview

In Programs Window user-defined measurement programs can be set and managed.

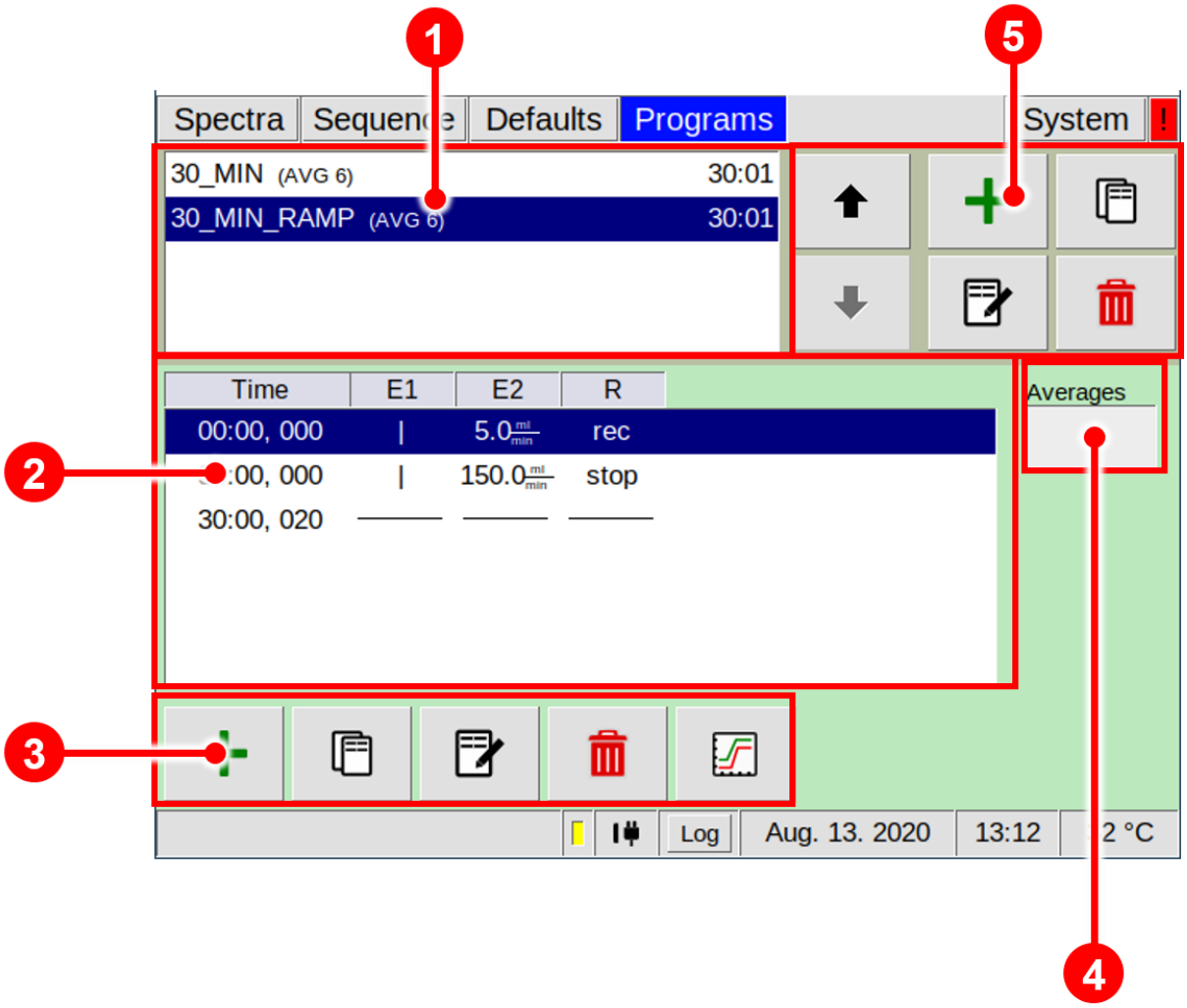
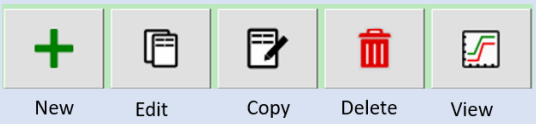
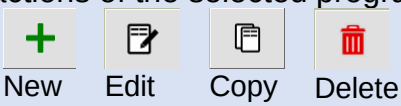


Figure 28: Operating Interface - Programs Window

1	**Measurement Program List area**	All created programs are listed in this box by name. The highlighted program is selected for execution or modification.
2	**Selected Program area**	All instructions of a selected program are listed here in a chronological order. For every device component that can be controlled by a program a separate column is displayed.
3	**Program Action Control Panel**	Buttons for creating, changing or deleting actions of the selected program

		
4	**Average Settings**	Average of the current selected program can be set. The current average is appended to the name of the measurement program.
5	**Program Control Panel**	Buttons for creating, changing or deleting actions of the selected program 

6.5.2 Create Measurement Programs

The Measurement Program List window displays all measurement programs currently existing. The measurement programs list can contain **up to 100 entries**. The current average value is part of the program name. The selected program can be edited.

Figure 29: Measurement Control Panel

Up	The list order of the selected program can be changed stepwise upwards
Down	The list order of the selected can be changed stepwise downwards.
New	The **New** button which will open a keyboard window for entering the program name.
Edit	By pressing the **Edit** button the program name for the selected entry can be edited into a keyboard window.
Copy	By pressing the **Copy** button the program of the selected program will be copied.
Delete	By pressing the **Delete** button the program of the selected program will be deleted.

In the Average field the average of the current selected program can be set.

6.5.3 Edit Measurement Programs

Each program consists of a list of chronological ordered steps, so called actions. The Selected Program Window displays the list of actions for the currently selected program. Each row in this list represents a step in the measurement program in which various changes to the device components are made.

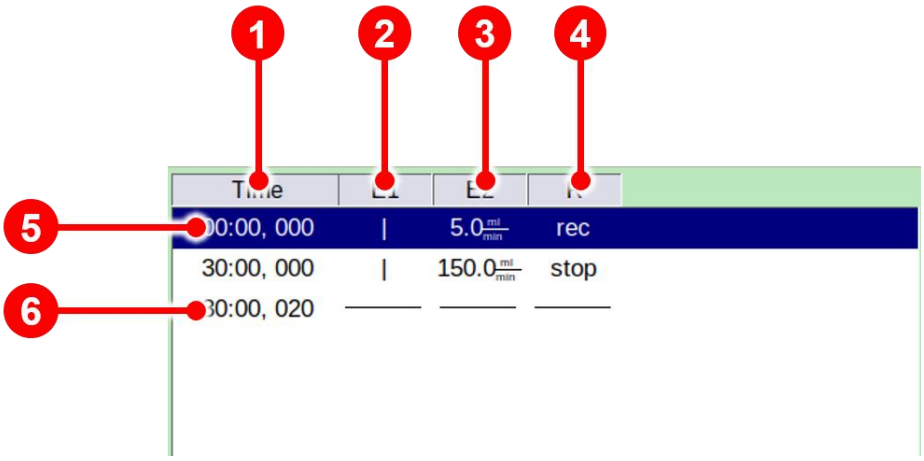


Figure 30: Selected Program Window

1	**Time:** Time point of action start
2	**E1:** Flow rate control for EPC1 drift gas **(0- 500 ml/min)**
3	**E2:** Flow rate control for EPC2 carrier gas **(0- 150* ml/min)**
4	**R:** Start / Stop recording spectra **(rec / stop)**
5	Selected program action line
6	End of Program line

INFORMATION!

The EPC2 maximum flow (carriergas) of 150 ml/min is restricted by the installed column dimemsions. It only can be attained if the

standard column is installed (15 m length, 0.53 mm inner diameter).

A value here determines the new state of the respective device component. A vertical line "|" indicates that the respective device component is not involved in this action.

The last row in this action list contains horizontal lines only. It indicates the end-of-program. The point of time of this end-of-program marker can be increased. This determines the duration of the program run.

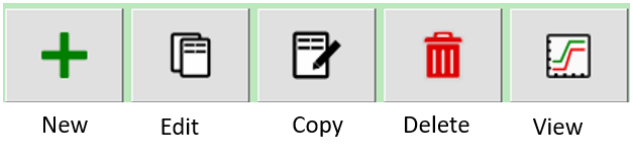


Figure 31: Program Action Control Panel

With the buttons in the Selected Program Window Control Panel the currently displayed program can be created, modified, deleted and viewed. A newly created action is positioned after the currently selected action. Pressing the **Copy** button copies the selected action and orders the copy behind the selected action. To maintain the chronological order of the actions the system may rearrange the actions by ordering them according to their numbers later on. By pressing the **Del** button the currently selected action is deleted.

Pressing the **Edit** button or the **New** button opens the Edit Action dialogue.

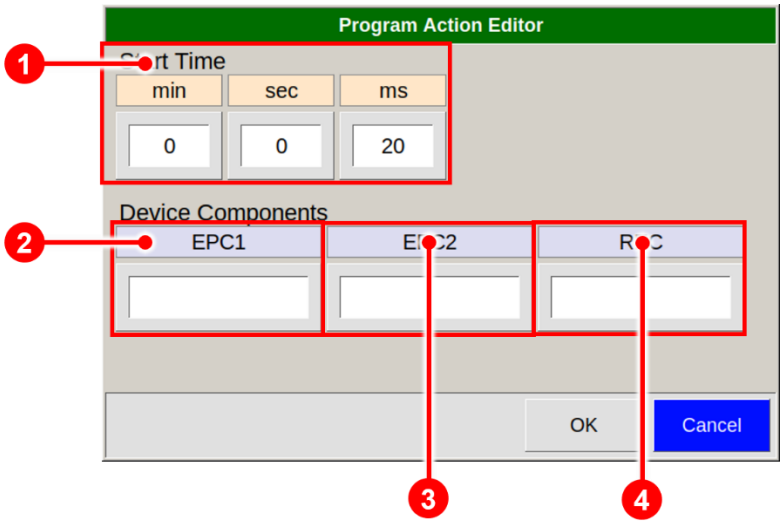


Figure 32: Program Action Editor

1	**Time**	Time point of action start
2	**Electronic pressure control 1**	Drift gas flow rate ramp set point (0-500 ml/min) (Standard: 150 ml/min)
3	**Electronic pressure control 2**	Carrier gas flow rate ramp set point (0-150 ml/min)
4	**Recording**	Start / Stop recording spectra (rec / stop)

Pressing the **View** shows a graphical view of the created program.

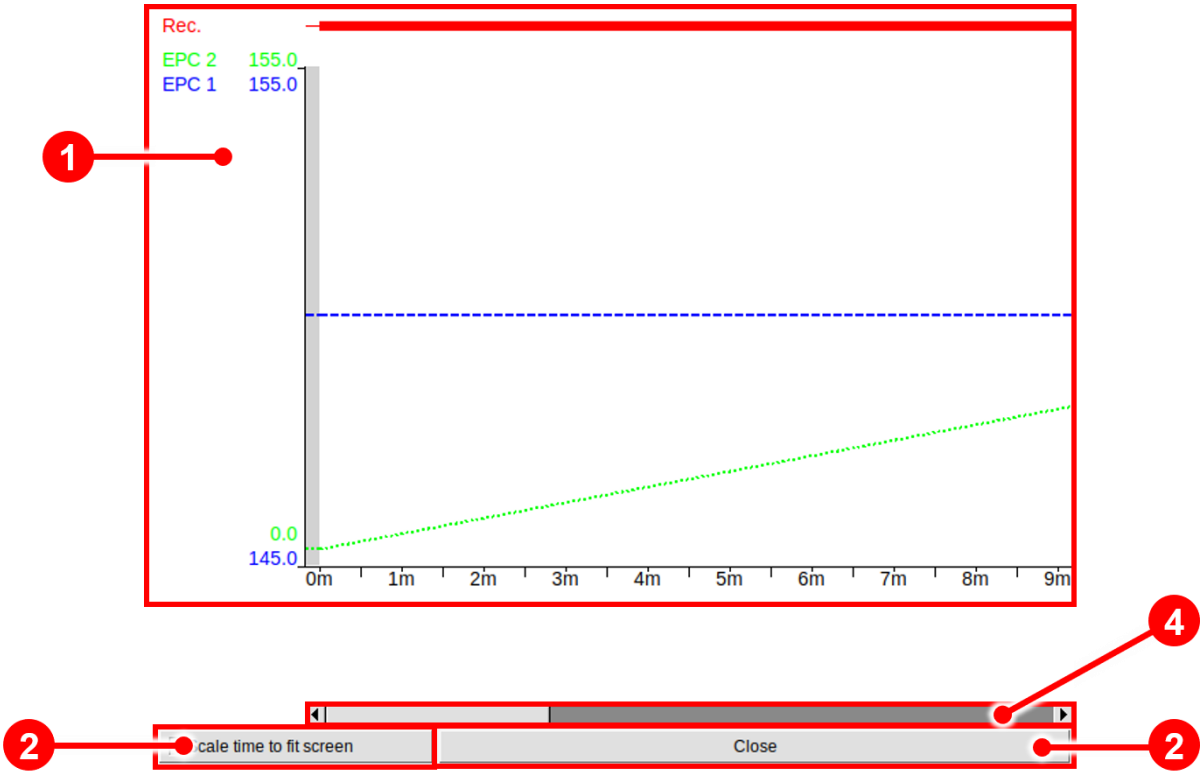


Figure 33: Program Action View

1	**Graphical View Display**	Displays the Program parameter EPC1, EPC2 and REC

2	**Scale time to fit screen Button**	Adjusts the display to the screen
3	**Close**	Closes the graphical view
4	**Scrollbar**	Shifts the current time view area

6.5.4 Flow Ramps

The flow rate set points in a measurement program determine the target flow rates at the specified time index. If set points differ from the default flow rate or varying flow rate set points are specified in a program, the course of the actual flows will be conducted as a linear ramp of the flow. Starting point of the ramp is the latest set point. If no earlier set point is given the ramp starts with program initialization using the default set point.

An exemplary program using a dynamic flow rates is visualized in the following figure:

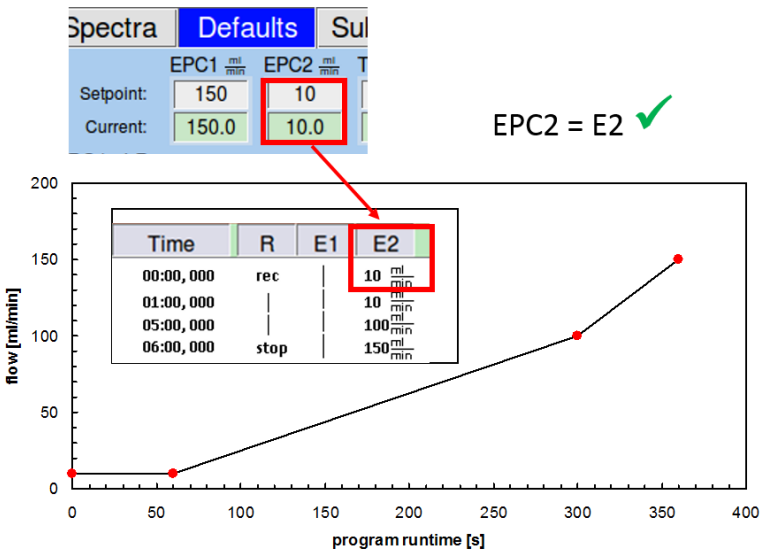


Figure 34: Flow Ramps

The E2 (carrier gas flow) value is initially set to 10ml/min. The flow is kept constant for one minute. Between runtime 1min – 5min the flow is linearly increased to the target value 100ml/min. In the following the flow is increased linearly to 150ml/min in one minute.

INFORMATION!

Before starting a measurement make sure that the highest flow set points can be achieved. Note that large changes in the flow set points will need finite time.

INFORMATION!

Please make sure that default values of EPC1 and EPC2 (Default window) corresponds with the start value of E1 and E2 in the program, otherwise the reproducibility of the measurement cannot be guaranteed.

INFORMATION!

Make sure that the EPC2 start pressure is reached again at the beginning of the next program run.

RECOMMENDATION:

Make sure that the initial flow at EPC2 is kept constant during the first 60 seconds after injection before starting a flow ramp, especially when a low flowrate is chosen.

6.6 System Window

In the System Window system specific information are displayed and can be set.

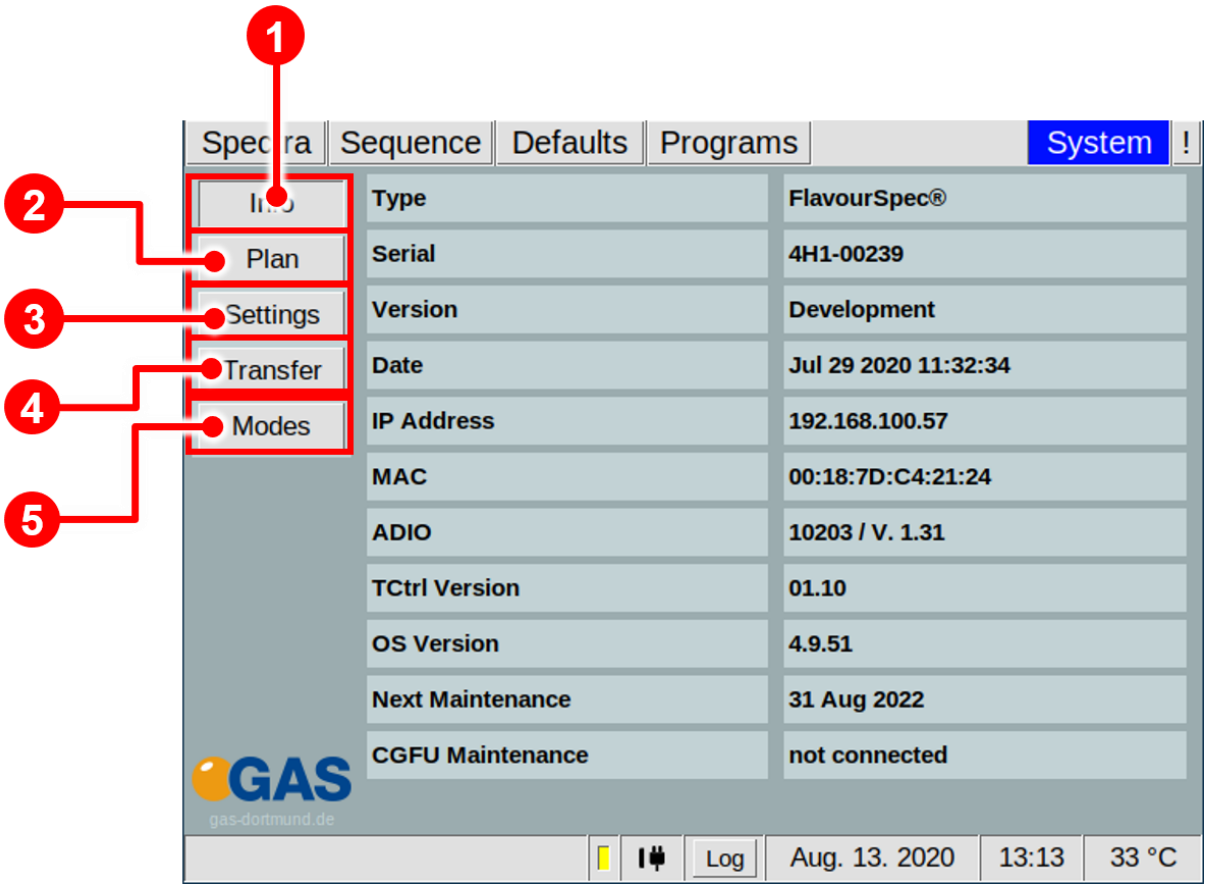


Figure 35: Operating Interface - System Window

1	**Info Button**	Displays the System Information Window
2	**Plan Button**	Displays the Device Plan Window
3	**Settings Button**	Displays the Settings Window. Various device parameter like Export Setting, Livedata output, Device attributes can be set.
4	**Transfer Button**	Displays the current data transfer settings. Data transfer settings can be set.
5	**Modes Button**	Special application modes can be set.

6.6.1 System Info Window

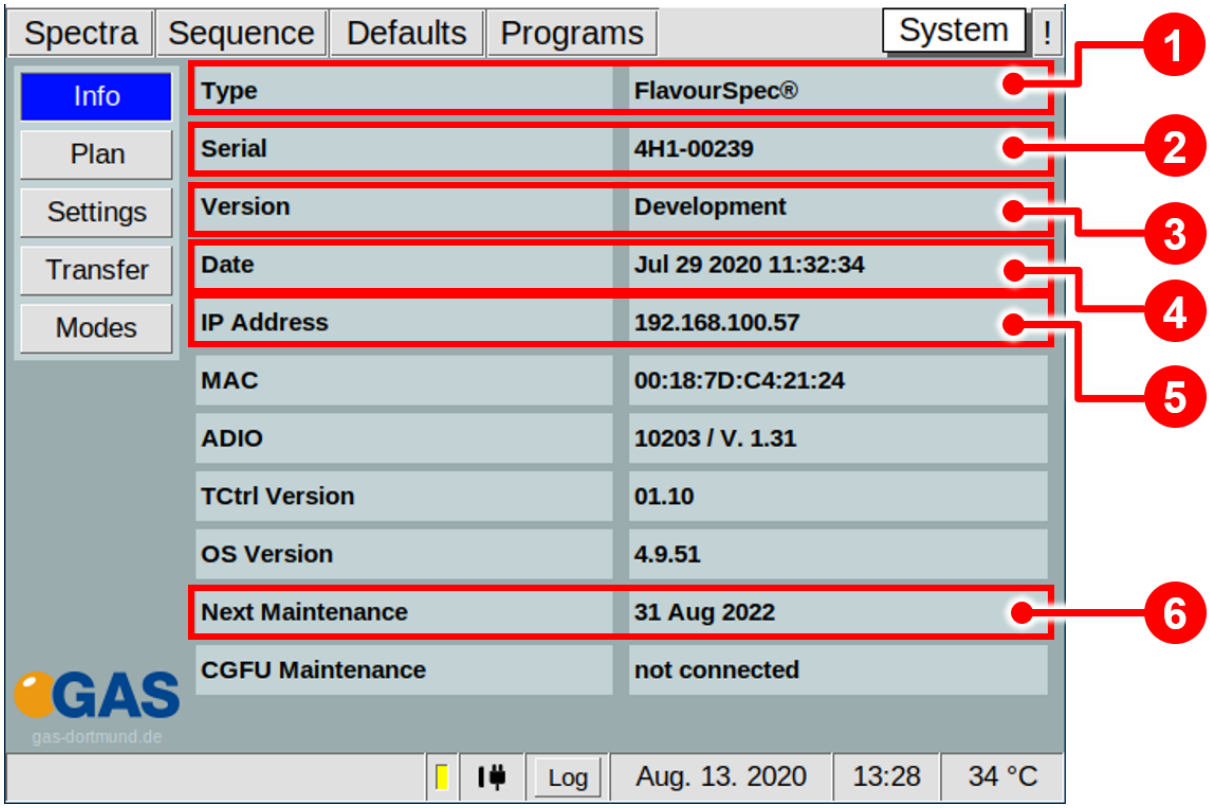


Figure 36: Operating Interface - System Info Window

1	**Type**	Device type.
2	**Serial**	Device Serial Number.
3	**Version**	Current Firmware Version.
4	**Date**	Date of current Firmware Version.
5	**IP-address**	Displays the current IPv4-Address.
6	**Next Maintenance**	Displays the next maintenance date.

6.6.2 System Plan Window

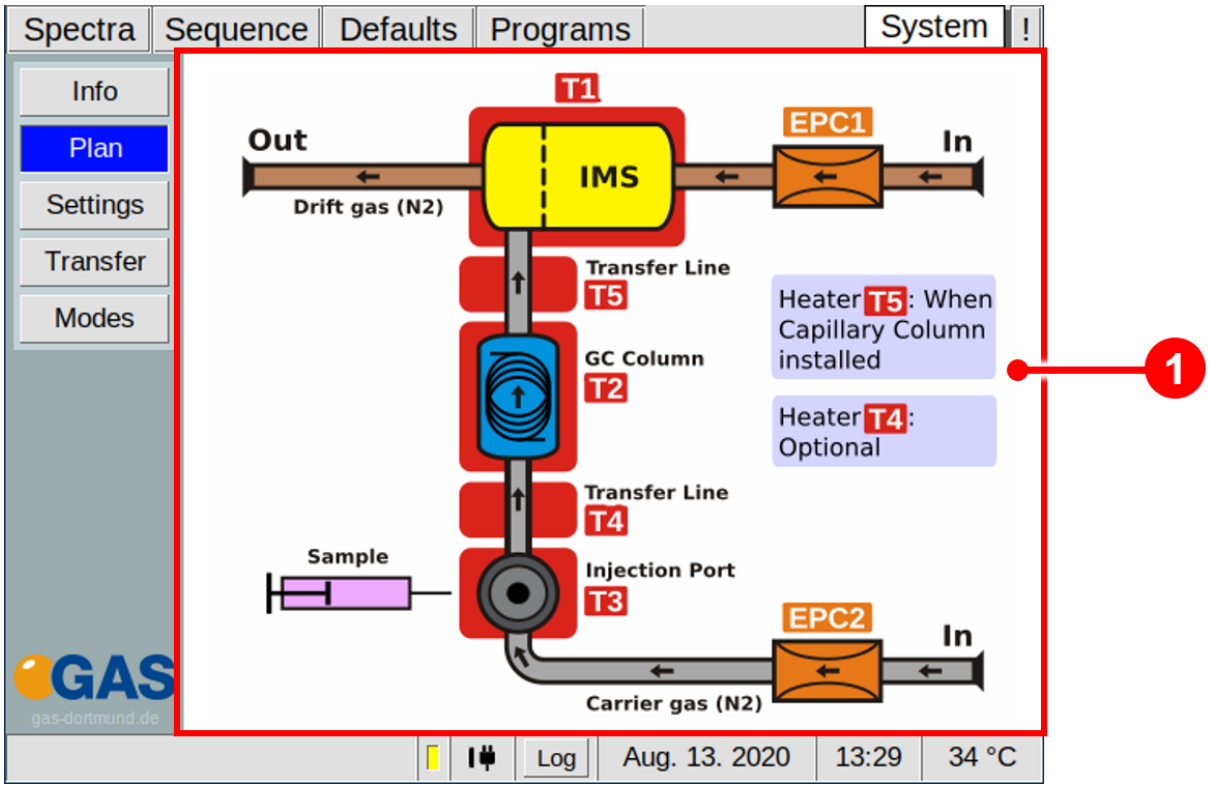


Figure 37: Operating Interface - System Plan Window

1	**Plan**	Displays an overview plan of the device

6.6.3 System Settings Window

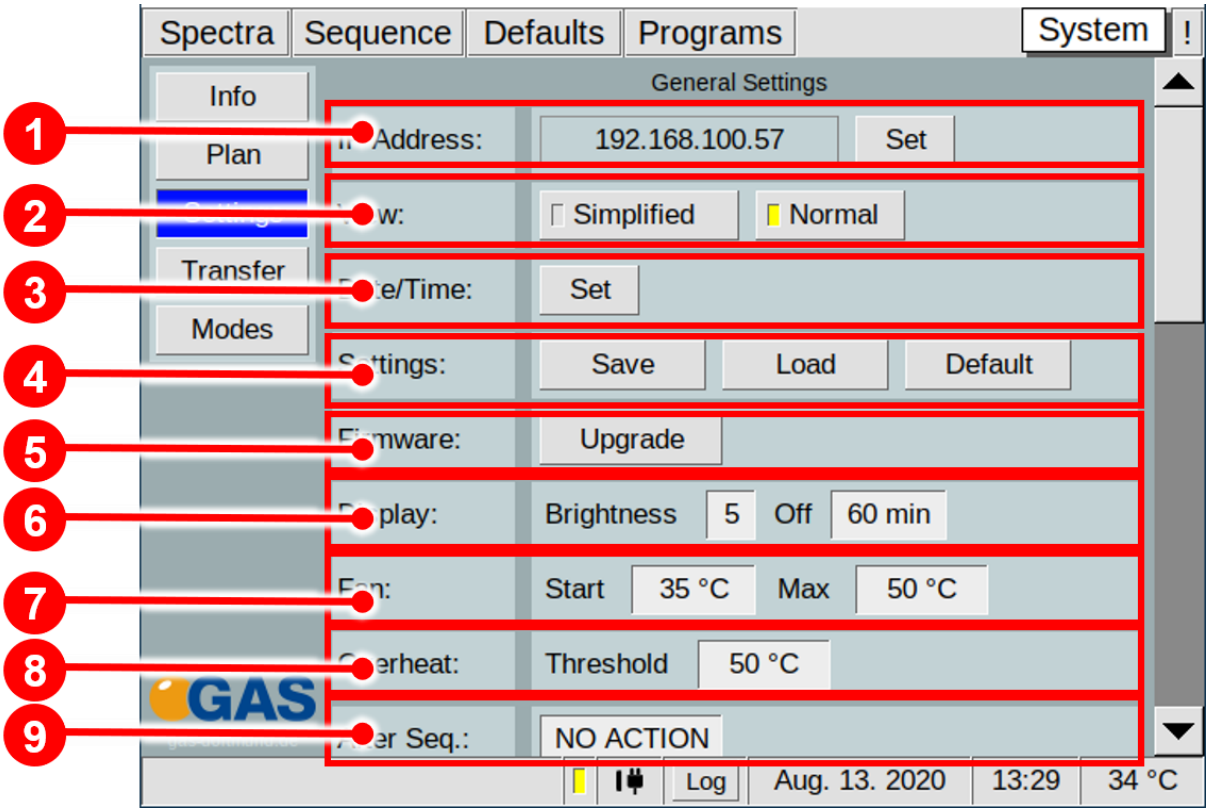


Figure 38: Operating Interface - System Settings Windows 1

1	**IP Adress**	Displays the current set IPv4-Adress of the device. With **Set-Button** the IPv4-adress can be set
2	**View**	Toggles between **simplified** and **normal** view.
3	**Date/Time**	With **Set-Button** the Date and Time can be set
4	**Settings**	**Save Button**: The system settings can be saved to a connected USB volume. **Load Button**: The system settings can be loaded from a connected USB volume. **Default Button**: Resets all system settings to factory default values. All measurement-programs and substance-entries set by user will be deleted.

5	**Firmware**	With **Upgrade-Button** a firmware upgrade can be performed from a connected USB volume.
6	**Display**	The display brightness and screen-saver time-out can be set.
7	**Fan**	The behaviour of the cooling fan can be set. When the temperature inside the device reaches the temperature in the field Start the cooler fan starts working. The power of the cooler fan is increased up to the desired temperature of the value in the field Max.
8	**Overheat**	The threshold temperature for the overheat alarm can be set.
9	**After Seq.:**	The **After Sequence Action** can be set. The following options are available: **No Action, Cleaning, Standby, Custom.**

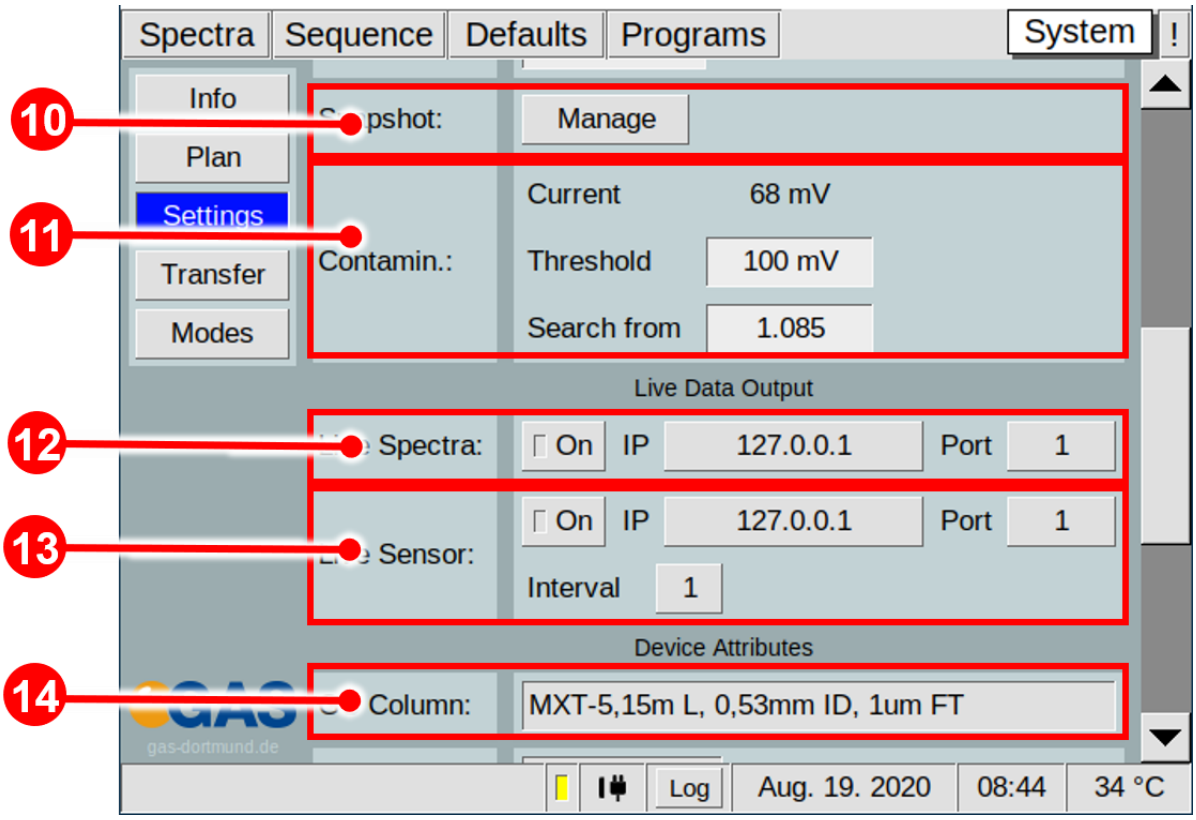


Figure 39: Operating Interface - System Settings Window 2

10	**Snapshot**	The **Manage** Button opens the snapshot window. User-specific target values can be set. A new snapshot can be recorded or can be imported Snapshot is a new function to allow automatic instrument performance checking
11	**Contamin**	Define the automatic search area for contamination. The search window can be defined by setting the Threshold (signal level in mV which is recognised as a contamination) and the Start of the search in the drift-time spectrum given as RIP relative proportional factor. • **Current:** Shows the currently detected contamination Shows the currently detected contamination. • **Threshold:** The set value from which an error is triggered. • **Search from:** The RIP-relative starting position of the search.
12	**Live Spectra:**	Prepared for further use! Currently not in function!
13	**Live Sensor:**	The settings for Live Data communication with G.A.S. Sequence Designer Software can be set. For detailed Information refer to the G.A.S. Sequence Designer Software Manual.
14	**GC Column:**	Input filed for Column ID. The value is stored with measurement file. This data is stored in the metadata of the measurement.

INFORMATION!

The device is delivered with an acceptance snapshot. This snapshot defines the system performance during device acceptance and is used to assess the readiness for measurement.

Any deviations from this are displayed in the Error Information Window. **The default values can be adjusted by the customer**.

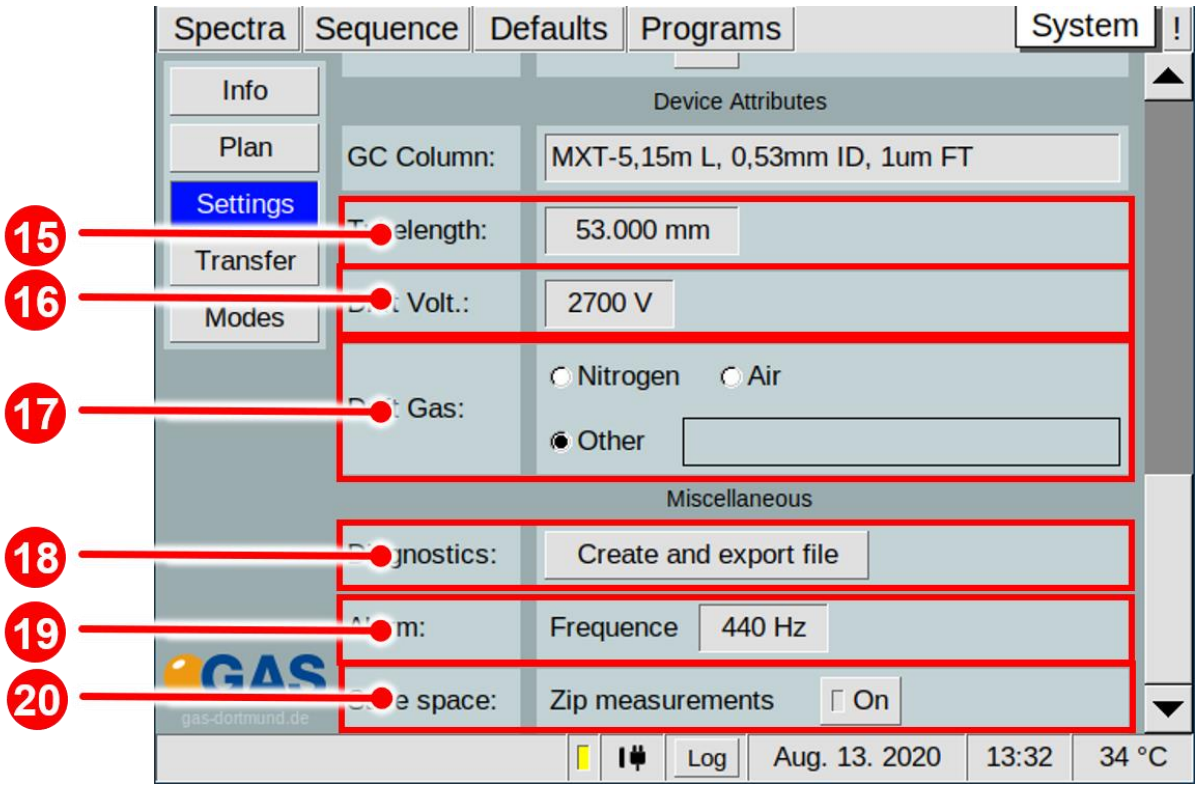


Figure 40: Operating Interface - System Settings Windows 3

15	**Tubelength:**	Prepared for further use! Currently not in function!
16	**Drift Volt.:**	Prepared for further use! Currently not in function!
17	**Drift Gas:**	Selection field for operating gas type. The value is stored with measurement file.
18	**Diagnostics:**	With the **Create and export file-Button** an encrypted diagnostic file is created which is intended to be analysed by the G.A.S Helpline for diagnostic purpose.
19	**Sound:**	The frequency of the warning sound can be set.
20	**Compression:**	Compresses the measurement data to a zip-file

6.6.3.1 Snapshot Window

The instrument performance and status can be monitored using recorded snapshots. It is an automatic comparison of current instrument settings versus the operator defined target settings which helps the operator to assess the readiness of the system for starting a measurement. This automatic monitoring can recognize among other a System contamination, insufficient gas quality or system leaking. For this purpose, the following parameters are constantly cross-checked against the target-settings:

- The carriergas pressure - EPC2 pressure (kPa)
- The height of the Reaction-Ion-Peak (RIP) - Rip-height (V)
- The position of the Reaction-Ion-Peak (RIP) normalized to normal pressure – Rip Pos at 101.33 kPa (ms)
- The full width at half maximum of the Reaction-Ion-Peak - FWHM (ms)
- The temperature values T1-T6
- The gasflow and pressure of Driftgas (EPC1) and Carriergas (EPC2)

The user can change the default factory settings for his needs. Error messages are displayed in the Error Information Window.

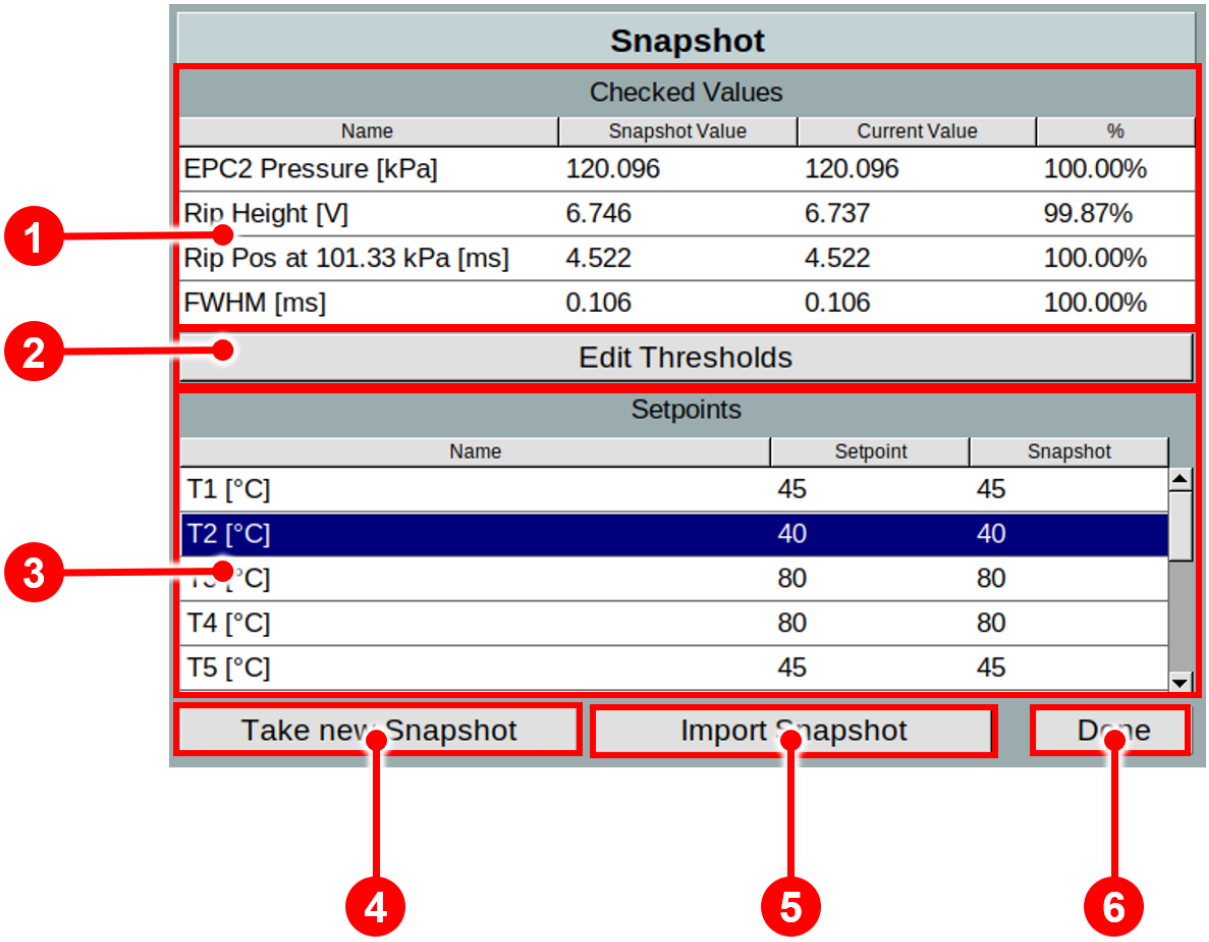


Figure 41: Operating Interface – Snapshot Window

1	**Checked values Area**	The checked Snapshot values (EPC2 Pressure; Rip Height, Rip-Position at 101,33 kPa, Rip-half-value width FWHM are displayed.
2	**Edit Threshold**	The selected Snapshot values (EPC2 Pressure; Rip Height, Rip-Position at 101,33 kPa, Rip-half-value width FWHM can be edited.
3	**Setpoints Area**	Display of the current setpoints and the corresponding snapshot values.
4	**Take new Snapshot Button**	Take a new snapshot of the current system status.
5	**Import Snapshot Button**	Import a Snapshot-file with prepared values by G-A.S.
6	**Done Button**	Closes the snapshot window

6.6.3.1.1 Snapshot window in detail

The system is delivered with standard limits for EPC2-Pressure, RIP-Height, RIP Position at 101.33 kPa and FWHM. The upper and lower limits of these parameters r can be adjusted by the customer.

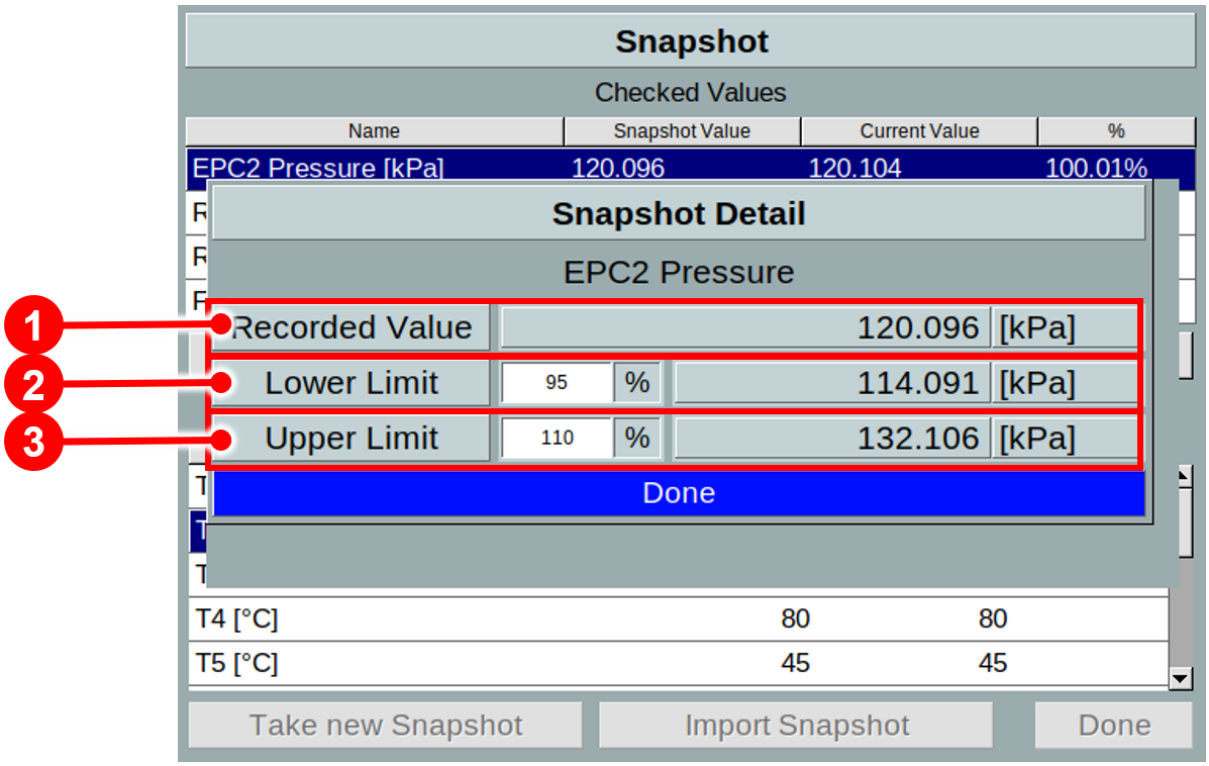


Figure 42: Operating Interface – Snapshot Window in detail (example EPC2 pressure)

1	**Recorded Value**	Displays the current recorded snapshot value (Example EPC2 pressure).
2	**Lower Limit**	The lower limit of the current recorded snapshot value (Example EPC2 pressure) is displayed. This limit can be specified by the user.
3	**Upper Limit**	The upper limit of the current recorded snapshot value (Example EPC2 pressure) is displayed. This limit can be specified by the user.

Factory default limits		
Name	**Lower limit (%)**	**Upper limit (%)**
EPC2-Pressure (kPa)	**95**	110
RIP Height (V)	**80**	150
RIP Position at 101.33 kPa (ms)	**95**	105
FWHM (ms)	**80**	120

INFORMATION!

The device is delivered with an acceptance snapshot. This snapshot defines the system performance during device acceptance and is used to assess the readiness for measurement. Any deviations from this are displayed in the Error Information Window. **The default values can be adjusted by the customer**.

6.6.3.2 Simplified View Window

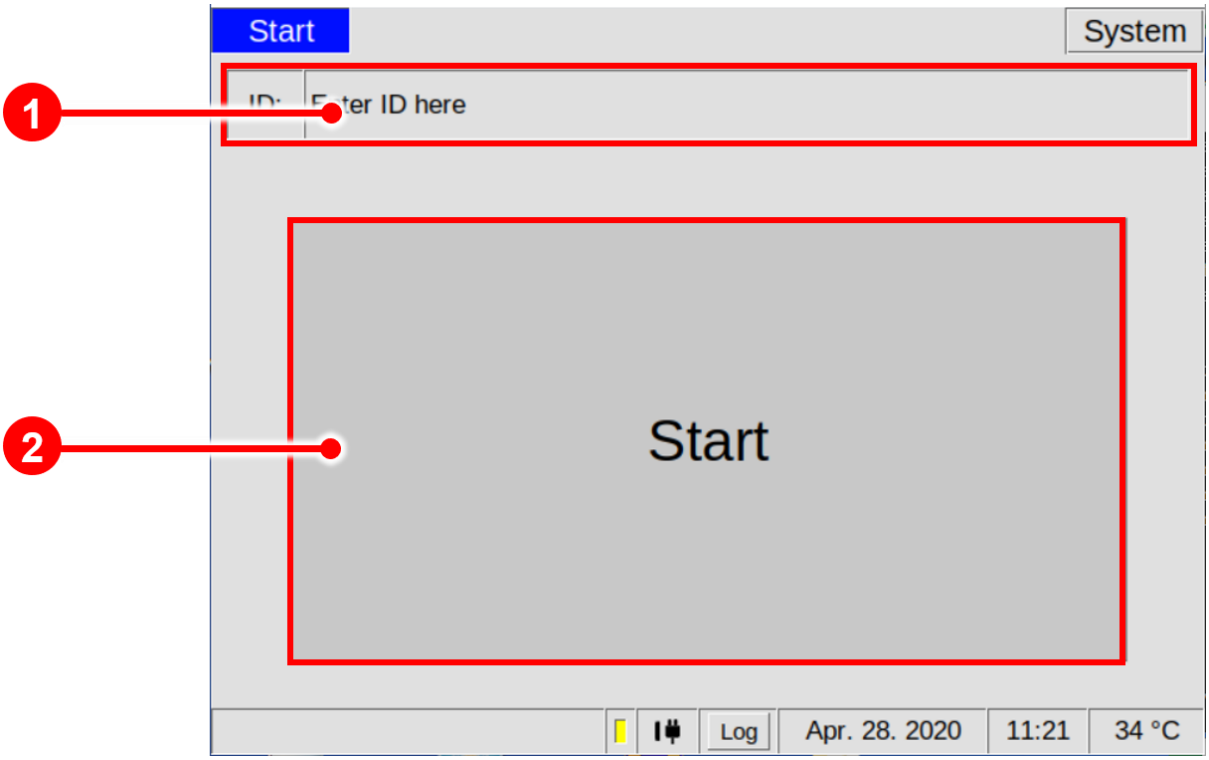


Figure 43: Operating Interface - Simplified View Window

1	**ID**	A measurement identification can be specified by the customer.
2	**Start Button**	By selecting this button the current program is started.

6.6.4 System Transfer Window

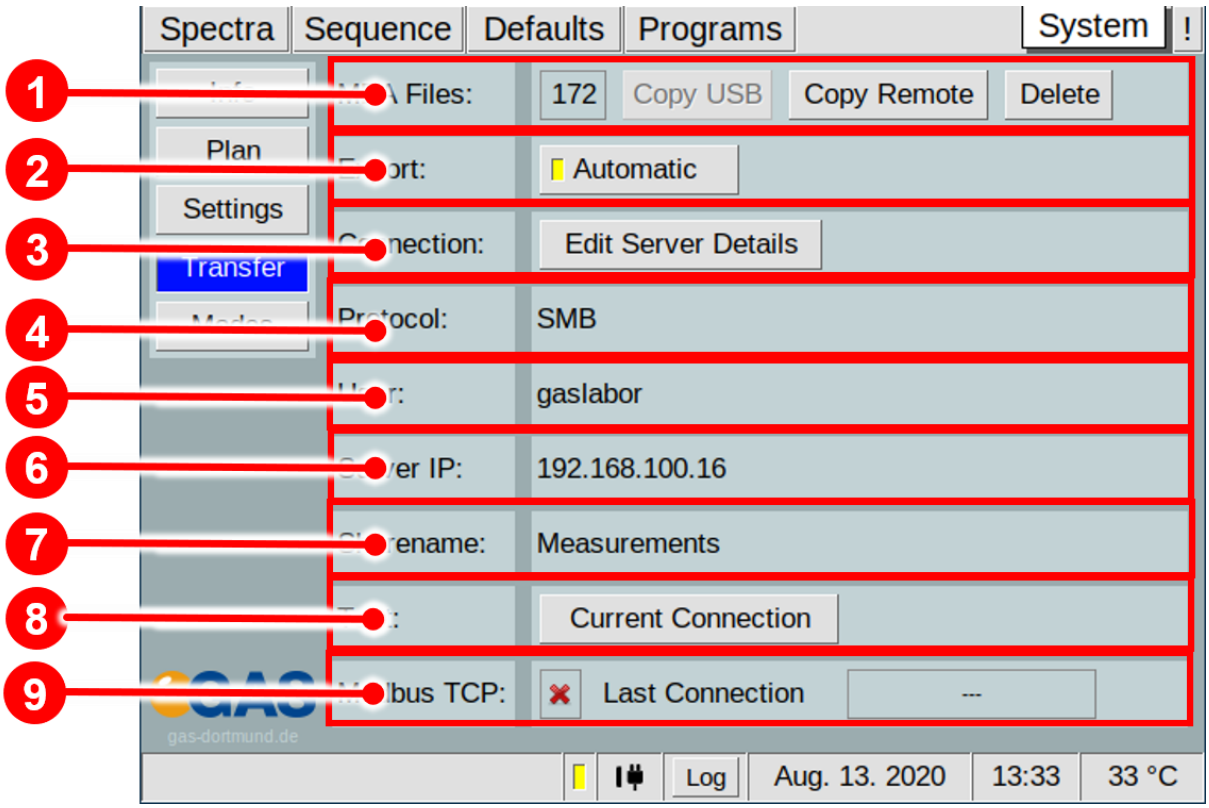


Figure 44: Operating Interface - System Transfer Window

1	**MEA Files:**	The current number of internal stored measurement files and the following measurement file managing options are displayed and available: **Copy to USB**: Copy all internal stored measurements to a connected USB device. **Copy to remote**: All internal stored measurement files will be copied to the connected shared folder. **Delete**: Deleting all internal stored measurement files.
2	**Export:**	Activating the automatic storage to a connected shared folder on a network as storage location for measurements.
3	**Connection:**	With **Edit Server Details Button** the Export settings (transfer protocol, IPv4-adress, shared folder name) can be set.

4	**Protocol:**	Displays the activated transfer protocol (smb, sftp or tftp).
5	**User:**	Displays the selected user name.
6	**Export:**	Displays the defined IPv4-address.
7	**Sharename:**	Displays the selected sharename of the storage folder.
8	**Test:**	The Current Connection button initiates the connection to the host-device and establishes the communication to the shared folder using the current export settings. A message will appear to indicate if the connection initiated successfully.
9	**Modbus TCP**	The last Modbus TCP connection can be checked. It will give you information on when and from which IP the last connection was made and whether it is still active.

6.6.5 System Modes Window

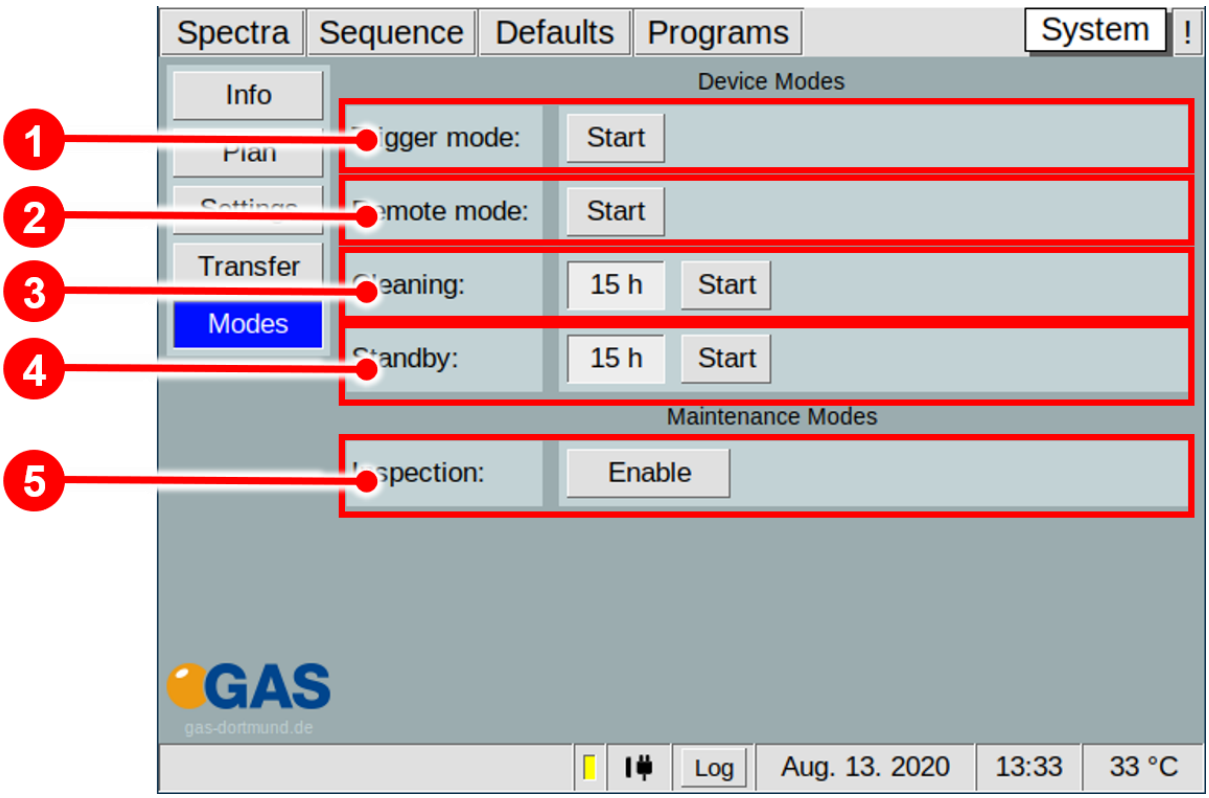


Figure 45: Operating Interface - System Modes Window

1	**Trigger mode:**	Activate trigger mode with **Start**.
2	**Remote mode:**	Activate remote mode with **Start**.
3	**Cleaning:**	Setup and activate of cleaning mode. With Start-Button the cleaning process is activated and the **Cleaning Mode Window** appears. Possible Values: (1-96 hours or infinity) Activate **Cleaning Mode** with **Start**.
4	**Standby:**	Setup and activate of standby mode. With Start-Button the standby process is activated and the **Standby Mode Window** appears. Possible Values: (1-96 hours or infinity). Activate **Standby Mode** with **Start**.

5	**Inspection**	With **Enable-Button** the access to the inspection and diagnostic functions of the device is allowed.

6.6.5.1 Trigger Mode Window

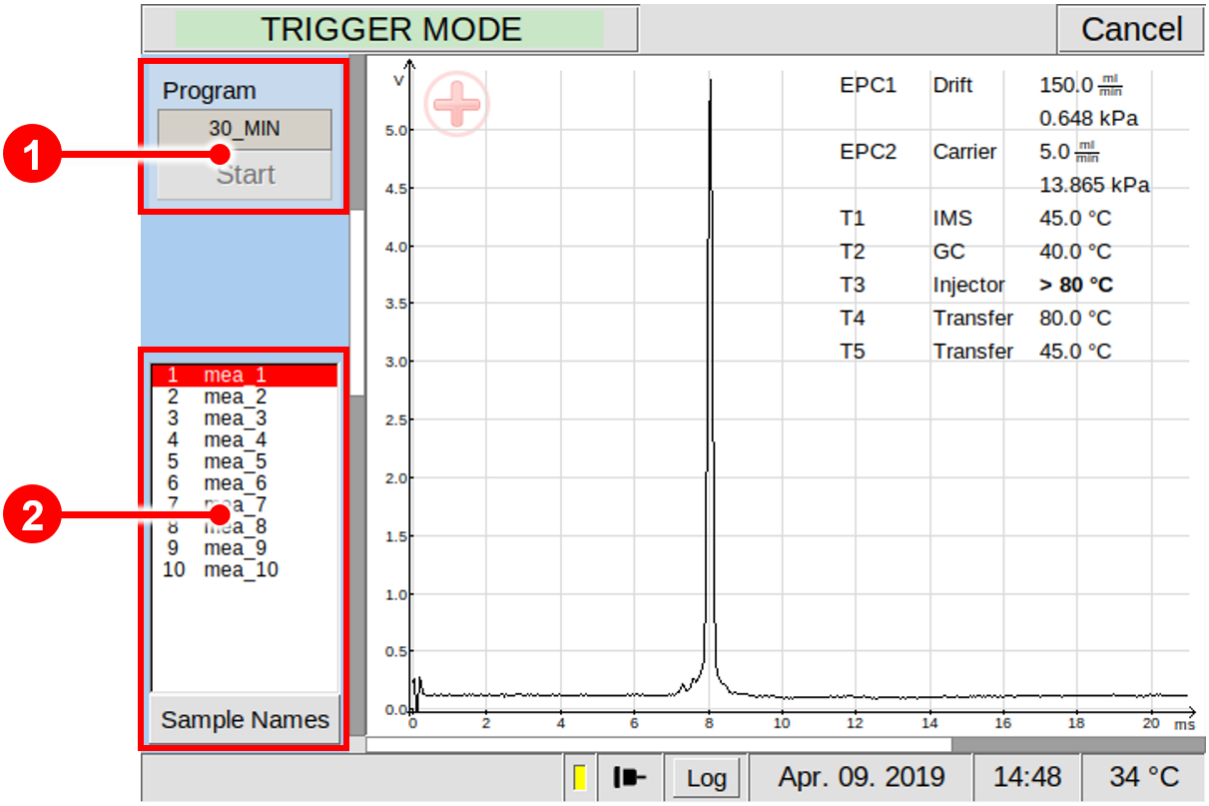


Figure 46: Operating Interface - Trigger Mode Window

1	**Program Start Area**	In Trigger mode the displayed program is started by a connected autosampler that operates as master device.
2	**Sample Names Area**	Displays the currently loaded sample names list. The current sample name is highlighted red. With this **Sample names button** the sample names list file **SampleNames.txt** can be imported

6.6.5.2 Remote Mode Window

By activating the Remote Mode, the **Remote Mode Window** appears. The windows is initially empty. The device is waiting for a sequence file to import.

INFORMATION!

The sequence file must be created with the **G.A.S. Sequence Designer Software**. For detailed Information refer to the **G.A.S. Sequence Designer Software Manual.**

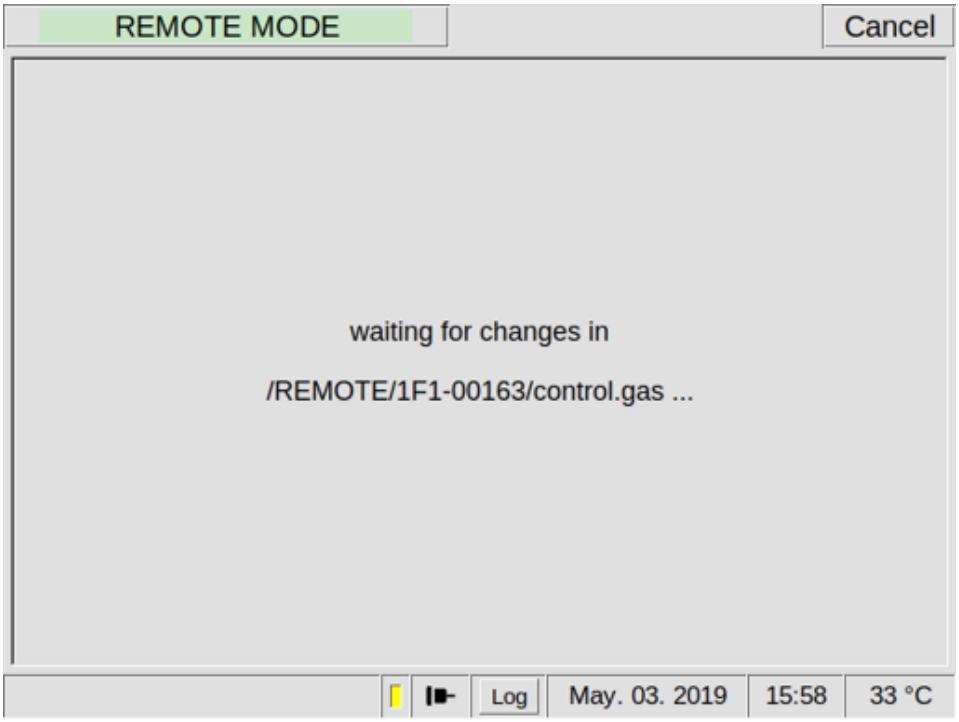


Figure 47: Operating Interface - Remote Mode Window

6.6.5.3 Cleaning Mode Window

By activating the Cleaning Mode, the **Cleaning Mode Window** appears. During the cleaning process the available system temperatures (T1-T6) are heated up to their maxima. The user default flow rates settings for Driftgas (EPC1) and Carriergas (EPC 2) setup in Defaults window are used. After the setup time has expired the cleaning process is terminated.

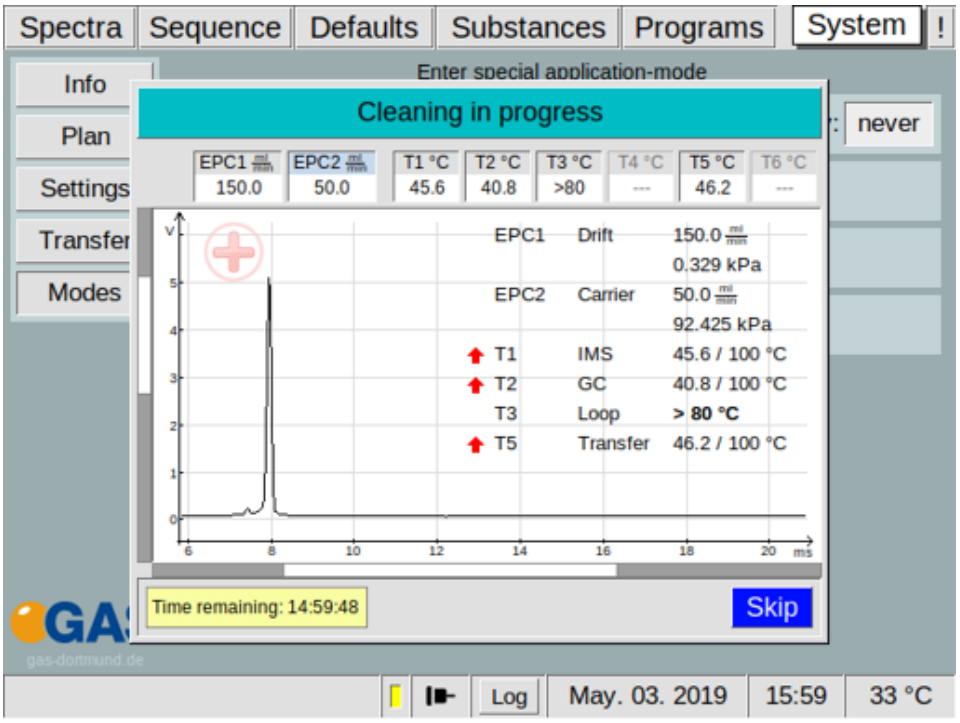


Figure 48: Operating Interface - Cleaning Mode Window

INFORMATION!

During the cleaning process the available heating module temperature (T1-T6) are set to their maxima. Values of more than 80 °C are displayed as >80°C.

6.6.5.4 Standby Mode Window

By activating the Standby Mode, the **Standby Mode Window** appears. The flowrate of the Drift gas (EPC1) and the carrier gas (EPC2) will be decreased to reduce gas consumption. The standby mode flowrate for drift gas (EPC1) is 10 ml/min and for carrier gas (EPC2) is 5 ml/min.

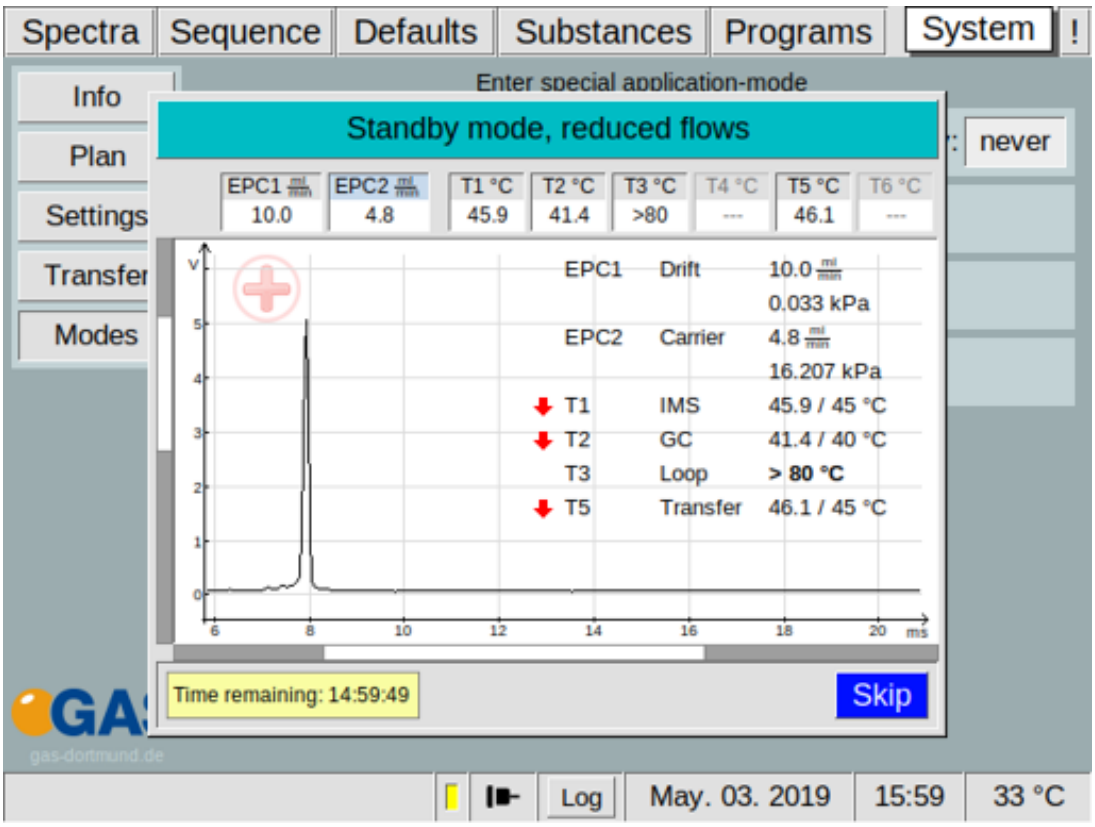


Figure 49: Operating Interface - Standby Mode Window

6.7 Error Information Window

In case if an Error the **!-Tab** is blinking red. The error window shows an overview of the current error events. When the device is restarted, the error events are deleted.

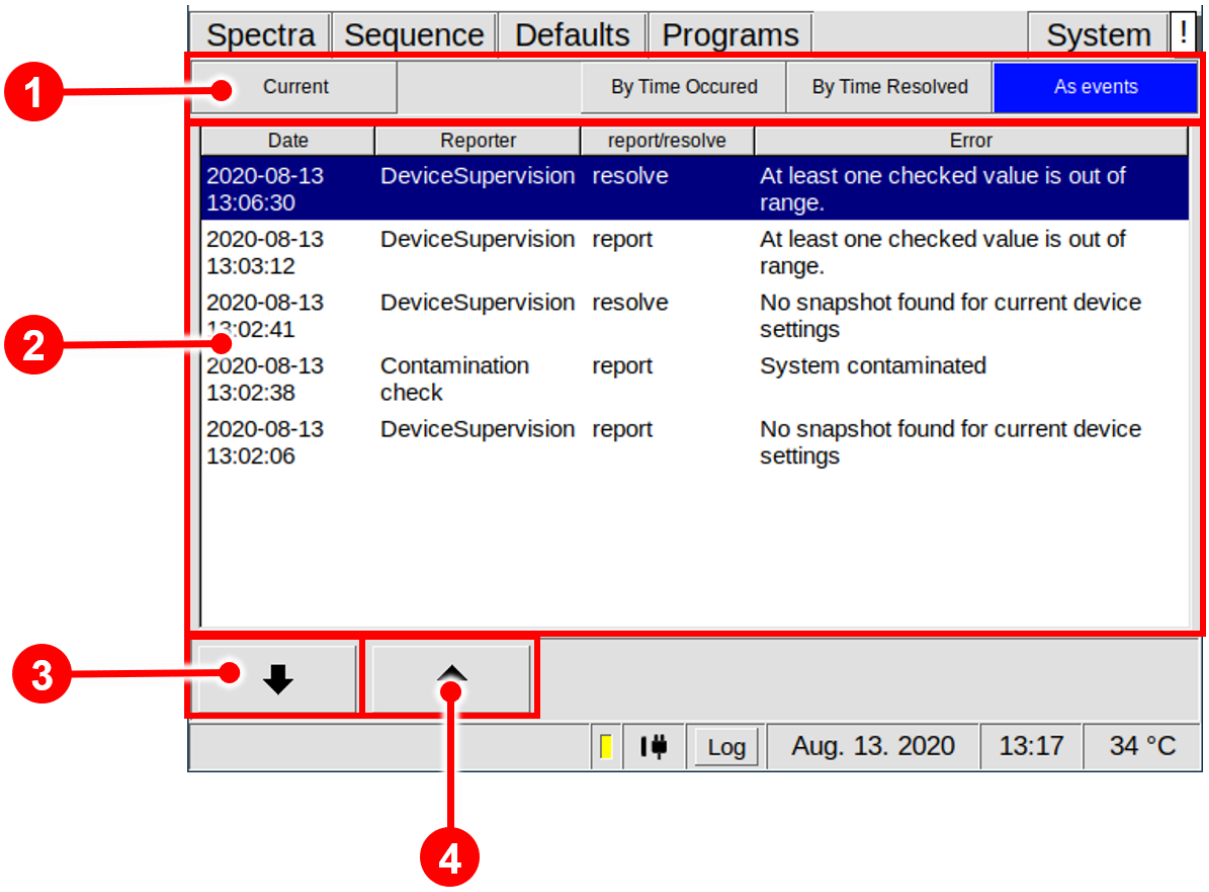


Figure 50: Error Information Window

1	**Selection Sort Order Bar**	Selects the following sort order: **Current**; **By Time Occurred**; **By Time Resolved**; **As Event**
2	**Entry List**	A list of system event messages. The display depends on the selected sort order
3	**Down Button**	Scrolls one message down.
4	**Up Button**	Scrolls one message up.

6.8 Additional Dialog Windows

6.8.1 Log Messages Dialog Window

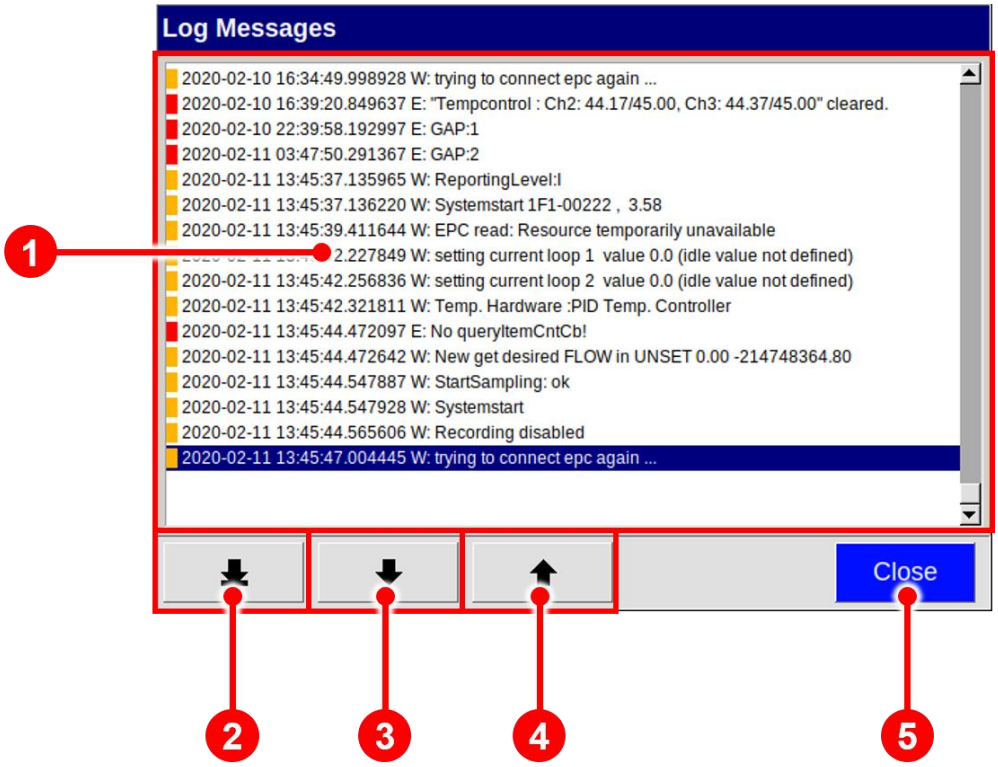


Figure 51: Log Messages Dialog Window

1	**Entry List**	A chronological list of system event messages. Warnings are marked orange, error messages are marked red.
2	**To Last Entry Button**	Scrolls down to the latest entry.
3	**Page Down Button**	Scrolls one page down.
4	**Page Up Button**	Scrolls one page up.
5	**Close Button**	Closes the dialog.

6.8.2 IP Adress Input Dialog Windows

The IP Address Input Dialog is used to edit the static IP address of the device and the IP address of a remote server. This is necessary when configuring the LAN file transfer.

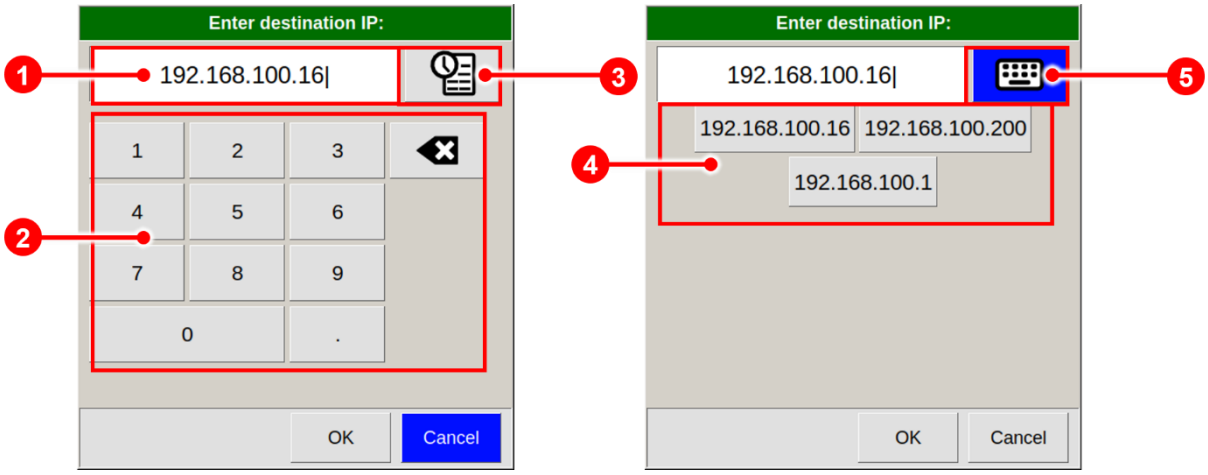


Figure 52: IP Adress Input Dialog Windows

1	**IP Address Field**	The current IP address.
2	**Digit and Dot Buttons / Backspace Button**	Use these buttons to enter an IP address.
3	**History Button**	Displays a menu of previously used IP addresses to choose from.
4	**History Entry Buttons**	Buttons for entering previously used IP addresses.
5	**Keyboard Button**	Displays the keyboard.

6.8.3 Date and Time Input Dialog Window

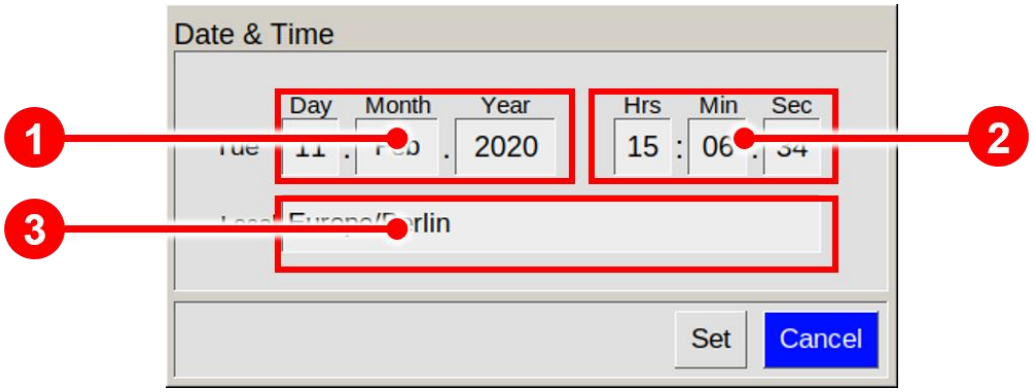


Figure 53: Date and Time Input Dialog Window

1	**Date Fields**	Fields displaying and modifying day, month and year.
2	**Time Fields**	Fields displaying and modifying hours, minutes and seconds.
3	**Timezone**	Field for selection of timezone.

6.8.4 Text Input Dialog Window

The Text Input Dialog is used to enter identifiers, e.g. shared folder name.

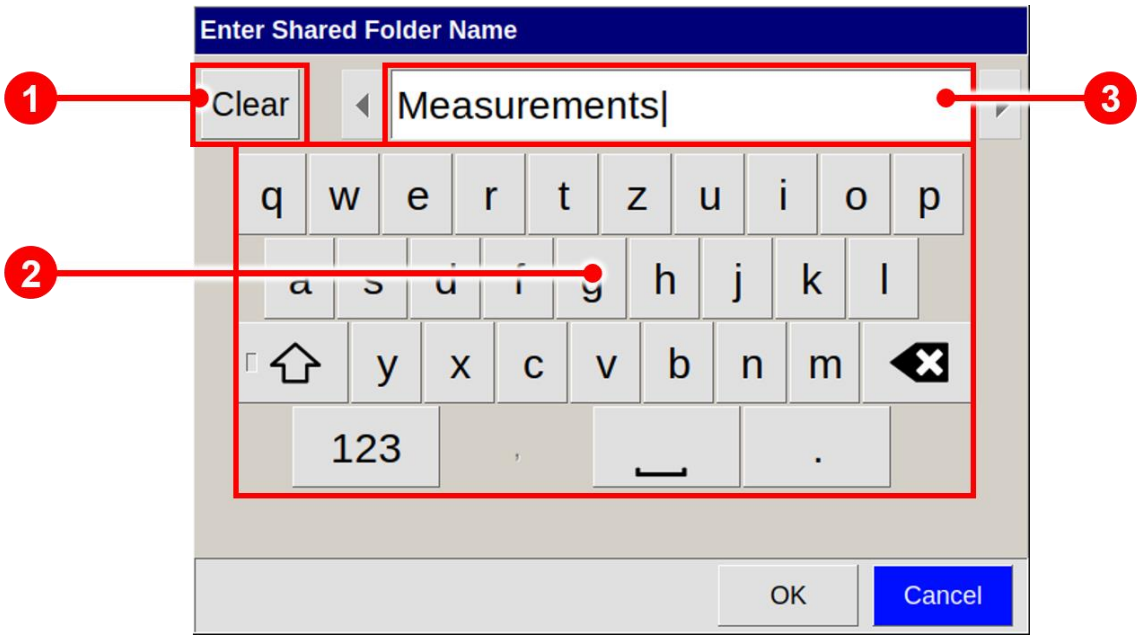


Figure 54: Text Input Dialog Window

1	**Clear Button**	Deletes the text in the current text field
2	**Keyboard Buttons**	Character and control buttons for entering a text. Depending on the context some buttons are disabled.
3	**Current Text Field**	The editable text.

6.8.5 Number Input Dialog Window

The Number Input Dialog is used in Program Window to enter number values, e.g. Start time, Flow Rates and Pump Power setpoints in Program Actions.

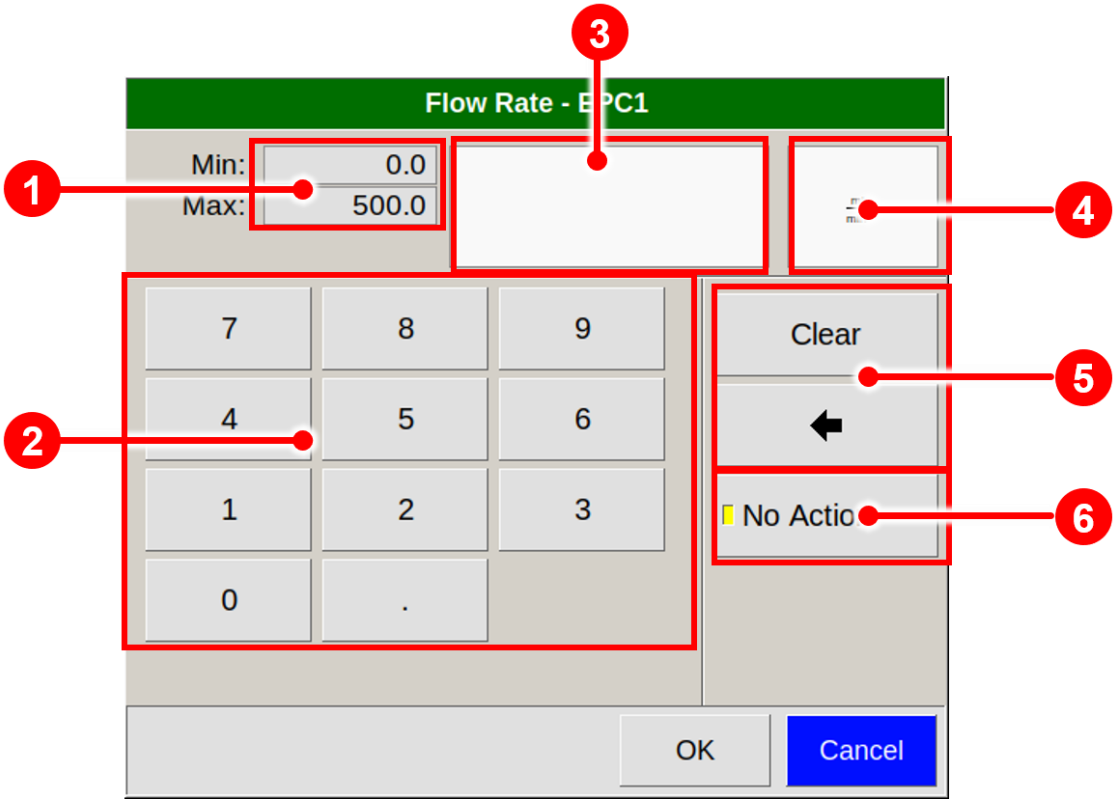


Figure 55: Number Input Dialog Window (Example)

1	**Range / Raster Info**	Displays the valid value range.
2	**Keyboard Buttons**	Buttons for entering a number.
3	**Value Field**	The entered numerical or selected special value.
4	**Unit**	Value unit name.
5	**Clear and Backspace Button**	Buttons for clearing the input field or deleting the last digit.
6	**Dedicated Values Buttons**	Dedicated value like **No Action** (only if available)

6.9 PAL3 Autosampler-Terminal

The Combi PAL Autosampler can be controlled by using Terminal. It is the main input unit for user interaction.

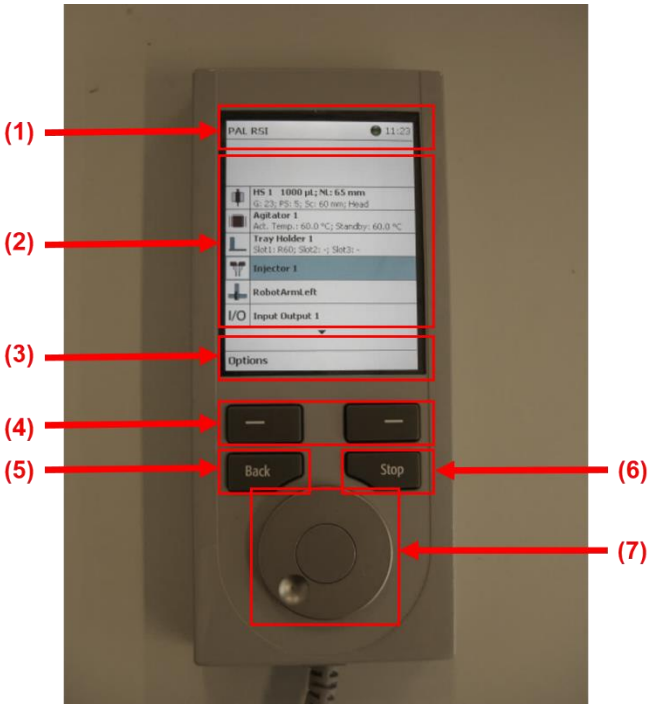


Figure 56: Autosampler Terminal

1	**Status Bar**	Selected section, the status and time are displayed
2	**Content Area**	Shows the list of selected items
3	**Menu Bar with Funktion Keys**	Shows the options for the function keys.
4	**Menu Buttons**	With the function keys the actual option in the menu bar can be selected.
5	**Back Button**	Press the Back Button to return to the previous page. If the Back Button is pressed continuously the cursor will jump back to the home screen.
6	**Stop Button**	Pressing the stop button will abort the ongoing activity.

7	**Pushable Rotary Knob**	Rotates the outer knob to move the cursor bars. Press the inner knob to selected an item or ENTER a selection.

INFORMATION!

For detailed Information refer the PAL RSI Operating Manual

7 Installation FlavourSpec Device

7.1 Installation Requirements

The following requirements must be fulfilled by the customer:

Location of Installation

- Available space of 1000 x 900 x 800 mm (W x D x H)
- Ambient temperature of 5 – 40 °C
- Humidity: 0-90 % RH, non-condensating
- Robust table with a minimum carrying capacity of >40kg

Electricity

- Electricity supply free of interferences
- Power Supply of 230 V ± 10%, 50- 60 Hz ± 1%

Gas supply

- Nitrogen (Quality 5.0 (99,999%) or Synthetic Air (Quality 5.0 (99,999%)
- Stainless steel pressure reducer with 3mm or 1/8“ Swagelok-Connector adjustable pressure range of 3 – 6 bar and 3 mm Swagelok connector

Safety

- Availability of exhaust system for device exhaust gas tubes (Gas out and Sample Gas out)

Computer

- Computer with current Microsoft Windows operating system

- Administrator right to install G.A.S. software

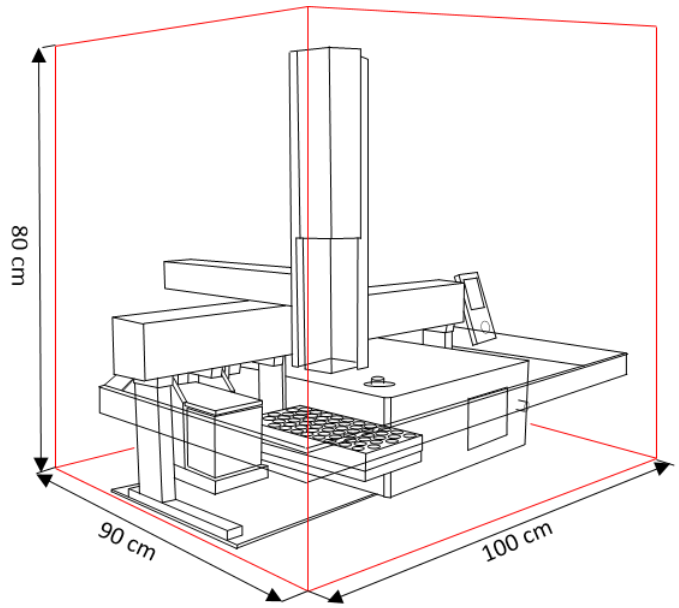


Figure 57: Space requirement FlavourSpec with Autosampler PAL RSI

INFORMATION!

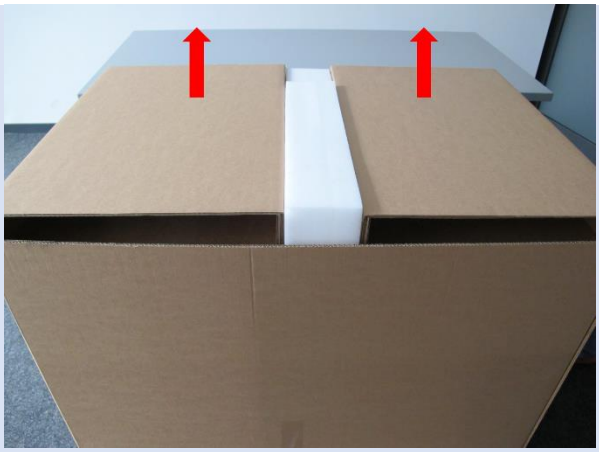
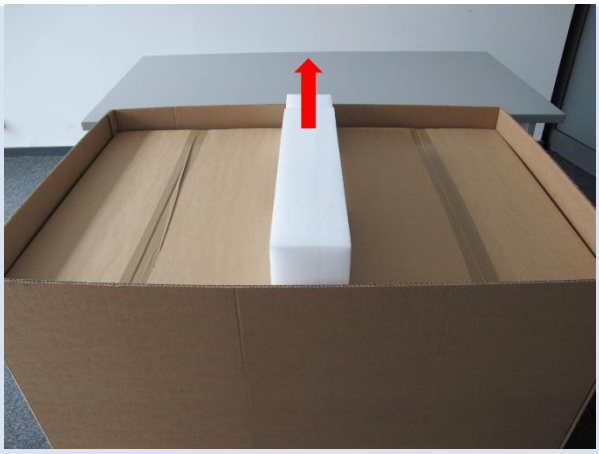
To ensure correct measurements it is absolutely necessary to **connect the supplied exhaust tubes** (Gas out and Sample gas out).

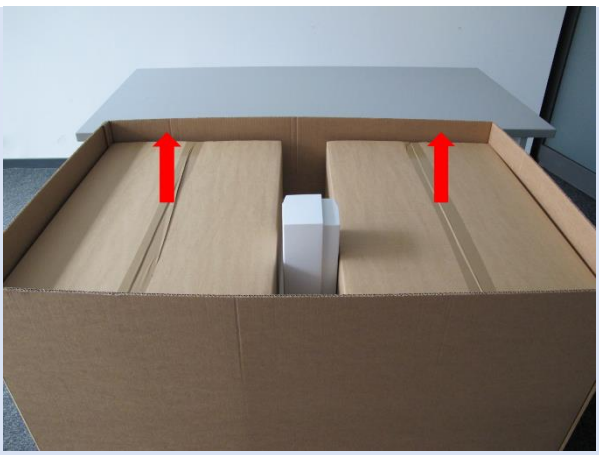
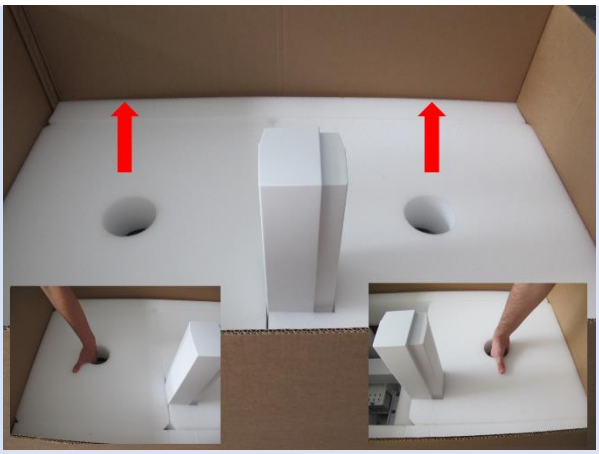
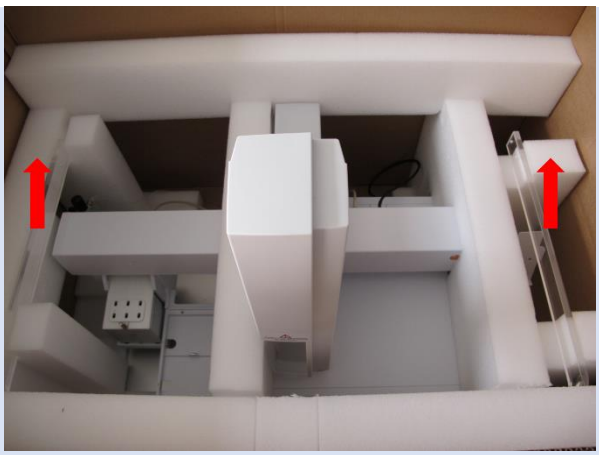
The exhaust tubes (Gas out and Sample gas out) **must be led separately into the exhaust system and must not be connected.**

The exhaust system must **not generate any negative pressure**.

7.2 Unpack the device

At least two people are necessary to unpack the device.

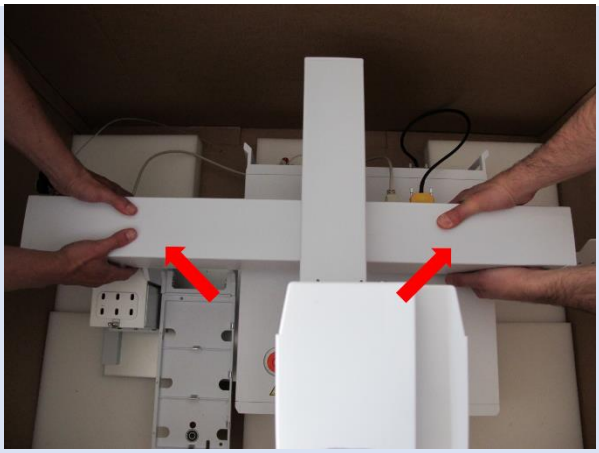
1		Remove the cover
2		Remove the cardboard spacers.
3		Remove the foam spacer.

4		Remove both Accessories boxes.
5		Remove both foam spacers.
6		Remove the safety guard.

7

Remove the big foam spacer.

8

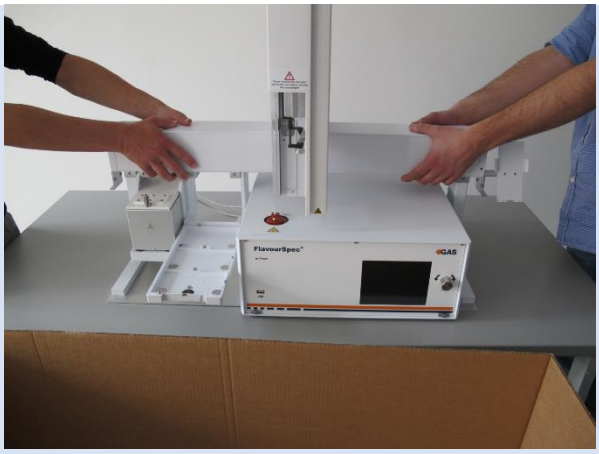


Lift the device carefully

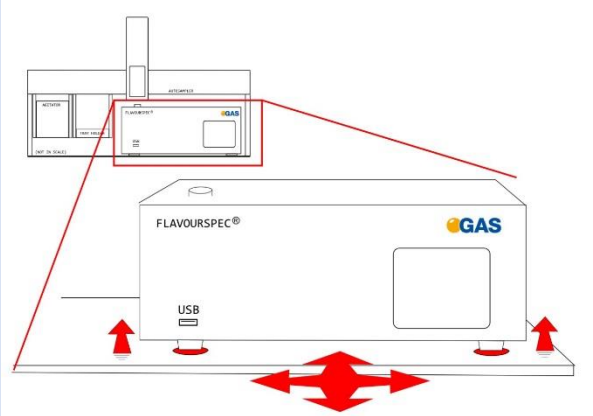
WARNING

The arm of the autosampler can move freely. It is recommended to hold the arm by a third person.

9



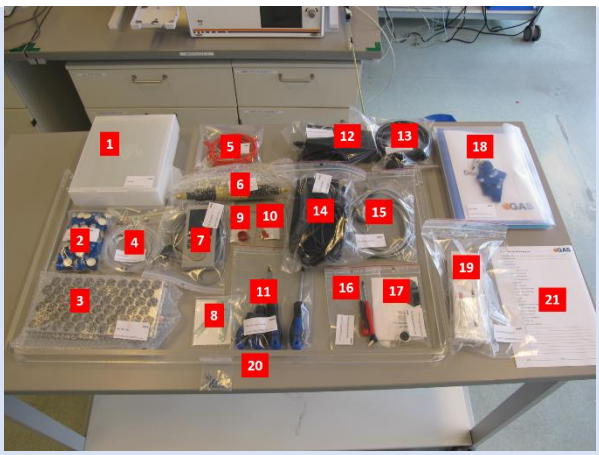
Put the device on a stable table.

10		Check the position of the instrument feet. The instrument feet and the position holes of the baseplate must fit.

7.3 Unpack the accessories

1		1 Safety guard 2 Accessories box 3 Packing list
2		The figure shows the opened box.

3



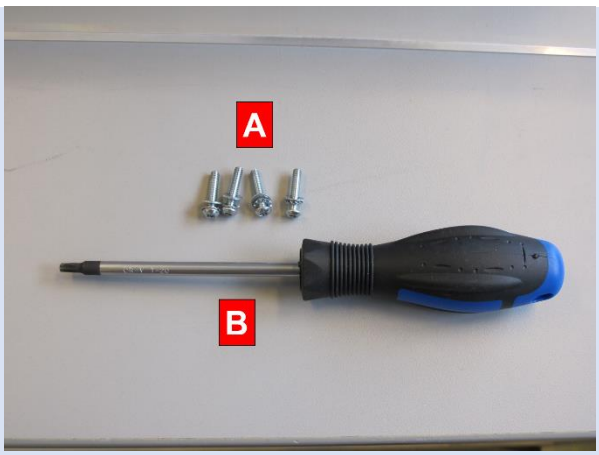
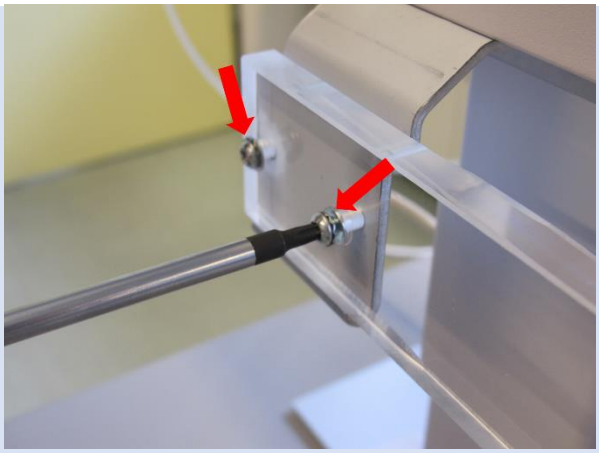
The figure shows the delivered standard components.

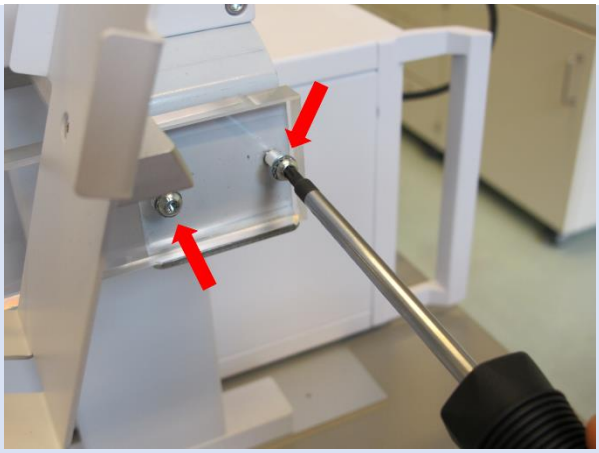
Check the entire delivery for completeness on basis of the packing list.

4

1 20 ml headspace vials
2 magnetic caps for headspace vials
3 Tray
4 Gas tubes with 3 mm Swagelok connection
5 LAN-Cable
6 Molecular sieve
7 Terminal
8 PAL RSI spanner
9 Injector adapter
10 Septa
11 PAL RSI torx screwdriver
12 FlavourSpec power supply
13 FlavourSpec power cable
14 PAL RSI power supply
15 PAL RSI power cable
16 FlavourSpec torx screwdriver
17 PAL RSI teaching tool
18 Documents / USB-memory stick
19 PAL RSI Syringe KIT
20 Safety guard
21 Packing list

7.4 Mount the Safety guard

1		The neccessary screws are included.
2		To connect the Safety Guard the following required: **A**: four M4 Torx screws with spring washer and washer **B**: Screwdriver Torx T20
3		Connect the Safety Guard to the Safety Guard Brackets on the left and …

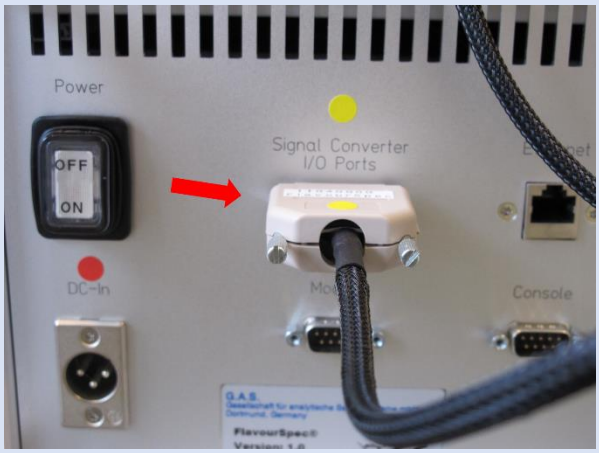
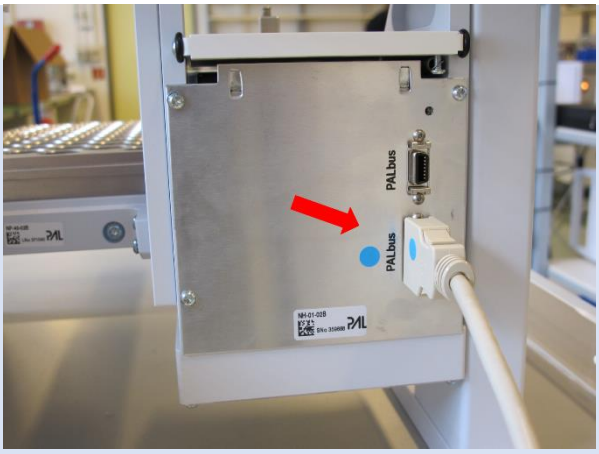
4		…right side of the X-Axis using the screws.
5		The figure shows the autosampler with installed Safety Guard.

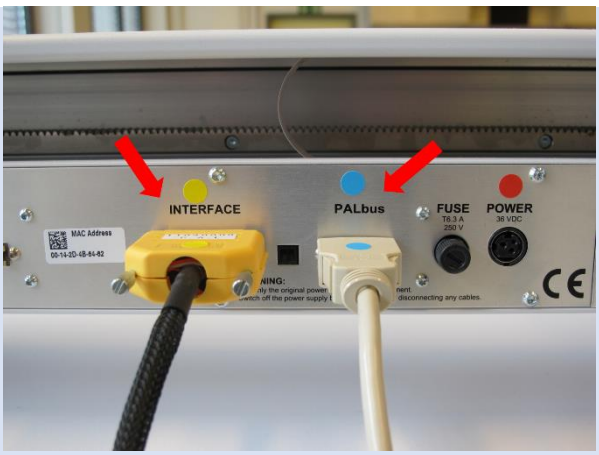
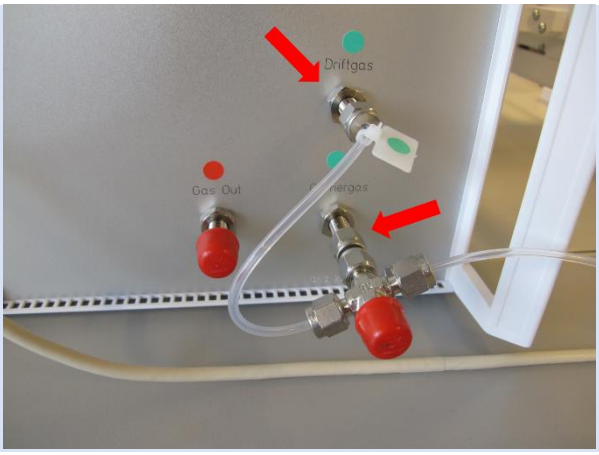
7.5 Connect the PAL RSI Terminal

1		Connect the Terminal cable to the Terminal Connector (green marking).

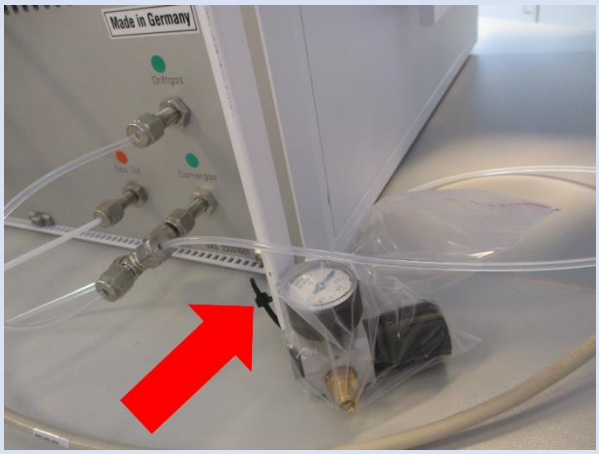
2		Place the Terminal into the Terminal Holder.

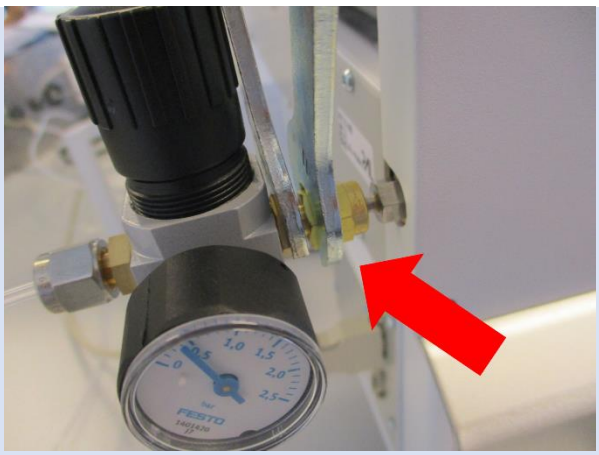
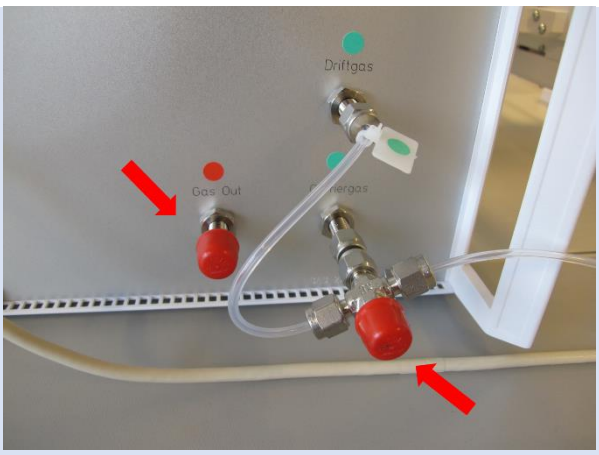
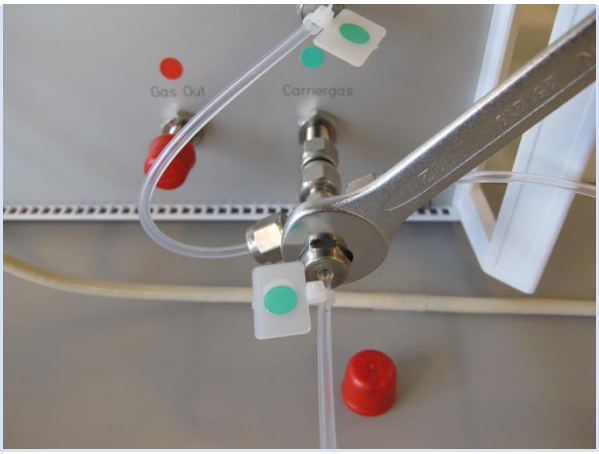
7.6 Check the Preinstalled Connecting Cable

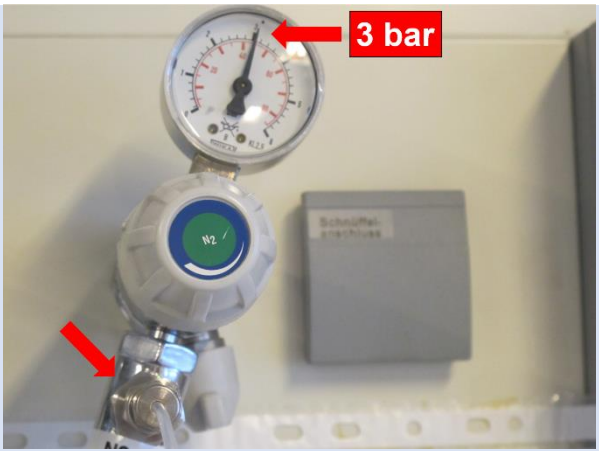
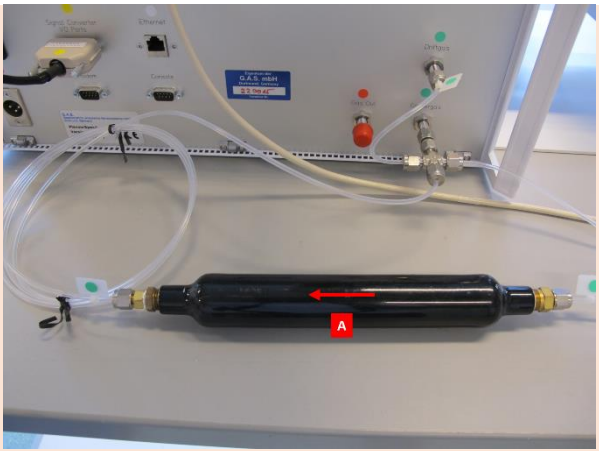
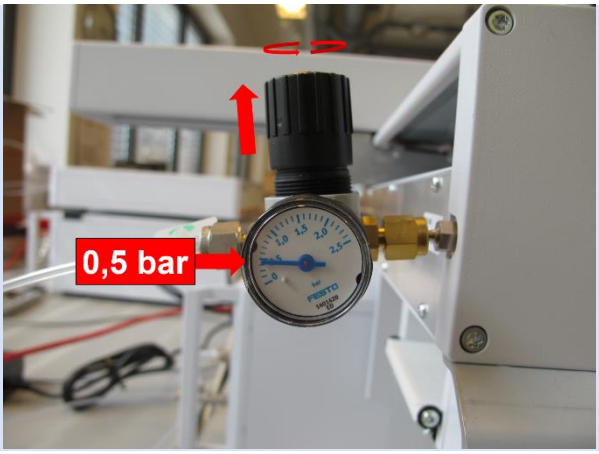
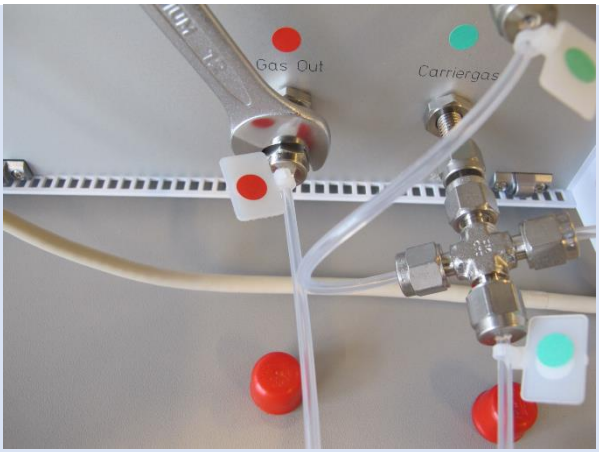
1		**Rear FlavourSpec:** Check the connection cable Autosampler/FlavourSpec (Grey Plug, Yellow marking) at the Signal Converter I/O Ports
2		**Rear Agitator:** Check the connection cable Agitator (blue marking) at the port PALbus.

3		**Rear Autosampler X-Axis:** Check the connetion cable Agitator (blue marking) at the port PALbus. Check the connection cable Autosampler/FlavourSpec (Yellow plug, yellow marking) at port Interface
4		**Rear FlavourSpec:** Check the 3mm Swagelok-Connection of the Driftgas-/Carriergas-Adapter-

7.7 Connect the Gas Supply

1		Release the pressure reducer.

2		Mount the pressure reducer at the rear of the autosampler.
3		Remove the red caps on the rear panel of the device. **Keep the red caps.**
4		Connect a tube (green marking) with 3 mm Swagelok-connection to the Driftgas/Carriergas-connection using a 12 mm spanner.

5		Connect the tube to a nitrogen or synthetic air gas supply. (Gasquality: nitrogen 5.0 or synthetic air 5.0). **Set up the back pressure to 3 bar.**
6		**OPTIONAL** To ensure a high purity of the gas install the delivered molecular sieve. **A** with another green marked tube.
7		Pull the button to unlock. Set the purge gas pressure to 0,5 bar. Press the button to lock
8		Connect a waste tube (red marking) with 3 mm Swagelok-connection to the Gas out-connection using a 12 mm spanner. Connect the other end of the tube to an adequate laboratory waste system.

INFORMATION!

Only use stainless steel pressure reducer, PTFE tubes with 3 mm outer diameter and 3 mm swagelok connectors.

To ensure a high purity of the gas install the provided moisture trap.

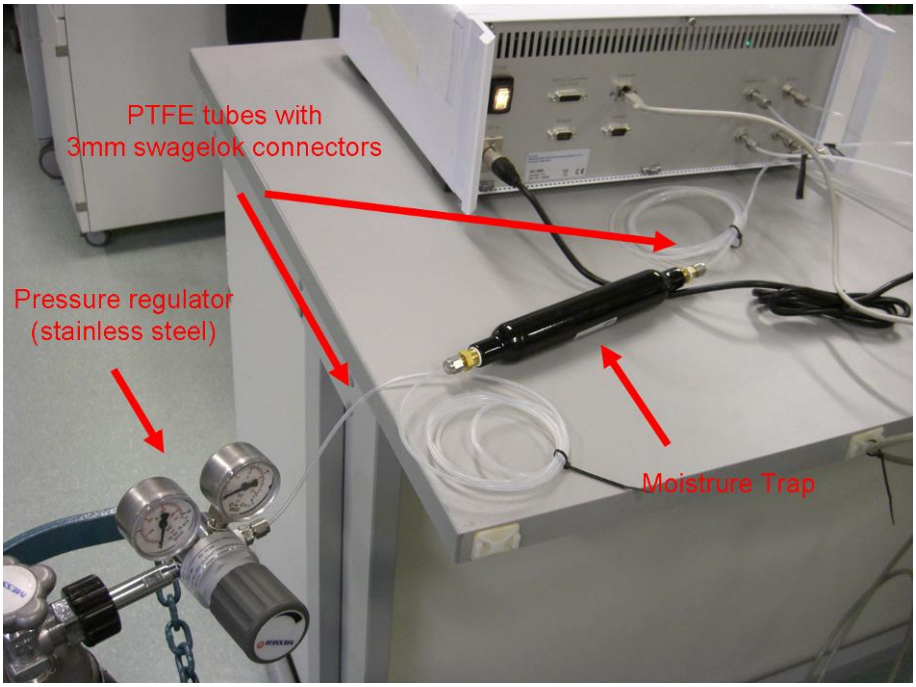


Figure 58: Gas supply installation

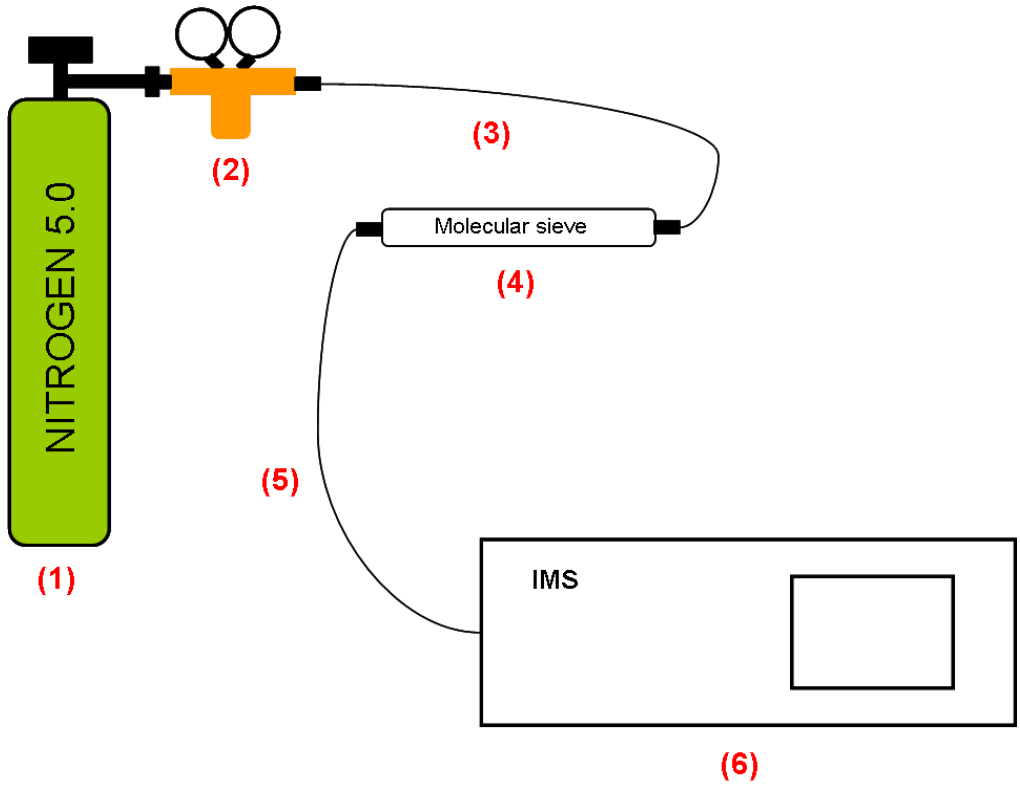
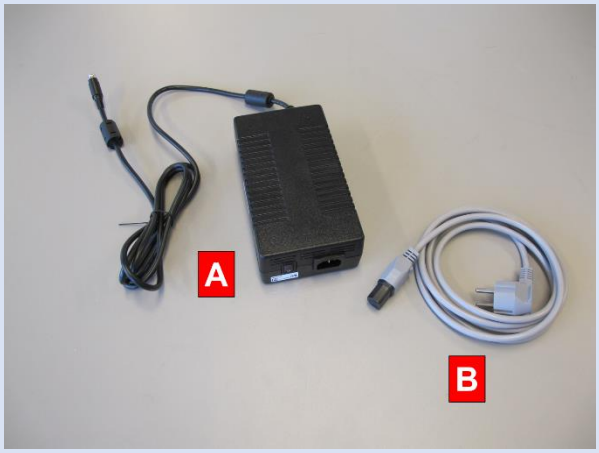
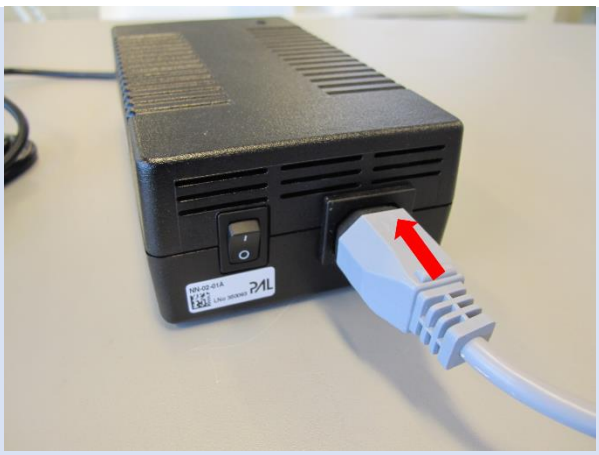
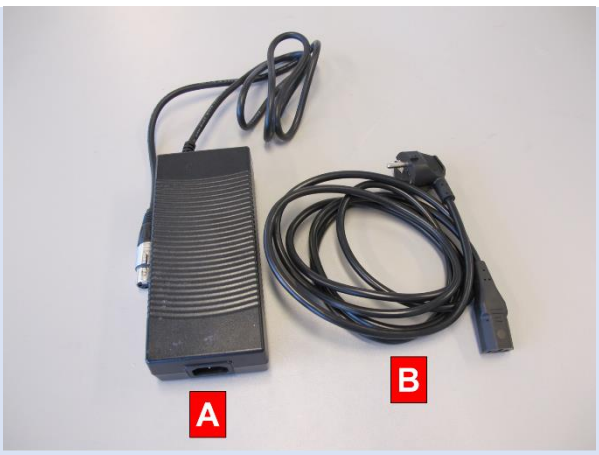


Figure 59: Gas supply installation (schematic)

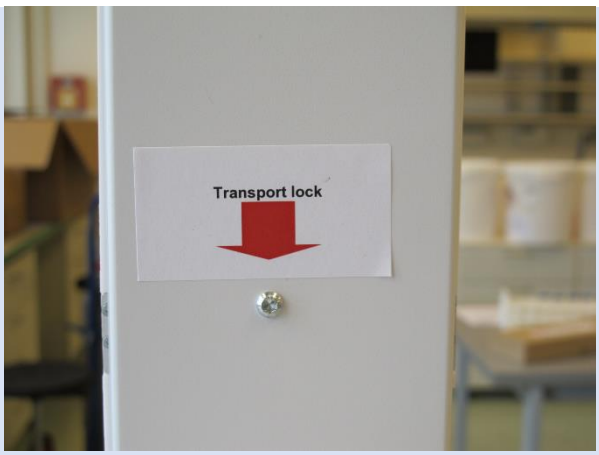
1	Gas supply e.g. gas bottle with Nitrogen 5.0 ***(provided by customer)***
2	Pressure reducer ***(provided by customer)***
3	2 m PFA gas tube with 3 mm Swagelock connector ***(provided by G.A.S.)***
4	Molecular sieve with 3 mm connection ***(provided by G.A.S.)***
5	2 m PFA gas tube with 3 mm Swagelock connector ***(provided by G.A.S.)***
6	Device ***(provided by G.A.S.)***

7.8 Connect the Power Supply

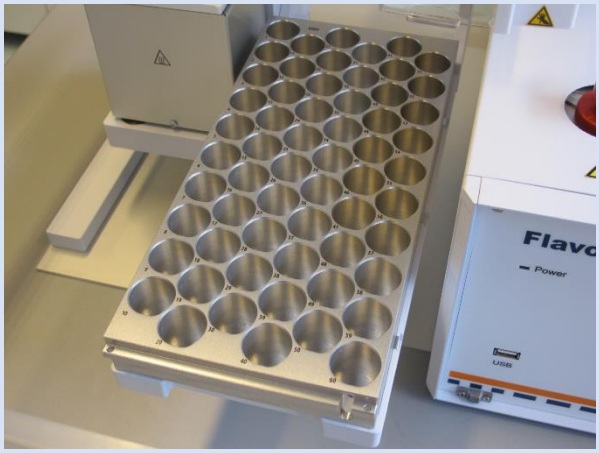
1		**Power supply Autosampler:** A: PAL RSI Autosampler Power Supply B: Country-specific Power Plug
2		Connect the Power supply unit with the power plug. Connect the power plug to a power supply.
3		Connect the power plug to the power connector at the rear of the Autosampler (red marking).

4		**Power Supply FlavourSpec:** A: FlavourSpec Power Supply B: Country-specific Power Plug
5		Connect the Power supply unit with the power plug. Connect the power plug to a power supply.
6		Connect the power plug to the power connector at the rear of the FlavourSpec (red marking).

7.9 Remove the Transport Lock

1		Transport Lock Sign at the front of the autosampler.
2		Transport Lock Sign at the rear of the autosampler.
3		Remove the transport lock screw with a screwdriver (Torx T20). Keep the screw for future use.

7.10 Complete the Device

1		Place the tray to the trayholder.

7.11 Switch on the Device

1		Switch on PAL RSI Autosampler.
2		Switch on the FlavourSpec.

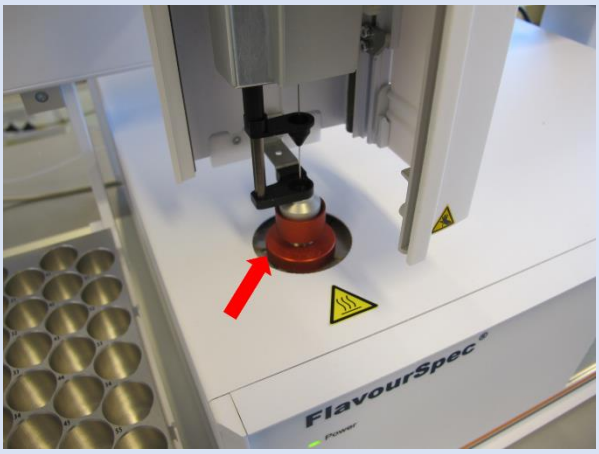
INFORMATION!

For detailed information concering the autosampler please refer the autosampler manual.

7.12 Check essential device postion

Before working with the intrument the position of the injector, agitator and the trayholder must be tested and if neccessary adapted.

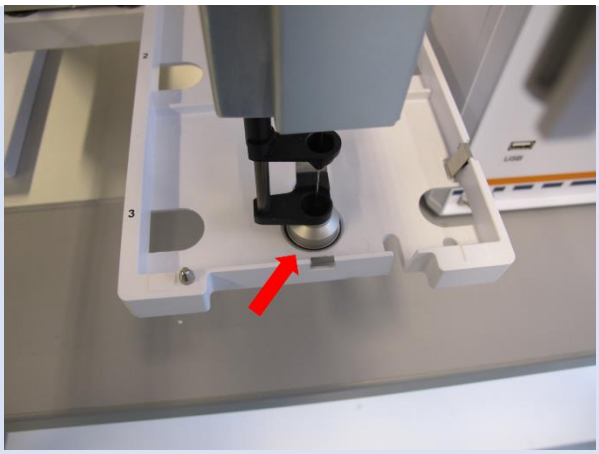
1



Check the position of the injector **(see chapter 8.2)**

OPTIONAL
Teach the position of the injector **(see chapter 8.3)**

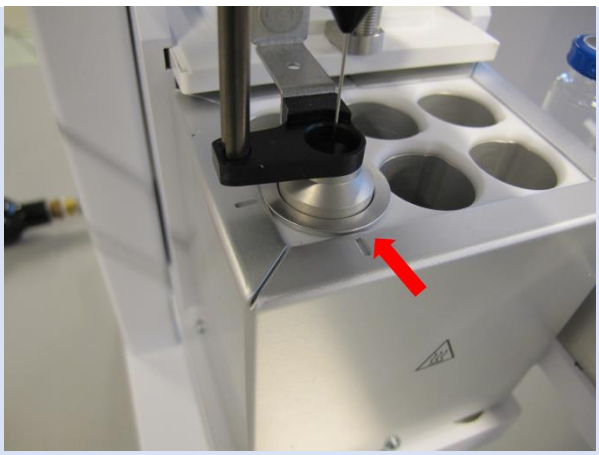
2



Check the position of the trayholder **(see chapter 8.6)**

OPTIONAL
Teach the position of the trayholder **(see chapter 8.7)**

3



Check the position of the agitator **(see chapter 8.4)**

OPTIONAL
Teach the position of the agitator **(see chapter 8.5)**

7.13 Prepare the device for operation

Before using the device for the first time or after being disconnected from the nitrogen source for some time it must be cleaned to ensure proper operating conditions. In this case start the **cleaning mode**.

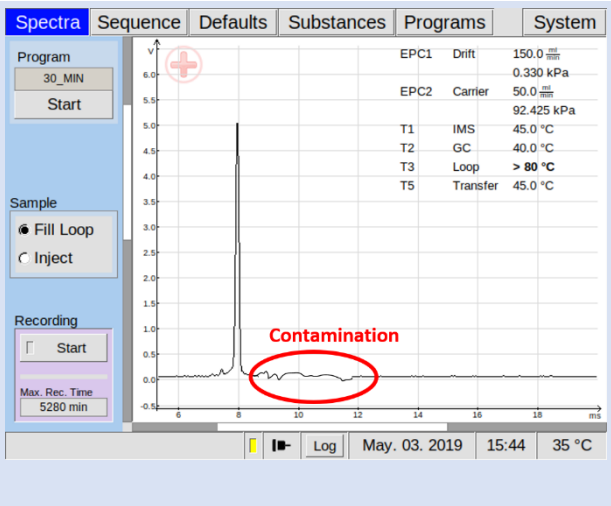
An appropriate cleaning period duration must be chosen depending on how long the device was switched off and on the extent of contamination. It is recommended to clean the device for at least **15 hours** before operating it for the first time. If the Spectrum is not clean repeat the process. A **reference spectrum** for the evaluation can be found in the supplied **Analytical Approval**.

INFORMATION!

After the cleaning process the device needs at least **2 hours** to cool down the internal components to their required temperatures.

The duration of the cool down process is depending on the temperature default settings.

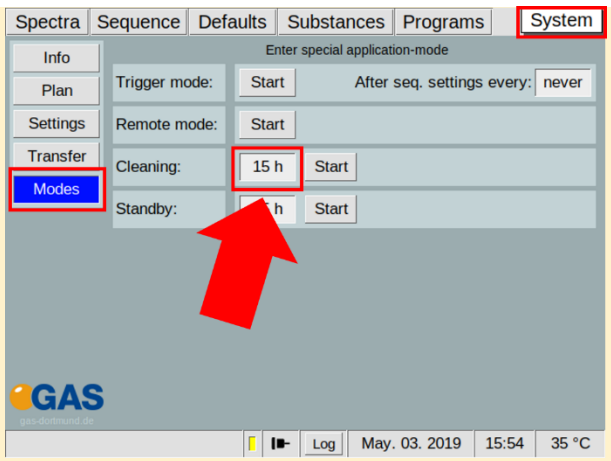
1



Inspect spectrum for contamination. Control the baseline. Start cleaning when contaminated. Contamination is indicated by peaks or the disappearing of the RIP.

2

Option

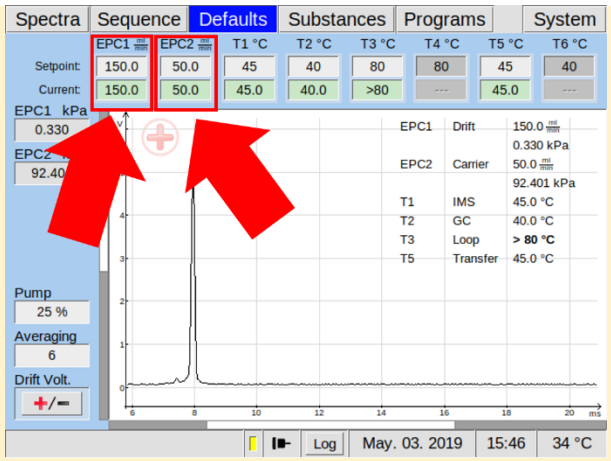


Select duration in hours:

System › **Modes** › **Cleaning Mode** › **x h**

3

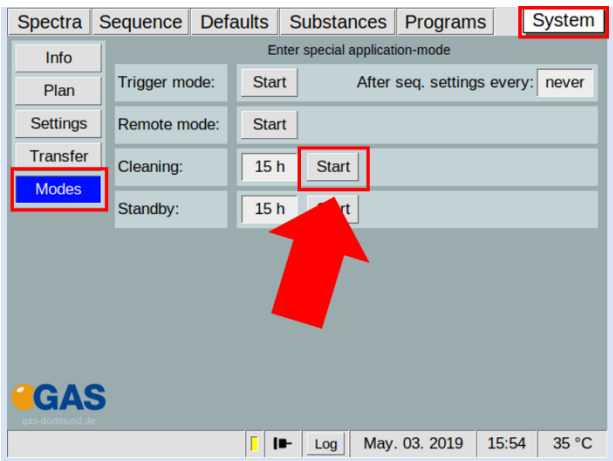
Option



To speed up this process, increase flow rate of EPC1 and EPC2 to their maximum values (e.g 500/150 ml/min):

Defaults › **EPC1** › **EPC2**

4

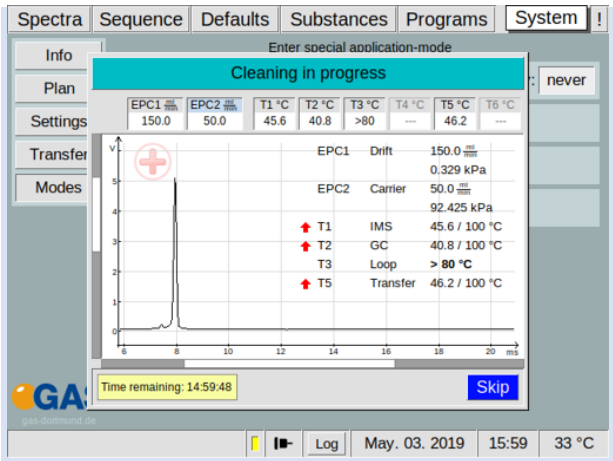


Start cleaning:

System › **Modes** ›

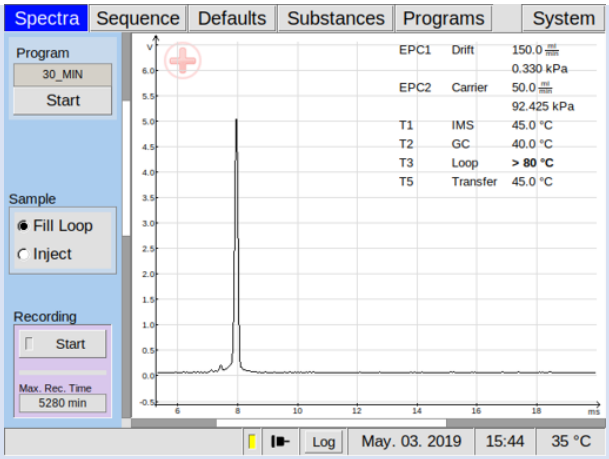
Cleaning Mode › **Start**

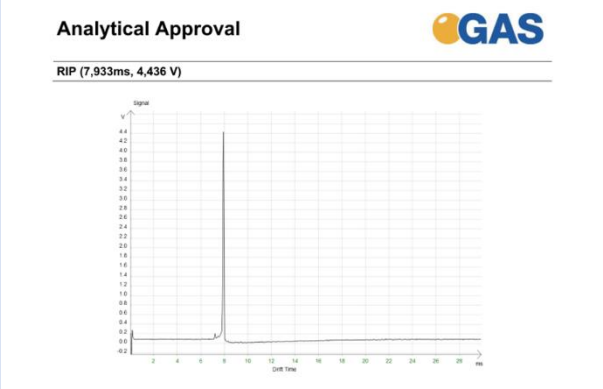
5



Wait until cleaning process is completed. The process can be stopped with **Skip**.

6





After all temperatures reached the default values inspect visually the current spectrum and compare it with the reference spectrum of the analytical approval. **The RIP should reach ~80% of the RIP height displayed in the delivered Analytical Approval of the device under same measurement conditions of G.A.S. The assessment of the readiness to measure is additionally supported by the system.**

If not check the gas quality and/or install additional purification cartridges and start the cleaning procedure again.

INFORMATION!

The device is delivered with an acceptance snapshot. This snapshot defines the system performance during device acceptance and is used to assess the readiness for measurement. Any deviations from this are displayed in the Error Information Window. **The default values can be adjusted by the customer**.

8 System Operation

8.1 Measurement Requirements

INFORMATION!

Only use the original accessories supplied with the device.

INFORMATION!

Make sure that the gas quality is 5.0 (99,999%) or better.

INFORMATION!

Only use stainless steel pressure reducer.

INFORMATION!

Make sure that the spectrum is clean a without contamination.

WARNING!

Do not introduce any liquids. This can destroy the device.

INFORMATION!

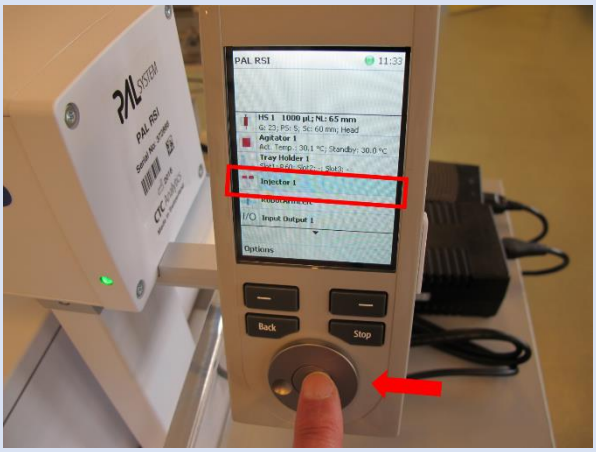
Make sure that that all temperature-, flow- and pressure values have reached their default value and are stabilized.

8.2 Workflow: Check Injector Position

INFORMATION!

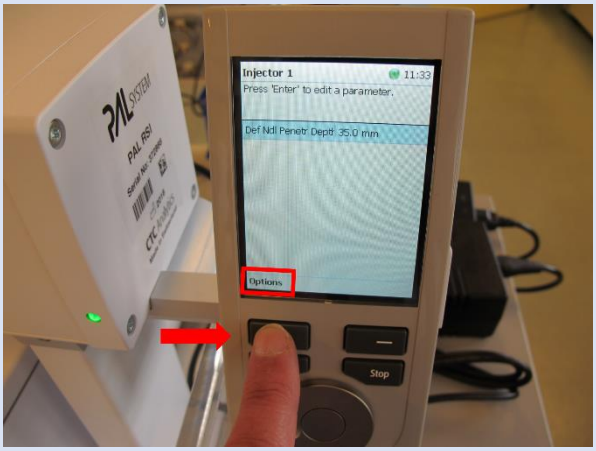
It is recommended to check the position of the injector after every transport of the device. A false position can damage the syringe. When using the Headspace-Tool it is recommended to use the Injector Adapter.

1

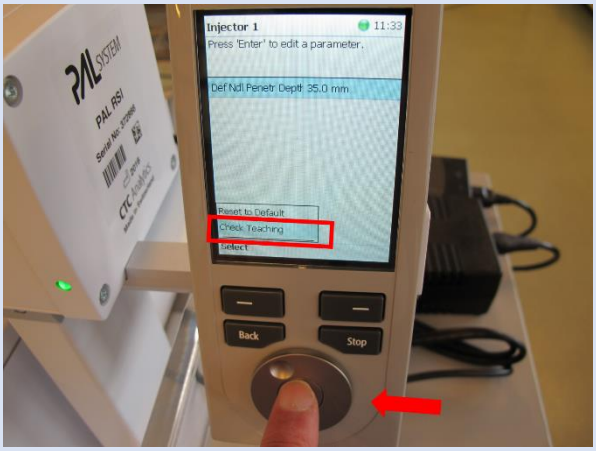
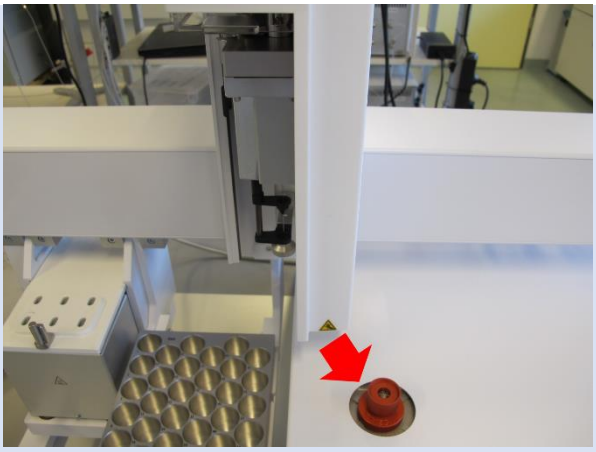


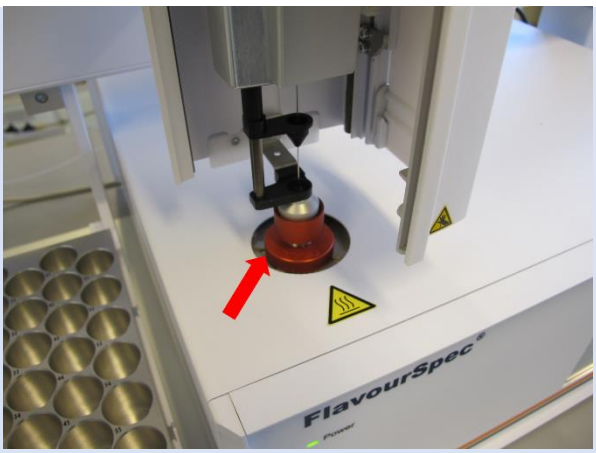
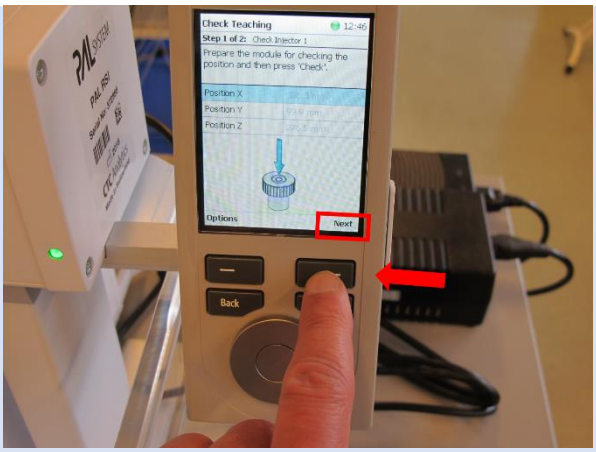
On the PAL RSI main screen select **Injector 1**.

2



With the **left function key** select **Options**.

3		In **options menu** select **Check Teaching**.
4		With the **right function key** select **Check**.
5		After a **warning signal** the **arm moves** to actual injector position.

6		The magnetic adapter of the tool and the injector adapter has to fit. Otherwise the injector position must be teached **(see chapter 8.3)**.
7		With the **right function key** select **Next**.
8		With the **right function key** select **OK**.

9

Select the **BACK-button** to go to the **main screen**.

8.3 Workflow: Teach Injector Position

INFORMATION!

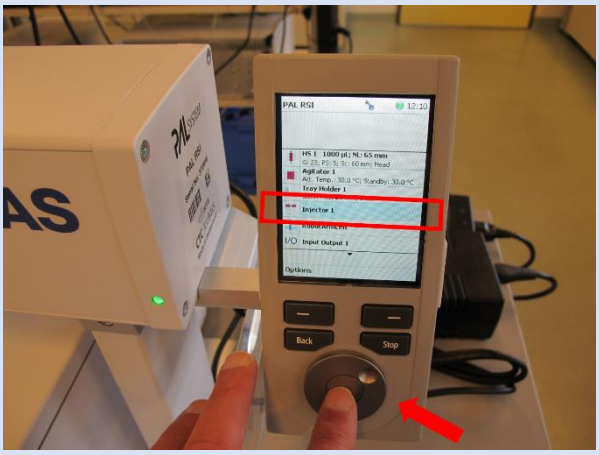
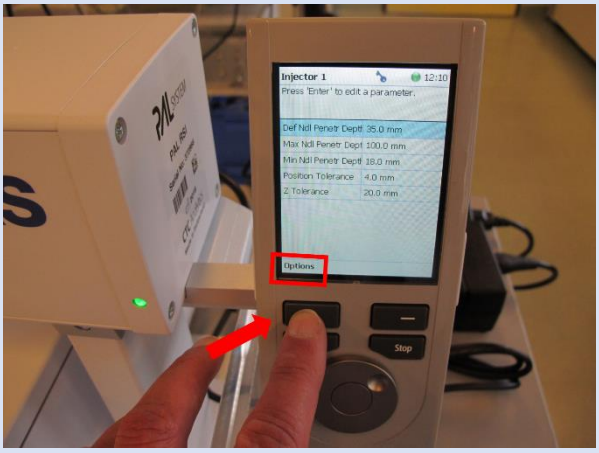
The teaching procedure is only available in **Extended User Level**.
When using the Headspace-Tool it is recommended to use the Injector Adapter. The Injection Penetration Depth Value must be 35 mm. Do not modify.
When using the ITEX-Tool (optional) the Injector Adapter needs to be removed. The Injection Penetration Depth Value must be 35 mm. Do not modify.
Teach the Injector Position after every tool change.

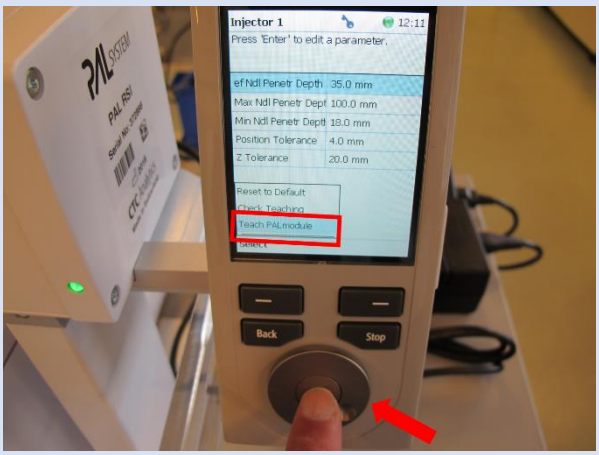
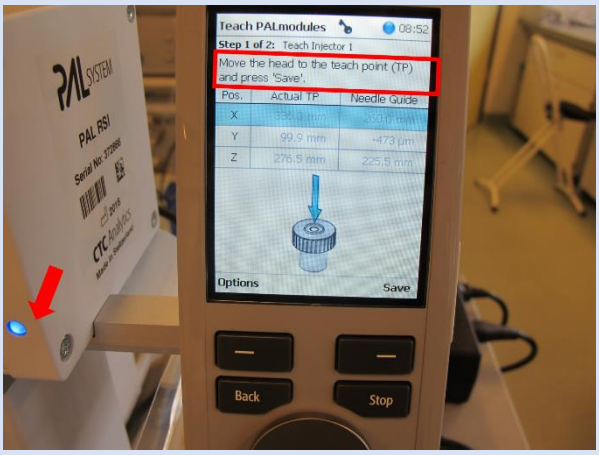
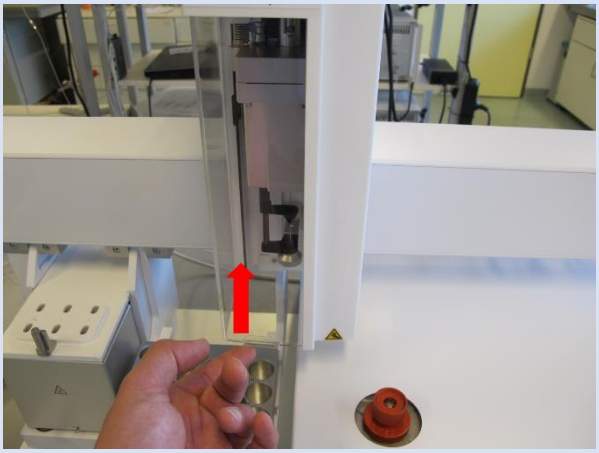
WARNING!

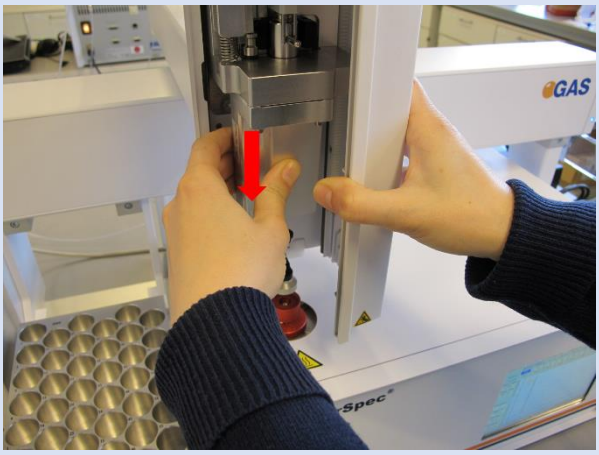
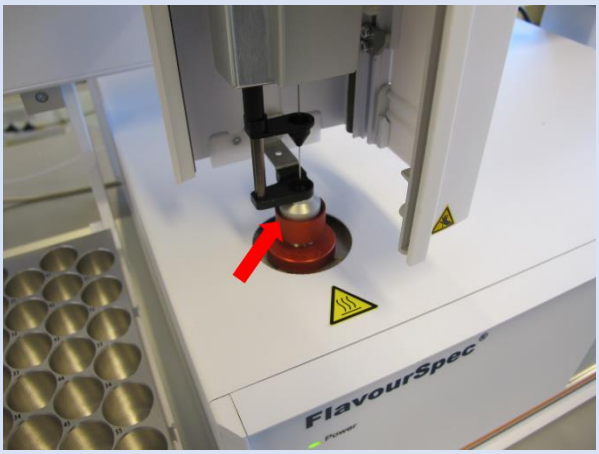
The Injector can become very hot. Risk of burning. Use heat-resistant gloves.

1

Press **both function keys** simultaneously to got to the **Change Access screen**

2		Select **Extended User Level**. Select **Back** to go to the main screen.
3		In **main screen** select **Injector1**.
4		With the **left function key** select **Options**.

5		In **options menu** select **Teach PALmodule**.
6		When the status light turns to blue, follow the instructions on the screen: *Move the head to the teach point.*
7		Move the protective cover to its top position.

8		Move the arm to the injector position, …
9		…move the tool down to the injector position…
10		…and position the magnetic ring into the injector adapter.

11		With the **right function key** select **Save**.
12		**OPTIONAL:** To manually adjust the position select the X-, Y- or Z-axis.
13		The values can be adjust in 0,1 mm steps.

14		Confirm the value by pressing the rotary button.
15		With the **right function key** select **Next**.
16		With the **right function key** select **OK**.

17

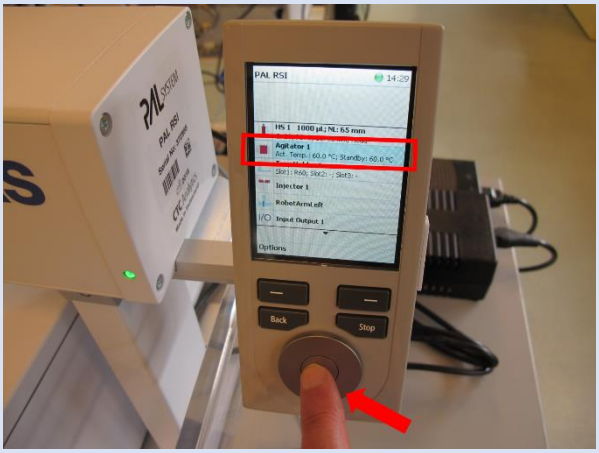
Select the **BACK-button** to go to the **main screen**.

8.4 Workflow: Check Agitator Position

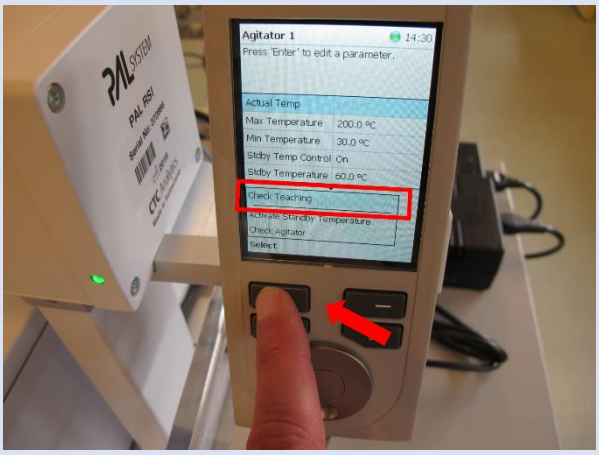
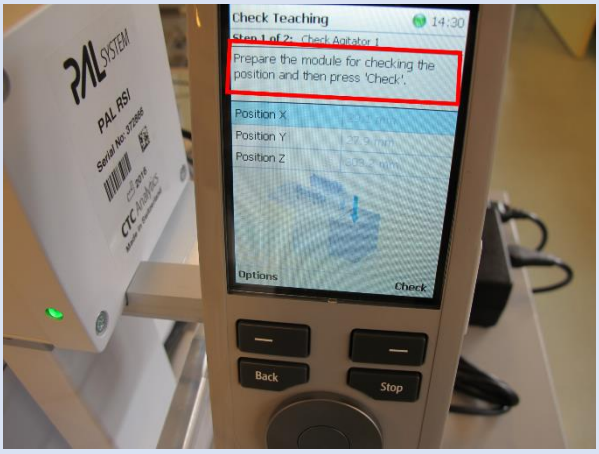
INFORMATION!

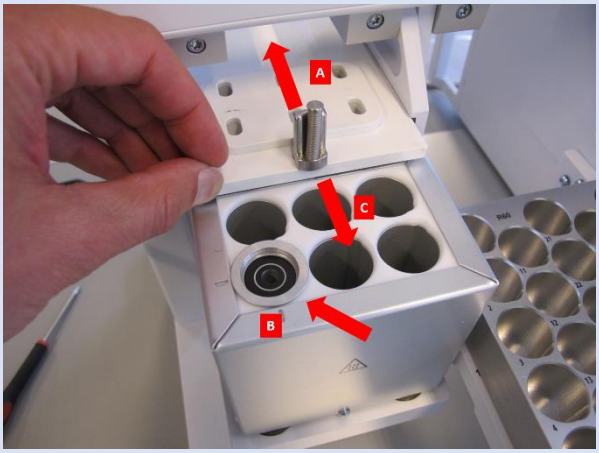
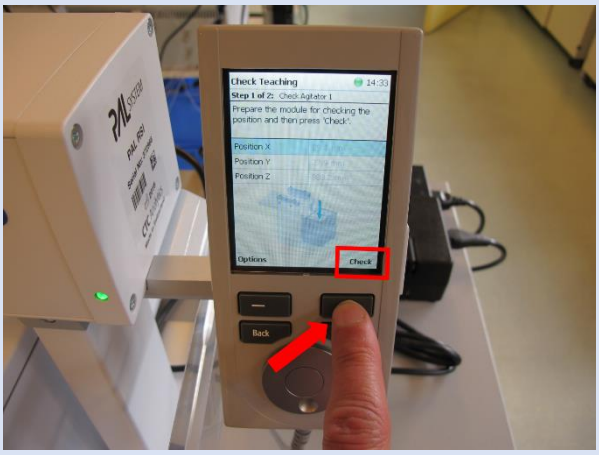
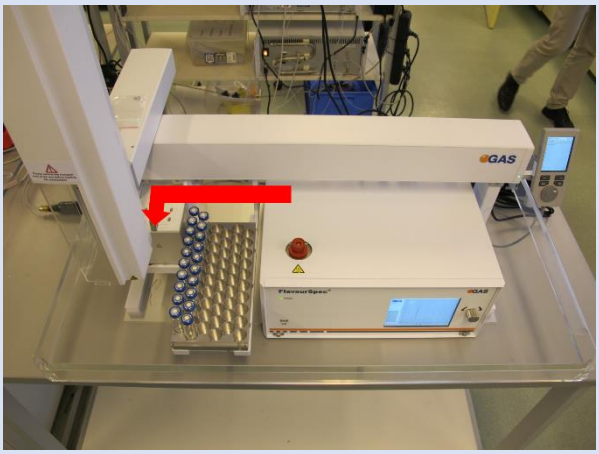
It is recommended to check the position of the agitator after every transport of the device.

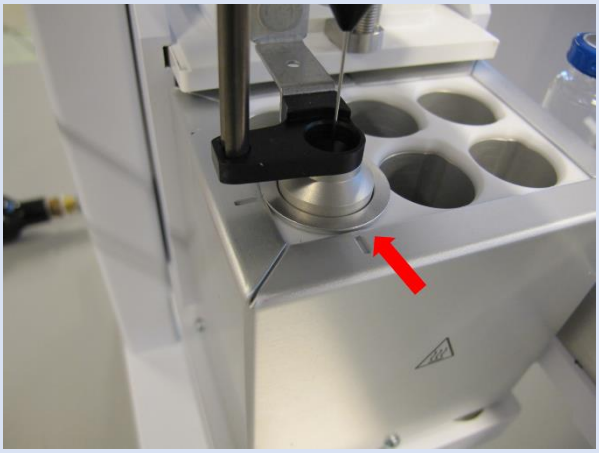
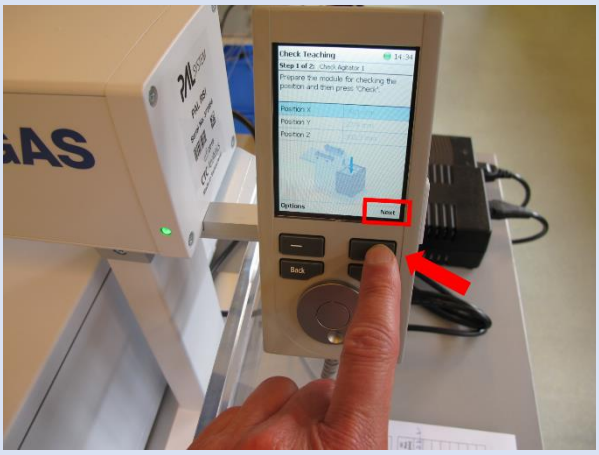
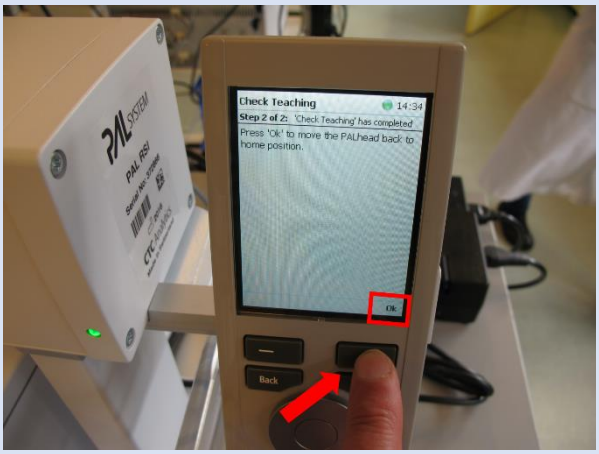
1



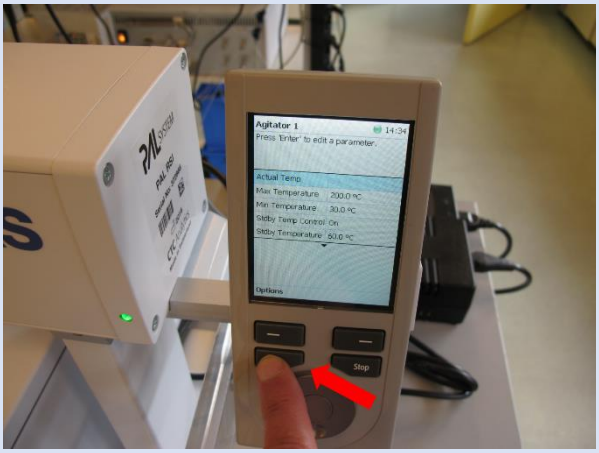
On the **PAL RSI main screen** select **Agitator 1.**

2		With the **left function key** select **Options**.
3		In **option menu** select **Check Teaching**
4		Follow the instruction on the screen: *Prepare the module…*

5		Move the cover back A, insert the teaching tool in position 1 B and close the cover. C.
6		With the **right function key** select **Check**.
7		After a **warning signal** the **arm moves** to the actual agitator position.

8		The magnetic adapter of the tool and the teaching tool has to fit. Otherwise the agitator position must be teached. **(see chapter 8.5)**
9		With the **right function key** select **Next**.
10		With the **right function key** select **OK**.

11



Select the **Back button** to go to the **main screen**.

8.5 Workflow: Teach Agitator Position

INFORMATION!

The teaching procedure is only available in **Extended User Level**.

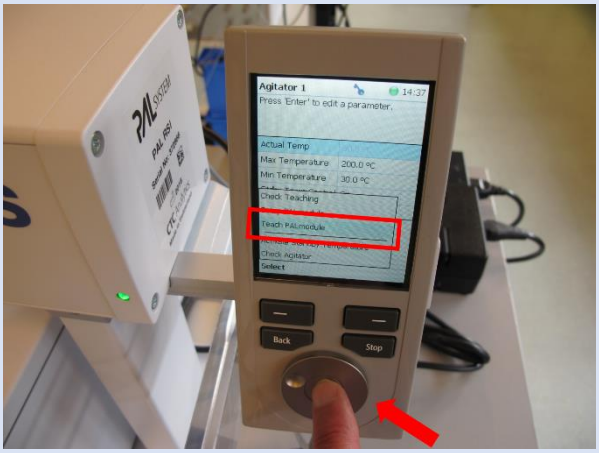
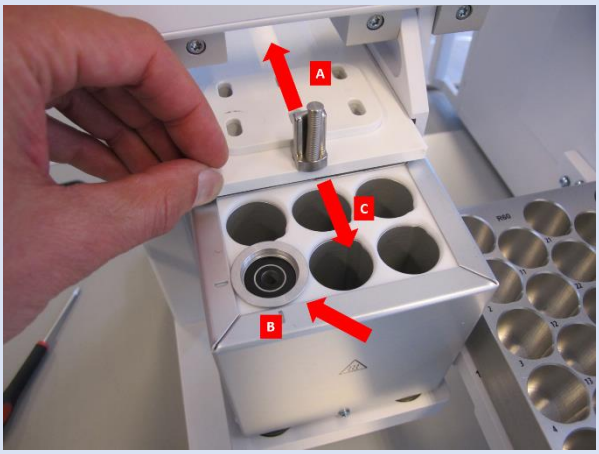
WARNING!

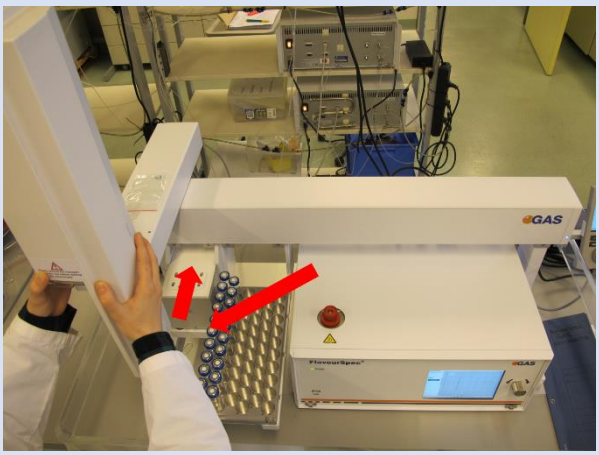
The Agitator can become very hot. Risk of burning. Use heat-resistant gloves.

1

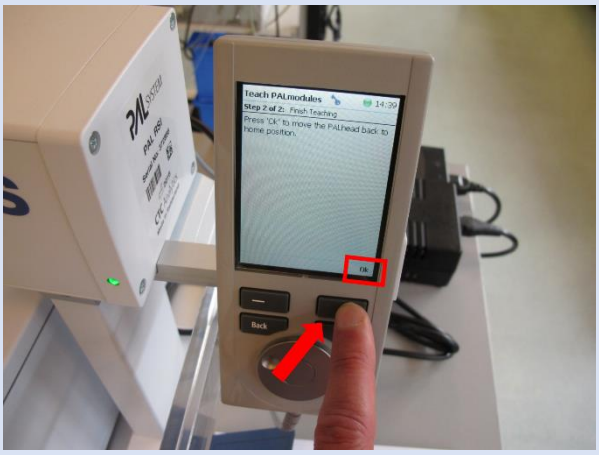
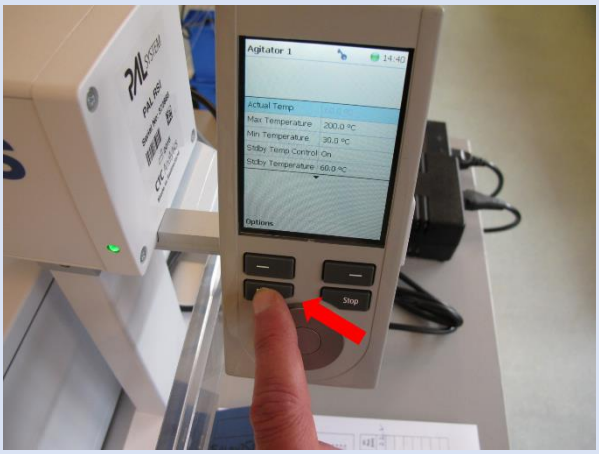
Press **both function keys** simultaneously to got to the **Change Access screen**

2		Select **Extended User Level**. Select **Back** to go to the main screen.
3		In **main screen** select **Agitator 1**.
4		With the **left function key** select **Options**.

5		In **options menu** select **Teach PALmodule**.
6		If the status light has change to blue follow the instructions on the screen: *Move the head to the teach point*
7		Move the cover back A, insert the teaching tool in position 1 B and close the cover. C.

8		Move the arm to the Agitator, …
9		…move the tool down to the agitator position, and position the magnetic ring into the teaching tool.
10		With the **right function key** select **Save**.

11		**OPTIONAL:** To manually adjust the position select the X-, Y- or Z-axis.
12		The values can be adjust in 0,1 mm steps.
13		Confirm the value by **pressing the rotary button**.

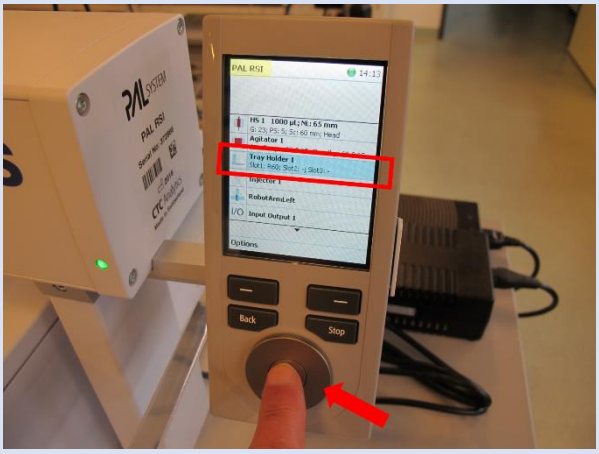
14		With the **right function key** select **Next**.
15		With the **right function key** select **OK**.
16		Select the **BACK-button** to go to the **main screen**.

8.6 Workflow: Check Tray Reference Position

INFORMATION!

It is recommended to check the position of the agitator after every transport of the device. A false position can damage the syringe.

1

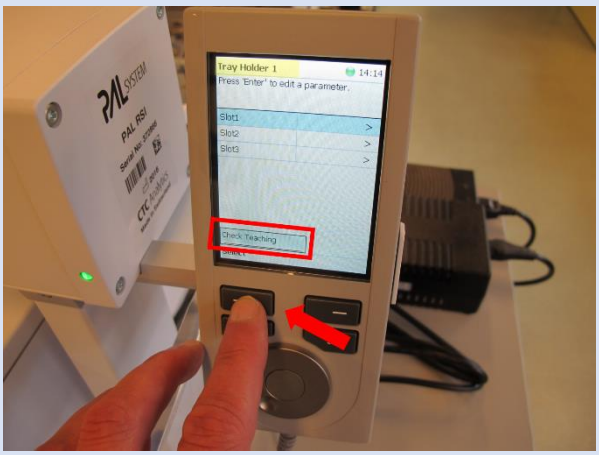


On the PAL RSI main screen select **TrayHolder 1**.

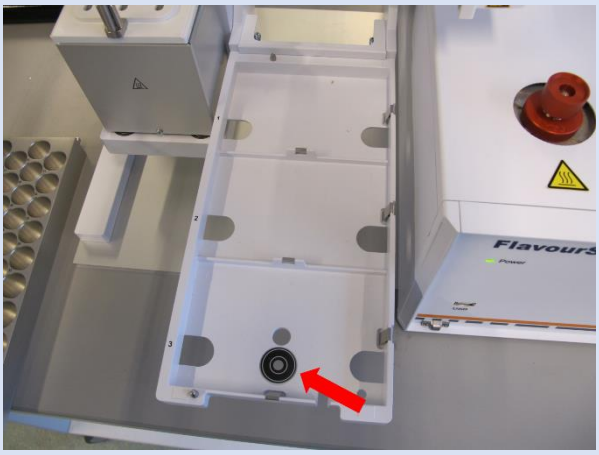
2

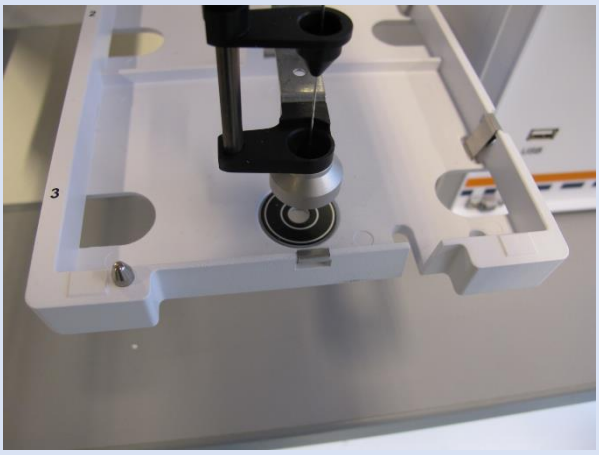
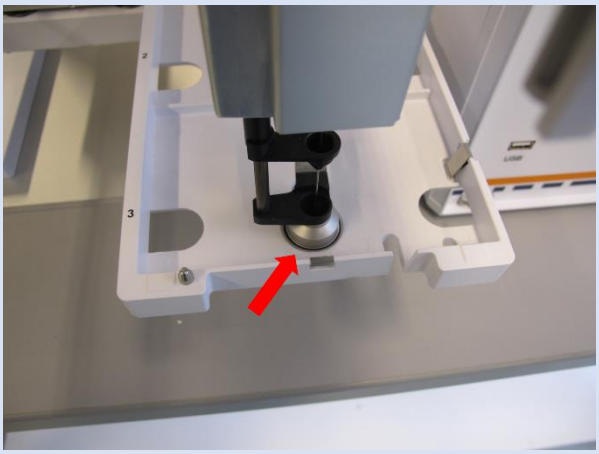
With the **left function key** select **Options**.

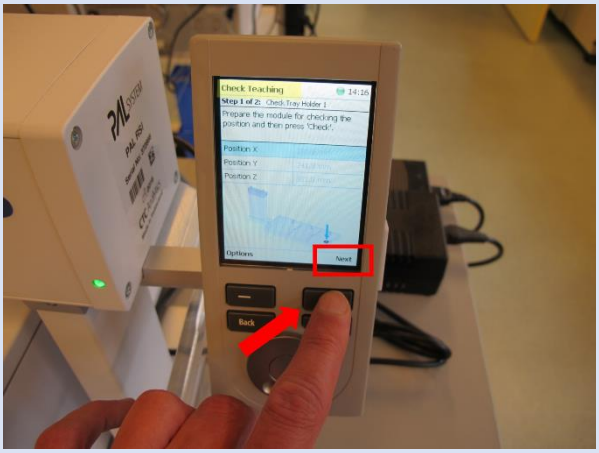
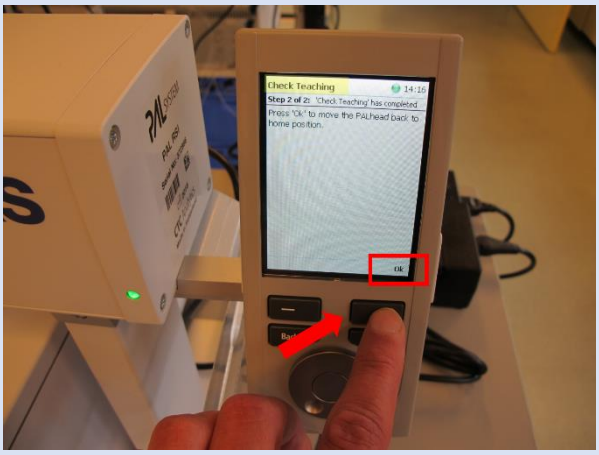
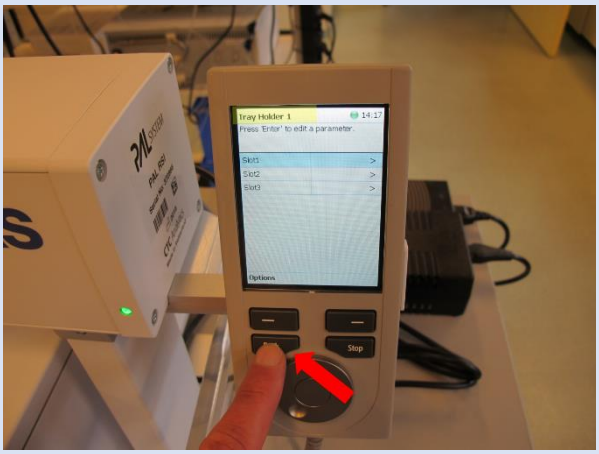
3



In **options menu** select **Check Teaching**.

4		Follow the instruction on the screen: *Prepare the module…*
5		Remove the tray.
6		The figure shows the teaching point of the tray holder.

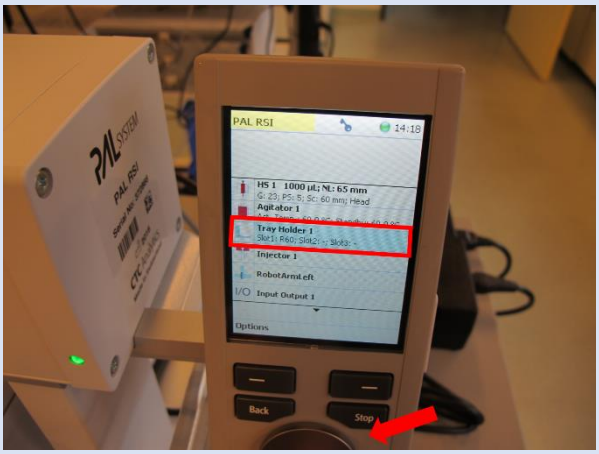
7		With the **right function key** select **Check**.
8	 	After a **warning signal** the **arm moves** to the actual teaching point. The magnetic adapter of the tool and the teaching point has to fit. Otherwise the tray reference position must be teached. **(see chapter 8.7)**.

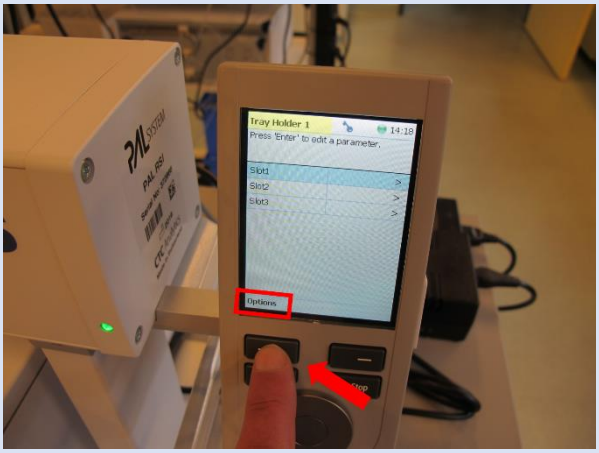
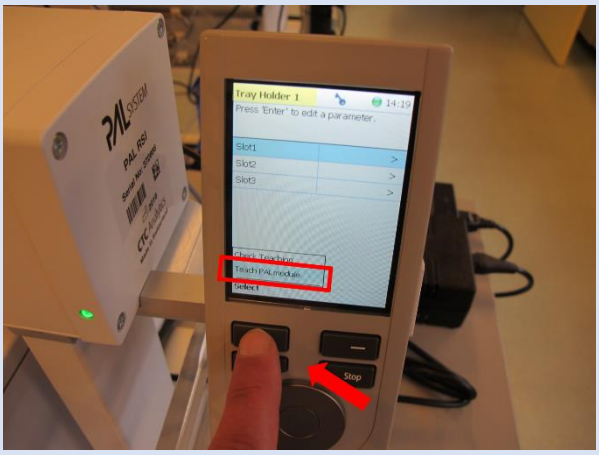
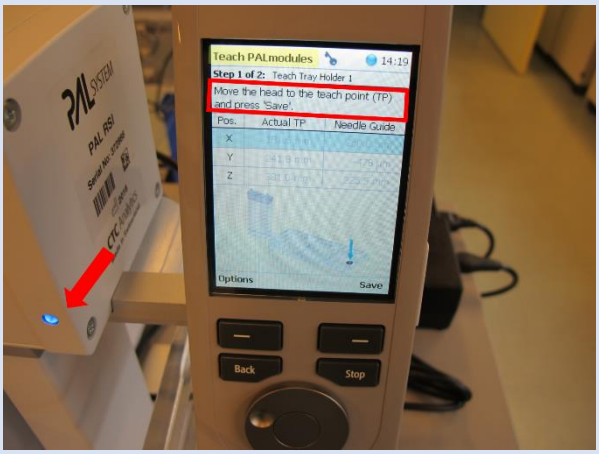
9		With the **right function key** select **Next**.
10		With the **right function key** select **OK**.
11		Select the **Back button** to go to the **main screen**.

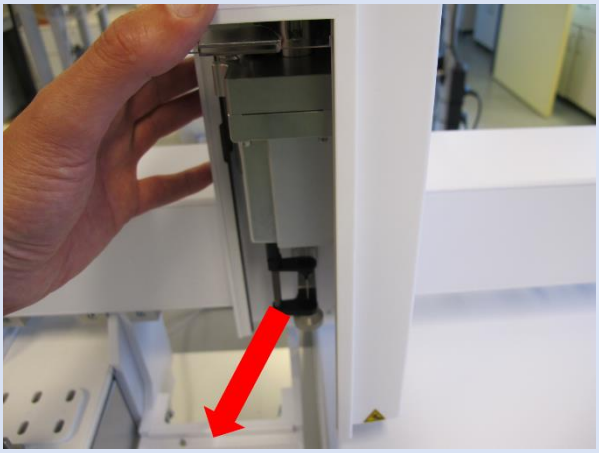
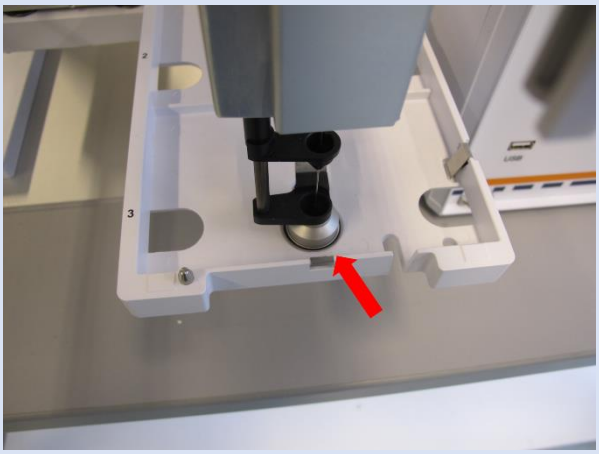
8.7 Workflow: Teach Tray Reference Position

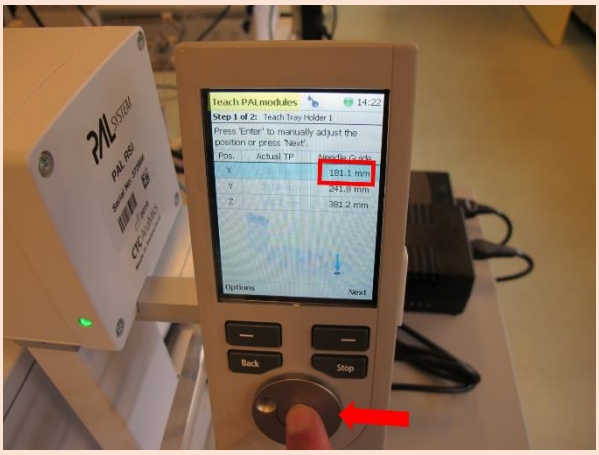
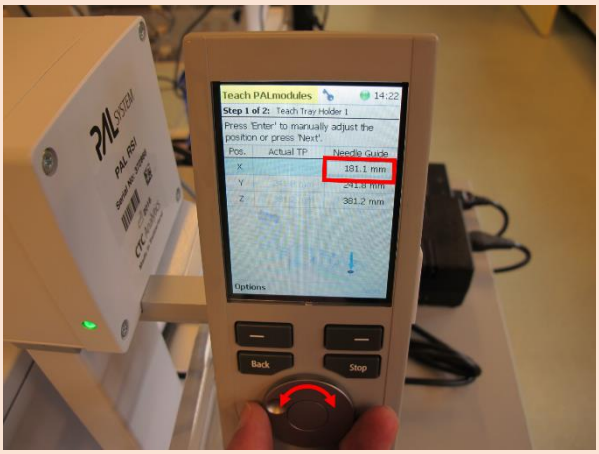
INFORMATION!

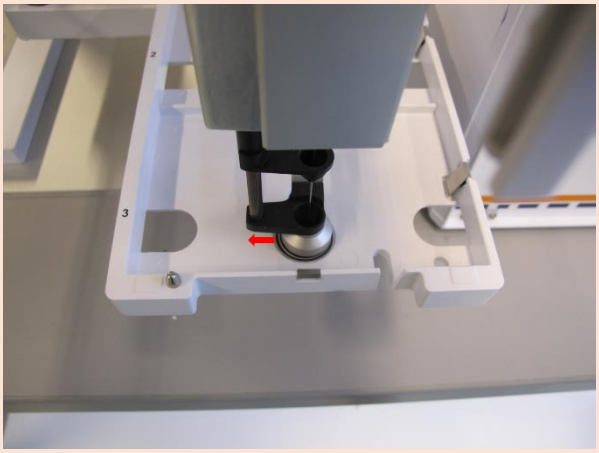
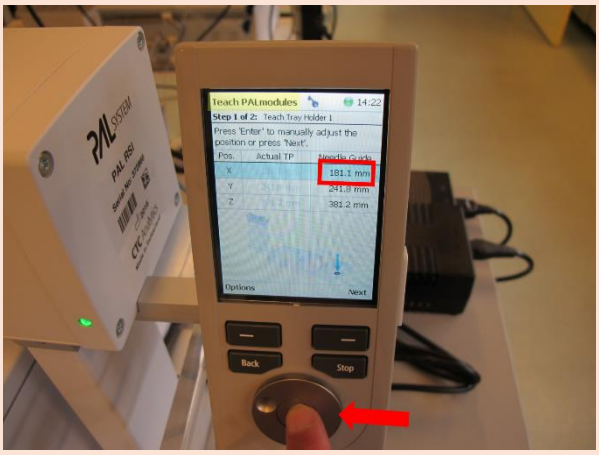
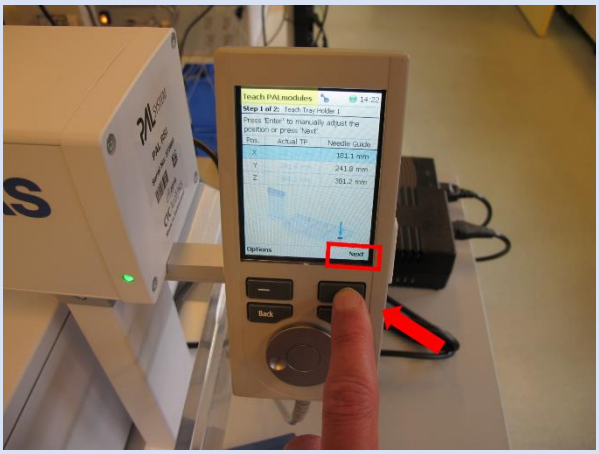
The teaching procedure is only available in **Extended User Level**.

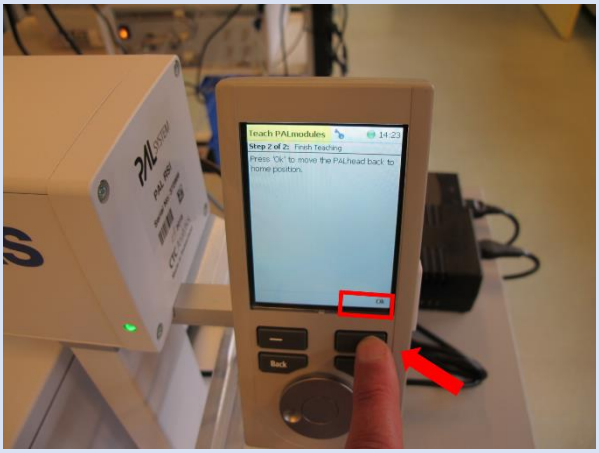
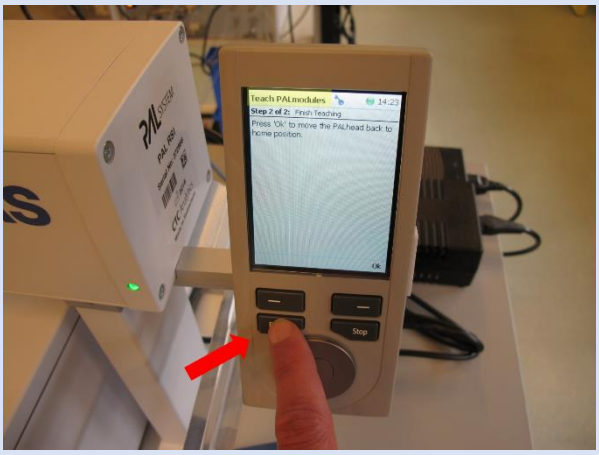
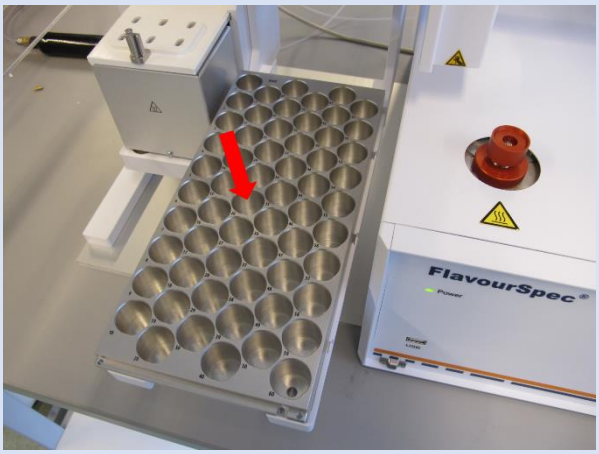
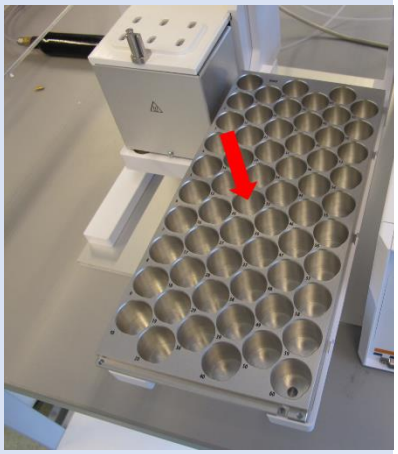
1		Press **both function keys** simultaneously to got to the **Change Access screen**
2		Select **Extended User Level**. Select **Back** to go to the main screen.
3		In **main screen** select **Tray Holder 1**

4		With the **left function key** select **Options**.
5		In **options menu** select **Teach PALmodule**.
6		If the status light has change to blue follow the instructions on the screen: *Move the head to the teach point*.

7		Move the arm to the tray holder position, ...
8		move the tool down to the teaching point …
9		and position the magnetic ring onto teaching point.

10		With the **right function key** select **Save**.
11		**OPTIONAL:** To manually adjust the position select the X-, Y- or Z-axis.
12		The values can be adjust in 0,1 mm steps.

13		The figure shows the x-axis adjustment.
14		Confirm the value by **pressing the rotary button**.
15		With the **right function key** select **Next**.

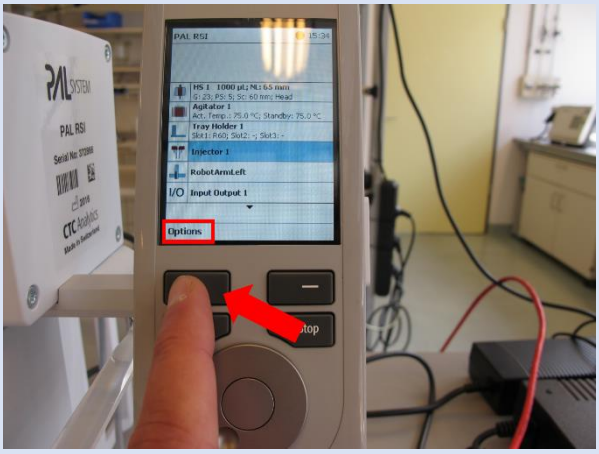
16		With the **right function key** select **OK**.
17		Select the **BACK-button** to go to the **main screen**.
18		

8.8 Workflow: Create a New Job

INFORMATION!

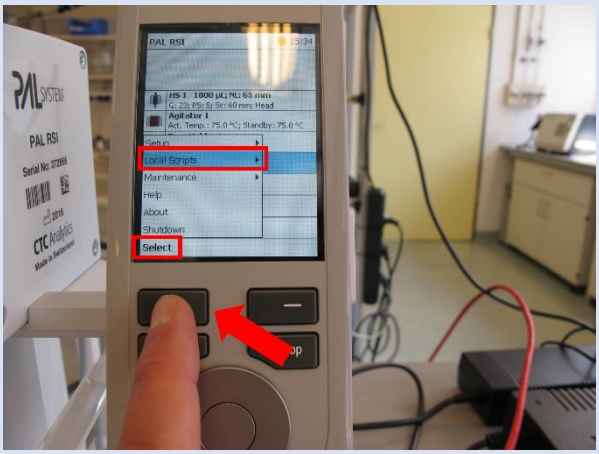
A job contains the amount the position of the sample vials in the tray and the sample volume that will be injected. A Job is always connected to a method **(see chapter 8.12 and chapter 8.13)**

1



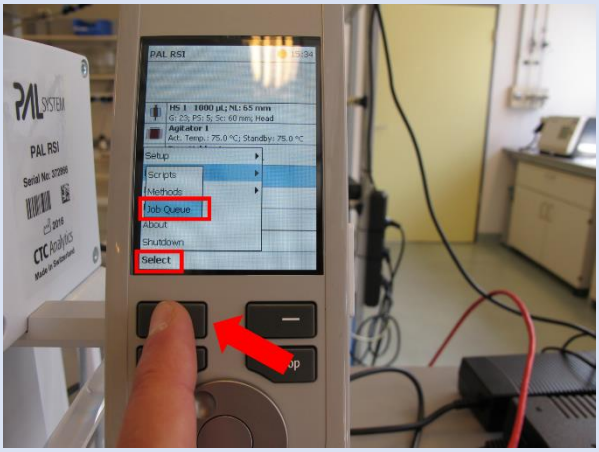
With the **left function key** select **Options**.

2

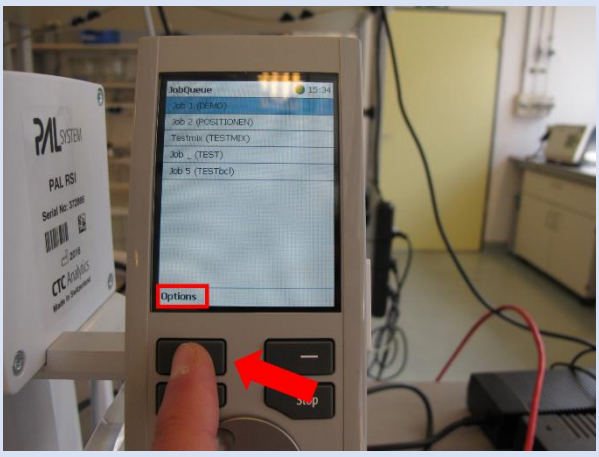
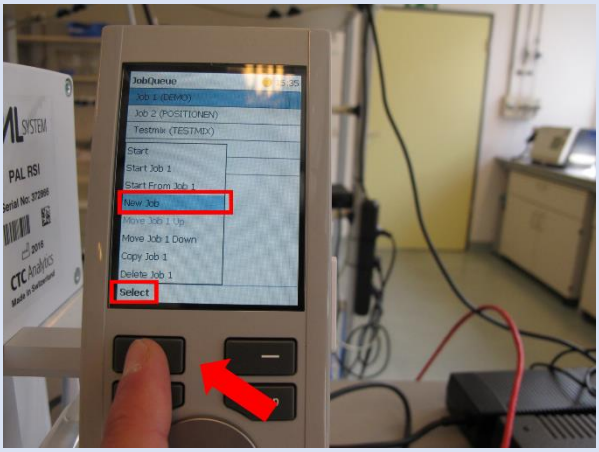
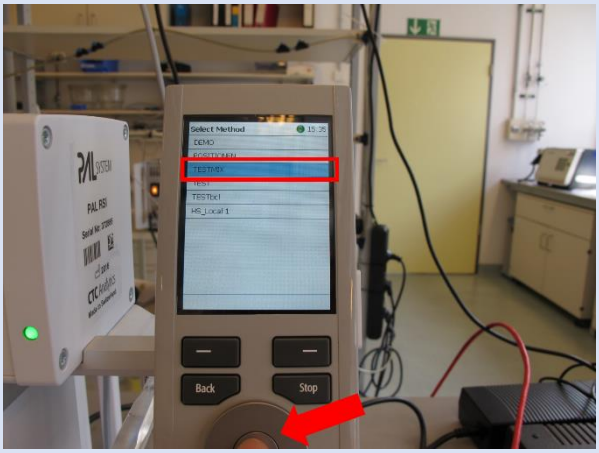


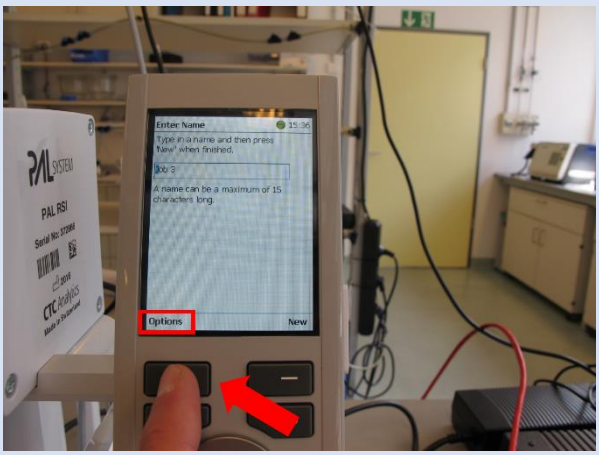
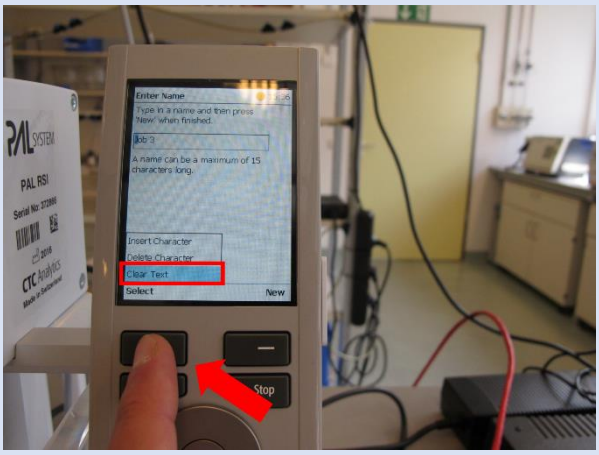
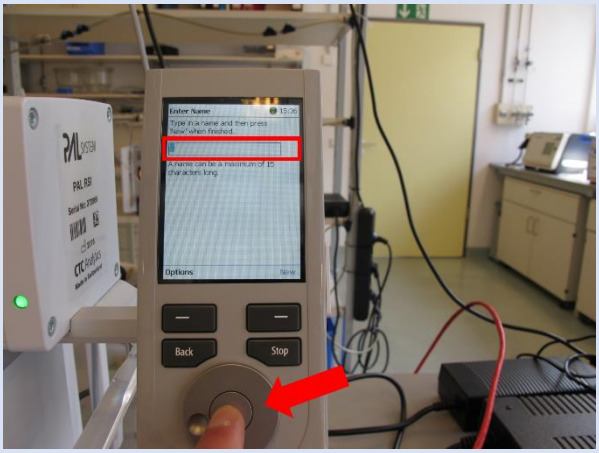
In **options menu** select **Local Scripts**.
With the **left function key** select **Select**.

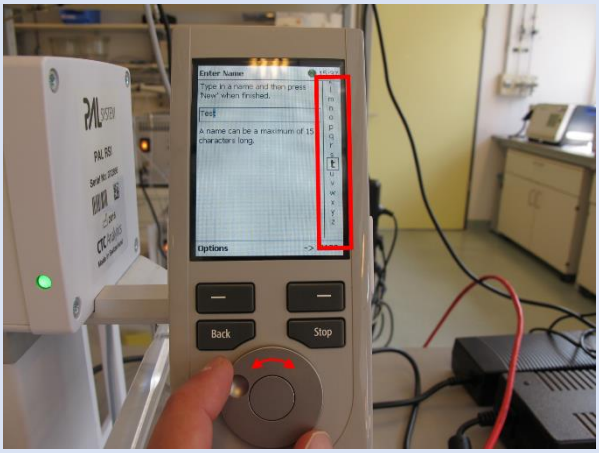
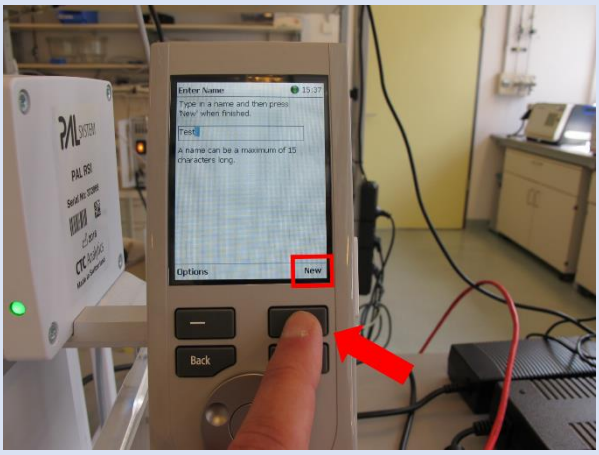
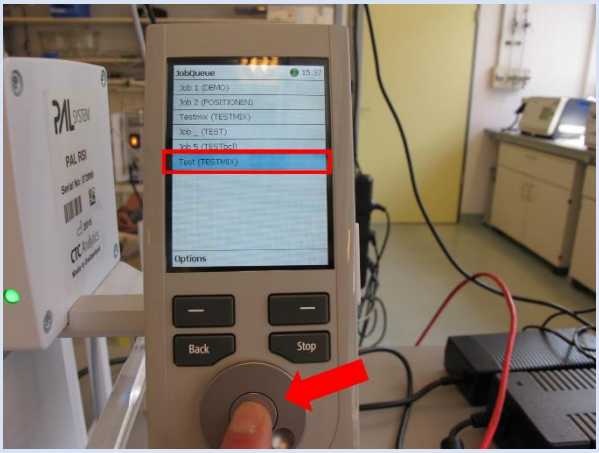
3

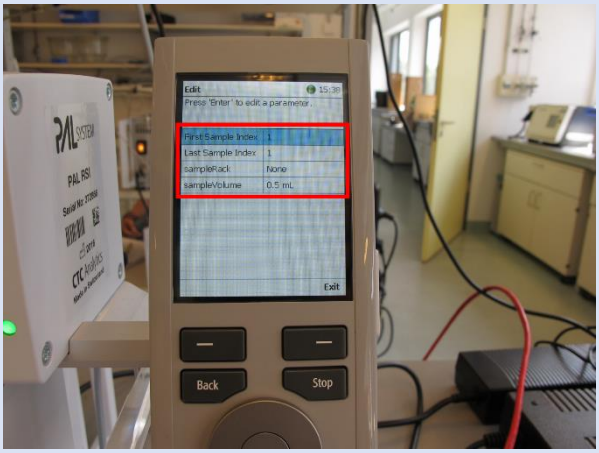
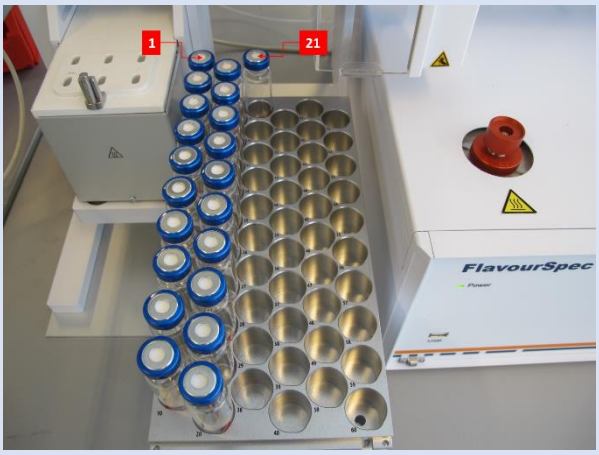
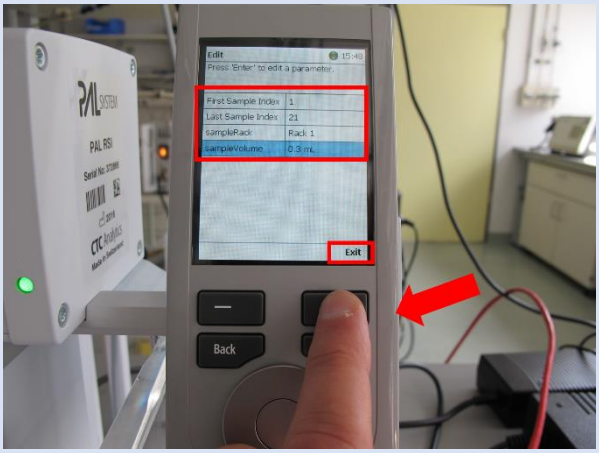


In **options menu** select **Job Queue**.
With the **left function key** select **Select**.

4		With the **left function key** select **Options**.
5		In **options menu** select **New Job**. With the **left function key** select **Select**.
6		Move to the **method** and select it by **pressing the rotary knob**.

7		With the **left function key** select **Options**.
8		In **options menu** select **Clear Text**. With the **left function key** select **Select**
9		Press the **Edit button** to edit the name.

10		Select **letters and numbers** with the **rotary knob**.
11		With the **right function key** select **New** to accept the new name and leave the screen.
12		Select the new job an press **Edit** to edit the job.

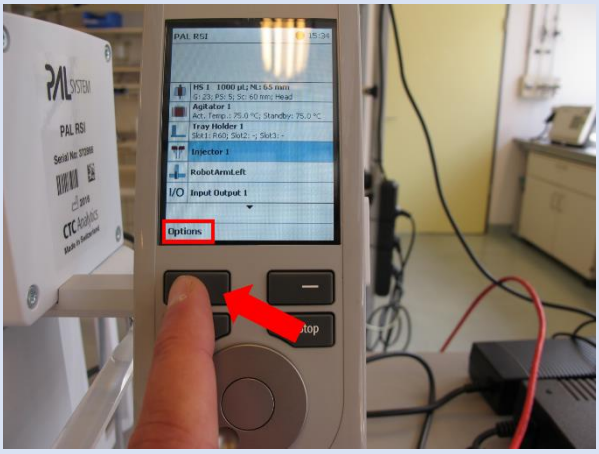
13		In job screen several parameters can be edit **(see chapter 9.12)**
14		**Example:** Sample 1 to 21should be measured. The position of the sample vials are 1 to 21 in the Tray. The Injection volume should be 300 µl.
15		The following values must be entered: First Sample Index: 1 Last Sample Index: 21 Sample Rack: Rack 1 Sample Volume: 0,3 ml

8.9 Workflow: Edit a Job

INFORMATION!

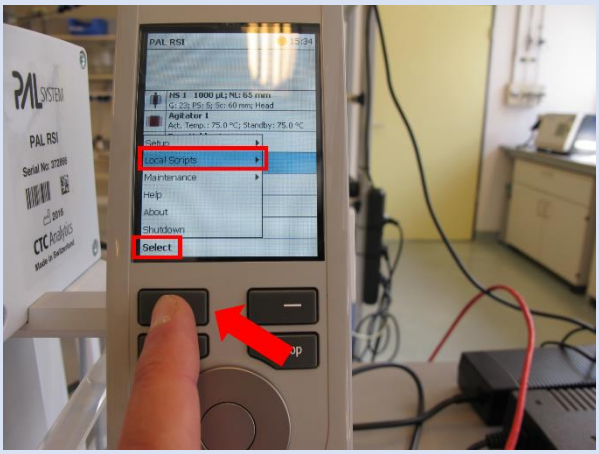
A job contains the amount the position of the sample vials in the tray and the sample volume that will be injected. A Job is always connected to a method **(see chapter 8.12 and chapter 8.13)**

1



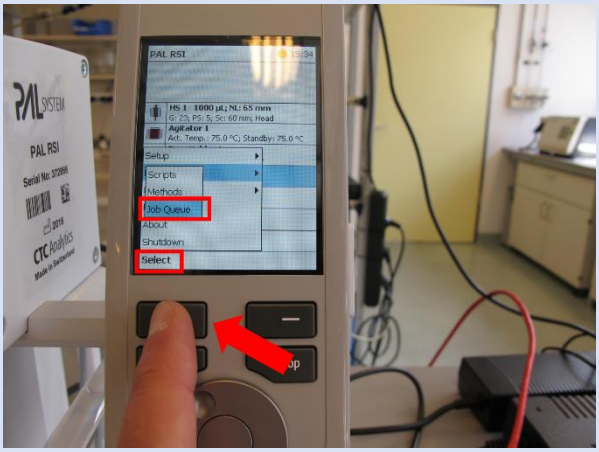
With the **left function key** select **Options**.

2

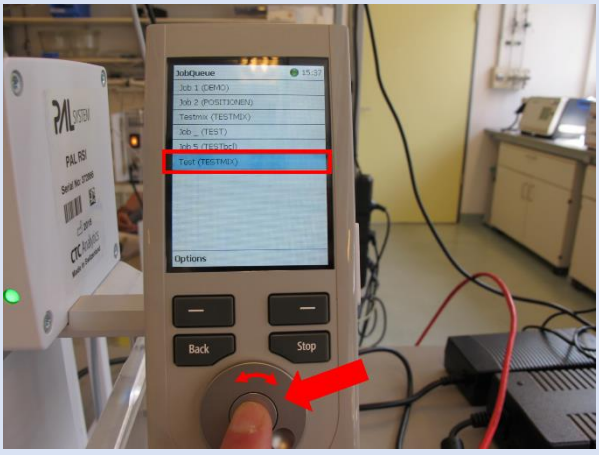
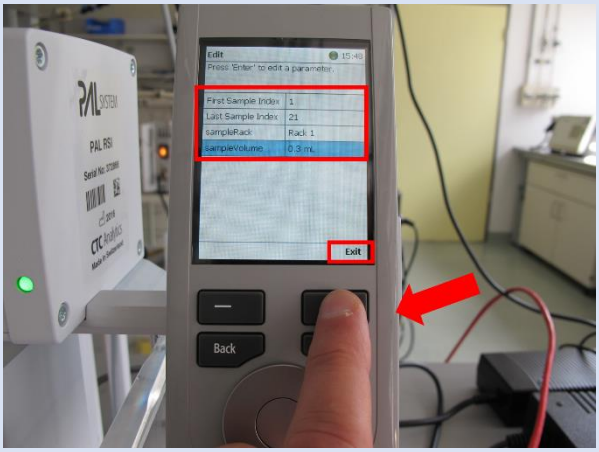
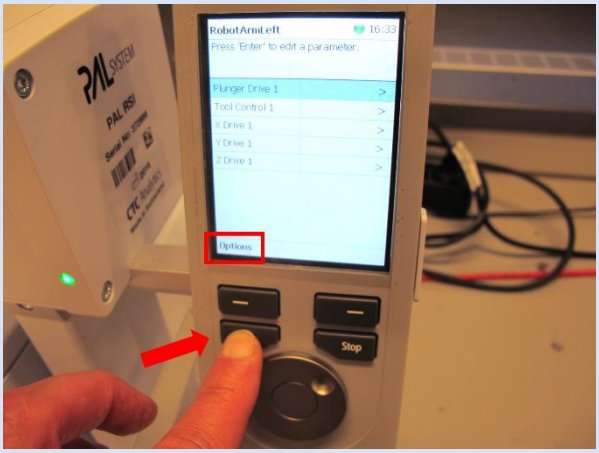


In **options menu** select **Local Scripts**.
With the **left function key** select **Select**.

3



In **options menu** select **Job Queue**.
With the **left function key** select **Select**.

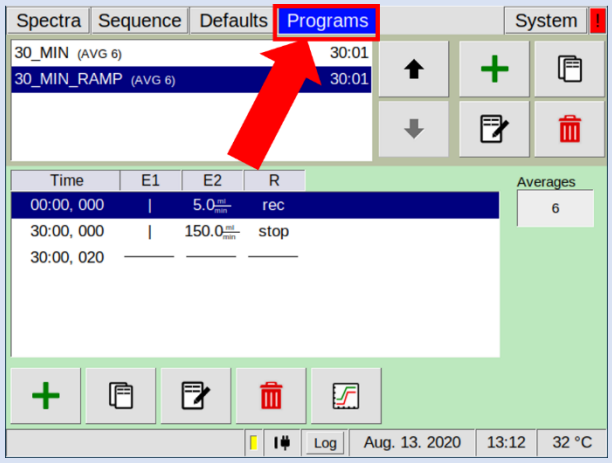
4		Move to the **job** and select it by **pressing the rotary knob**.
5		In **job screen** several parameters can be edit **(see chapter 9.12)**
6		Select the **BACK-button** to go to the **main screen**.

8.10 Workflow: Select Measurement Program

INFORMATION!

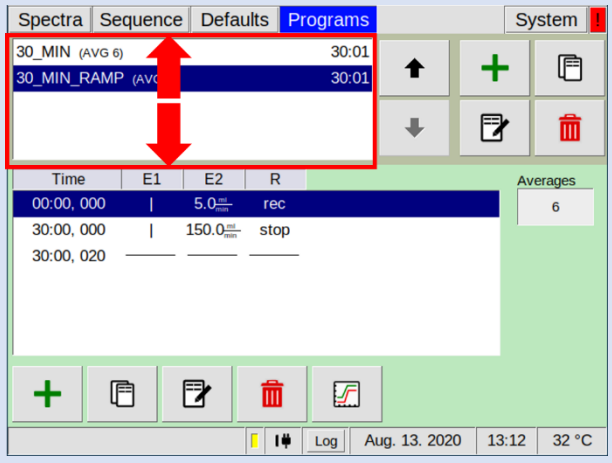
Selection and input of a measurement program is possible via graphical user interface of the FlavourSpec using the Touchscreen and/or rotary knob at the front of the device.

1



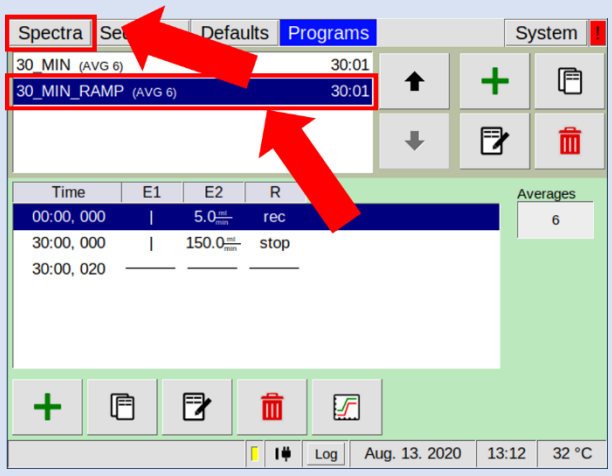
Select the **program window**

2



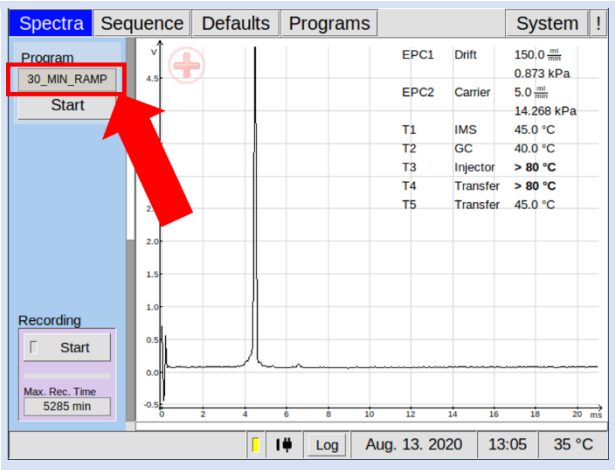
Scroll through the programs with the **rotary knob**.

3



Select a measurement program. Select Spectra to move to the Spectra window.

4



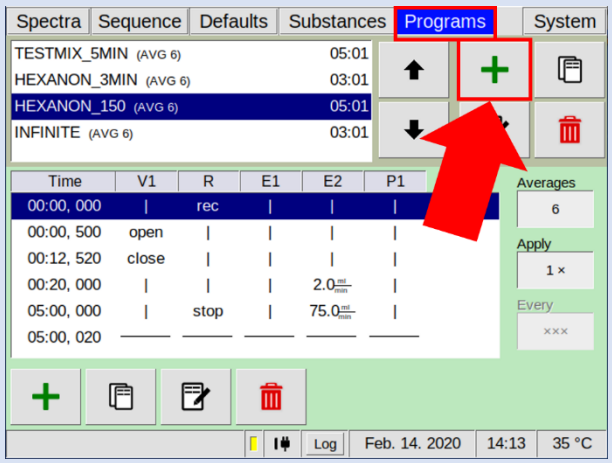
The **actual measurement program** is shown.

8.11 Workflow: Create a Measurement Program

INFORMATION!

Selection and input of a measurement program is possible via graphical user interface of the FlavourSpec using the Touchscreen and/or rotary knob at the front of the device.

1

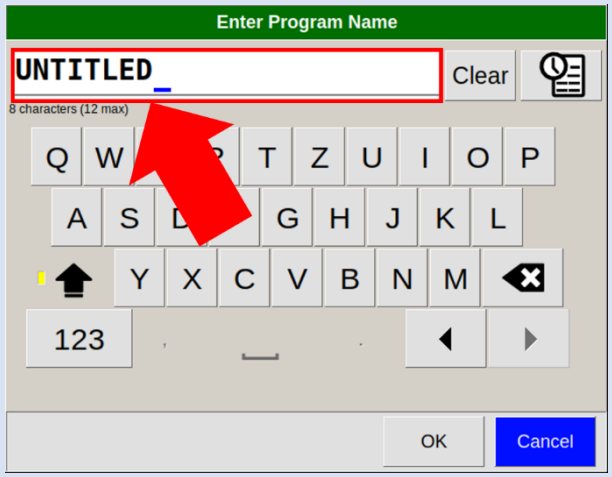


Select:

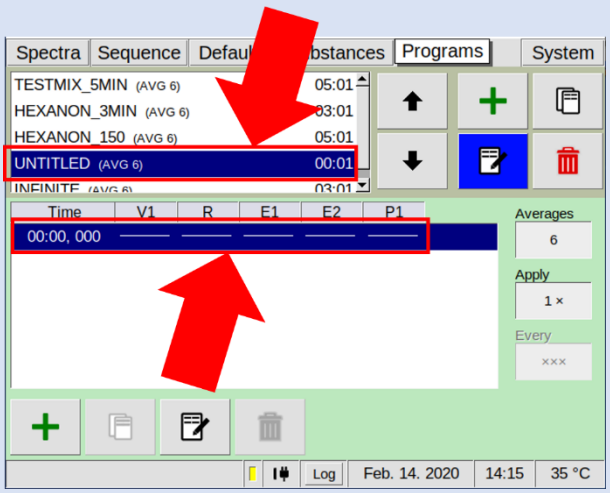
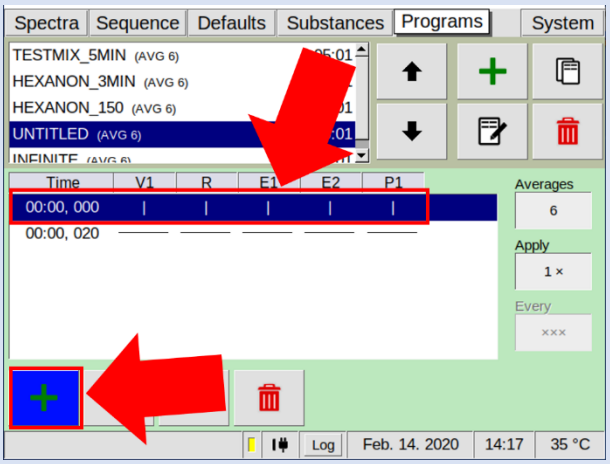
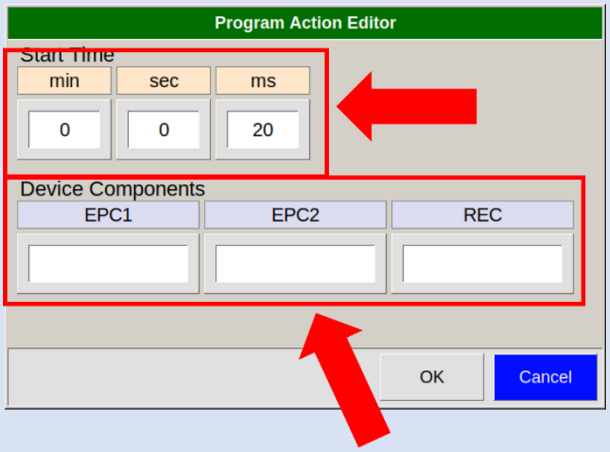
Programs

To create a new program select the Button +

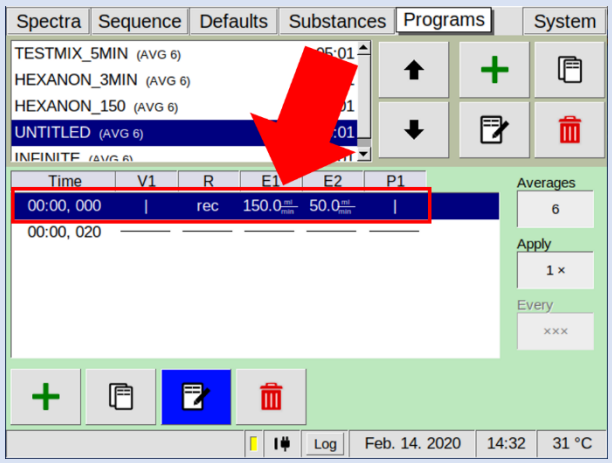
2



Enter a new program name or use the default name.

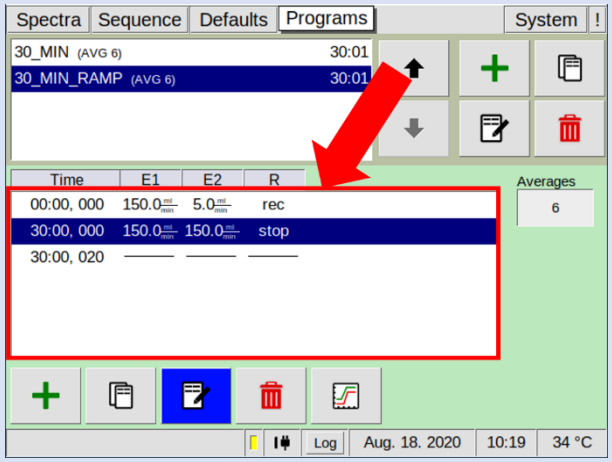
3		The program end time is displayed as the final line
4		To create a new program action line select the Button +
5		This line can be filled with values. For more information see also **Chapter 6.5.3 Edit Measurement Programs**

6



After the necessary values have been entered, repeat step 4 and 5 to create the next program action line.

7



A complete program sequence can be created line by line.

INFORMATION!

The device is delivered with standard programs that can be adapted to your needs.

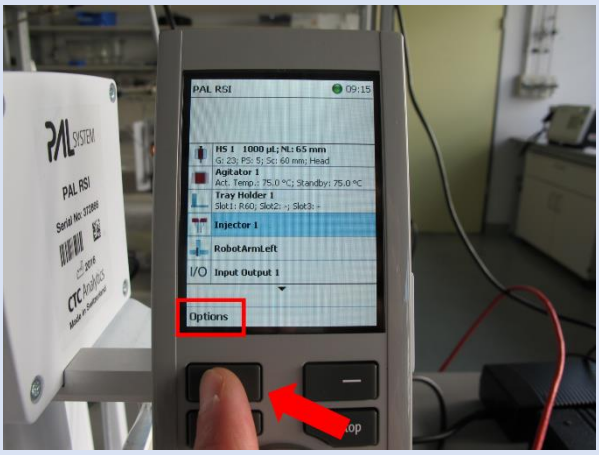
Customer-specific programs can also be created optionally.

8.12 Workflow: Create a New Method

INFORMATION!

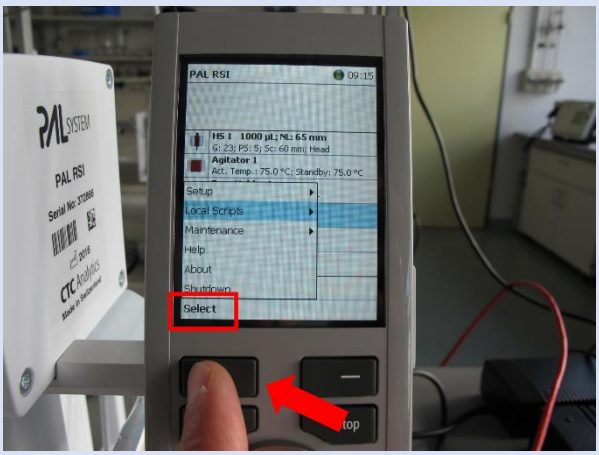
A method contains Incubation time and -temperature, the analyte time … **(see chapter 9.10 and 9.11)**. A method is required for a job.

1



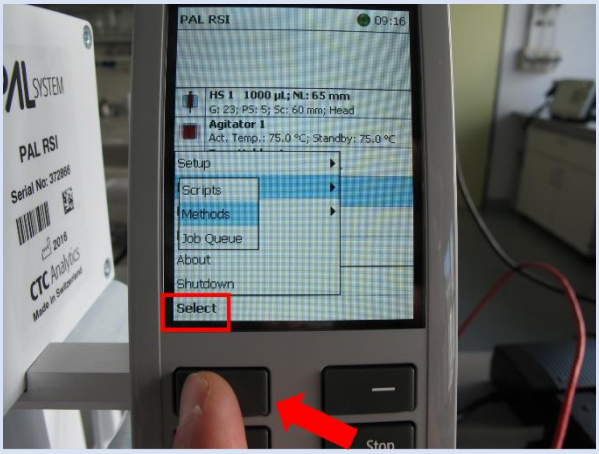
With the **left function key** select **Options**.

2

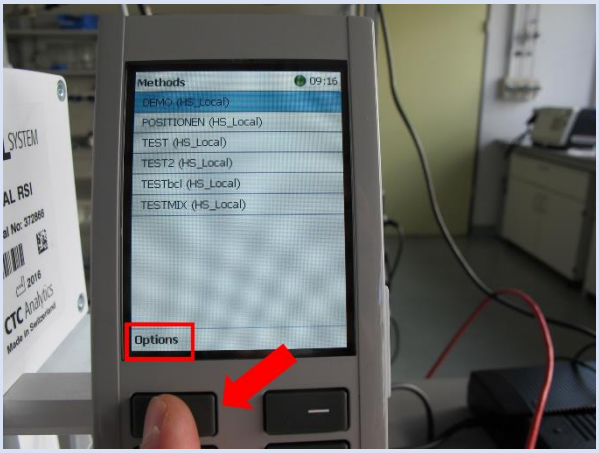
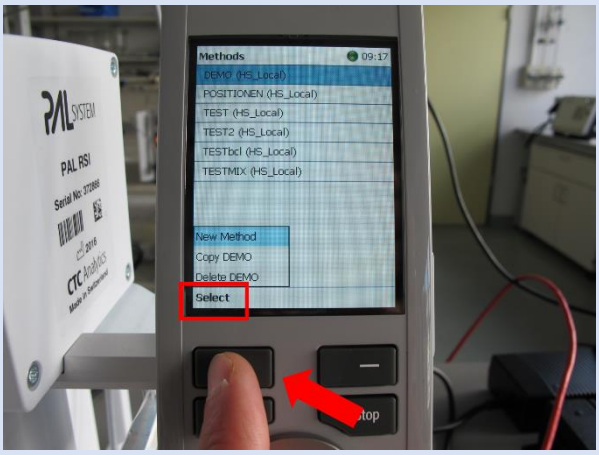
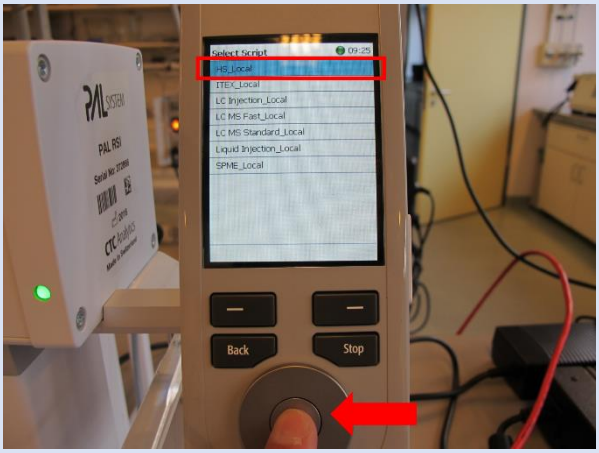


In **options menu** select **Local Scripts**.
With the **left function key** select **Select**.

3

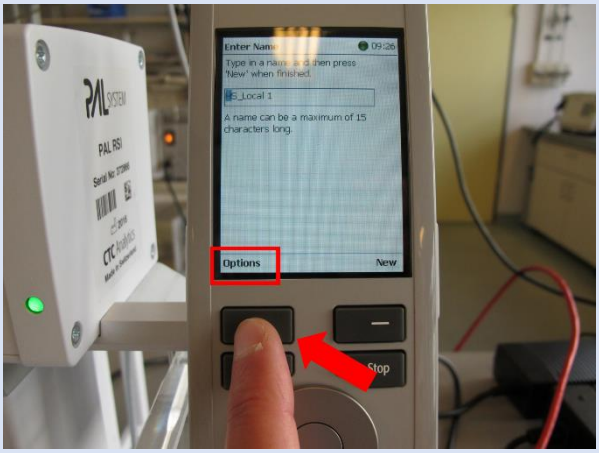
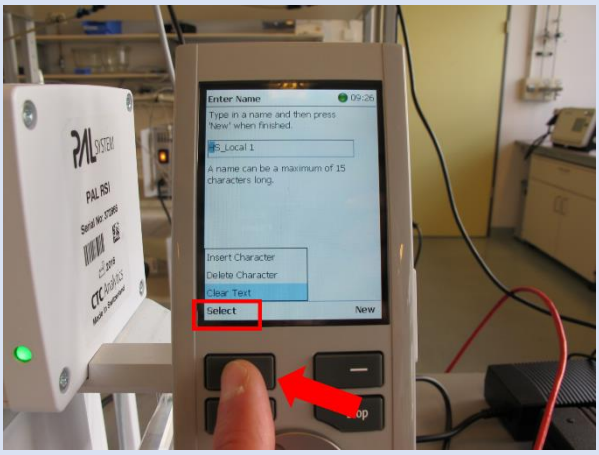
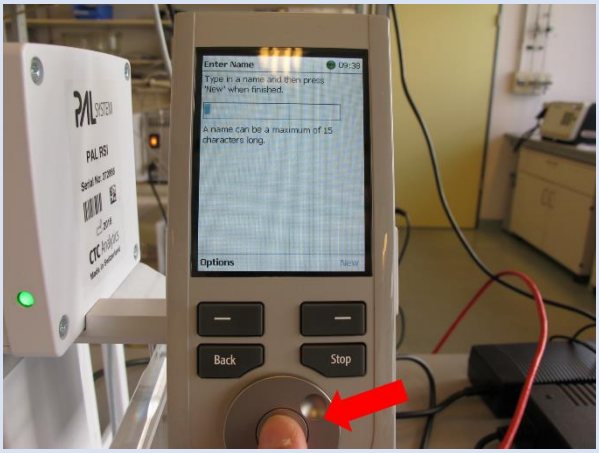


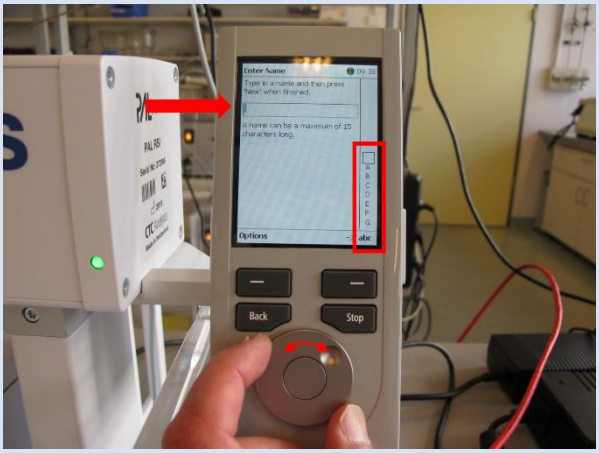
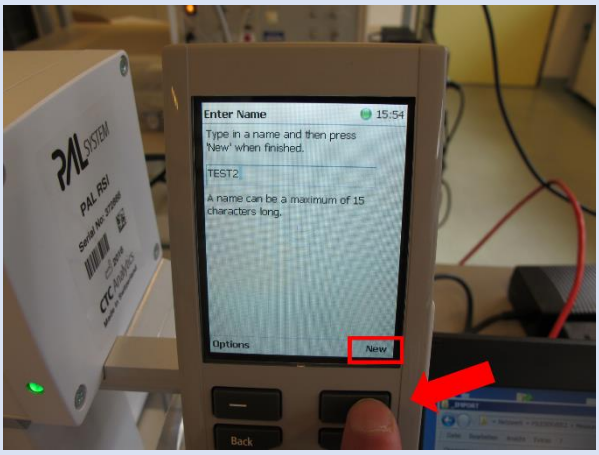
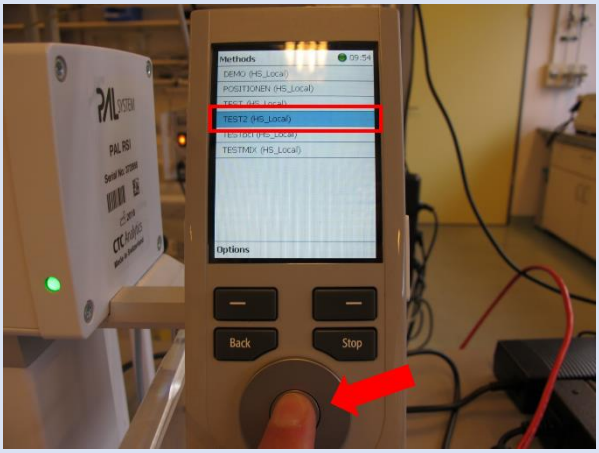
In **options menu** select **Methods**.
With the **left function key** select **Select**.

4		With the **left function key** select **Options**.
5		In **options menu** select **New Method**. With the **left function key** select **Select**.
6		Select the script HS Local.

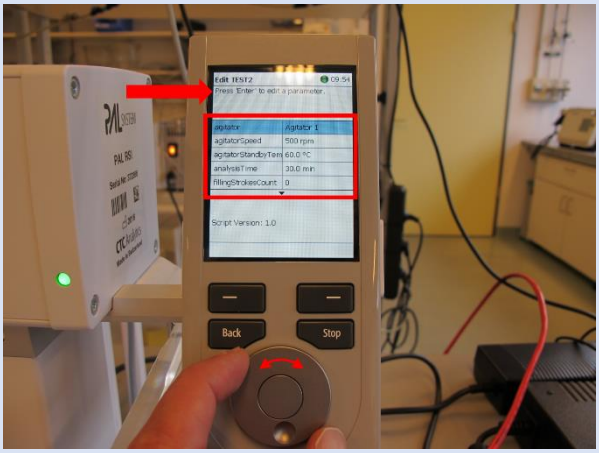
INFORMATION!

The intended use of the FlavourSpec is only headspace measurement. Only the script HS Local will work..

7		With the **left function key** select **Options**.
8		In **options menu** select **Clear Text**. With the **left function key** select **Select**.
9		Press the **EDIT Button** to enter a new name.

10		Select **letters and numbers** with the **rotary knob**.
11		With the **right function key** select **New** to accept the new name and leave the screen.
12		Select the new method and press **Edit** to edit the method.

13



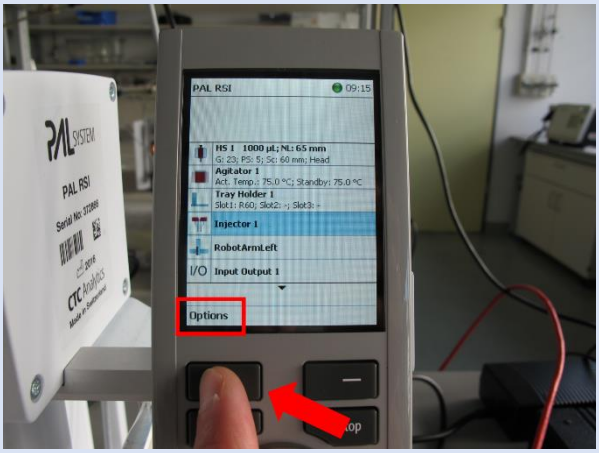
In **method screen** several parameters can be edit. **(see chapter 9.10 and 9.11)**

8.13 Workflow: Edit a Method

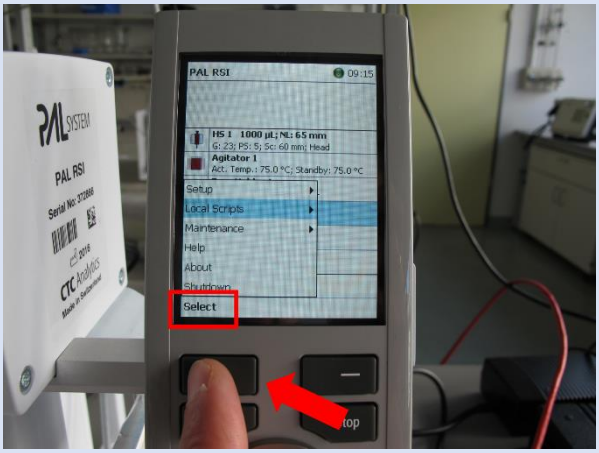
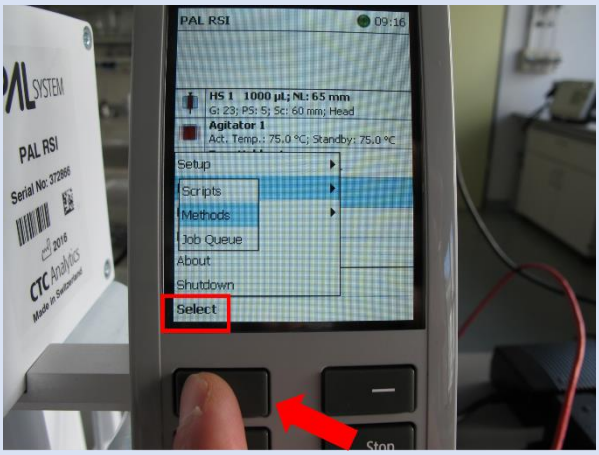
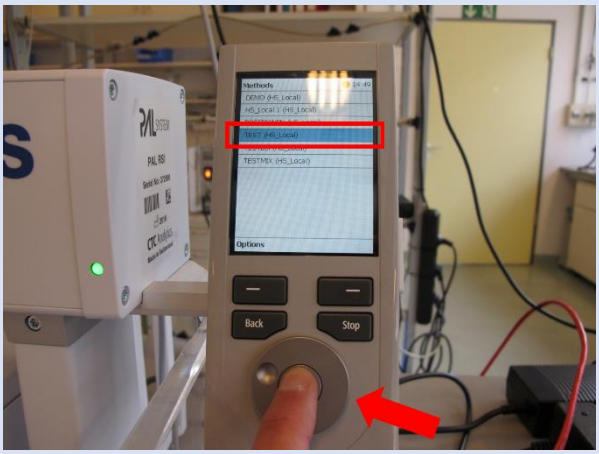
INFORMATION!

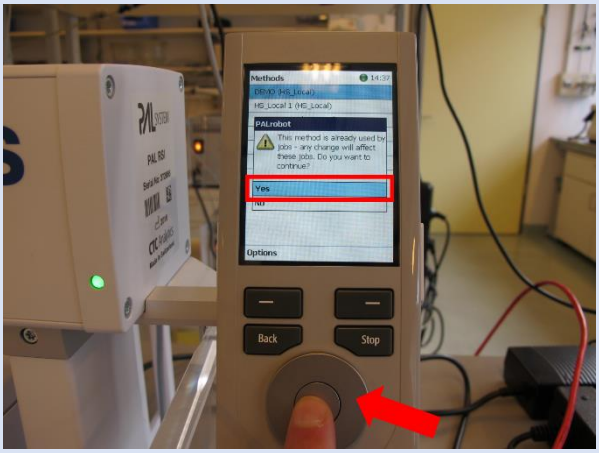
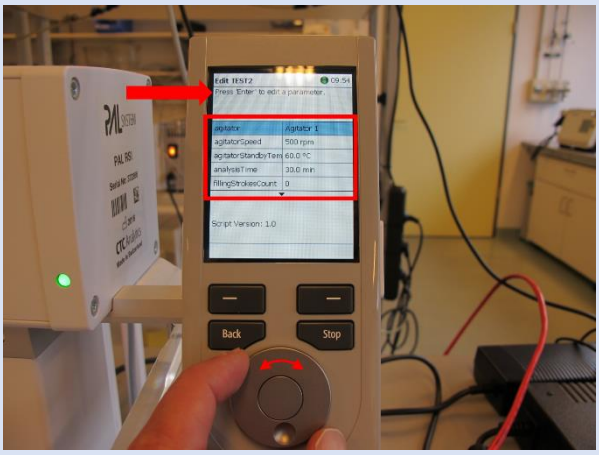
A method contains Incubation time and -temperature, the analyte time … **(see chapter 9.10 and 9.11)**. A method is required for a job.

1



With the **left function key** select **Options**.

2		In **options menu** select **Local Scripts**. With the **left function key** select **Select**.
3		In **options menu** select **Methods**. With the **left function key** select **Select**.
4		Select the **new method** and press **Edit** to edit the method.

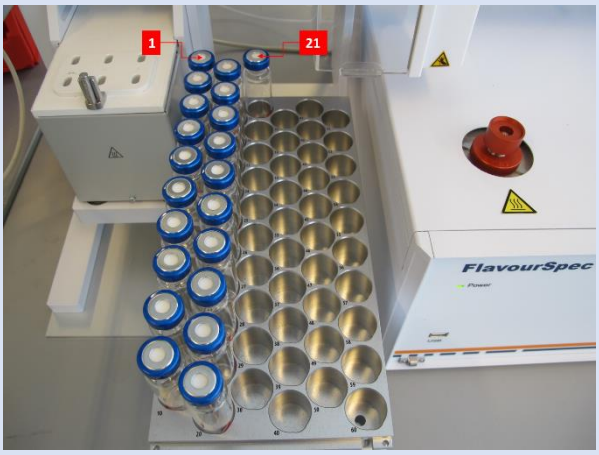
5		In the Information windows select **YES**.
6		In **method screen** several parameters can be edit. **(see chapter 9.10 and 9.11)**

8.14 Workflow: Run a measurement with autosampler

INFORMATION!

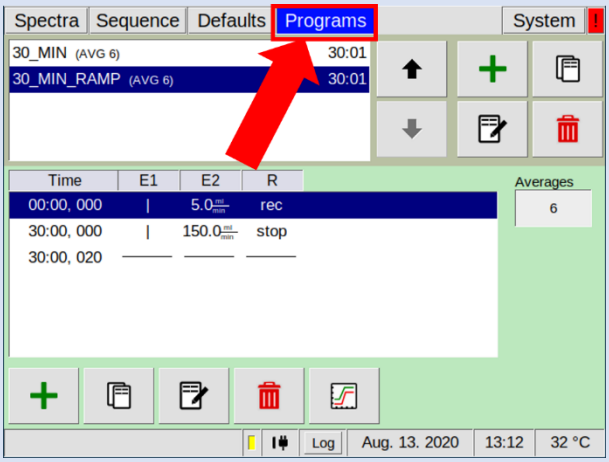
To run measurements with an autosampler the following steps are required.

1



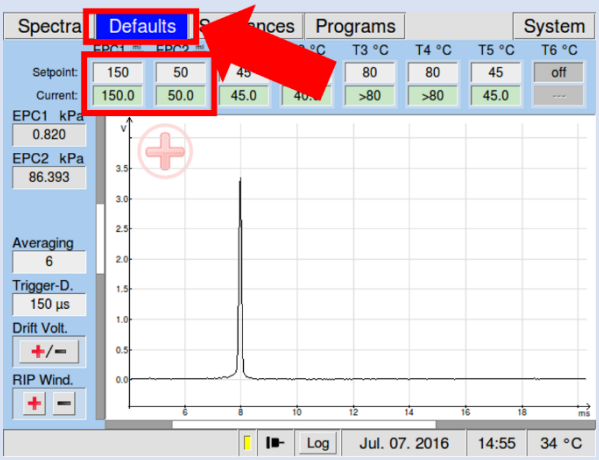
Put the sample into the tray.

2

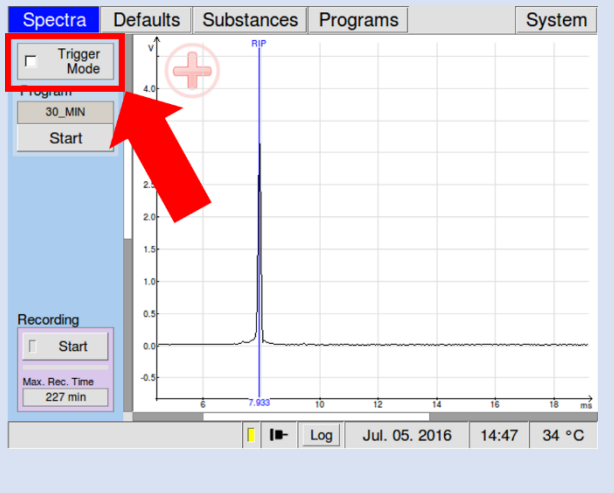
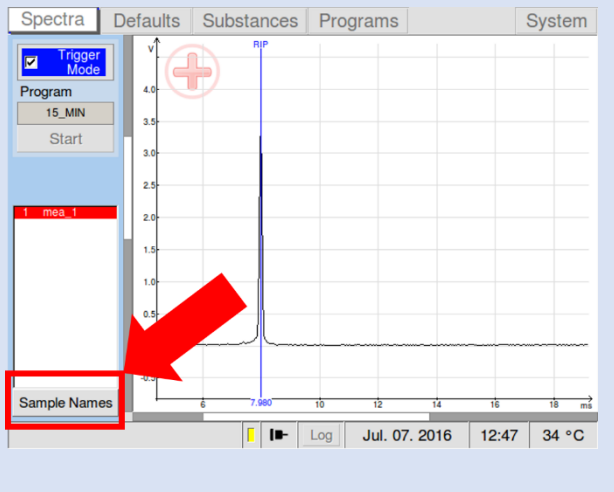
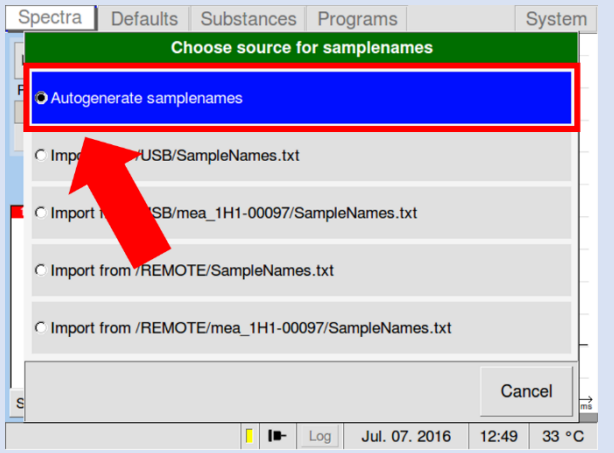


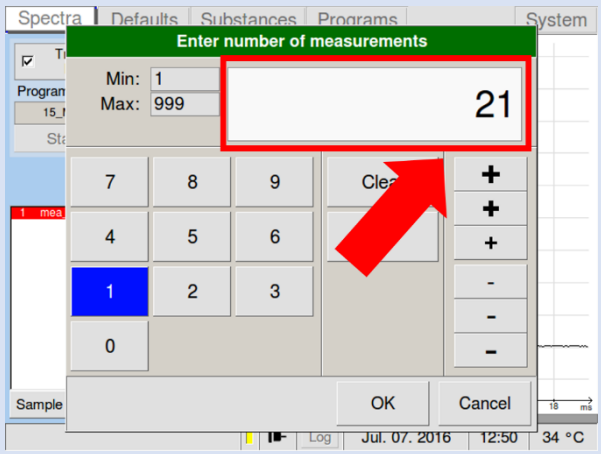
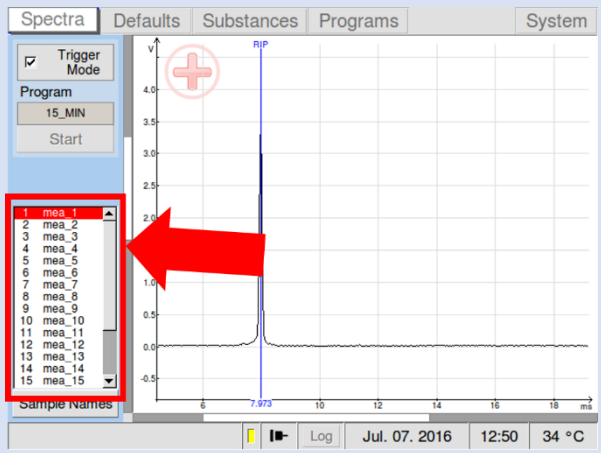
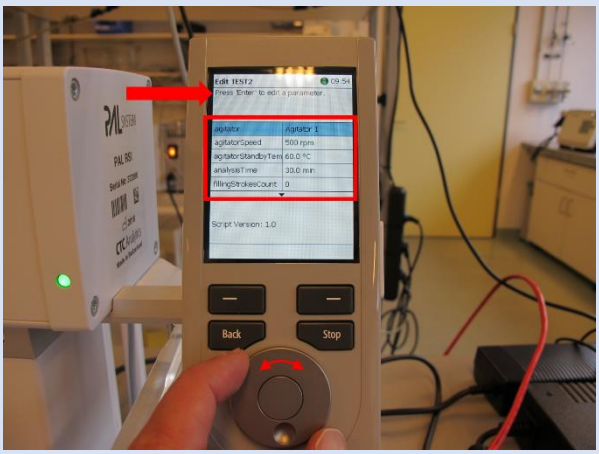
Create a measurement program (see chapter 6.5.2) or select one (see chapter 8.10)
The start values for E1 and E2 must correspond…

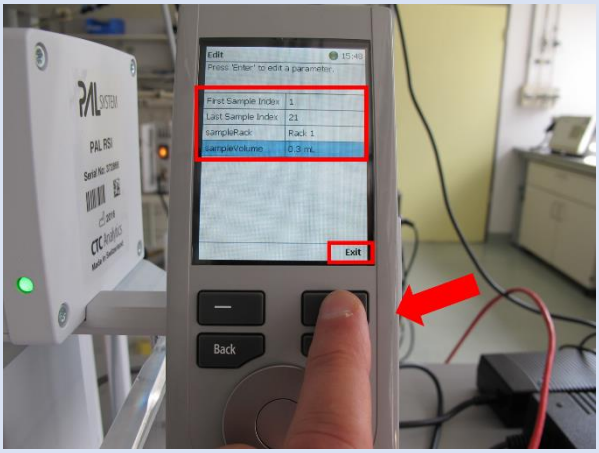
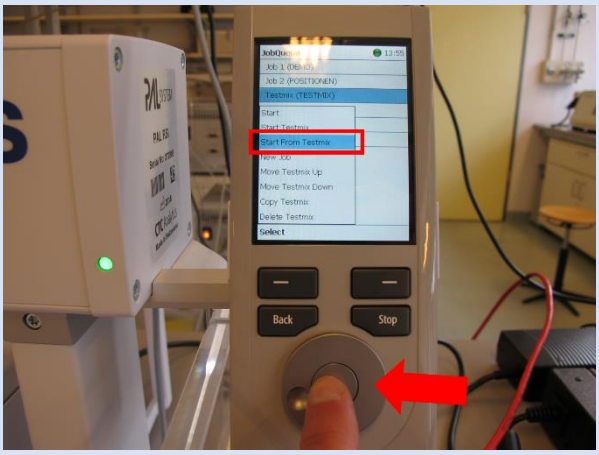
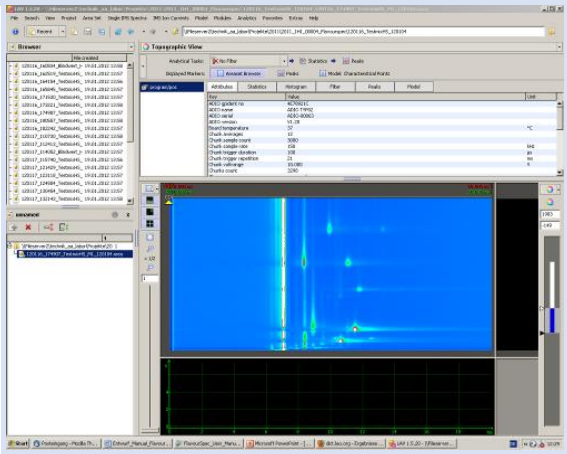
3



…to the values for EPC1 and EPC2 in Defaults window.

4		In **spectra window** select **Trigger mode**.
5		Select Sample Names.
6		To generate an automatic samplelist select autogenerate samplelist.

7		Enter the number of samples.
8		The actual samplelist is shown.
9		Create a new method **(see chapter 8.12)** or edit a method **(see chapter 8.13)**

10		Create a new job **(see chapter 8.8** or edit a job **(see chapter 8.9)** Enter the number of samples.
11		Select the job and start.
12		View and analyze the measurement files with the VOCAL software.

INFORMATION!

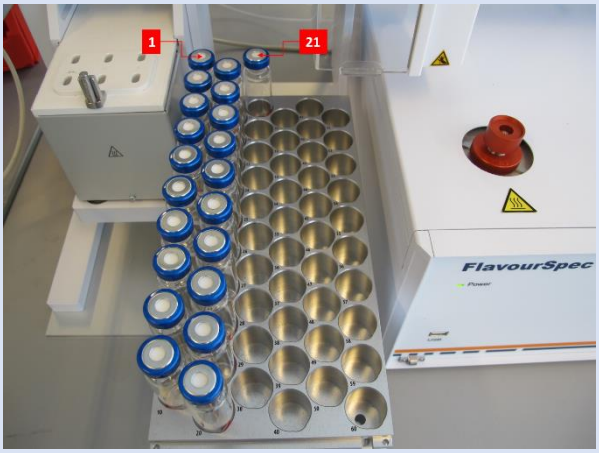
For detailed information about the Laboratory Analytical Viewer LAV refer the VOCAL Software Manuals and Tutorials

8.15 Workflow: Run a measurement with manual injection

INFORMATION!

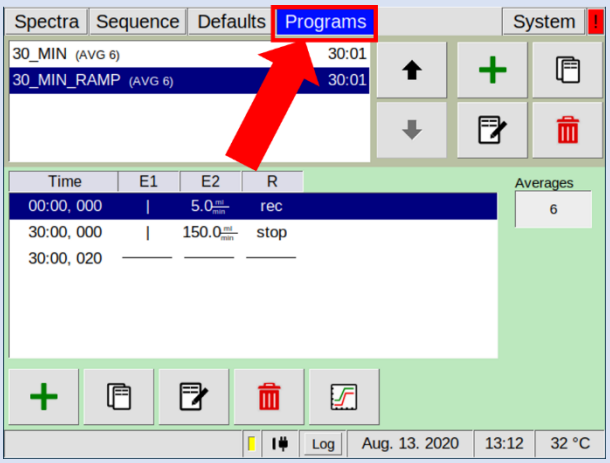
Measurements can also be done without autosampler. The headspace-sample must be inject manually and the device has to be start manually too.

1



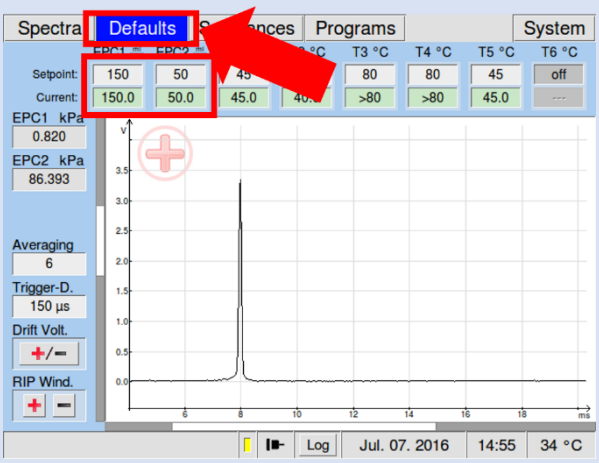
Put the sample into the tray.

2

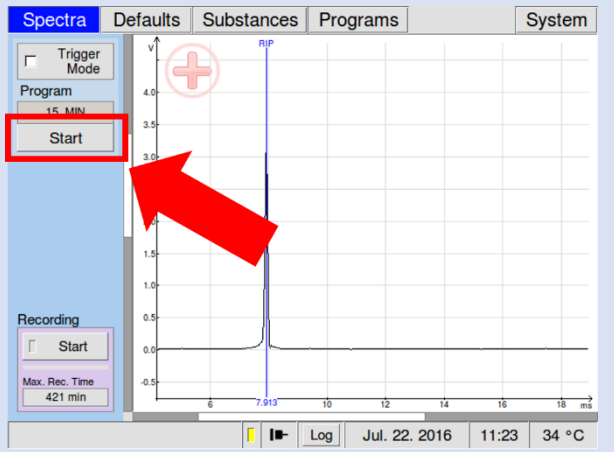
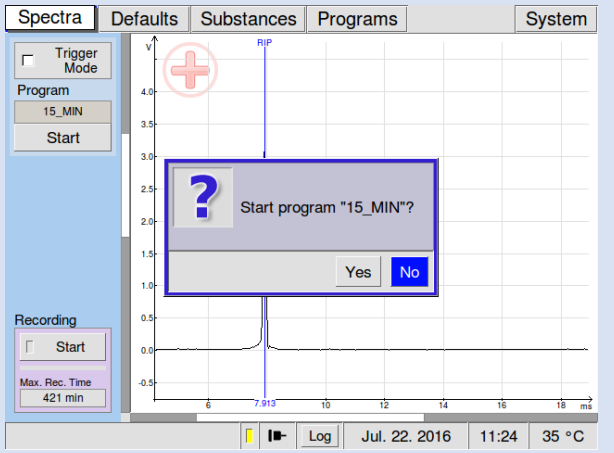
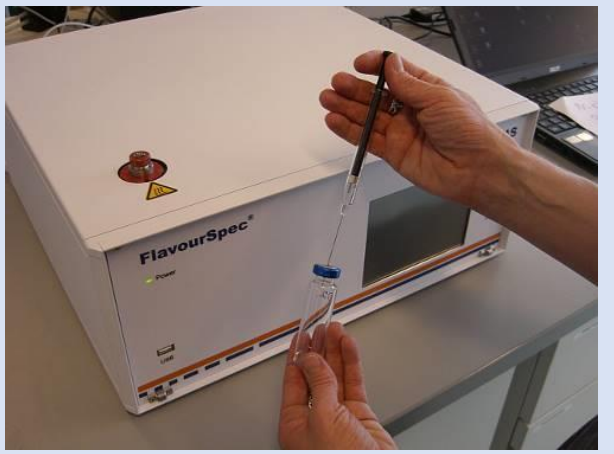


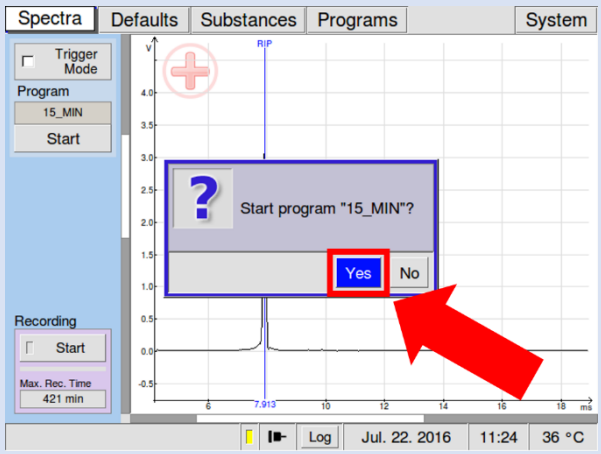
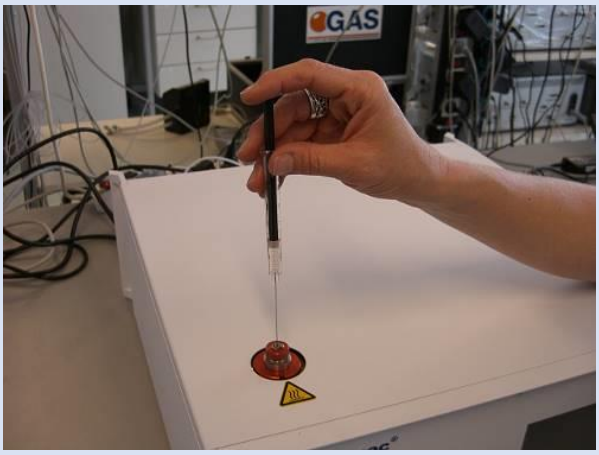
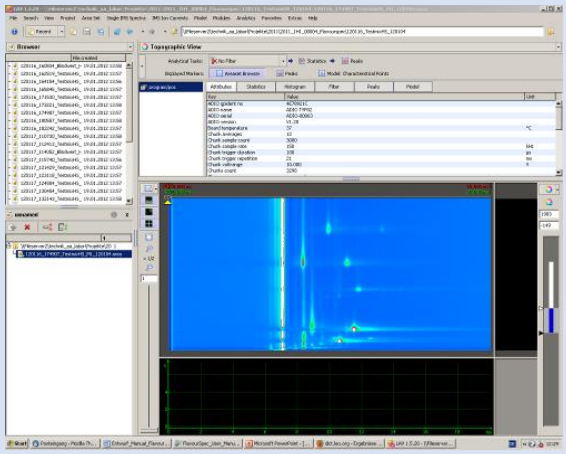
Create a measurement program (**see chapter 6.5.2**) or select one (**see chapter 8.10**)
The start values for E1 and E2 must correspond…

3



…to the values for EPC1 and EPC2 in **Defaults window.**

4		Go to **Spectra window** and **press start**.
5		An information windows appears.
6		Select the headspace sample with a proper gastight syringe.

7		**Select YES** in the information window.
8		Inject the headspace sample into the sample injector port.
12		View and analyze the measurement files with the VOCAL software.

INFORMATION!

For detailed information about the Laboratory Analytical Viewer LAV refer the VOCAL Software Manuals and Tutorials

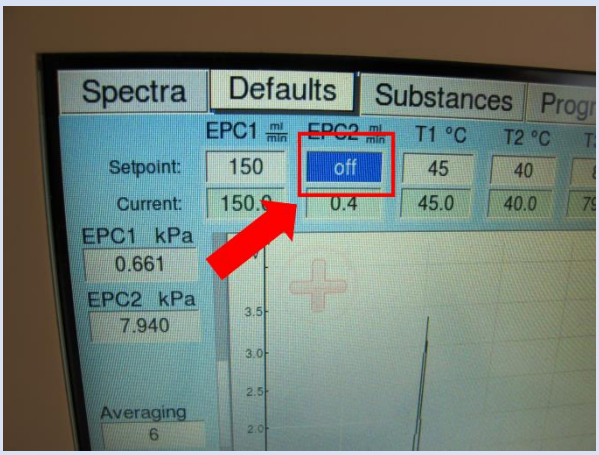
8.16 Workflow: Change Septa

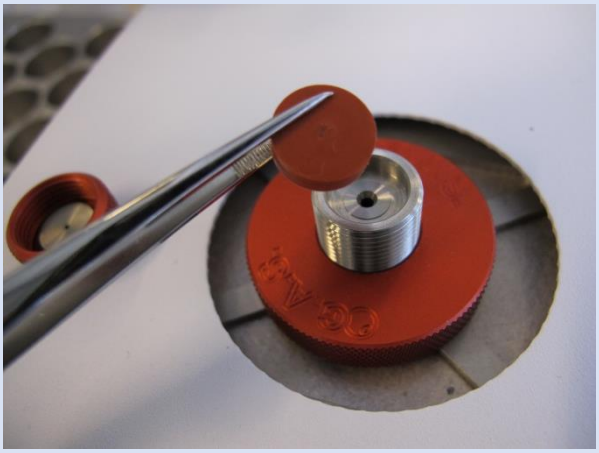
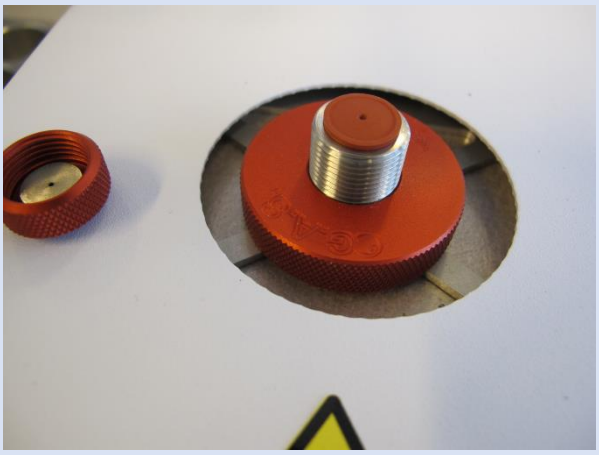
INFORMATION!

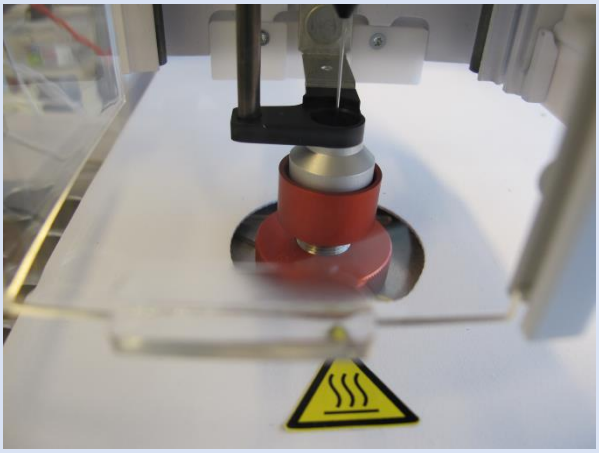
Typically modern septa can last 100 injections or more. Factors that affect the septa lifetime are syringe size, inlet temperature etc.

WARNING!

The Injector can become very hot. Risk of burning. Use heat-resistant gloves.

1		Set off the Carriergas flow (EPC2 = off).
2		Unscrew the injector adapter with septum retainer nut.

3		Remove the old septa, insert a new septa. (11-mm Septs, high temperature, low-bleed).
4		Press the septa into the injector.
5		Hand screw the injector adapter with septum retainer nut.

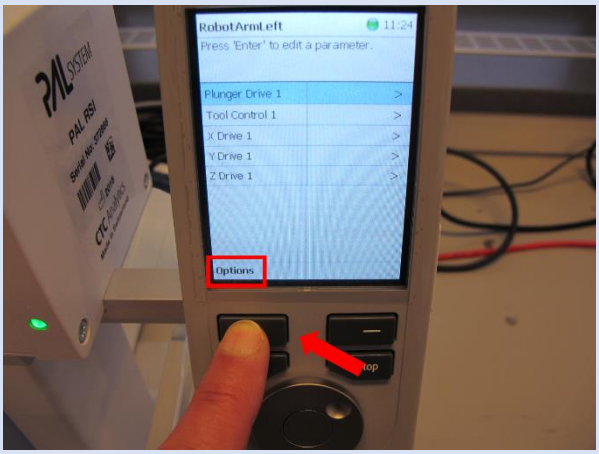
6		Check the Injector position. **(see chapter 8.2)**

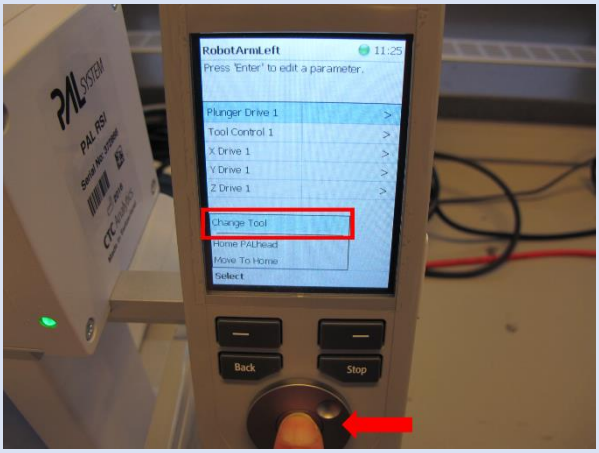
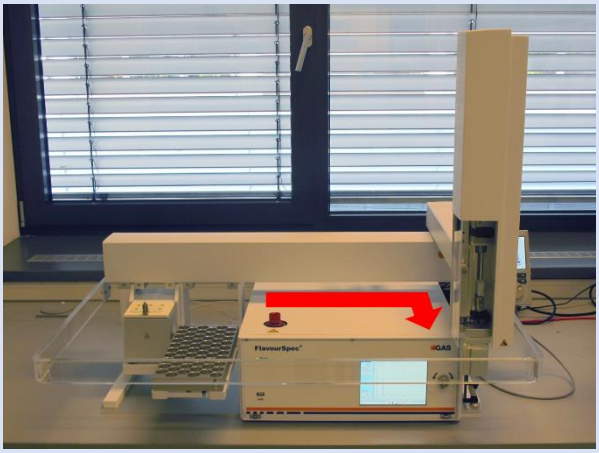
8.17 Workflow: Change syringe

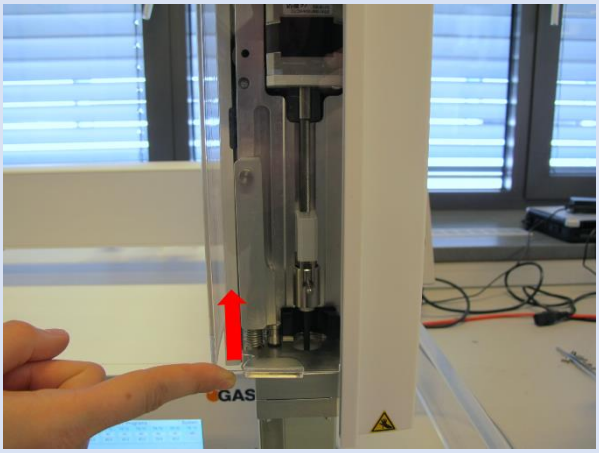
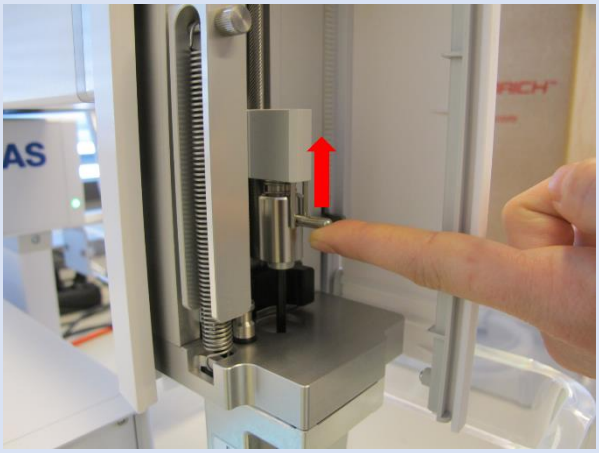
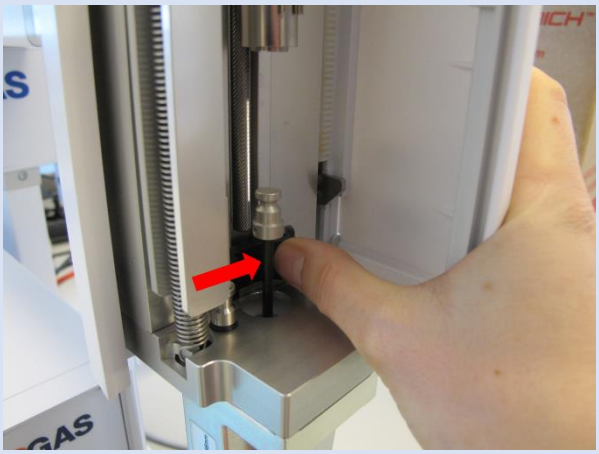
INFORMATION!

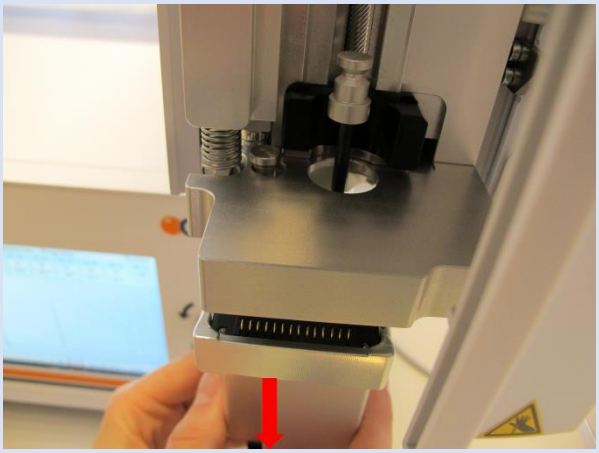
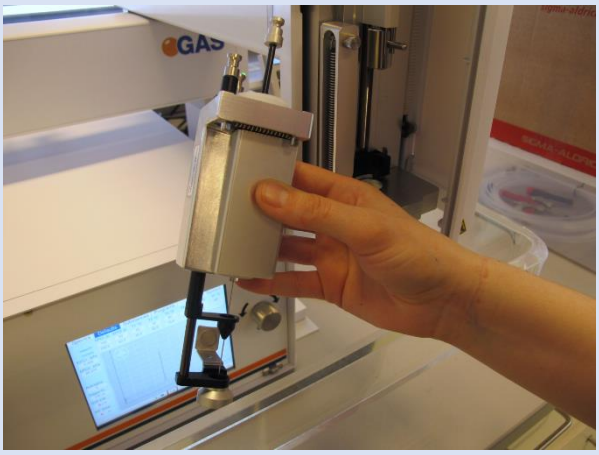
The FlavourSpec®, in combination with the autosampler PAL RSI, is delivered with a gastight 1 ml syringe. To change a syringe do the following:

8.17.1 Disambling the Syringe tool

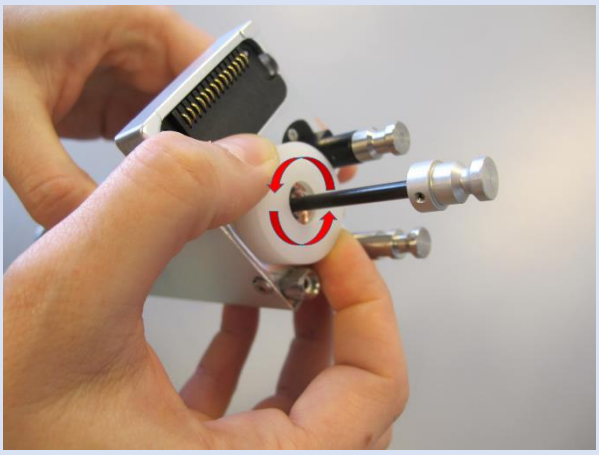
1		On the **PAL RSI main screen** select **RobotArmLeft**
2		With the **left function key** select **Options**.

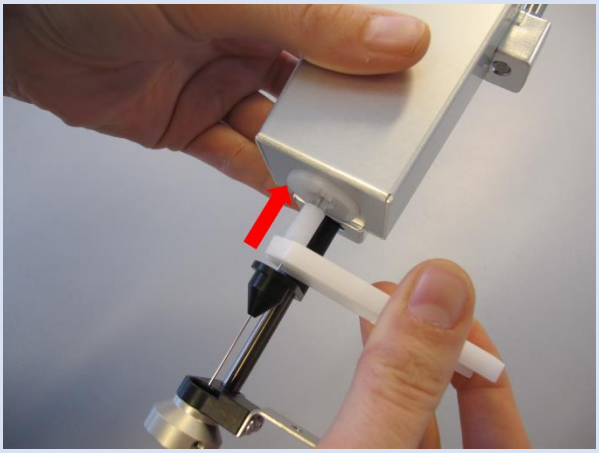
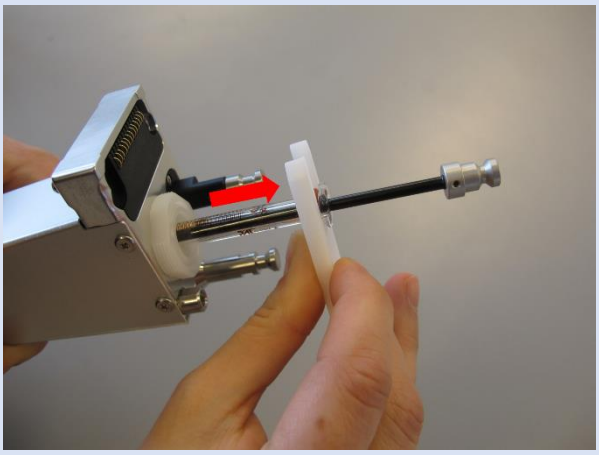
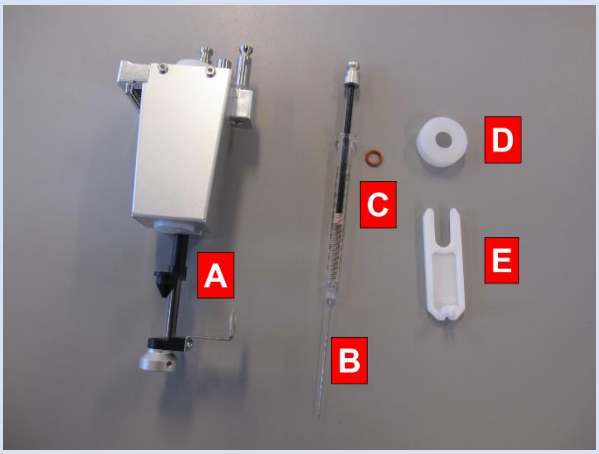
3		In **options menu** select **Change Tool**.
4		With the **right function key** select **Move**.
5		After a **warning signal** the **arm moves** to the actual change tool position.

6		Move the protective cover to its top position.
7		Move the holder upwards.
8		Push the locking...

9		…and remove the syringe tool.
10		The figure shows the syringe tool.

8.17.2 Disambling the Syringe

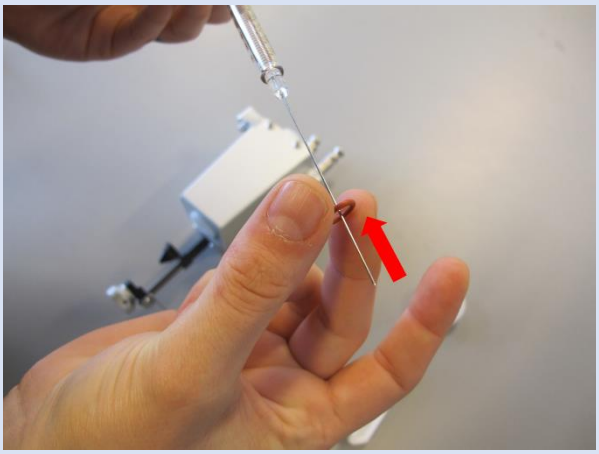
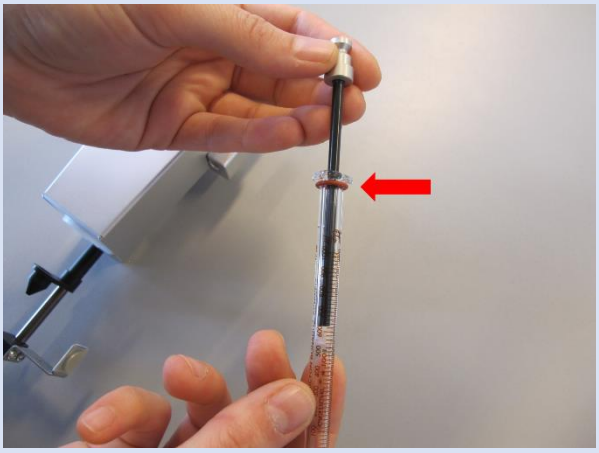
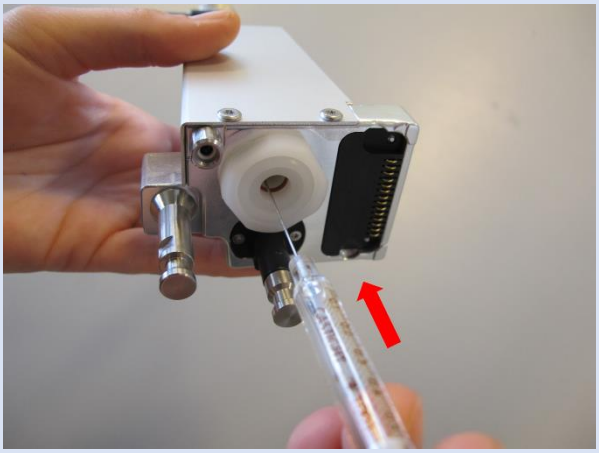
1		Unscrew the white plastic retainer.

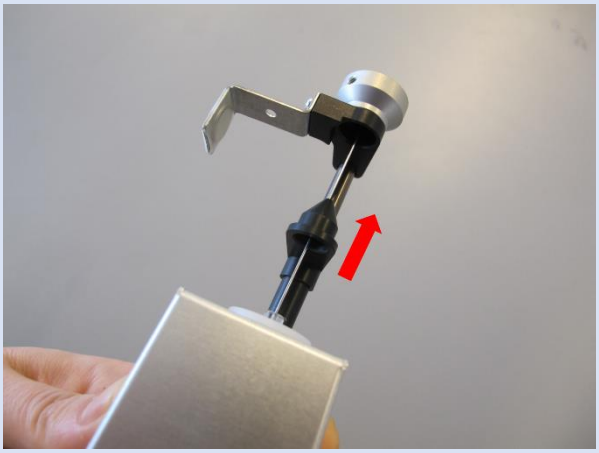
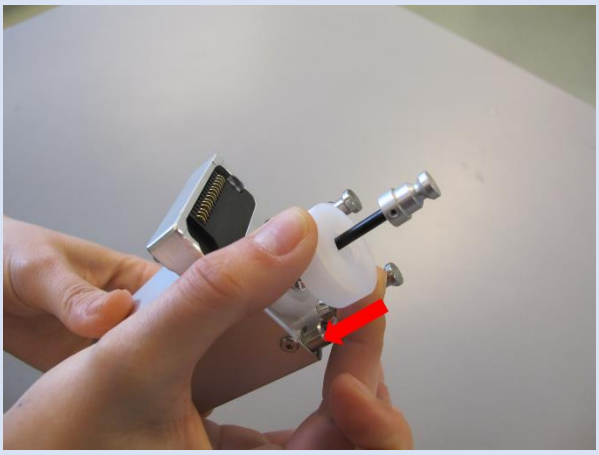
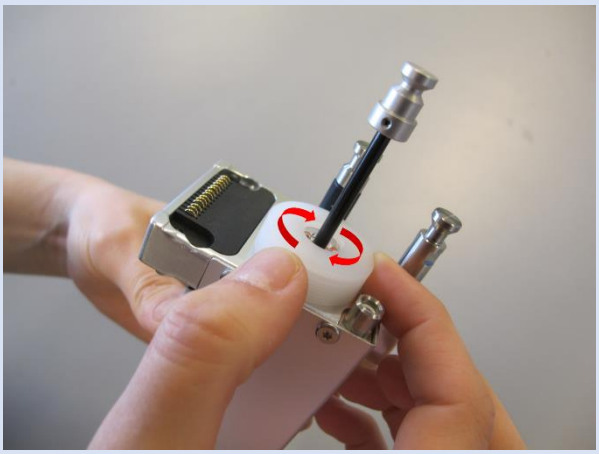
2		Use the syringe auxilliary tool to remove the syringe.
3		Use the syringe auxilliary tool to remove the syringe.
4		A: Syringe tool with heater B: Syringe (gastight) C: O-ring for syringe D: Plastic retainer E: Syringe auxilliary tool

8.17.3 Install a syringe

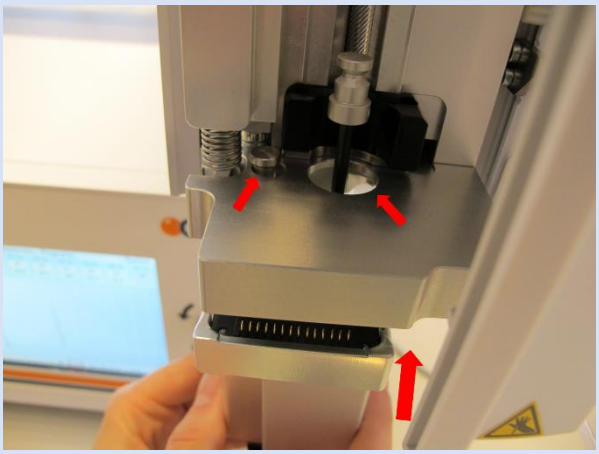
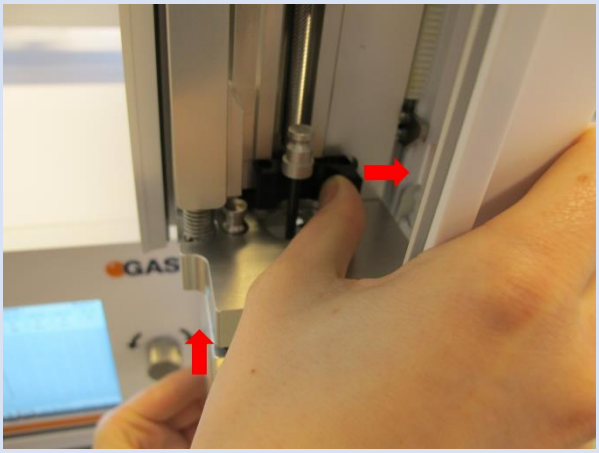
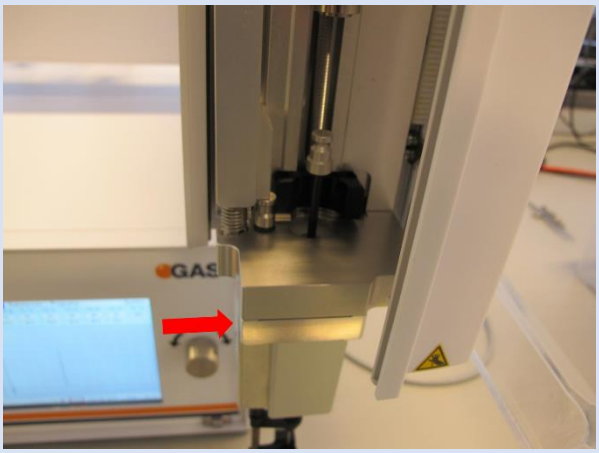
WARNING!

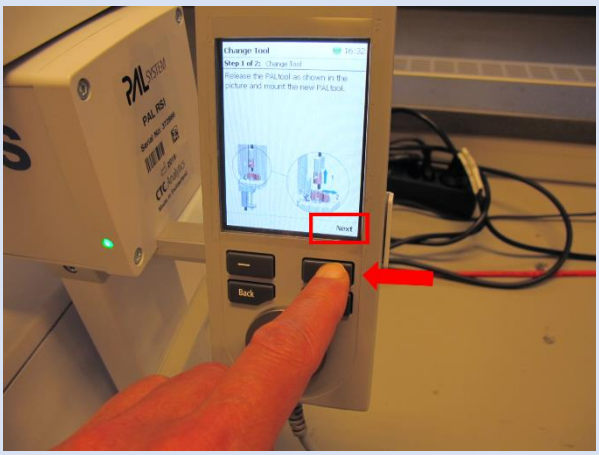
Be careful when installing a syringe, to avoid injuries.

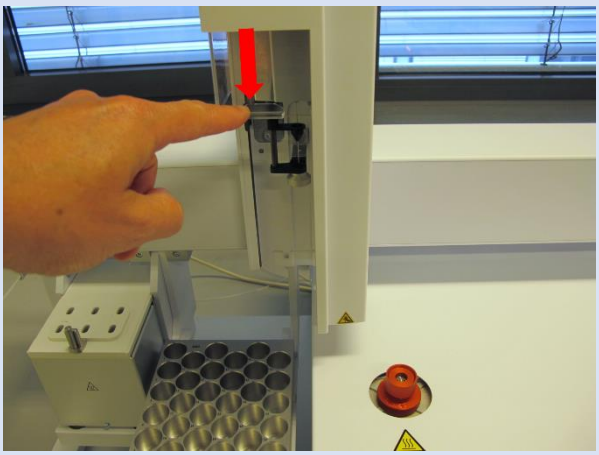
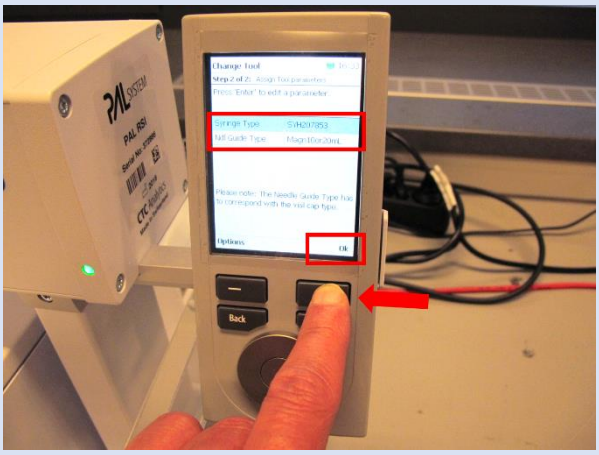
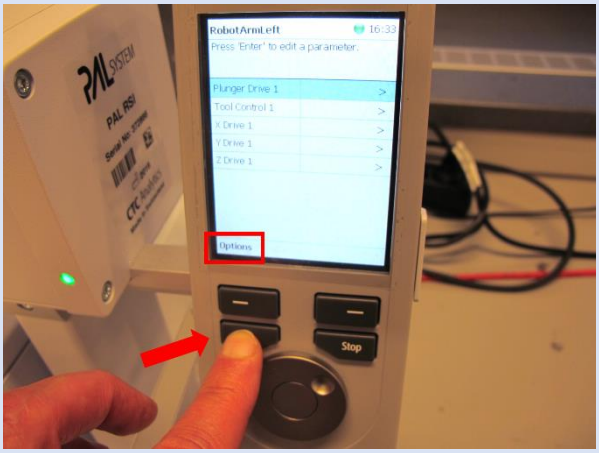
1		Install a new O-ring.…
2		… install a new O-ring
3		Install the syringe with O-ring into the syringe tool.

4		Pay attention to a proper needle guide.
5		Put on the white plastic retainer and…
6		… fix the syringe.

8.17.4 Install the syringe tool

1		Place the syringe tool back into its holder.
2		Push the locking and insert the tool and release the locking.
3		The figure shows the installed syringe tool.

4		With the **right function key** select **Next**.
5		The syringeholder moves down …
6		… and after a **warning signal** the **arm moves** to the home position.

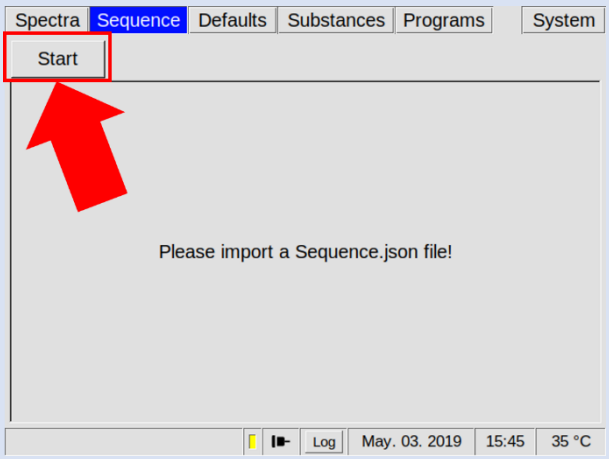
7		Move the protective cover downwards.
8		Check the syringe identification: Syringe Type: SH1000-65-T-23-SP NdlGuideType: Magn.10or20ml With the **right function key** select **OK**.
9		Select the **BACK-button** to go to the **main screen**.

8.18 Workflow: Start Sequence

INFORMATION!

The sequence file must be created with the **G.A.S. Sequence Designer Software**. For detailed Information refer to the **G.A.S. Sequence Designer Software Manual.**

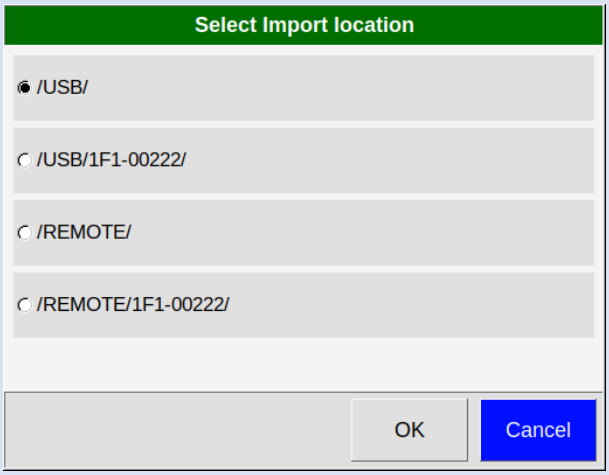
1



To start a sequence select:

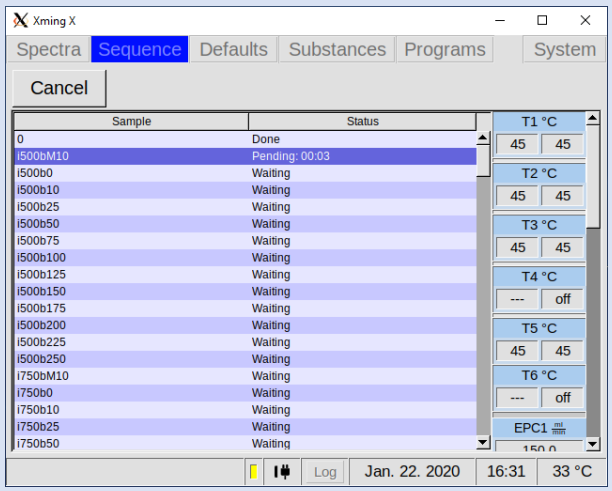
Spectra › **Start**

2



Select the import location pf the sequence file named **Sequence.json**

3



The Sequence will be executed.

INFORMATION!

The file has to be named **Sequence.json** for the software to recognize it. Make sure, that the parameters specified in the programs and after-run settings are within your devices permitted regions.

WARNING!

Be careful when changing device critical parameters by applying **After Run Settings**. A device can become inoperable with faulty IMS parameters. After Run settings are also applied if the Sequence is cancelled by the user. In case of cancellation, the devices default parameters will be the same as if the sequence had successfully finished, taking all previous After Run Settings into consideration.

8.19 Workflows: File Transfer Setup

8.19.1 Overview

Files can be transferred to and from the device by LAN connection and by USB device connected to the USB port at the front of the housing.

INFORMATION!

A connected USB device is always preferred to a LAN connection when exporting or importing files manually.

INFORMATION!

The USB device must be formatted to FAT32. Consult your system administrator on formatting USB devices.

Generated measurement files and measurement result files are stored on the internal storage volume of the device.

The following file types are generated from measurements:

File Type	Description
MEA Measurement Files	Contains the complete data of one single measurement including the raw sampling data.

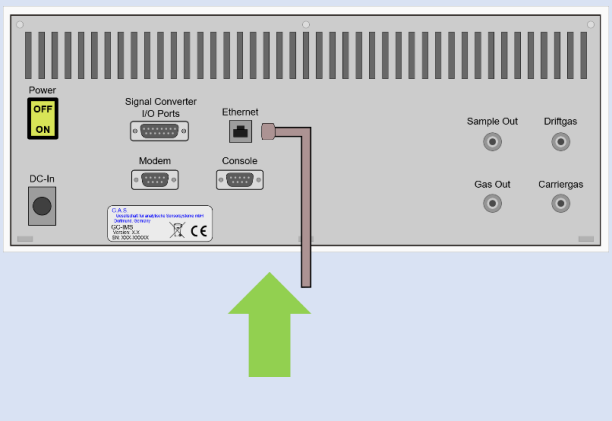
When a connection to a server is established and the export is activated these files are copied to this server when created in the workflow. Measurement files once copied to one of these locations are marked and will be overwritten in case the internal storage is full.
By default the **Service Message Block Protocol (SMB)** also known as Common Internet File System (CIFS) is used. The **Secure File Transfer Protocol (SFTP)** or a modified version of the **Trivial File Transfer Protocol (TFTP)** can also be used.
LAN file transfer settings can be modified in **System** › **Transfer** › **Connection** › **Edit Server Details**.
Manual transfer of measurement files stored on the device can be done **System** › **Transfer** › **Mea Files** › **Copy to Remote**.
Manual transfer of measurement files stored on the device can be done **System** › **Transfer** › **Mea Files** › **Delete**.

8.19.2 Connecting to a Server in a LAN

INFORMATION!

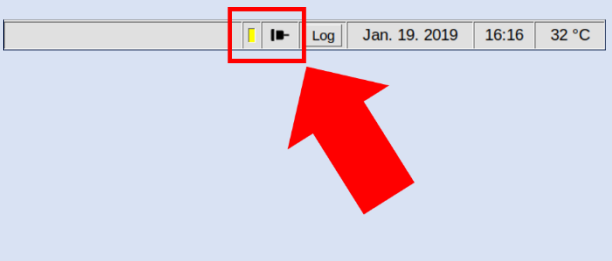
Some PC Ethernet interfaces may not be suited for a direct connection to the device. In that case consider using an Ethernet switch to connect both devices.

1a



Connect the device with a standard Ethernet cable (LAN cable) to the LAN or directly to a computer.

1b



In the status bar the connection icon is displayed.

INFORMATION!

Make sure that any firewall present in the network does not block necessary traffic. Consult your system administrator on how to configure your firewall.

INFORMATION!

Consult your system administrator on how to set up a server with one of the protocols SMB and SFTP. The TFTP protocol requires the G.A.S. TFTP Server software to run on a Microsoft® Windows® computer.

2a

Option

For SMB set up a SMB share on a server. Consult your system administrator on how to do that.

2b

Option

For **SFTP** set up a SFTP server. Consult your system administrator on how to do that.
For an example SFTP server for Microsoft® Windows® PCs see: **http://www.coreftp.com/server**

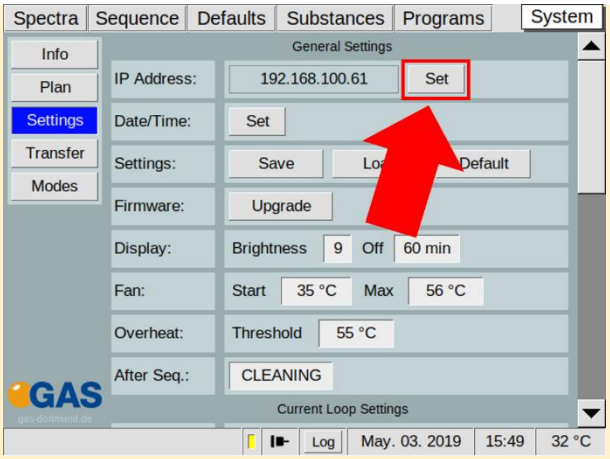
2c

Option

For **TFTP** install the G.A.S. IMS-Control TFTP-Server on the PC. For detailed information see the **IMS Software Suite IMScontrol TFTP-Server manual.**

3a

Option

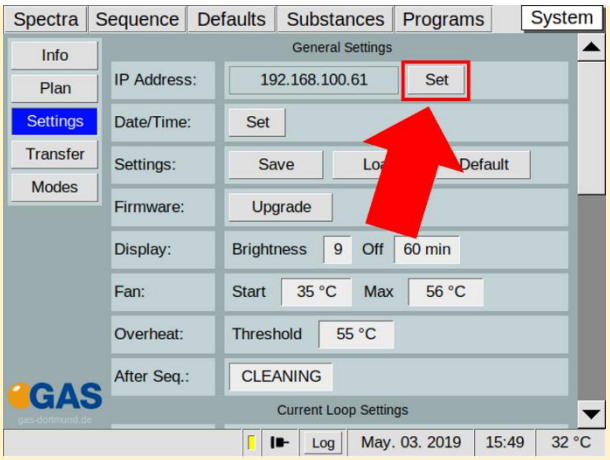


Set a static device IP (Recommended for direct connection of PC and device):
Use System › **Settings** › **Set**

In the next dialogbox select: **Yes**

3b

Option

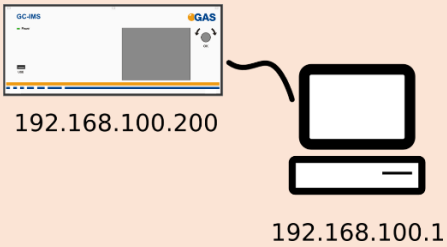


Get device IP From DHCP Server (Recommended for LAN integration of the device):
Use System › **Settings** › **Set**

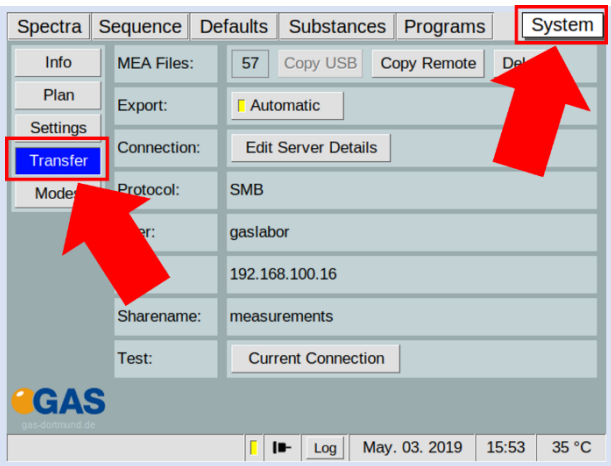
In the next dialogbox select: **No**

INFORMATION!

Note that both devices must be in the same subnet mask area of **255.255.255.0** i.e. only differ in the fourth number of the four-part IPv4 address.

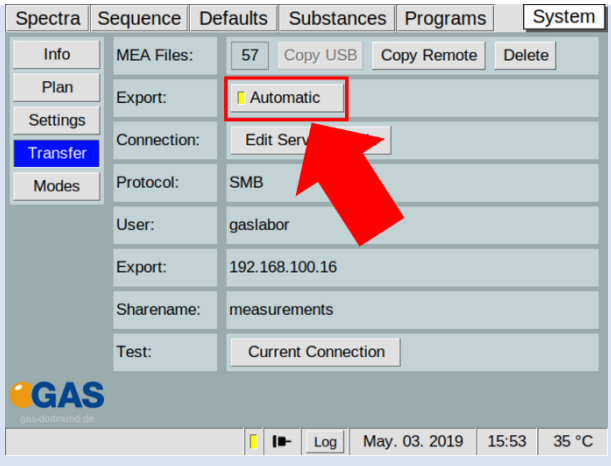


4



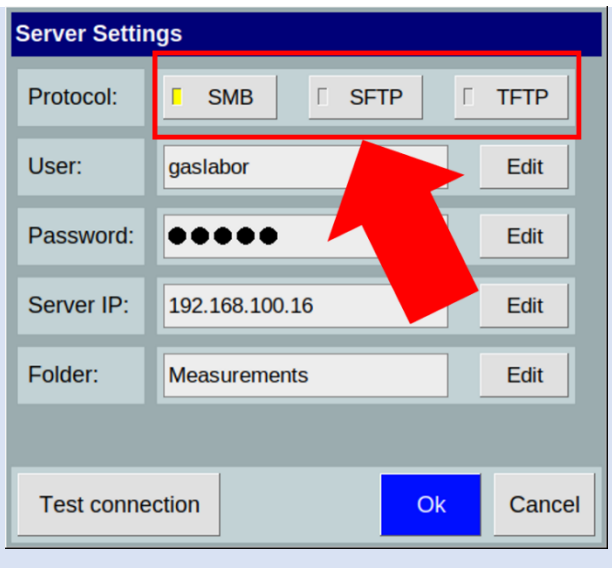
Open **System** › **Transfer**

5



Activate or deactivate automatic file transfer to the server with **Automatic Export**.

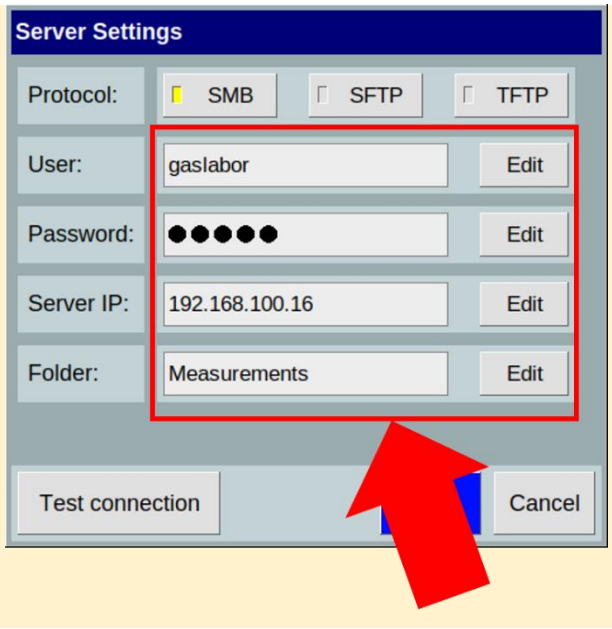
6



Select the desired protocol **SMB**, **SFTP** or **TFTP**.

7a

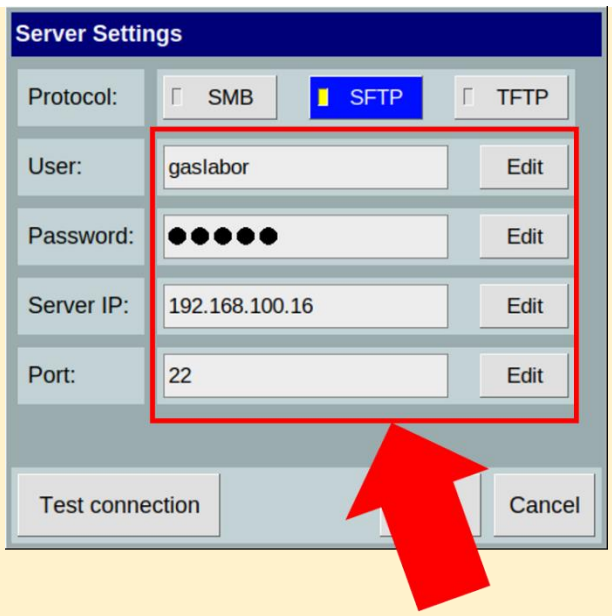
Option



For **SMB** enter **Server IP Address**, **Folder** name, **User** name and **Password** for the SMB share on the server.

7b

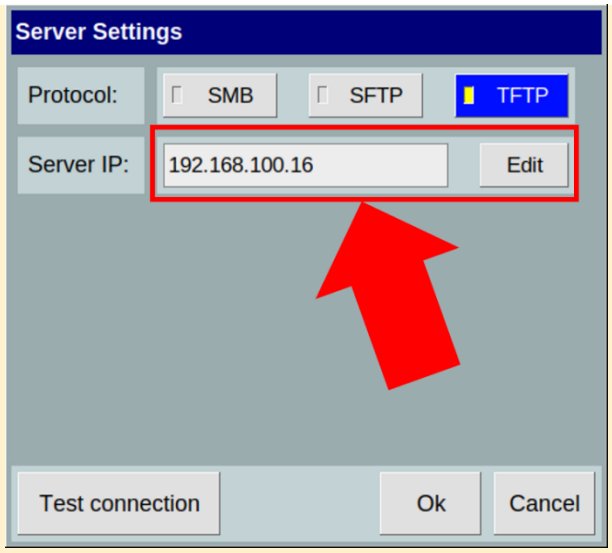
Option



For **SFTP** enter **Server IP Address**, **IP Port**, **User** name and **Password** for the SFTP server.

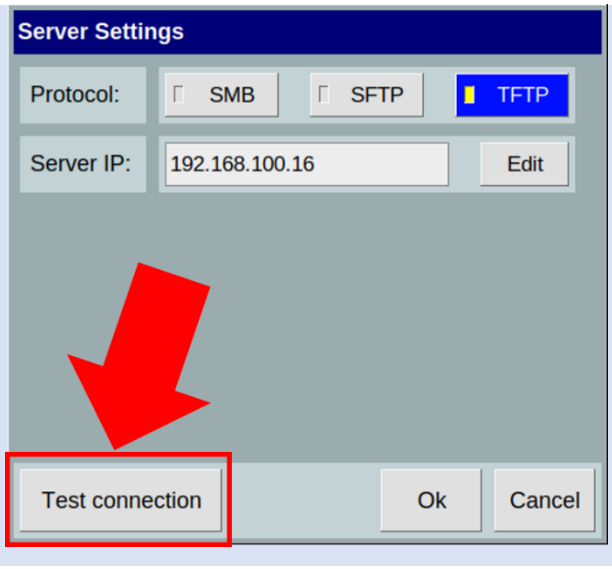
7c

Option



For **TFTP** enter the **Server IP Address**.

8

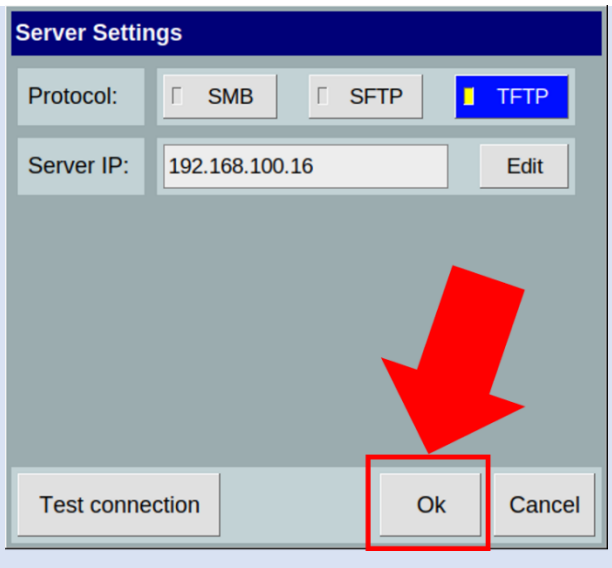


Test the connection with **Test Connection**.

INFORMATION!

When the connection cannot be established check the Ethernet cable connection. Main the network IP address of the server, the used protocol, the name of the shared folder (SMB) on the server and the server account login data (SMB, SFTP). Consult the manuals of your server operating system and your system administrator.

9



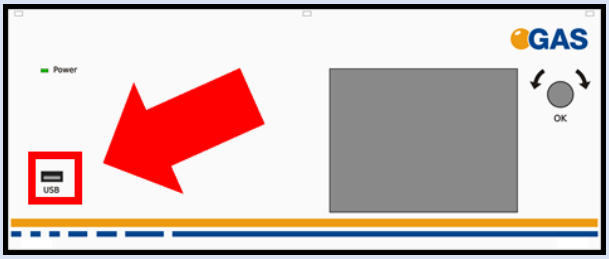
Close Dialog with OK.

8.19.3 Workflow: Manual Transfer of measurement files to USB-Stick

INFORMATION!

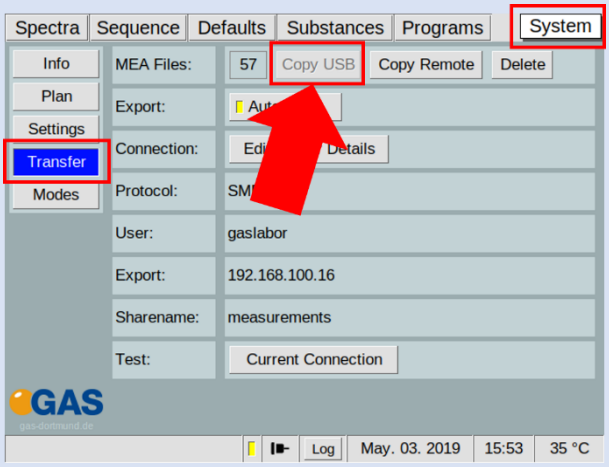
Do not turn off the device during the download process!

1



Connect the USB device (FAT32-formatted) to the USB socket at the front side of the housing.

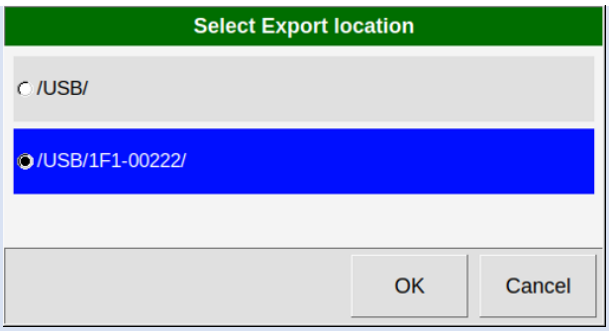
2



Open page:
System › Transfer.

Press:
Copy USB.

3



A confirmation dialog opens.
Select the storage location.

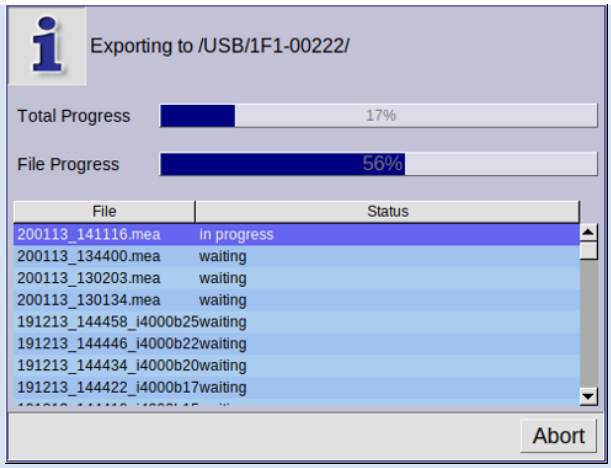
Press OK to start the process.

INFORMATION!

All internally stored measurements are transferred.

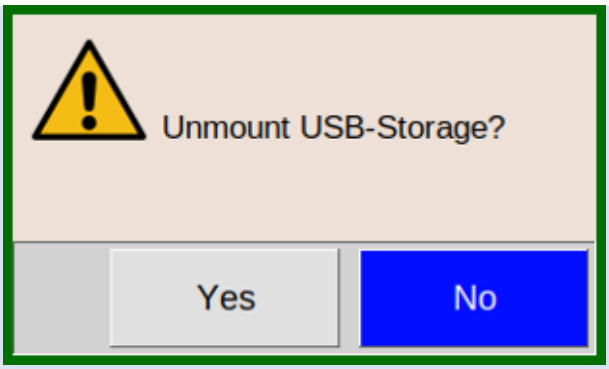
The process can be stopped at any time

4



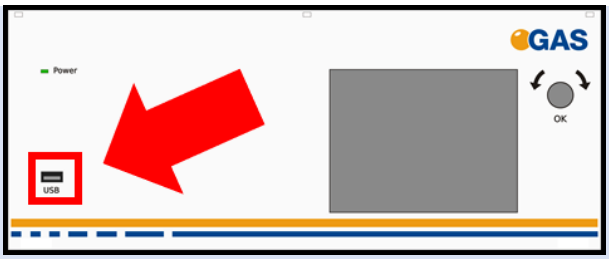
Wait until the exporting process is completed.

5



A confirmation dialog opens.
Press **OK** to unmount the USB-Stick

6



Remove the connected USB device from the **USB** socket at the front side of the housing.

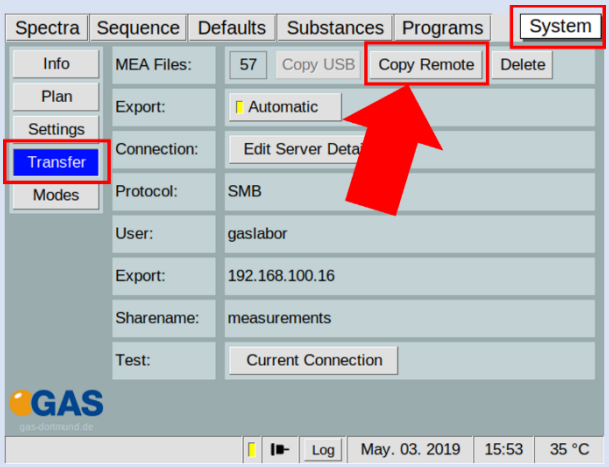
The measurement files has been downloaded.

8.19.4 Workflow: Manual Transfer of measurement files to connected server

INFORMATION!

Do not turn off the device during the download process!

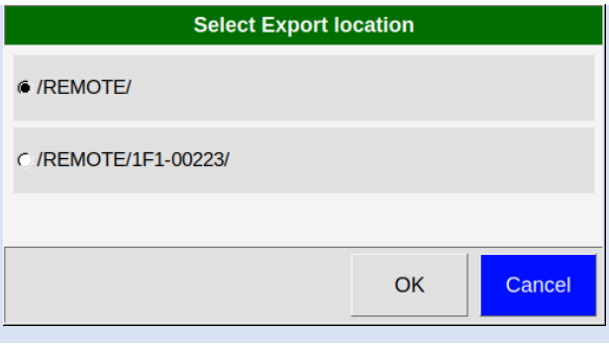
1



Open page:
System › **Transfer**.

Press:
Copy Remote.

2



A confirmation dialog opens.
Select the storage location.

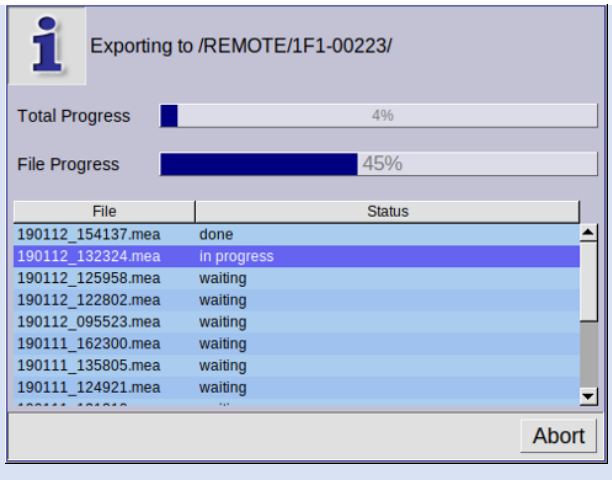
Press **OK** to start the process.

INFORMATION!

All internally stored measurements are transferred.

The process can be stopped at any time

3



Wait until the exporting process is completed.

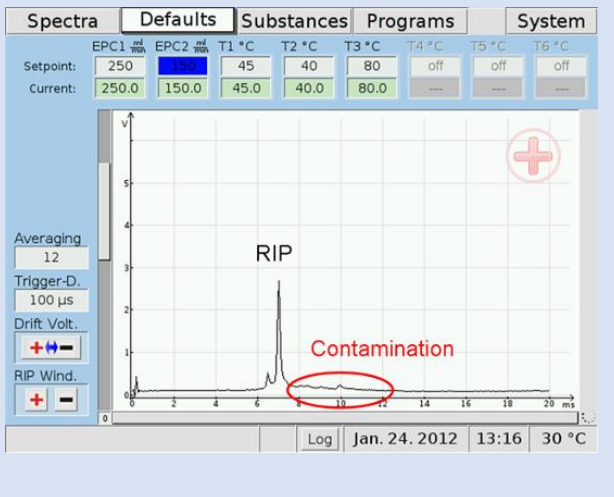
The measurement files has been downloaded.

8.20 Workflow: Start Cleaning mode

INFORMATION!

In case of contamination it is helpful to activate the cleaning mode to clean the system.

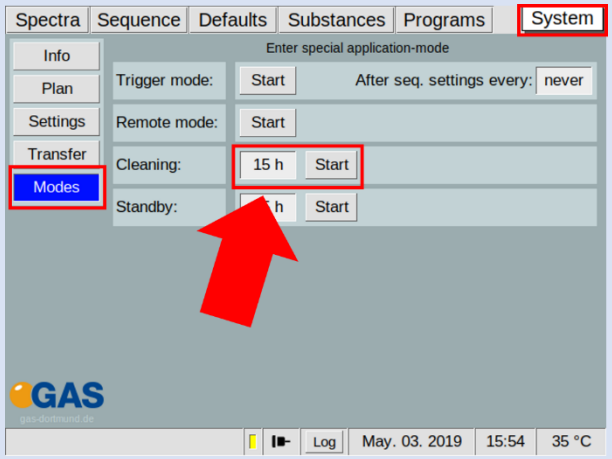
1



In case of contamination it is helpful to activate the cleaning mode to clean the system.

The frequency of cleaning interval is depending on the character and quantity of the samples.

2

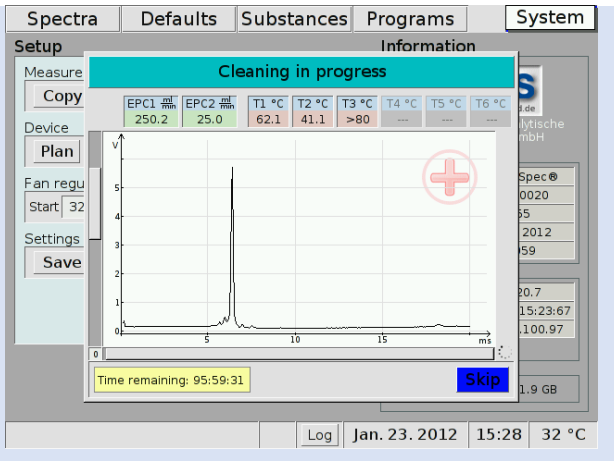


Select **System** › **Modes** › **Cleaning [x h]** and set the cleaning duration time.

Select **Start** to start the cleaning process.

All temperatures are set up to their maxima.

3



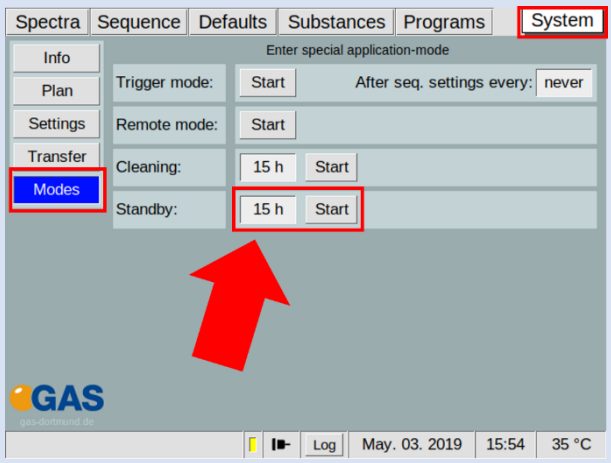
During the cleaning process a Cleaning window appears.
During this process no other activities can be executed.
This process can be skipped at any time.

8.21 Workflow: Start Standby mode

INFORMATION!

It is recommended not to switch off the device during measurement breaks. Using the Standby mode ensures the cleanness of the system and a quick readiness to measure.

1

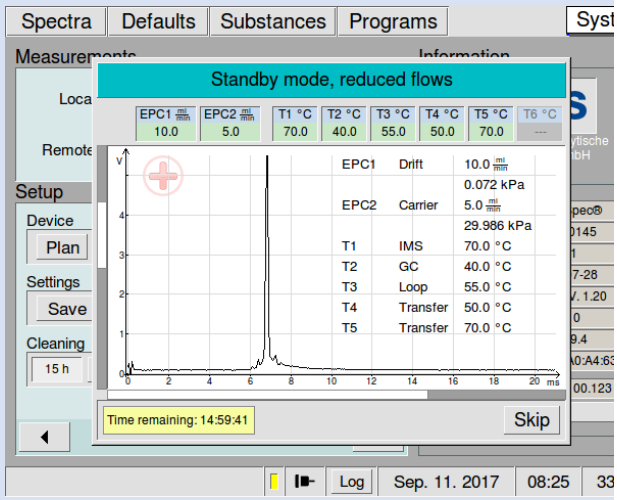


Select **System** › **Modes** › **Standby [x h]** and set the standby duration time.

Select **Start** to start the Standby process.

Driftgas (EPC1) is set to **10 ml/min** and Carriergas (EPC2) is set to **5 ml/min**.

2



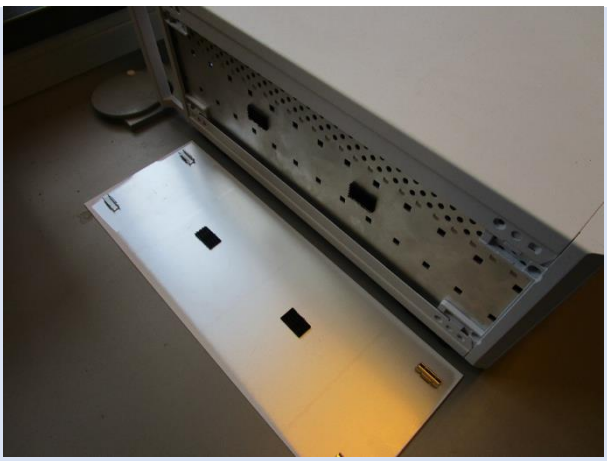
During the standby process a **Standby Window** appears.
During this process no other activities can be executed.
This process can be skipped at any time.

8.22 Workflow: Remove the Housing Cover

DANGER!

Before all work on the device switch off the device and pull out the power plug!

1		Switch off the device and pull out the power plug.
2a		Open the side-covers of the case carefully using a screwdriver.
2b		Remove the side-covers of the case carefully

2c		Removed side-cover.
3a		Open the top-cover of the case carefully using a screwdriver.
3b		Remove the top-cover of the case carefully.

4		Device without top cover.

8.23 Workflow: Change Capillary Column

DANGER!

Before all work on the device switch off the device and pull out the power plug!

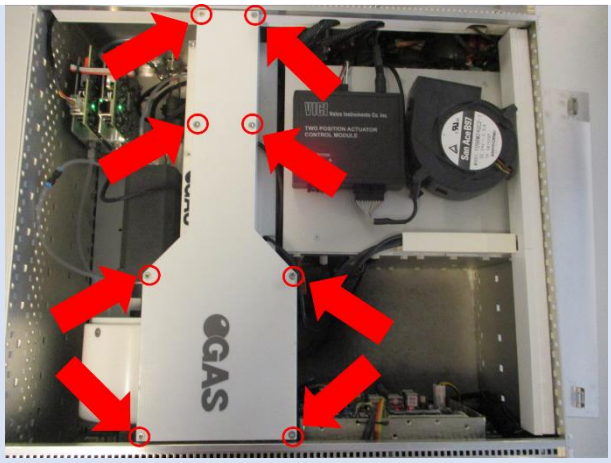
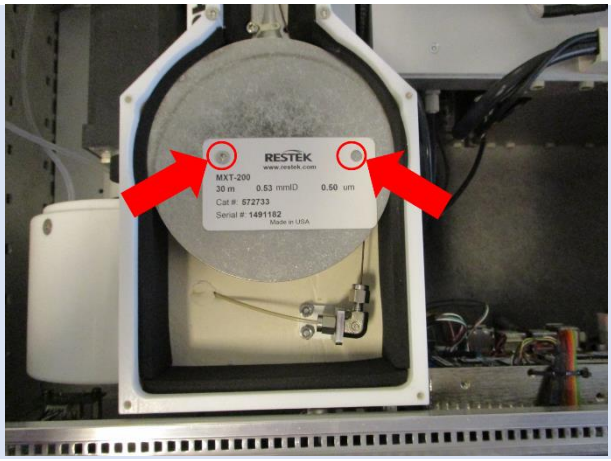
1

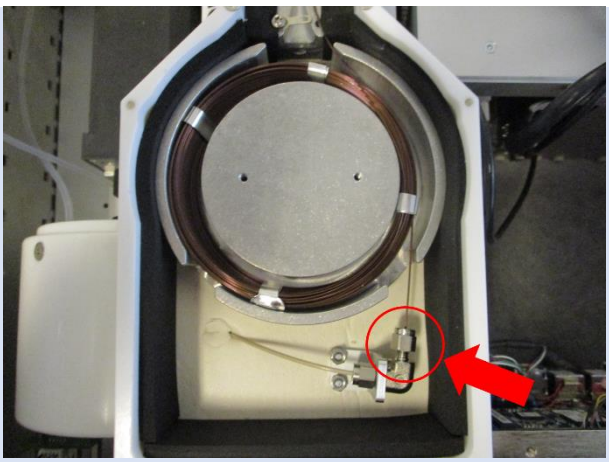
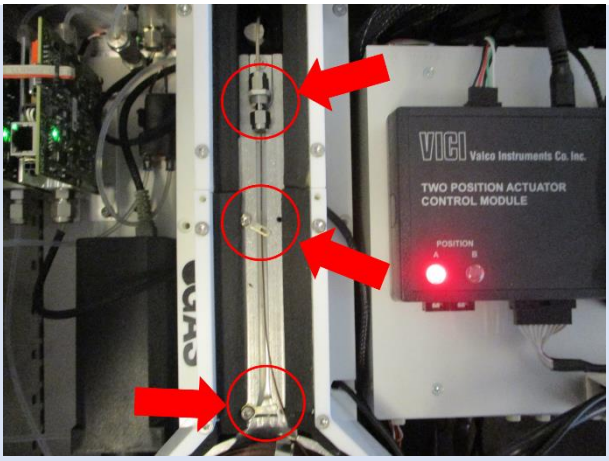
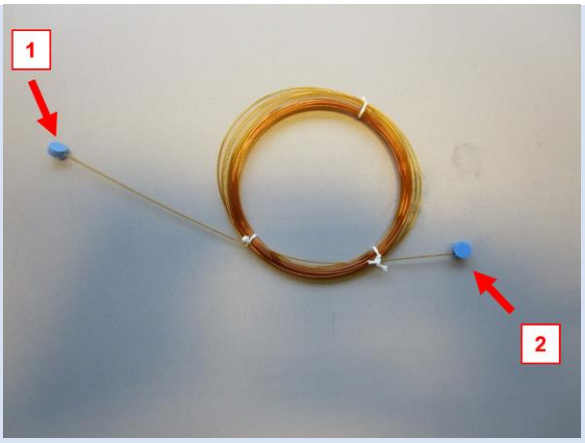
Necessary tools:

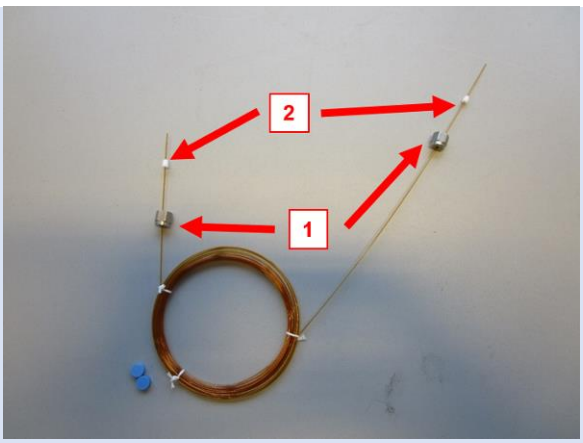
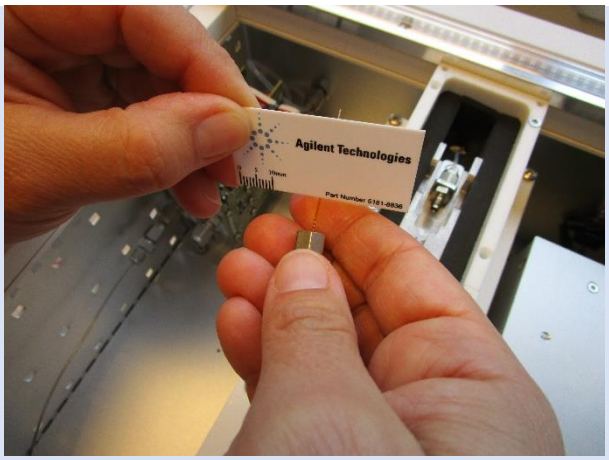
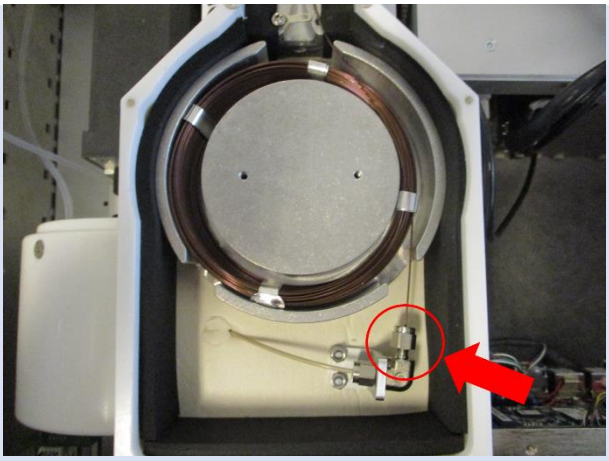
1. Small slotted screw driver
2. T10 Torx screwdriver
3. 8mm wrench
4. 1/16 “ Swagelok srew connections
5. Teflon Ferrule with hole (depending on the column dimensions)
6. Column cutter
7. Capillary column

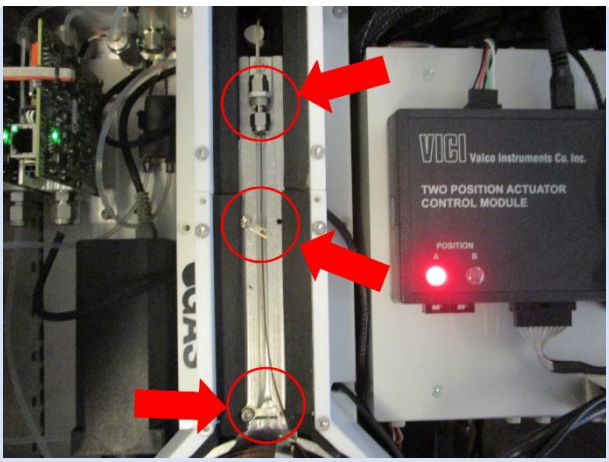
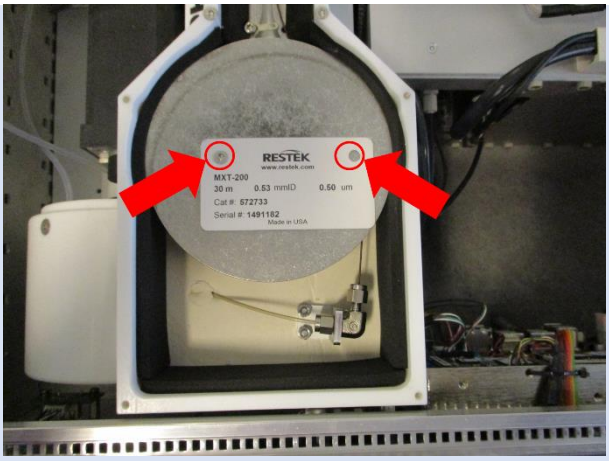
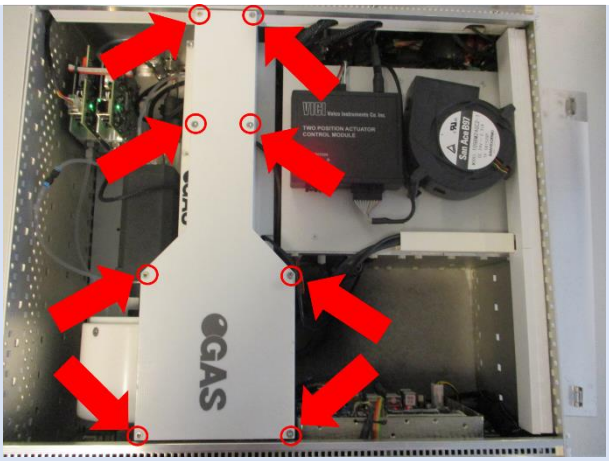
2

Switch off the device and pull out the power plug.

3		Remove the top cover. For detailed information see **Workflow: Remove Housing Cover**
4		Release all screw of the oven-cover and remove it.
5		Release all screw of the inner oven-cover and remove it.

6		Open the capillary-column-connectors using a 8 mm open-end-wrench.
7		Open the capillary-column-connectors using a 8 mm open-end-wrench. Also open the transfer line securing holder. Remove the capillary column.
8		Remove the blind bolts (1) + (2) of the capillary column

9		Insert the 1/16“ screw connectors und the Teflon-ferrules with hole. **Ensure that the distance between ferrule and column end is about 5 mm.**
10		Put the new capillary column into the oven. If necessary cut the ends of the column.
11		Connect the capillary-column-connector using two 8 mm open-end-wrench.

12		Connect the capillary-column-connector using two 8 mm open-end-wrench. Also close the transfer-line securing holder.
13		Mount the screws of the inner oven cover. Make sure that the column labeling is screwed on.
14		Mount the screw of the oven cover. Attach the top cover, the bottom cover and the side cover. Install all connections and switch on the device.

8.24 Workflow: Change high voltage circuit board

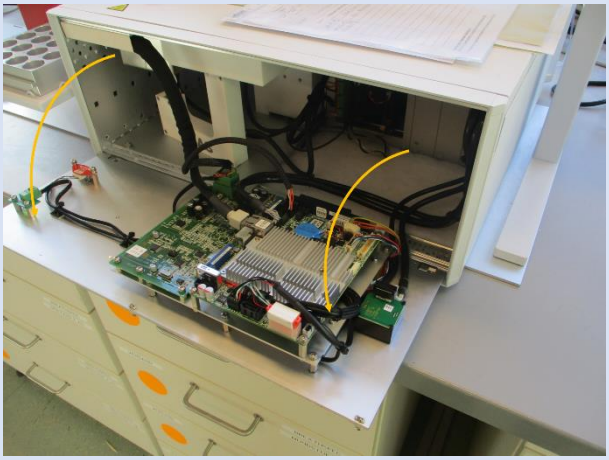
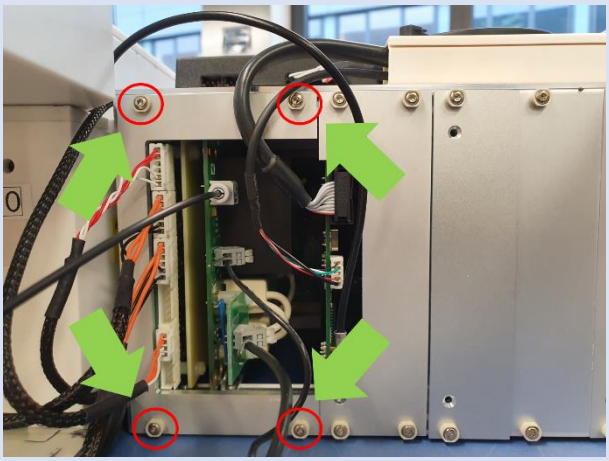
INFORMATION!

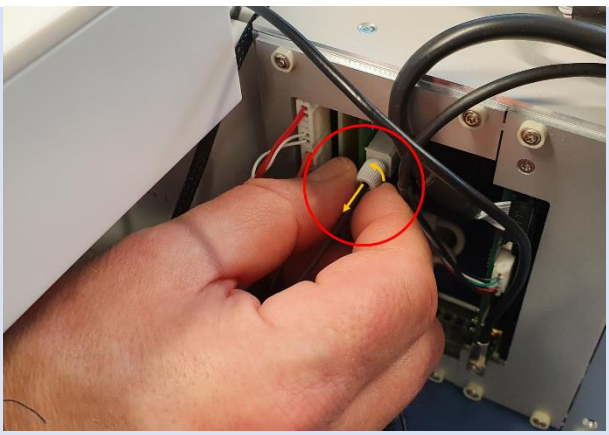
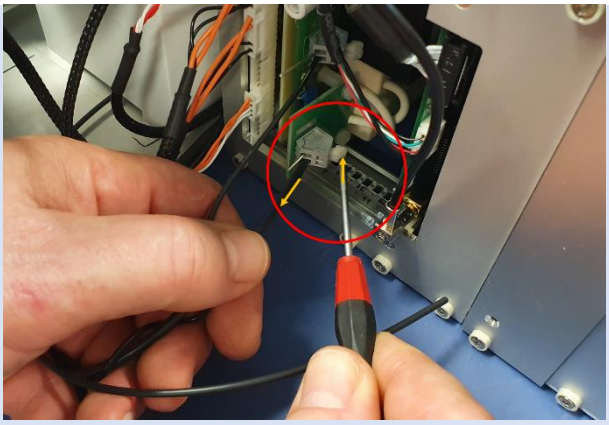
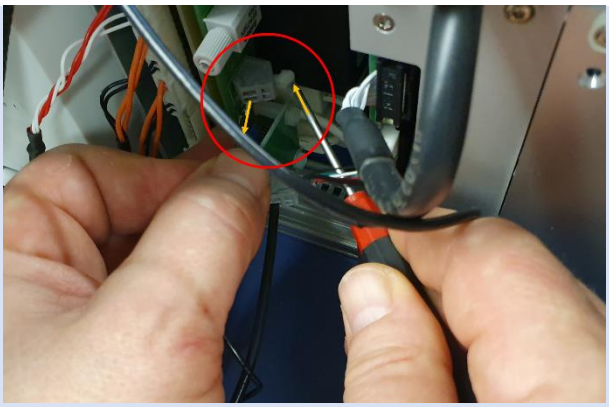
Only authorized, trained and technically instructed people are allowed to do these work steps.

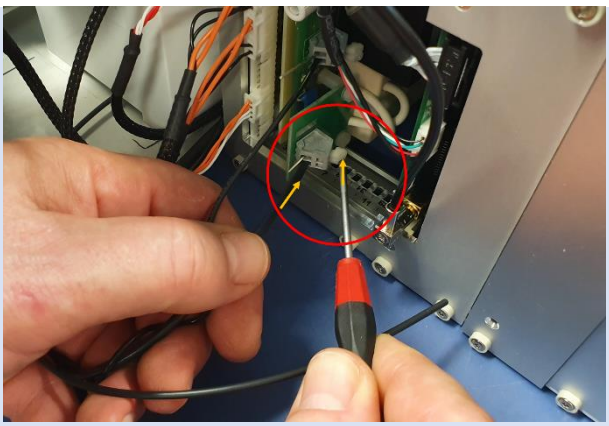
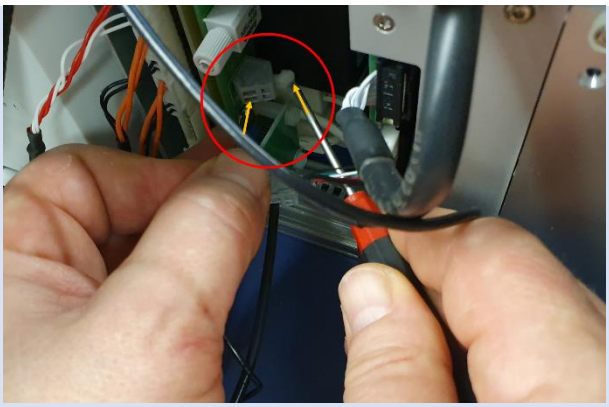
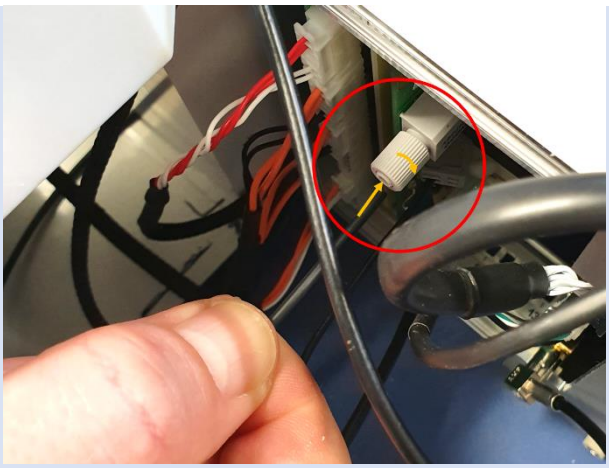
DANGER!

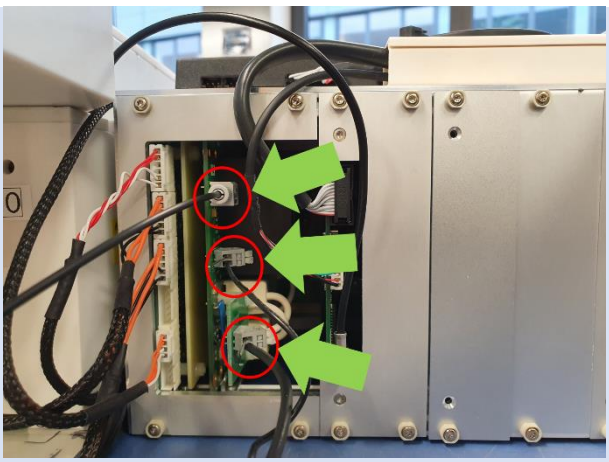
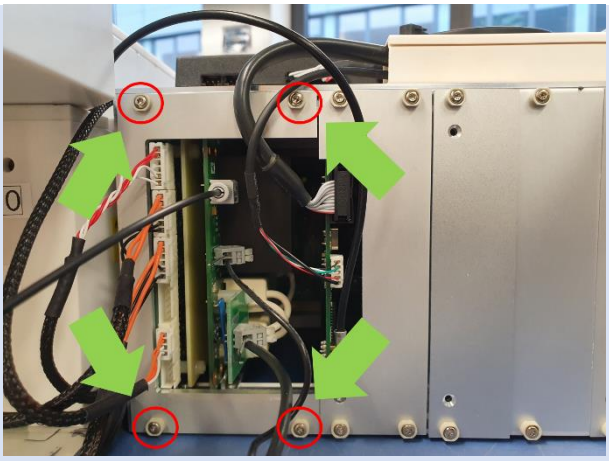
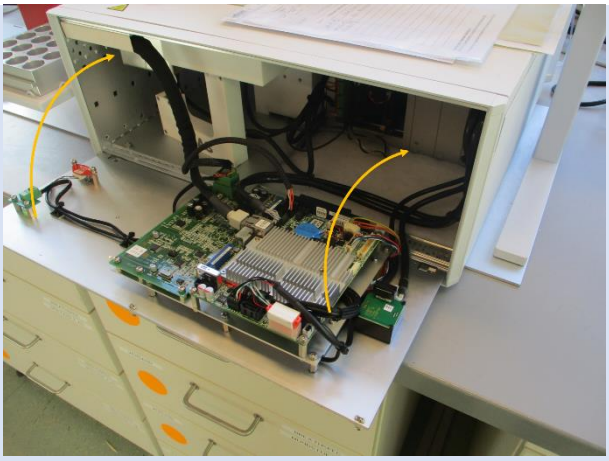
Before all work on the device **switch off the device** and **pull out the power plug!**

1		Switch off the device and pull out the power plug.
2		Loosen three Screws at the front of the device.

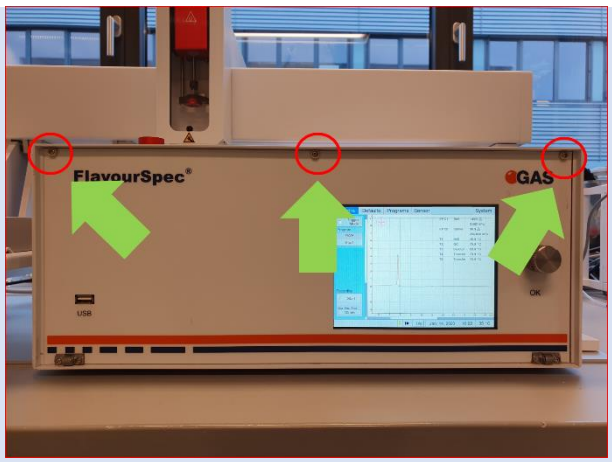
3		Remove the top cover. For detailed information see **Chapter 8.22 Workflow: Remove Housing Cover** .
4		Open the front panel.
5		Loosen four srews with T8 screwdriver and remove the coverplate.

6		Loosen the nut from transmitter and pull out fibre-optical-cable.
7		Push the button and pull out high voltage wire
8		Push the button and pull out ground wire
9		Pull the circuit board out of the casing profile

10		Insert the new circuit board
11		Push the button and reinsert the ground wire
12		Push the button and reinsert the high voltage wire
13		Reinsert the optical fiber cable and tighten the screw connection.

14		View of the three connected wires.
15		Replace the cover plate and tighten the four screws.
16		Close the front plate and attach the top cover..

17



Tighten the three screws of the frontplate.

8.25 Workflow Firmware Upgrade

The firmware of G.A.S. IMS devices can be upgraded by the user with an upgrade file – named update.gas - provided by G.A.S.

This file has to be put on an empty USB storage device (e.g. ‘USB stick’ / ‘USB thumb drive’) formatted as a FAT32 file system.

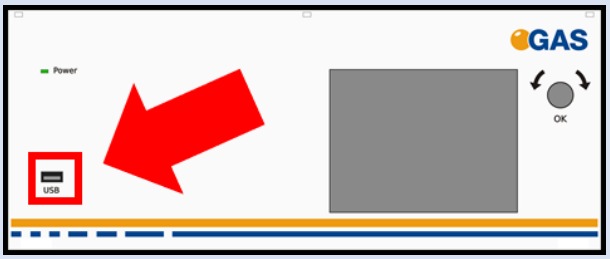
INFORMATION!

The USB storage device must be formatted to FAT32. Consult your system administrator on formatting USB devices.

INFORMATION!

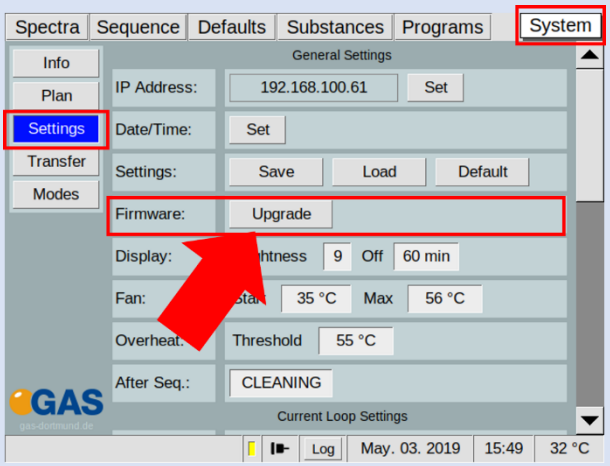
Do not turn off the device during the upgrade process!

1



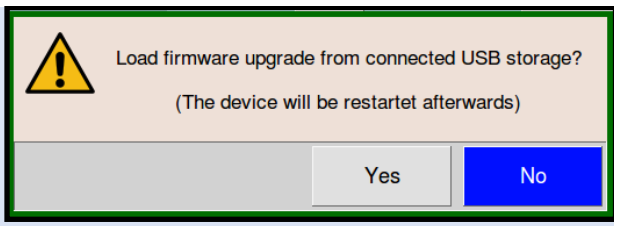
Connect the **USB device** (**FAT32-formatted**) with the upgrade file – named **update.gas** - provided by G.A.S. to the **USB socket** at the front side of the housing.

2



Open page:
System › **Settings**.

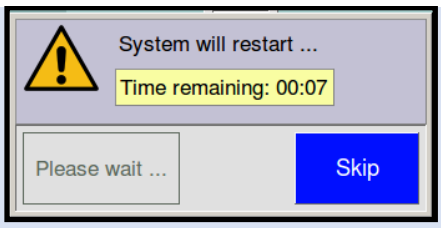
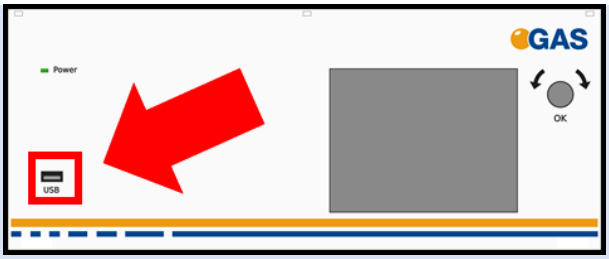
Press:
Firmware › **Upgrade**.

3		A confirmation dialog opens. Press **Yes** to start the process.

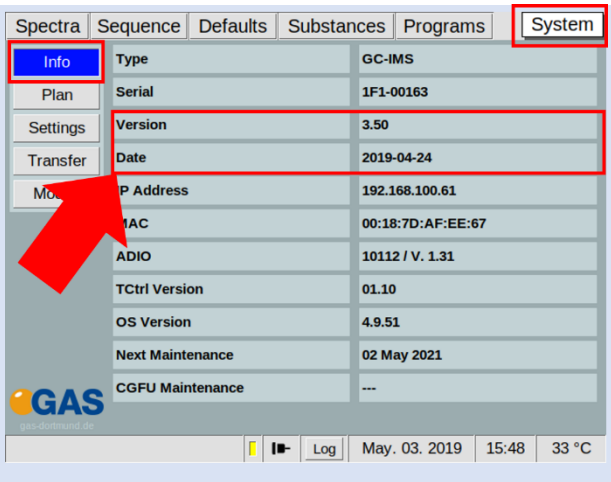
INFORMATION!

Do not turn off the device during the upgrade process!
Do not remove the USB device!

The upgrade process will take one minute or more depending on the tasks that are perfomed during the process.

4		Wait until the process is completed and a system restart dialog opens.
5		Wait for the device to restart or press **Skip** to restart the device immediately.
6		**Now:** Remove the connected USB device from the **USB** socket at the front side of the housing.
7		Wait until the device has started and the user interface is visible on the screen.

8



Open page:
System › **Info**.

Verify that the new firmware version has been installed.

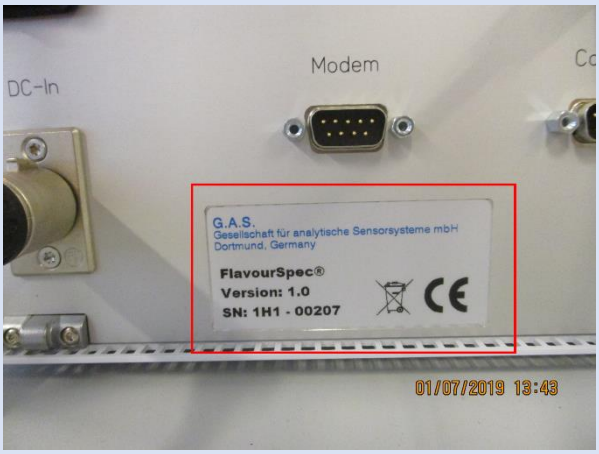
The device firmware has been upgraded.

8.26 Workflow: Creating diagnostic information for support

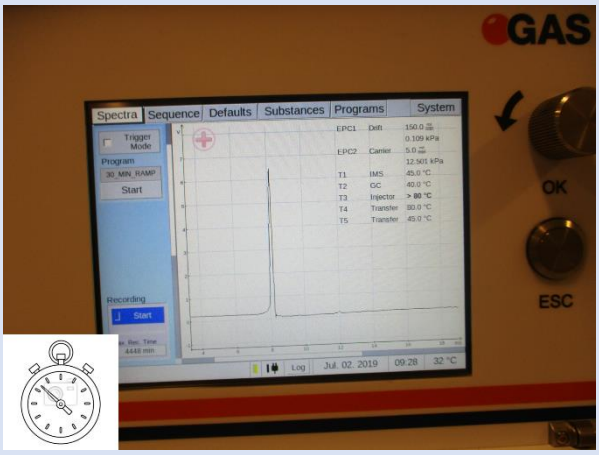
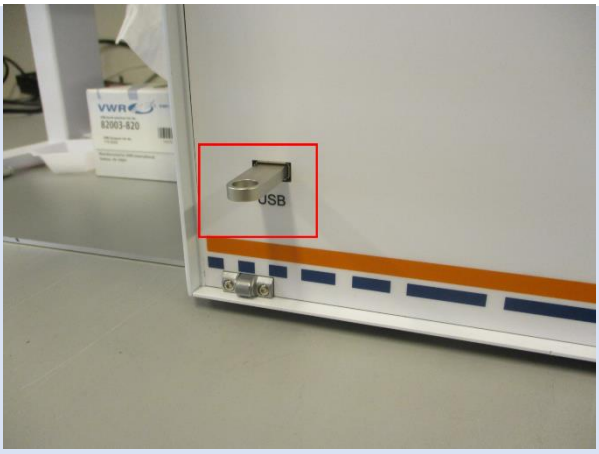
INFORMATION!

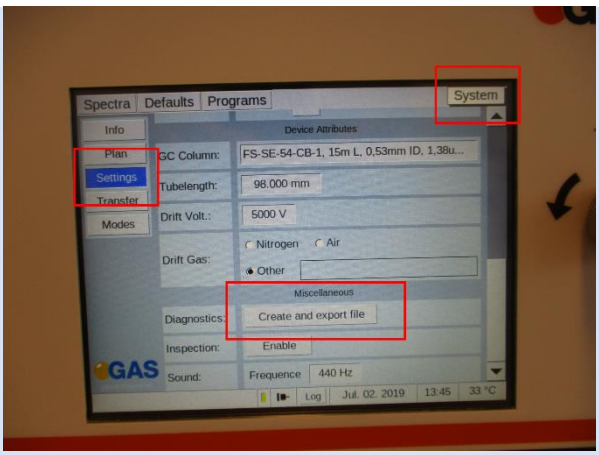
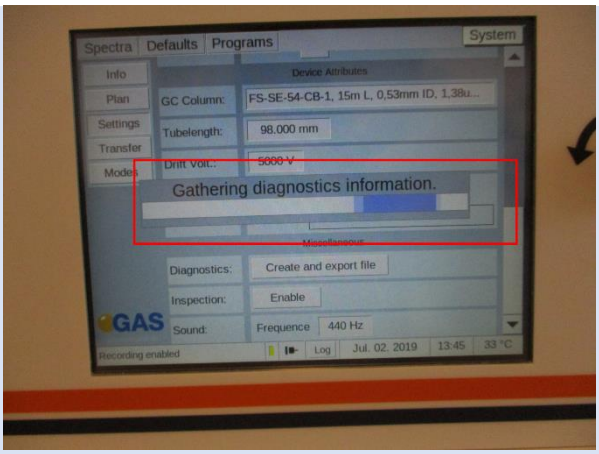
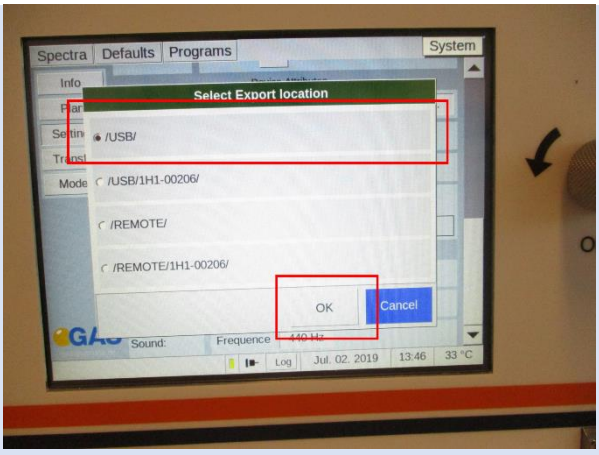
The following steps are necessary to compile the required diagnostic information. Please stick on consecution as listed below.

1

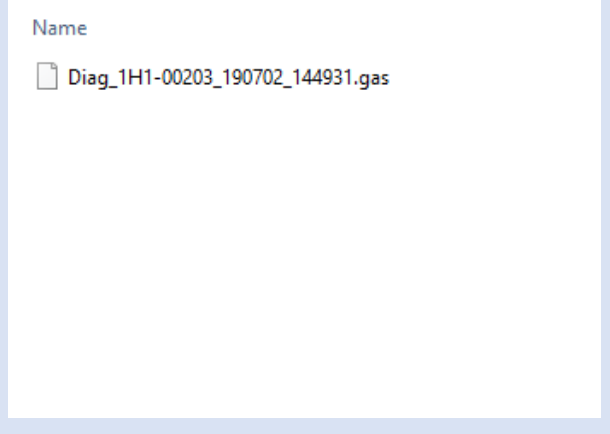


Take a picture of the instrument label on the rear side.

2		Switch on the device. Power LED front and switch (rear) have to be illuminated.
3		Inform how long it takes to boot up and to display of GUI in seconds. In case of error take a photo of the display.
4		Insert a **FAT32 formated USB-stick** into the **USB slot** at the front of the device.

5		In **System Window** > **Transfer** select Settings and start the diagnostic file compilation by selecting the **Create and Import file Button**.
6		The diagnostic file is created.
7		Select Export Location /USB/ and press **OK**.

8



Send the **diagnostic file** and the **photos** taken by user by data transfer to support@gas-dortmund.de

8.27 Workflow: Packing the FlavourSpec unit for return transport

INFORMATION!

It is recommended to **use the original transport box** for a safety return transport.

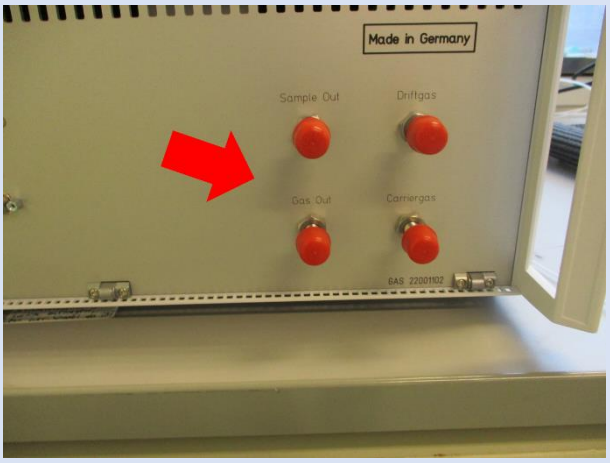
INFORMATION!

A suitable transport carton is available from G.A.S.

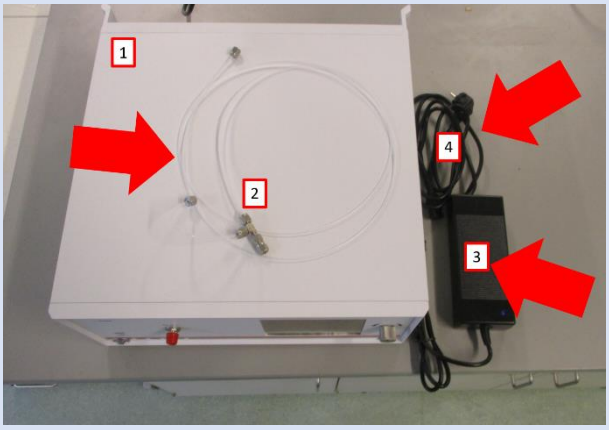
INFORMATION!

It is recommended **to send the transport box on palett** for a safety return transport.

1



Close all gas connections with the red caps on the rear side of the device.

2		Minimum scope of delivery for the return transport: Device 1, Hoses 2, power supply 3 and plug 4
3		It is recommended to return the system in the original box and on palett. Further accessories can be supplied optionally.

8.28 Workflow: Packing the FlavourSpec unit with PAL3 autosampler for return transport

INFORMATION!

It is recommended to **use the original transport box** for a safety return transport.

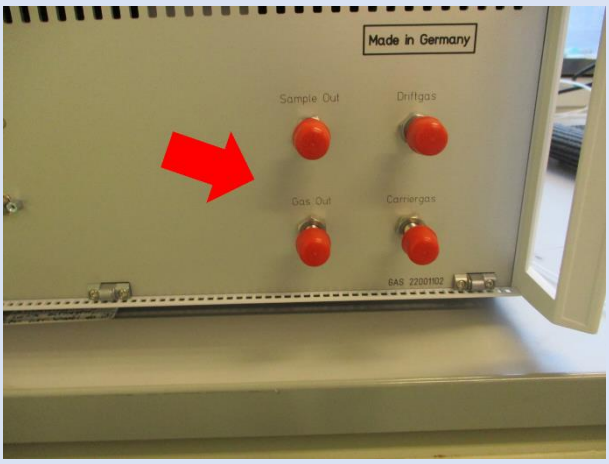
INFORMATION!

A suitable transport carton is available from G.A.S.

INFORMATION!

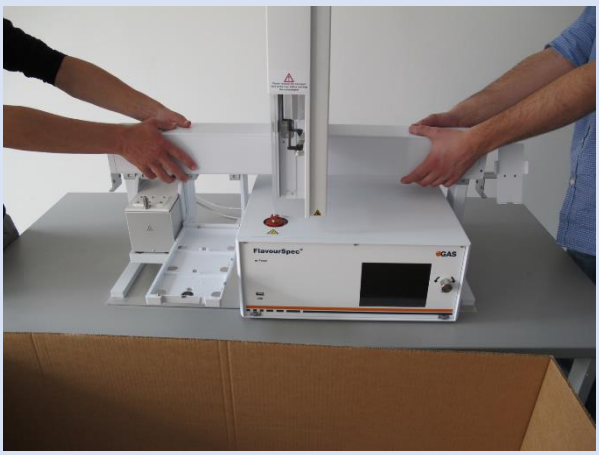
It is recommended to **to send the transport box on palett** for a safety return transport.

1

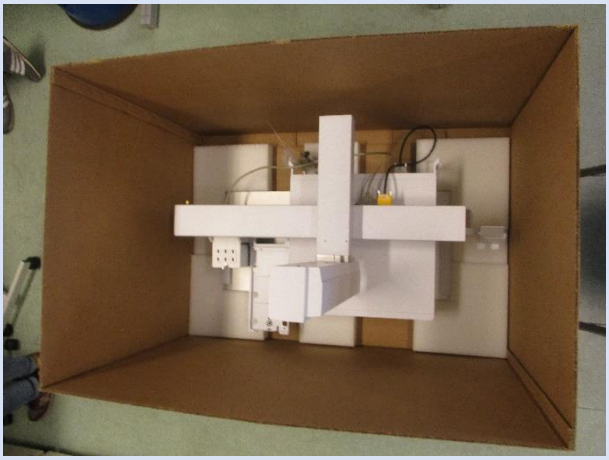
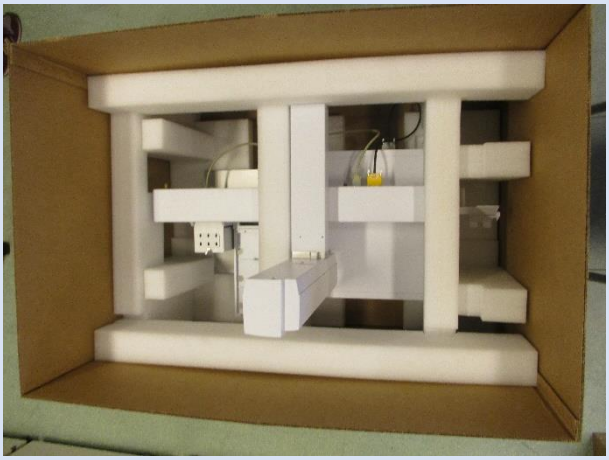
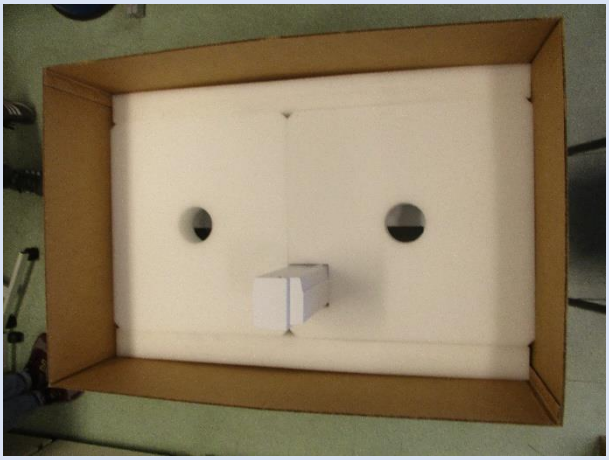


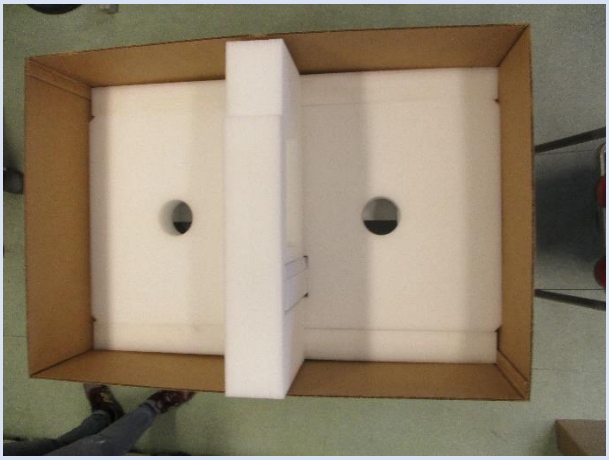
Close all gas connections with the red caps on the rear side of the device.

2



Lift the device into the box

3		Place the device into the box.
4		Insert the big foam spacer.
5		Insert both foam spacers.

6		Insert the foam spacer.
7		Insert both accessories boxes,
8		Insert both cardboard spacers and put the cover on.

INFORMATION!

Please supply both power supply units, all connecting cables and the complete tubing with the unit.

8.29 Workflow: Manual modification of the sample description attribute.

The attribute sample description can be changed manually in the measurement file. For this purpose a text editor is required, e.g. the free editor **Notepad++** [https://notepad-plus-plus.org/].

INFORMATION!

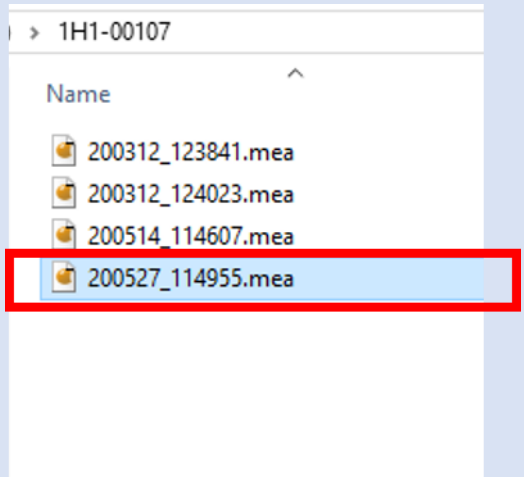
Only authorized, trained and technically instructed people are allowed to do these work steps. Please contact us in any case before you start working.

Only use the recommended text editor notepad++ [https://notepad-plus-plus.org/].

Wrong input can corrupt the measurement file.

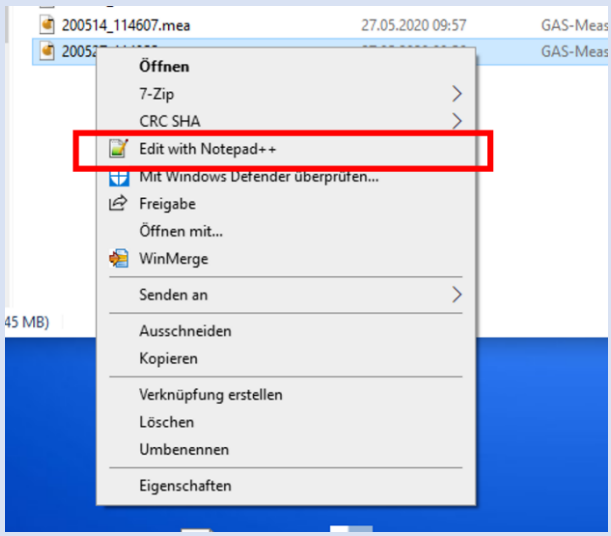
Only work with a copy of the measurement file.

1



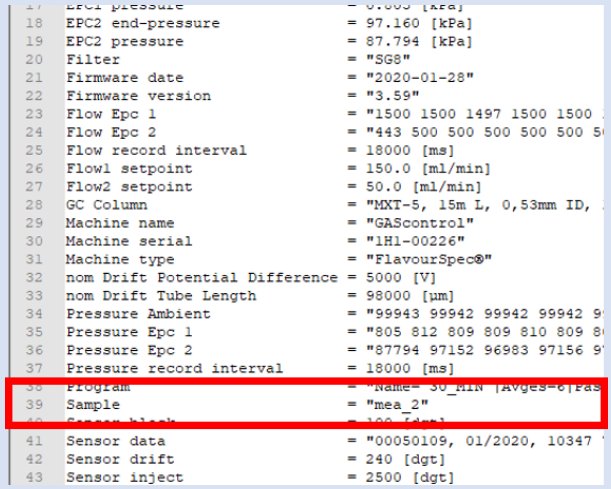
In windows explorer **select a copy** of the measurement file.

2



With **right click** on measurement file select **Edit with Notepad++**.

3



In the opened measurement file find the attribute **Sample**.

4

Change sample description **(Entry between the quotation marks).**

Save the measurement file.

9 Appendix

9.1 Technical data: FlavourSpec

Dimensions	• Housing: 19”-compatible • Height: 184.5 mm • Width: 449 mm • Depth 435 mm • Weight: ca. 15 kg
Operational conditions	• Temperature range: +5 °C … +40°C • Humidity: 0-90 % RH, non-condensating
Electrical Connectors	• 2 x RS232 DE9 plug • 1 x I/O DA15 socket • 1 x Ethernet RJ45 IEEE 802.3 100BASE-T • 1 x USB 2.0 Host (USB A Connector) • 1 x XLR 3-pole male, for power supply
Power Supply	• Input line voltage: Grounded AC, 85 to 264V • Input line frequency: 47-63 Hz • Input current: < 2.8 A • Output voltage: 24 VDC • Output current: 9.2 A internal • Power consumption: < 221 Watt
Cooling	• Axial ventilator, temperature-controlled, max. 5.5 m^3/h
Gas connectors	• 3 mm stainless steel Swagelok-connector.
Internal hoses	• PFA
IMS-parameters	• Drifttube lenght: 53 mm • Electrical field strenght: 500 V/cm • Resolution: ~ 45 • Operating temperature: 35–80°C
Ionisation source	• Radioactive - Tritium H^3 (ß⁻ Radiation)

Data aquistion	• Sample-Rate: 150 kHz • Resolution: 14 bits • Trigger-duration: 100 µs • Trigger-repetition rate: 30 ms • Transimpendance: 3 V/nA typ.
Drift voltage	• 2,7 kV Positive/negative Driftvoltage switchable
Sampling system	• Injector - Splitless • Operation temperature: 35 – 80 °C (default 45 °C) • Temperature display accuracy: ± 1°C • Temperature control accuracy: ± 0,1 K
Data storage	• Internal storage volume • Data transfer via LAN-connection via SMB, SFTP or TFTP (G.A.S. variant of TFTP)
Operation	• 6.4” TFT Touchscreen • Pushable rotary knob

Standard Gaschromatic Capillary Column (Other Column types only on request)	• **Standard Stationary Phase:**
	  • (5%-diphenyl, 95% dimethylpolysiloxane)
	• **Capillary column**
	  • Identification: MXT-5
	  • Film thickness: 1 µm
	  • Column lenght: 15 m
	  • ID: 0.53 mm
	  • OD: 0.68 mm

Column oven	• Operation temperature: 35 – 80 °C • Temperature-display accuracy: ± 1°C • Temperature-control accuracy: ± 0.1 °C
Flow Control EPC1 **Driftgas**	• Type: Differential pressure control • Input Pressure: 3.0 bar (300 kPa) – 6.0 bar (600 kPa) • Output Pressure Stability: 0.01% • Output Pressure Linearity: 0.05%

	• Operation flow rates: 0 – 500 mL/min
Flowcontrol EPC2 **Carriergas**	• Type: Differential pressure control • Input Pressure: 3.0 bar (300 kPa) – 6.0 bar (600 kPa) • Output Pressure Stability: 0.01% • Output Pressure Linearity: 0.05% • Operation flow rates: 0 – 150 mL/min (depending on the GC-Column dimensions)
Consumables	• Gas nitrogen 5.0 quality or Synthetic air 5.0 quality
Cleaning mode	• IMS, column and sampling system are heated up to > 80°C (~ 100 °C). • Injector is heated up to > 80°C (~ 160°C).

9.2 Technical data: PAL 3 Series II

Dimensions	• Height: 770 mm • Width: 795 mm • Depth: 990 mm • Weight: ca. 24 kg
Operational conditions	• Temperature range: +5 °C … +40°C • Humidity: 0-80 % RH, non condensing
Power Supply	• Input line voltage: Grounded AC, 100 - 240 V • Input line frequency: 50-60 Hz • Input power: ~4 A • Output voltage: 36 VDC • Output current: 5,555 A • Power consumption: 200 Watt (max.)
Agitator	• Temperature controlled, 35–200 °C, 250–750 rpm

Sample capacity	• 60 Positions (6 x 10) for 20 ml Headspace Vials with 23 mm OD; 78 mm Height(Standard) and for 10 ml Headspace Vials with 23 mm AD; 47 mm Height (optional)
Syringe	• Syringe size: 1,0ml (Standard); 2,5 / 5,0 ml (optional)
Consumables	• Gas Nitrogen 5.0 or synthetic air 5.0 • Gastight syringe • 20 ml Headspace Vials • Magnetic caps for 20 ml Headspace Vials

9.3 Technical data: I/O Interface

Device Connector Specification		
Analog output	Output type Non-loaded voltage Maximum output signal Maximum output load (burden resistance) Accuracy Linearity error Temperature coefficient Output Ripple (RMS)	Isolated active current output 0-22 mA < 20 V < 25 mA 500 Ohm better than 0.5 % (t.b.d) (t.b.d. 0,02%K) T (.b.d. < 10 µA)
	INFORMATION! Output can be set to 0-10 V voltage output by connecting internal 500 Ohm shunt restor.	
Digital input	Input type Off-state voltage On-state voltage Input current	Isolated opto-coupler input < 1 V 5 .. 30 V < 20 mA depending on input voltage
Digital output	Output type Maximum open circuit voltage Maximum on-state saturation voltage Maximum on-state current	Isolated passive transistor output 30 V 2 V 20 mA
Isolation	Isolation type[1] Surge voltage category Pollution degree Rated insulation voltage [1] All in-/outputs are isolated from instrument	basic insulation according to EN 61010 II 2 100 V DC or 100 Vrms AC
Device Connector Pinout		

Connector type	D-Sub DA-15 female	
Analog output	Return Internal shunt Current output [2] Connect to Pin 9 to select 0-10 V voltage output	Pin 1 Pin 2[2] Pin 9
Digital input	Negative Positive	Pin 13 Pin 5
Digital output	Negative Positive	Pin 6 Pin 4

INFORMATION!

- Do not connect any other pins.

9.4 Ionisiation Source Specification

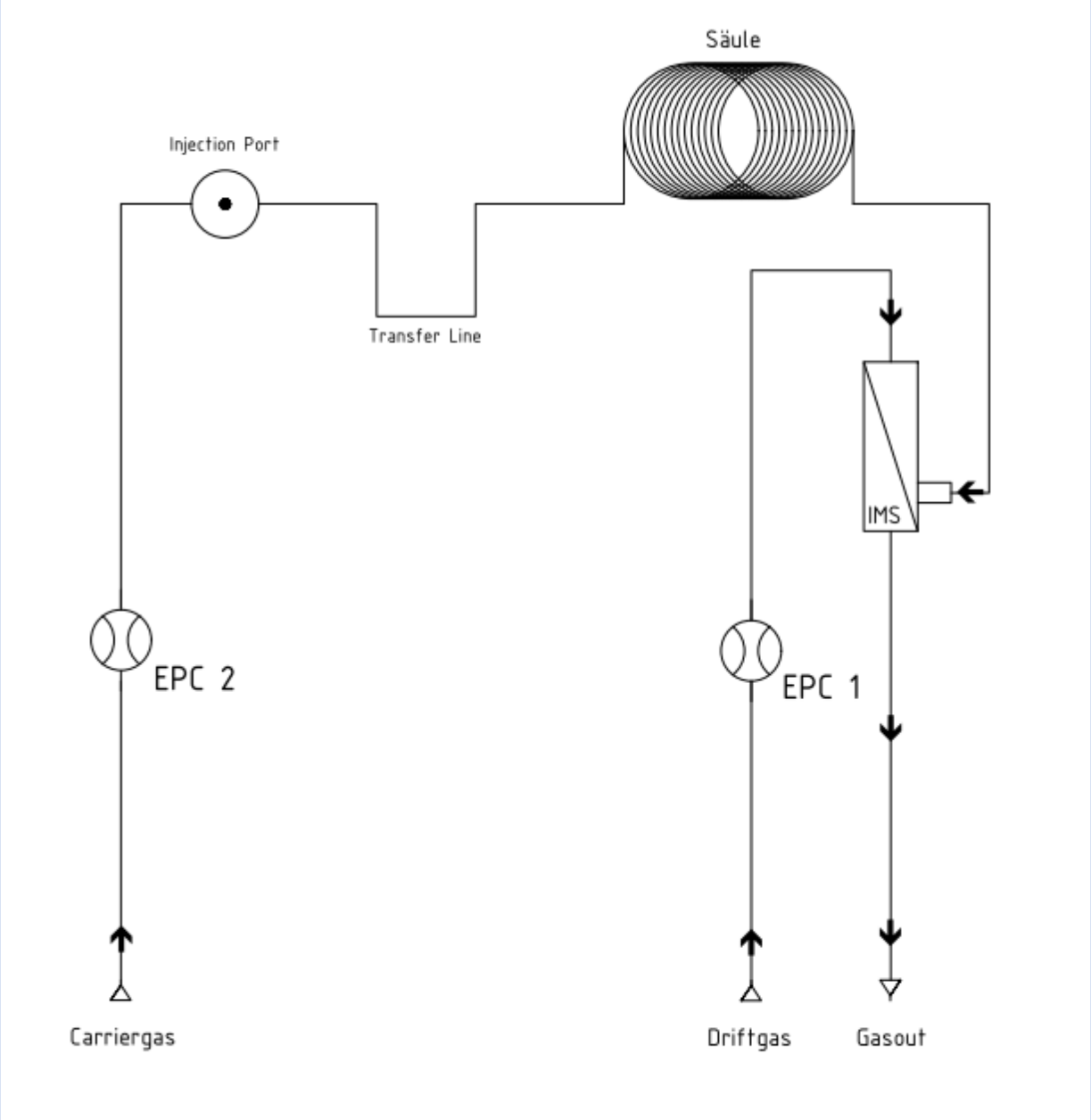
INFORMATION!

The permission and exemption limits are regulated by the Radiation Protection Ordinance and the European Union Council Directive 96/26/EURATOM in accordance with the regulations of the International Atomic Energy Authority (IAEA).

Source Type	**Tritium H^3, Solid-state bonded**
Activity	Below the exemption limit of 1 GBq for tritium acc. to Table B (column 2) of Article 26, of the Directive 2013/59 EURATOM of December 5th, 2013
Radiation Type	**β^--Radiation**
Radiation Energy	**Average energy: 5.68 keV** Maximum energy: 18.7 keV
Full Duration Half Maximum (FDHM)	**12.3 years**
Bracking radiation	**2×10^{-7} (mSv / h x GBq)** $H_{Brake} = A \times h_{Br} \times (1m / r)^2$ $hBr = 0.257 \times 10^{-4} \times (E\beta max / MeV) \times 2$
Attenuation of Radiation	**Air: 4 mm** Water: < 100 µm Tissue: < 100 µm

	Below the exemption limit of a dose rate of 1 µSv/h at a distance of 0.1 m from any accessible surface of the apperatus acc. to Article 26, of the Directive 2013/59 EURATOM of December 5th, 2013
Mounting Location and Type	**Fixed inside the device and not accessible from the outside. The source cannot be touched directly.**

9.5 Technical drawing: Internal Gasflow



9.6 PAL LED Status LED

INFORMATION!

For detailed information refer the CTC PAL RSI User Manual

LED Color	LED Status	Specification
Successful Booting Process		
Off	Off	Off
Yellow	Blinking fast	PALsystems booting
Blue	Blinking fast	Updating Software
Yellow	Blinking normal	Application software initialized
Green	Blinking normal	Application working
Green	Steady ON	Application Ready
Yellow	Steady ON	Booting Process Errors
LED Status during Operation		
Yellow	Blinking normal	Configuration error
Yellow	Steady ON	Activity execution error
Blue	Blinking normal	Backup / Restore executed
Blue	Steady ON	Manual operation (waiting for inputs)
Green	Blinking normal	PALsystem working
Green	Steady ON	PALsystem Ready / Idle
Yellow	Steady ON	Fatal error

9.7 LED Status at PAL Control PCB

INFORMATION!

For detailed information refer the CTC PAL RSI User Manual

LED Color	LED Status	Specification
Successful Booting Process		
Off	Off	Off
Red	Steady ON	PALsystems booting
Red	Blinking fast	Software OS Initialized
Green	Blinking normal	Application software initialized
Green	Steady ON	PALsystem Ready

9.8 FlavourSpec Defaults – Parameter

Parameter	G.A.S. Standardvalue	Range
EPC1	**150 ml/min**	Off; 1ml/min – 500 ml/min
EPC2	**5 ml/min**	Off; 1ml/min – 150 ml/min
T1	**45 °C**	Off; 5 °C – 80 °C
T2	**40 °C**	Off; 5 °C – 80 °C
T3	**80 °C**	Off; 5 °C – 80 °C
T4	**80 °C**	Off; 5 °C – 80 °C
T5	**45 °C**	Off; 5 °C – 80 °C
T6	**off**	Off; 5 °C – 80 °C
Averaging	**6**	Off; 1 - 99
Trigger-D.	**100 µs**	10 µs – 2000 µs

9.9 FlavourSpec Program – Parameter

Parameter	G.A.S. Standardvalue	Range
Time	**---**	00 min 00 sec 000 ms – 59 min 59 sec 980 ms
E1	**150 ml/min**	0 ml/min – 500 ml/min
E2	**5 ml/min**	0 ml/min – 150 ml/min
R	**---**	0,0 ml – 5,0 ml

9.10 PAL RSI Headspace Methodsparameter

Parameter	G.A.S. Standardvalue	range
Agitator	**Agitator 1**	None; Agitator 1
AgitatorSpeed	**500 rpm**	60 rpm – 750 rpm
AgitatorStandbyTemp	**60,0 °C**	30,0 °C – 200,0 °C
FillingStrokesCount	**0**	0 – 15
FillingStrokesVolume	**1,0 ml**	0 – 2,2 ml
GasChromatograph	**GC1**	None; GC1
IncubationTemperatures	**60,0 °C**	30,0 °C – 200,0 °C
IncubationTime	**20,0 min**	0,1 min – 600,0 min
InjectionFlowReate	**51,0 ml/min**	1,0 ml/min – 100,0 ml/min
InjectionSignalMode	**PlungerUp**	PreInject, PlungerUp
Injection	**Injector 1**	None; Injector 1
InjectionPenetrationDepth	**35,0 mm**	15,0 mm – 50,0 mm
PostInjectionDwellTime	**0,5 s**	0,0 s – 60,0 s
PostInjectionPurgeTime	**10,0 s**	0,0 s – 600,0 s

PreInjectionDwellTime	**0,5 s**	0,0 s – 60,0 s
PerInjectionPurgeTime	**5,0 s**	0,0 s – 60,0 s
SampleVialDepth	**15,0 mm**	10,0 mm – 50,0 mm
Syringe	**HS 1**	None; HS 1
SyringeTemperatures	**80,0 °C**	40,0 °C – 150,0 s

INFORMATION!

- Teach the Injector Position after every tool change.
- The Injection Penetration Depth Value must be 35 mm. Do not modify

9.11 PAL RSI ITEX Methodsparameter

Parameter	**G.A.S. Standardvalue**	**range**
ITEX Tool	**ITEX 1**	None; ITEX 1
Analysis Time	**5,0 min**	0,0 min – 600,0 min
Sync Before Incubation End	**0,0 min**	0,0 min – 600,0 min
GasChromatograph	**GC1**	None; GC1
Trap Pre Cleaning Temp	**320 °C**	100 °C – 350 °C
Trap Pre Cleaning Time	**200,0 s**	0,0 s – 86400 s
IncubationTime	**20,0 s**	0,1 min – 600,0 min
IncubationTemp	**72 °C**	30,0 °C – 200,0 °C
Agitator	**Agitator 1**	None; Agitator 1
Heat Agitator	**X**	X; ☐

Wait for Readiness Agitator	**X**	X; ☐
AgitatorSpeed	**500 rpm**	60 rpm – 750 rpm
Extraction Strokes	**50**	0 - 1000
Trap Extraction Temp	**40°C**	30,0 °C – 150,0 °C
Syringe Temp	**45°C**	40,0 °C – 150,0 °C
AgitatorStandbyTemp	**60,0 °C**	30,0 °C – 200,0 °C
Wait for Readiness Syringe	**X**	X; ☐
Extracton Volume	**1000,0**	0,0 ml – 1300 ml
Extraction Aspirate Flow Rate	**15,0 ul/s**	10,0 ul/s – 1000,0 ul/s
Extraction Dispense Flow Rate	**200,0 ul/s**	10,0 ul/s – 1000,0 ul/s
Sample Refill Ratio	**10,0 %**	-
Vial Penetration Depth	**12,0 mm**	10,0 mm – 35,0 mm
Water Removal	**Disabled**	Disabled; Enabled
Water Removal Trap Temp	**90,0 °C**	40,0 °C – 150,0 °C
Water Removal Purge	**300,0 s**	0,0 s – 600,0 s
Water Removal Position	**None**	-
Desorb Temp	**300 °C**	50,0 °C – 350 °C
Injection	**Injector 1**	None; Injector 1
InjectionAspirate Flow	**10,0 ml/s**	1,0 ml/s – 1000,0 ml/s
Post Inject Delay	**5,0 s**	0,0 s – 600,0 s
Desorb Flow Rate	**100,0 ul/s**	5,0 ul/s – 1000,0 ul/s
Injection Penetration Depth	**35,0 mm**	10,0 mm – 35,0 mm s

Injection Penetration Speed	**50,0 mm/s**	1,0 mm/s – 100,0 mm/s
Injection Signal Mode	**Plunger Up**	Pre Inject; Plunger Up; Plunger Down
Trap Post Cleaning Time	**300,0 s**	0,0 s – 86400,0 s
Trap Post Cleaning Temp	**320,0 °C**	100,0 °C – 350,0 s

INFORMATION!

- Teach the Injector Position after every tool change.
- The Injection Penetration Depth Value must be 35 mm. Do not modify

9.12 PAL RSI Jobparameter

Parameter	G.A.S. Standardvalue	Range
First Sample Index	**1**	1 - 60
Last Sample Index	**60**	1 - 384
SampleRack	**Rack 1**	None; Rack1
SampleVolume	**0,3**	0,0 ml – 5,0 ml

INFORMATION!

- The Injection Penetration Depth Value must be 35 mm. Do not modify. The values for First Sample Index, Last Sample Index and SampleVolume must be set by the user.
- Set the Parameter SampleRack to Rack1.

9.13 Troubleshooting

9.13.1 Error message list

Error message	**Drift voltage supply.**
Description	*Drift voltage error*
Action	Fatal Error! Contact the G.A.S. service hotline.
Error message	**Can't save measurement.**
Description	*The measurement file could not be saved to the internal memory.*
Action	Export and save all Measurement of the internal storage and clear the storage. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**smb connection failed:**
Description	*Samba (Service Message Block SMB) connection failed.*
Action	Check network cable, network shares and IP-address. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**sftp connection failed:**
Description	*Secure File Transfer Protocol (SFTP) connection failed.*
Action	Check network cable, network shares and IP-address. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**No USB-Storage found.**
Description	*Mounting of the USB-Stick failed.*
Action	Ensure that a USB-Stick is insert.

	Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. If that still does not help contact the G.A.S. service hotline.
Error message	**Unable to unmount USB-Storage.**
Description	*Unmounting of the USB-Stick failed.*
Action	Remove the USB-Stick and restart the device. Check the USB-Stick, optionally reformat it. Insert the USB-Stick and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**No program selected.**
Description	*At program start no program was detected*
Action	Create and select a program. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Drift gas flow too low. Aborting…**
Description	*At program start the drift gas flow is too low. Programstart will be refused.*
Action	Increase the back pressure. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Stop recording first.**
Description	*If recording is activ a programstart is refused.*
Action	Deactivate recording and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Can’t initalize drift supply. Program can not be started.**
Description	*Drift voltage error*

Action	Fatal Error! Contact the G.A.S. service hotline.
Error message	**Invalid program.**
Description	*The selected program has no instructions.*
Action	Complete the program and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Not enough storage space left. Please delete or copy measurement or choose a shorter program.**
Description	*The internal storage has not enough storage space left.*
Action	Export and save all Measurement of the internal storage and clear the storage. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Hardware access failure**
Description	*Error when switching the drift voltage polarity.*
Action	Fatal Error! Contact the G.A.S. service hotline.
Error message	**Valve set to Inject. Loop not filled! Proceed? OK or Chancel**
Description	*Valve start position is set to Inject instead of Fill loop.*
Action	Set valve start position manually to Fill loop. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Can’t import calibration.gsd**
Description	*The file „calibration.gsd“ was not found.*
Action	Create the file „calibration.gsd“ and import it with an USB-Stick. Repeat the procedure.

	If that still does not help contact the G.A.S. service hotline.
Error message	**No measurements stored.**
Description	*No measurements stored on the internal storage.*
Action	Do a measurement. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Folder cannot be created :**
Description	*When exporting the device subfolder could not be created.*
Action	Check the external storage. Check network cable, network shares and IP-address. Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**No measurement files transferred**
Description	*No measurement are transferred to an external storage.*
Action	Check the external storage. Check network cable, network shares and IP-address. Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**No measurements stored.**
Description	*No measurements were deleted, because no measurements are available.*

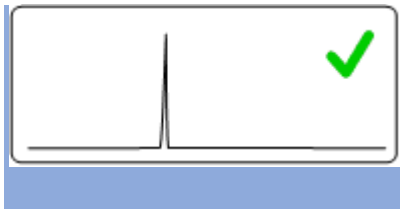
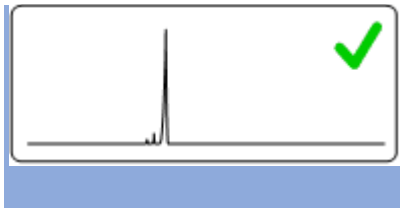
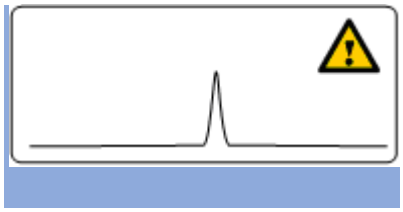
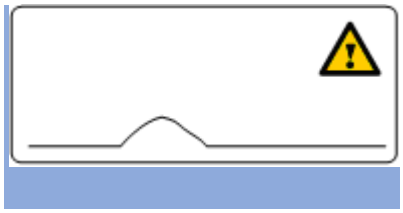
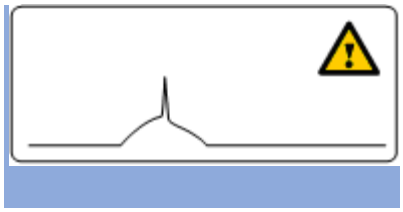
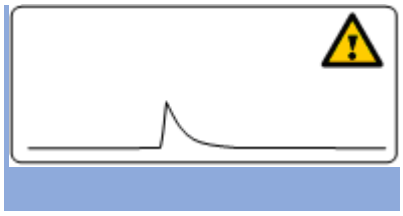
Action	Do a measurement. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**RTC read error.**
Description	*Date and time setting failed.*
Action	Restart the system and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Save settings failed.**
Description	*Setting data could not be save on a USB-stick.*
Action	Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Load settings failed.**
Description	*Setting data could not be load from a USB-stick*
Action	Repeat the procedure. Restart the system and repeat the procedure. Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Do you really want to relabel loop volume? It will be stored in all following measurements.**
Description	*Sample loop setting is change manually.*
Action	Confirm or abort the dialog.

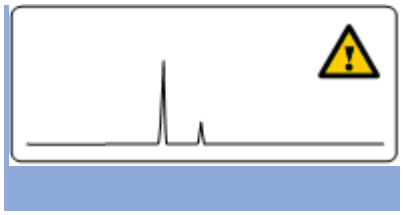
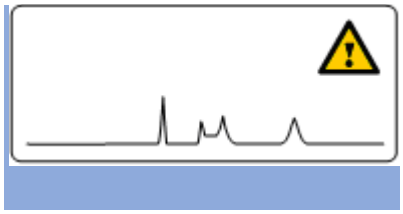
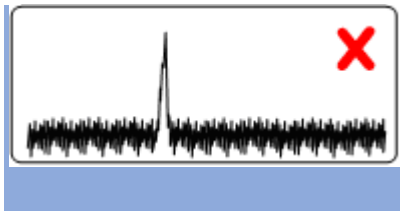
Error message	**Can't set static ip!**
Description	*Setup of the static IP-address failed.*
Action	Check the network settings. Contact your adminstrator. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Can't request DHCP:**
Description	*Setup of the dynmaic IP-address failed.*
Action	Check the network settings. Check DHCP-server. Contact your adminstrator. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Valve set to Inject. Loop not filled**
Description	*Valve setting is set to position “Inject” and not to “Fill loop”. Sample loop could not be filled.*
Action	Abort program and set valve to position „Fill loop‟ manually.
Error message	**Trigger recieved while running program.**
Description	*During the program run a new trigger signal will be received. The program run is aborted.*
Action	The device get a wrong trigger signal. Check the external trigger programming. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	**Stop recording first.**
Description	*When starting the trigger mode recording is activated.*
Action	Deactivate recording and repeat the procedure. If that still does not help contact the G.A.S. service hotline.

Error message	**Select program first.**
Description	*When starting the trigger mode no program is activated.*
Action	Select a program and repeat the procedure. If that still does not help contact the G.A.S. service hotline.

Error message	**Can’t read calibration.gsd**
Description	*The import of the calibration.gsd. file failed. The file was not found.*
Action	Ensure that the file calibration.gsd exist and is placed in the measurement subfolder of the device. Check network cable, network shares and IP-address. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.

9.13.2 IMS-Spectrum Examples

Schematic of IMS spectrum	Spectrum description	reasons / suggestions
	Clean spectrum	Perfect
	Clean spectrum, up to two extra signals left hand side of the RIP	Perfect
	RIP shifted to lower drift times	- elevated temperature - reduced pressure
	RIP shifted to higher drift times	- low temperatures - elevated pressure
	RIP deformed	- gas quality out of specifications - device needs to be flushed for some time - flows not in range
	RIP base deformed yet visible	- gas quality out of specifications - device needs to be flushed for some time - flows not in range
	RIP deformed towards tailing	- gas quality out of specifications - device needs to be flushed for some time - flows not in range

	Minor impurities	- gas quality out of specifications - device is polluted > run system cleaning
	Major impurities	- gas quality out of specifications - device is polluted > run system cleaning
	Elevated noise	Contact G.A.S. support
	No signal	Contact G.A.S. support

9.13.3 Troubleshooting / How to…

INFORMATION!

This chapter is a collection of possible practical problems and serves as a guide for making an initial assessment. It makes no claim to completeness.

Symtom	**Device does not start**
Possible Cause	*Problem with the electrical power supply*
Action	Check the current power supply and restart the system. If that still does not help contact the G.A.S. service hotline.
Symtom	**Device freezes during start procedure.**
Possible Cause	*Problem with the Firmware*
Action	Restart the system. If that still does not help contact the G.A.S. service hotline.
Symtom	**Start procedure paused**
Possible Cause	*Hardwarecheck during the start procedure*
Action	Wait up to 5 min. Normally the start procedure continues. Restart the system. If that still does not help contact the G.A.S. service hotline.
Symtom	**Temperature and/or gas flow values will not be displayed**
Possible Cause	*Problem with hardware/firmware communication*
Action	Restart the system. If that still does not help contact the G.A.S. service hotline.
Symtom	**Screen is black while device is on.**
Possible Cause	*Screensaver is active*

Action	Using the pushable rotary knob to active the screen. If the screen can't be reactivated then restart the system. If that still does not help contact the G.A.S. service hotline.
Symtom	**Gasflow set-values cannot be achieved.**
Possible Cause	*Backpressure to low*
Action	Set up the back pressure at least to 3 bar. If that still does not help contact the G.A.S. service hotline.
Possible Cause	*Hardware failure*
Action	Contact the G.A.S. service hotline.
Symtom	**Temperature set-values cannot be achieved.**
Possible Cause	*Hardware failure*
Action	Contact the G.A.S. service hotline.
Symtom	**No display of measurement values during monitoring**
Possible Cause	*Hardware failure*
Action	Contact the G.A.S. service hotline.
Symtom	**No Reaction Ion Peak (RIP) will be displayed.**
Possible Cause	*Device is in negative mode*
Action	Switch the drift voltage into positive mode. If that still does not help contact the G.A.S. service hotline.
Possible Cause	*Hardware failure*
Action	Contact the G.A.S. service hotline.
Symtom	**No or small Reaction Ion Peak (RIP) will be displayed.**
Possible Cause	*Insufficient gas quality*
Action	Check quality of operating gas (5.0 or better) and use moisture trap.

Action	When using the CGFU-unit, replace the CGFU-filters.
Possible Cause	*System contamination*
Action	Start cleaning mode.
Symtom	**Find signals from the prior measurement run in the chromatogram**
Possible Cause	*The measurement runtime is too short.*
Action	Increase the measurement run time
Symtom	**The actual size of the measurement file is to large**
Possible Cause	*Average setting too low.*
Action	Increase the Average setting or shorten the runtime (recommended averaging: 6).
Symtom	**The measurement signals cannot mapped well.**
Possible Cause	*Average setting is too high.*
Action	Decrease the Average setting (recommended averaging: 6).
Symtom	**EPC2 Maximum flow of 150 ml/min is not reached.**
Possible Cause	*The reachable maximum flow depends on the dimensions of the installed column.*
Action	Get the specified maximum flow from Analytical approval. If that still does not help contact the G.A.S. service hotline.
Possible Cause	When using a CGFU unit the total flow (EPC1 and EPC2) is limited to 400ml/min.
Action	No Action
Symtom	**Six-Port-valve doesn’t switch**
Possible Cause	*Lost connection*

Action	Restart the system. If that still does not help contact the G.A.S. service hotline.
Symtom	**Six-Port-valve switching noise sounds strange**
Possible Cause	*Initialization lost*
Action	Reintializise the Six-Port-Valve
Symtom	**No sample signals are displayed during a measurement.**
Possible Cause	*Sample-Pump has failed*
Action	Set pump capacity to 100%. The pump device must be audible loud. Turn the pumping power back to the working flow. In addition, the flow can be measured using a flowmeter at the sample inlet and outlet. If that still does not help change sample pump.
Symtom	**Drift time fluctuates**
Possible Cause	*System is untight*
Action	Check all gas supply connections of operating gas.
Action	Check all gas supply connections of GC-column.
Symtom	**Retention time fluctuates**
Possible Cause	*System is untight*
Action	Check all gas supply connections of operating gas.
Action	Check all gas supply connections of GC-column.

9.14 Consumables / Spare Parts

Part number: 4000 1000

Power supply with Power plug

Part number: 9510 1081

Gas tube Kit: (FlavourSpec)

- Driftgas/Carriergas Adapter with 0,15 m and 0,65 m PFA-Tubes with 3mm Swagelok Connectors (1piece)
- 2 m 3mm PFA Tubes with 3 mm Swagelok-Connector (3 Pieces)

Part number: 8900 1094

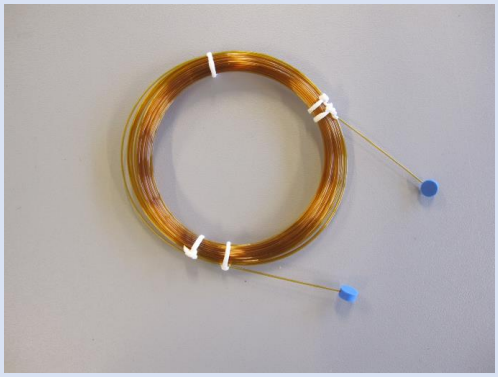
Molecular sieve 200 ml with 1/8” connections (1 piece)

(Labuse)

Part number: 8900 1101

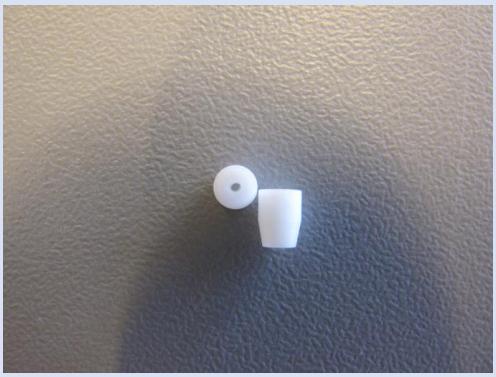
Molecular sieve 120 ml with 1/8” connections (1 piece)

(Attachable to device)



Part number: 8101 1524
Standard-capillary column MXT-5
Lenght 15 m, ID 0,53 mm, Filmthickness 1 µm, Winding ID 80 mm

(Other column types only on request)



Part number: 8103 1001

Teflon Ferrules for capillary column with ID 0,53 mm
Connection 1/16", Hole 0,8mm, T max. = 250°C

Package size: 10 Pieces

Part number: 1303 0036

Connection Kit for capillary column connection 1/16"

Package size: 2 Pieces

Part number: 9510 0000
LAN Cable

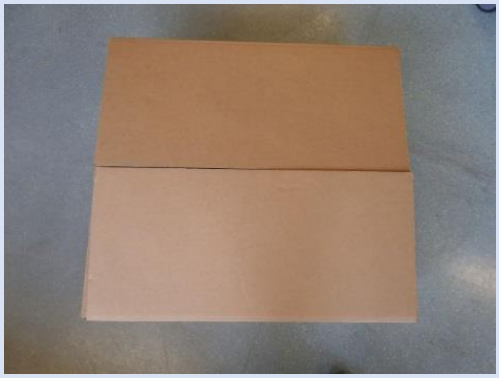
Part number: 1303 0006

GC-IMS Blind plug Set (4 pieces)

Part number: 1305 0013

Torx Tool Kit

- Torx Screwdriver 8 mm (1 piece)
- Torx Screwdriver 10 mm (1 piece)



Part number: 8001 1706

FlavourSpec Transport box Length = 110 cm, Height = 80 cm, Width = 77 cm
(1 piece)

Part number: 8003 0002

GC-IMS Transport palett (120 x 80 cm)

Part number: 26030200

FlavourSpec-PAL3 Connection Cable

Part number: 82021023

1000 ul Smart Headspace Syringe with fixed needle for Tool HS1000 (PAL3 SII)

Part number: 4600 500 000

Nitrogen Generator with accessories (example picture)

Part number: 89001021

Crimper for H20 ml Headspace Vials

Part number: 89001022

Septa BTO, Silicon red, 3mm size, 11mm Ø

Package size: 25 Pieces

Part number: 89001008

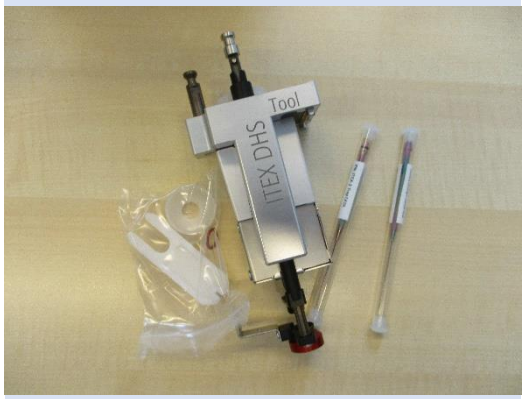
Headspace vials, glas 1. hydrolyt. class DIN ISO 719
Volume: 20 ml, Beading Ø x Height: 20x3,6 mm, Vial height x OD: 75,5 x 22,5 mm

Package size: 100 Pieces

Part number: 89001011

Magnetic Cap Aluminium, Hole-Ø 7 mm gasket Silica, PTFE 3 mm, for beading 20 x 3,6 mm

Package size: 100 Pieces



Part number: 82021041
PAL ITEX-Kit

Part number: 82021024

Smart ITEX Syringe 1300 ul for Tool ITEX (PAL3 SII)

Part number: 82021025

ITEX-2 Trap (G23) Siliconert 2000 Tenax TA 80/100

Part number: 8205 0000

Laptop Computer (different design) including software for control and evaluation

9.15 Corresponding G.A.S. Documents and Tutorials

INFORMATION!

- FlavourSpec Quickstart Manual
- PAL3 System User Manual
- Sequence Designer Manual
- IMS Control TFTP-Server Manual
- Tutorials Sequence Designer
- Tutorials VOCal
- Manuals VOCal

9.16 Table of Figures