

Vision Air Local Pharma



Tutorial

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2.0

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Vision Air Local Pharma

1 Overview

1.1 What is Vision Air?

Vision Air is a modern, intuitive and easy-to-use software solution for routine Vis-NIR analysis and quality assurance. Vision Air is divided into 2 dedicated software parts.

While **Vision Air Routine** puts a focus on the needs of routine users, **Vision Air Manager** provides administrative functions to meet the requirements of laboratory managers and division managers.

Vision Air is available in 2 versions: **Vision Air Local** and **Vision Air Network**. Vision Air Local includes all the necessary routine applications as well as numerous management functions and enables the control of 1 Vis-NIR spectrometer.

In contrast to Vision Air Local, Vision Air Network enables users to control and configure any number of spectrometers. All data produced can be saved automatically, both locally and globally.

Vision Air Local



In Vision Air Local, the program parts Vision Air Routine and Vision Air Manager Local are both installed on 1 single computer.

This computer is directly connected to the instrument. The configuration of the instrument, which includes information such as new operating procedures and new parameters, is done by the local administrator in Vision Air Manager Local. All data, e.g. configurations, results and spectra is stored on the local PC.

Acquisitions are performed in Vision Air Routine.

1.2

The product is available in the following versions:

Table 1 Product versions

Art. no.	Designation
6.6072.201	Vision Air 2.0
6.6072.202	Vision Air 2.0 Pharma
6.6072.203	Vision Air 2.0 Network Pharma
6.6072.204	Vision Air 2.0 Server
6.6072.205	Vision Air 2.0 Server Pharma
6.6072.206	Vision Air 2.0 Network
6.6072.207	Vision Air 2.0 Network Complete
6.6072.208	Vision Air 2.0 Complete
6.6072.209	Vision Air 2.0 Pharma Complete
6.6072.210	Vision Air 2.0 Pharma Network Complete

1.3

The following formatting may appear in the documentation:

(5-12)	Cross-reference to figure legend
	The first number refers to the figure number. The second number refers to the product part in the figure.
1	Instruction step
	Numbers indicate the order of the instructions steps.
Method	Names of parameters, menu items, tabs and dialogs
File ► New	Menu path
[Continue]	Button or key

2 Safety

2.1 Intended use

Metrohm products are used for the analysis and handling of chemicals.

Usage therefore requires the user to have basic knowledge and experience in handling chemicals. Knowledge regarding the application of fire prevention measures prescribed for laboratories is also mandatory.

Adherence to this technical documentation and compliance with the maintenance specifications make up an important part of intended use.

Any utilization in excess of or deviating from the intended use is regarded as misuse.

Specifications regarding the operating values and limit values of individual products are contained in the "Technical specifications" section, if relevant.

Exceeding and/or not observing the mentioned limit values during operation puts people and components at risk. The manufacturer assumes no liability for damage due to non-observance of these limit values.

The EU declaration of conformity loses its validity as soon as modifications are carried out on the products and/or the components.

2.2 Responsibility of the operator

The operator must ensure that basic regulations on occupational safety and accident prevention in chemical laboratories are observed. The operator has the following responsibilities:

- Instruct personnel in the safe handling of the product.
- Train personnel in the use of the product according to the user documentation (e.g. install, operate, clean, eliminate faults).
- Train staff on basic occupational safety and accident prevention regulations.
- Provide personal protective equipment (e.g. protective glasses, gloves).
- Provide suitable tools and equipment to carry out the work safely.

The product may be used only when it is in perfect condition. The following measures are required to ensure the safe operation of the product:

- Check the condition of the product before use.
- Remedy defects and malfunctions immediately.
- Maintain and clean the product regularly.

2.3 Requirements for operating personnel

Only qualified personnel may operate the product. Qualified personnel are persons who meet the following requirements:

- Basic regulations on occupational safety and accident prevention for chemical laboratories are known and complied with.
- Knowledge of handling hazardous chemicals is present. Personnel have the ability to recognize and avoid potential dangers.
- Knowledge regarding the application of fire prevention measures for laboratories is available.
- Safety-relevant information is communicated and understood. The personnel can operate the product safely.
- The user documentation has been read and understood. The personnel operate the product according to the instructions in the user documentation.

2.4 Safety instructions

2.4.1 Danger from electrical potential

Contact with electrical potential can cause serious injuries or death. To avoid danger from electrical potential, observe the following:

- Operate the product only if it is in perfect condition. The housing must also be intact.
- Only use the product with the covers fitted. If covers are damaged or missing, disconnect the product from the energy supply and contact the regional Metrohm service representative.
- Protect live components (e.g. power supply unit, power cord, connection sockets) against moisture.
- Always have maintenance work and repairs on electrical components carried out by a regional Metrohm service representative.
- Disconnect the product from the energy supply immediately if at least one of the following cases occurs:
 - The housing is damaged or open.
 - Live parts are damaged.
 - Moisture penetrates.

2.4.2 Danger from biological and chemical hazardous substances

Contact with biological hazardous substances may cause poisoning from toxins or infections from microorganisms. Contact with aggressive chemical substances may cause poisoning or chemical burns. To avoid danger from biological or chemical hazardous substances, observe the following:

- Label the product according to regulations if it is used for substances that have a potential for chemical hazards and are generally subject to the Hazardous Substances Ordinance.
- Wear personal protective equipment (e.g. protective glasses, gloves).
- Use exhaust equipment when working with vaporizing hazardous substances.
- Dispose of hazardous substances in accordance with regulations.
- Clean and disinfect contaminated surfaces.
- Only use detergents that do not cause any unwanted side reactions with the materials to be cleaned.
- Dispose of chemically contaminated materials (e.g. cleaning material) in accordance with regulations.
- Proceed as follows in case of a return shipment to Metrohm AG or a regional Metrohm representative:
 - Decontaminate the product or product component.
 - Remove the labeling for hazardous substances.
 - Create a declaration of decontamination and enclose it with the product.

2.4.3 Danger from highly flammable substances

Using highly flammable substances or gases may cause fires or explosions. To avoid danger from highly flammable substances, observe the following:

- Avoid ignition sources.
- Use protective grounding.
- Use exhaust equipment.

2.4.4 Danger during transport of the product

Chemical or biological substances may be spilled during the transport of the product. Parts of the product may fall down or may be damaged. There is a risk of injury from chemical or biological substances and pieces of broken glass. To ensure safe transport, observe the following:

- Remove loose parts (e.g. sample racks, sample vessels, bottles) before transport.
- Remove liquids.
- Lift and transport the product with both hands on the base plate.
- Lift and transport heavy products only according to instructions.

2.5 Design of warning messages

There are 4 hazard levels for warning messages. The following signal words are used for classifying the hazard levels in warning messages:

- **DANGER** indicates a hazardous situation which, if not avoided, will result in serious injury or death.
- **WARNING** indicates a hazardous situation which, if not avoided, could result in serious injury or death.
- **CAUTION** indicates a hazardous situation which, if not avoided, could result in minor or moderate injury.
- **NOTICE** indicates a hazardous situation which, if not avoided, could result in property damage.

Warning messages differ in design (color and warning sign) depending on the hazard level:



DANGER

Type and source of danger

Consequences when not observing the notice: An irreversible injury that may result in death is very probable.

- Measures to avoid the danger



WARNING

Type or source of danger

Consequences when not observing the notice: A serious injury that may result in death is probable.

- Measures to avoid the danger



CAUTION

Type or source of danger

Consequences when not observing the notice: A minor to moderate injury is probable.

- Measures to avoid the danger

2.6 Meaning of warning signs

This documentation uses the following warning signs:

Table 2 Warning sign according to ISO 7010

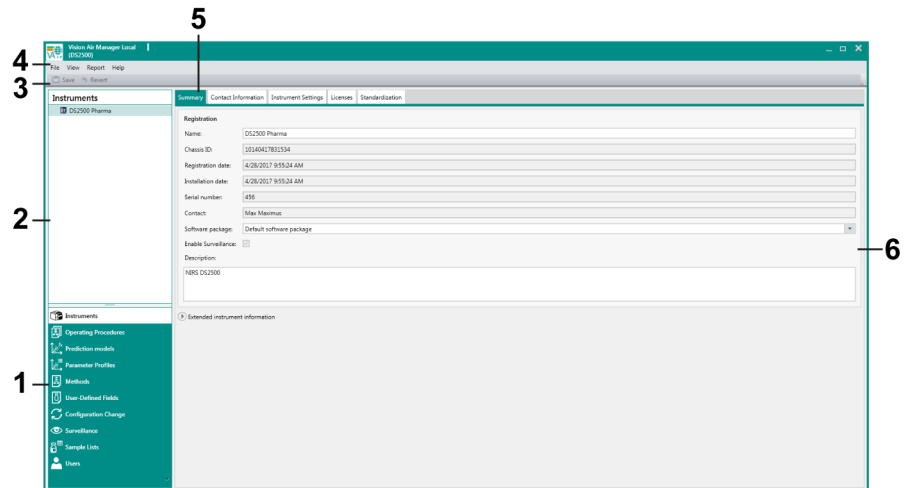
Warning sign	Meaning
	General warning sign
	Warning of electrical voltage
	Warning of hand injuries
	Warning of sharp object
	Warning of hot surface
	Warning of biological hazard
	Warning of toxic materials
	Warning of flammable materials
	Warning of corrosive substances
	Warning of optical radiation
	Warning of laser beams

Depending on the intended use of the product, the corresponding warning sign stickers must be placed on the product.

3 Vision Air – Functional description

3.1 Vision Air Manager

3.1.1 User interface



1 Navigation window

Options that enable the user to navigate through Vision Air Manager (*see "Navigation window", page 10*).

2 Structure window

The information in this window varies depending on the selection in the navigation window, e.g. for the navigation window **Prediction models** all available prediction models are displayed.

3 Toolbar

4 Menu bar

5 Work window

The information in the work window varies depending on the selection in the navigation window and the structure window. The text fields in the work window are either editable (white) or read-only (grey).

6 Functional area

The work window can be divided into several functional areas.

7 Configuration Change

The Configuration Change section lists the current system configuration and all previous configurations. New configurations are signed and published in this section.

9 Sample Lists

Sample lists are used to organize collected spectra and results. Sample lists are also used to conduct slope corrections and bias corrections.

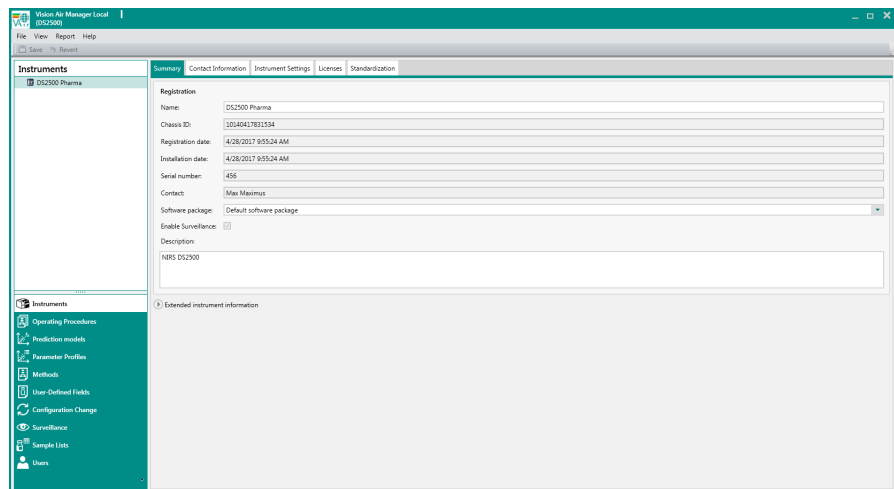
8 Surveillance

Overview of all measurements, events and instrument tests.

10 Users

User management for access to Vision Air Manager and Vision Air Routine.

3.1.2 Instruments section



All instrument related settings are made in the **Instruments** section in Vision Air Manager.

The **Instruments** section contains the following work window tabs:

Summary

Summary	Contact Information	Instrument Settings	Licenses	Standardization
Registration				
Name:	NIRS DS2500			
Chassis ID:	10140417831534			
Registration date:	06.12.2017 08:09:57			
Installation date:	06.12.2017 08:09:57			
Serial number:	456			
Contact:	System Administrator			
Software package:	Default software package			
Enable Surveillance:	☒			
Description:	NIRS DS2500			
▶ Extended instrument information				

The **Summary** tab contains the general information on the instrument. Here, the instrument name can be defined and a description of the instrument can be added. The following instrument specific information is displayed as read-only:

Chassis ID

Specific instrument ID.

Registration date

Date of the registration of the instrument with the server. In Vision Air Local, the registration date is identical to the installation date.

Installation date

Date of the first connection of the instrument with Vision Air Routine.

Serial number

Serial number of the monochromator.

Contact

The contact person is set in the **Contact information** tab.

Software package

Only 1 default software package is available for Vision Air.

Enable Surveillance

In the **Instruments** section, the setting **Enable surveillance** is read-only.

In the **Surveillance** section, the user can check/uncheck the check box **Enable surveillance**. After disabling, the instrument is not flagged any more, for example after a failed instrument diagnostic test.

Contact information

The screenshot shows the 'Contact Information' tab selected in a multi-tabbed interface. The 'Contact Information' section contains the following fields:

- First name: System
- Last name: Administrator
- Office Phone: (empty)
- Cell Phone: (empty)
- E-mail: (empty)
- Address: (empty)
- Description: (empty text area)

Below the contact information is the 'Instrument Location' section:

- Decimal Degrees (DD):
 - Latitude: (empty)
 - Longitude: (empty)
- Timezone: (UTC) Koordinierte Weltzeit (dropdown menu)
- Translation: Standard (dropdown menu)

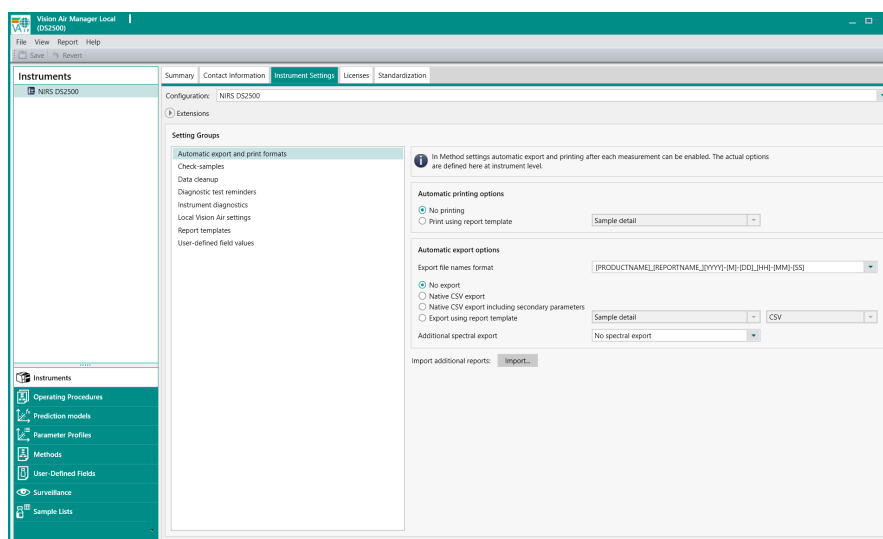
A button labeled 'Pick Another Contact...' is located at the bottom right of the contact information section.

The **Contact information** functional area contains information about the person who is responsible for the instrument.

Contact persons are created in the **Users** section. To select a contact, click on **[Pick another contact]**, select a contact in the pop-up window and press **[OK]**.

In the **Instrument location** functional area, it is possible to enter the GPS location and time zone of the instrument:

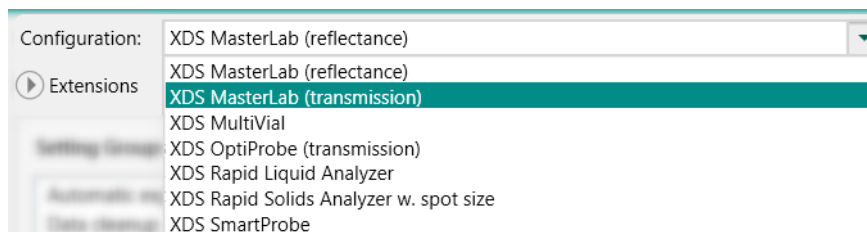
Instrument settings



Details on the instrument settings are displayed under the Instrument settings tab. Some settings are read-only.

Advanced settings can be displayed by activating the advanced view under **View ► Options ► Display advanced settings**. Advanced settings are only active for the current session. After a restart of Vision Air Manager, the display is reverted to the basic view. Advanced settings should only be modified by Metrohm representatives or after consultation with a Metrohm representative.

If different XDS modules have been used with Vision Air in the past, the individual modules are selectable in the configuration drop-down list.



The following instrument settings are available:

Automatic export and print formats

Settings to define which templates should be printed automatically and which templates should be created automatically after a measurement in Vision Air Routine. Set the storage location and the final activation of this procedure in Vision Air Routine under **Tools ► Settings ► Export or print**.

You can import additional report templates for automatic export options with the **[Import]** button. The newly imported reports are available for

selection for automatic export. Only sample related templates can be imported in this section.

Check samples (only available for DS2500)

Settings to define the behavior when using operating procedures with check samples.

If **Check sample reminders enabled** is checked, the user is reminded to analyze a check sample in the given interval (default setting: every 48 hours). The user has a grace period in which a successful check sample should be analyzed (default setting: 2 hours). If the user fails to analyze a successful check sample, the normal samples are marked with a warning if **Mark samples after unsuccessful check sample** is checked.

Check samples are physical samples that can be considered stable over some period of time. They are used as an additional verification of the instrument performance (*see "Check samples", chapter 3.3.4, page 62*).

Common hardware self-test limits (only available for DS2500)

Read-only view for self-test limits. These parameters are defined within the firmware of the instrument.

Data cleanup

Settings to define if and when normal samples or check samples should be automatically deleted.

Diagnostic test limits

In this setting, a Metrohm representative can add different configurations for the test limits.

Diagnostic test parameters

Settings where the number of test runs for low-flux tests and for wavelength certification tests is defined. Reference correction files are stored on the USB flash drive that is delivered with the individual standard sets, for example standard set 6.7450.010. These reference correction files can be stored permanently in Vision Air Manager. With this, the user does not need to insert the USB flash drive and select the file during diagnostic tests. The validity of files and standards is typically 1 year and can be renewed by a recertification. Contact your local Metrohm agency for details regarding a recertification.

The following options are available:

- Number of reference subsamples: Average of subsamples (read-only).
- Number of WSR (wavelength standard reflectance) subsamples: Average of WSR subsamples (read-only).
- Number of low-flux test runs: Average of low-flux test runs.
- Number of wavelength certification test runs.

- Show only valid standard sets in Vision Air Routine: Standards have a due date. If the check box is active, only standards where the due date is OK are displayed.
- External references: Add additional reference files here.

Diagnostic test reminders

Settings to enable an automatic reminder in Vision Air Routine to conduct a low-flux test, a wavelength certification or a photometric test. The following options are available:

- Enabled: If active, the user is reminded to perform the instrument diagnostic test.
- Interval: Frequency of instrument diagnostic tests (in days).
- Grace period: Time that remains until the user has to perform the instrument diagnostic test (in hours).
- Action on expiration or failure: Definition of what happens if no test was performed after the defined time. This ensures that data is only measured with properly working instruments. The user can either disable the measurement completely or flag the measured samples with an error.

Hardware self-test limits (only available for DS2500)

Read-only view for instrument specific settings. The settings are defined within the firmware of the instrument.

Hardware sensor limits (only available for DS2500)

Read-only view for instrument specific settings. The settings are defined within the firmware of the instrument. The current DS2500 product line does not use the settings.

Instrument calibration settings (only available for DS2500)

Read-only view for instrument specific settings. The settings are defined within the firmware of the instrument.

Instrument diagnostics

Settings for the instrument diagnostic test that is conducted in Vision Air Routine. If the automatic instrument diagnostic test is deactivated, then the automatic test does only run if the last conducted test failed, was canceled or was never performed.

If the instrument diagnostic test reminder is enabled, it reminds the user to perform an instrument diagnostic test in the given interval (default setting: every 8 days). The user has a grace period to perform a successful test (default setting: 2 hours). If the user fails to perform a successful test, the normal samples are marked with a warning or the measurement is disabled. This depends on the selected option in Vision Air Manager.

Run start-up test.

- XDS:
Always: The start-up test runs on every startup of Vision Air Routine.
After unsuccessful diagnostic test: The start-up test only runs if a diagnostic test failed.
- DS2500:
After unsuccessful diagnostic test or instrument restart: The start-up test only runs if a diagnostic test failed or the instrument has been restarted.
After unsuccessful diagnostic test: The start-up test only runs if a diagnostic test failed.

Local Vision Air settings

Read-only view for file storage options in Vision Air Routine. Define the settings directly in Vision Air Routine.

Performance test parameters (only available for XDS instruments)

Settings for the total amount of test runs, noise (reference) and number of wavelength (WSR) scans that are performed during the instrument diagnostic test.

Report templates

Section for the import of report templates that are available in the **Tools** section in Vision Air Routine. Only sample-related templates can be imported in this section (the same restrictions apply as for report templates that are imported in the automatic export and print format sections).

Stability test limits (PbS, Si or InGaAs)

Noise test limits for the individual detectors.

- Drift noise limit
- Random noise limit

Do not change factory settings yourself. Ask a Metrohm representative for assistance.

Stability test parameters

Settings for duration and acceptance limits for stability tests that are conducted during the instrument diagnostic test. The following options are available:

- Maximum test time: Maximum run time for the stability test. The maximum test time defines the maximal testing time for both stability tests: The lamp temperature stability test and the stability test (noise values).
- Number of reference subscans: Average of subscans.
- Number of scans: Number of measurements.
- Wait for a stable bias timeout (only available for XDS instruments): Noise test.

The tests can end before the total test time is reached if the test values, for example noise values, are below the set acceptance criteria. The maximum test time includes the test time for lamp stabilization and for noise bias.

With the DS2500 series, the number of scans and subscans can be defined.

Subscan settings (only available for DS2500)

Read-only view for subscan settings. The settings are defined within the firmware of the instrument.

User-defined field values

Handling of values in user-defined fields. If the check box is active, the values entered by the user are stored. Set the period how long a user-defined value is stored in the input field during sample registration.

Wavelength test limits (PbS, Si or InGaAs)

Wavelength test limits for the individual detectors. For the DS2500 series, the bandwidth limits can also be set. The following options are available:

- Bandwidth accuracy limit
- Bandwidth repeatability limit
- Wavelength accuracy limit
- Wavelength repeatability limit

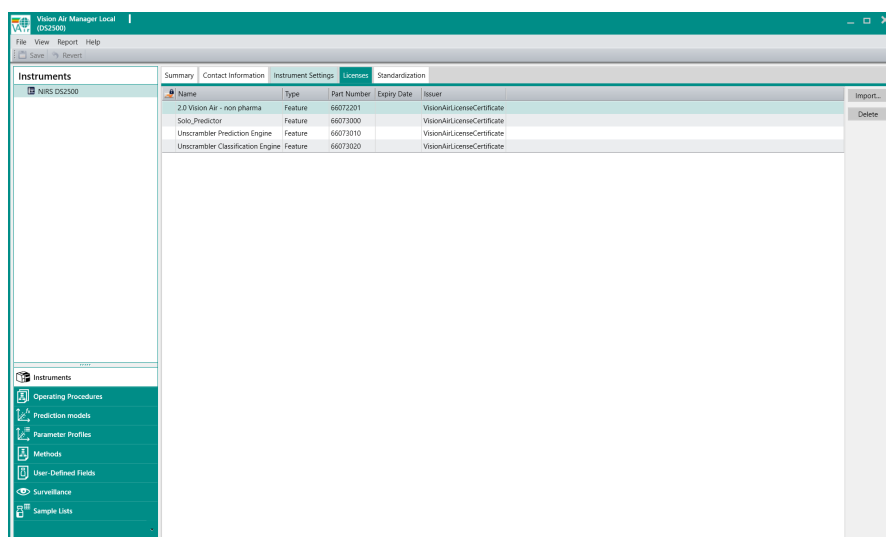
Do not change factory settings yourself. Ask a Metrohm representative for assistance.

Wavelength test parameters (only available for DS2500)

Settings for the instrument diagnostic test. The following options are available:

- Number of reference scans: Average of scans.
- Number of test runs: Number of measurements.
- Number of WSR (wavelength standard reflectance) subsans: Average of WSR scans.

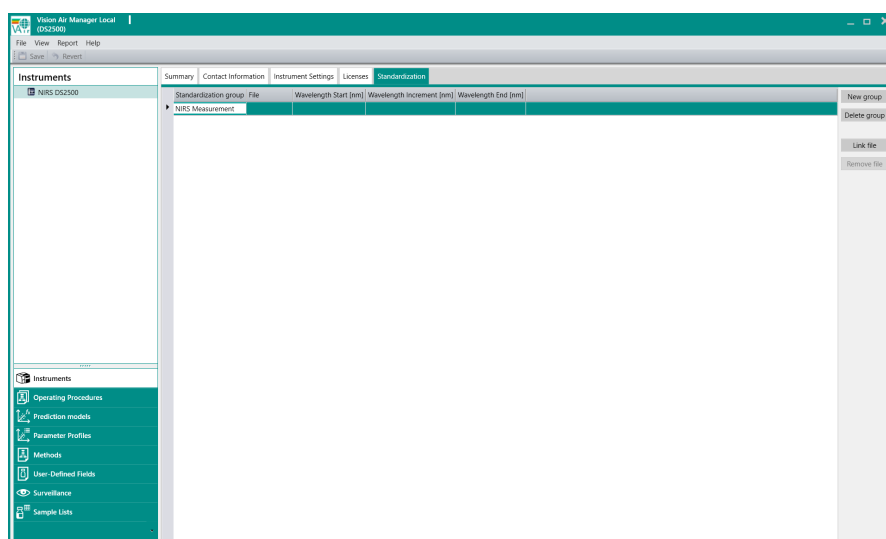
Licenses



In this section, licenses for the instrument can be imported and deleted.

Licenses can be imported to enable routine measurement and to activate secured prediction models that are provided with Metrohm pre-calibrations. Licenses, except demo licenses, are always instrument (monochromator) specific.

Standardization (DS2500 only)



By using a standardization file, it is possible to apply instrument adjustments to prediction models that were developed in other softwares. Prediction models that can be used in more than 1 software are called combined prediction models. When a standardization file is imported, it is linked to the prediction model of the instrument.

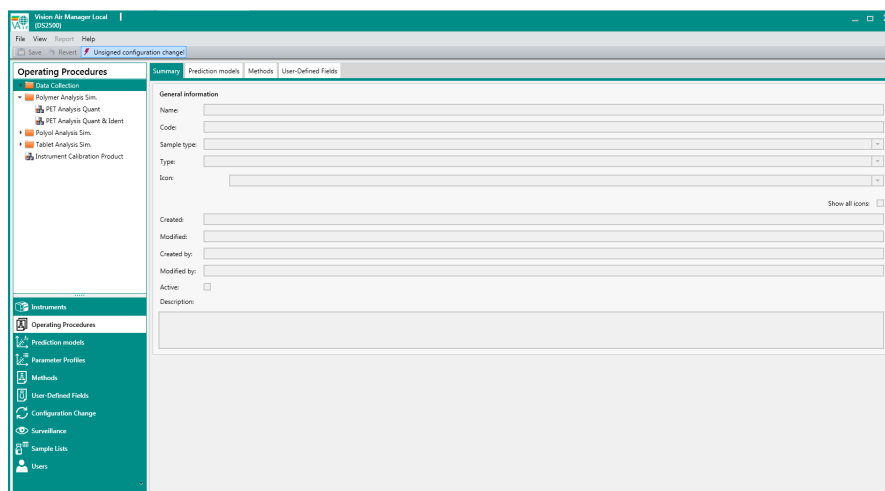
Click on **[New group]** if multiple instruments should use the same standardization. Delete groups by clicking **[Delete group]**.

Clicking on **[Link file]** to browse and link a prediction model to a standardization file (*.std).

Remove a linked file by selecting a file under the standardization tab and click on **[Remove file]**.

This functionality is not used with the current Metrohm product line.

3.1.3 Operating procedures section



All settings related to operating procedures are set in the **Operating procedures** section.

Prediction models, methods and user-defined fields are linked with the respective operating procedure in the **Operating procedures** section.

Lower and upper warning limits and intervention limits are defined in the **Operating Procedures** section.

The structure window lists all available operating procedures and operating procedure groups (📁) of the instrument.

Operating procedure groups can be created by right-clicking on the structure window and selecting **New operating procedure group**. Operating procedures can be assigned to operating procedure groups by right-clicking on the individual operating procedure and selecting **Move to operating procedure group**. Operating procedure groups allow to structure operating procedures.

The **Operating procedures** section contains the following work window tabs:

Summary

The **Summary** tab shows the following general information on the highlighted operating procedure in the structure window.

- The name of the selected operating procedure.
- The operating procedure code. It must be defined to export operating procedures via **File ► Export ► Configuration**. We recommend naming the code identically to the operating procedure.
- The sample type. It defines the kind of sample to be measured. The following sample types are available.
 - Normal: Standard samples for quality control.
 - Check sample (only available for DS2500): Physical samples that can be considered stable over a period of time. Check samples are used as an additional verification of the instrument performance (*see "Check samples", chapter 3.3.4, page 62*).
 - Standardization (only available for DS2500): Standardization samples are used for instrument calibration. Currently, Vision Air does not support this functionality.

Select the appropriate operating procedure type from the drop-down list **Type**.

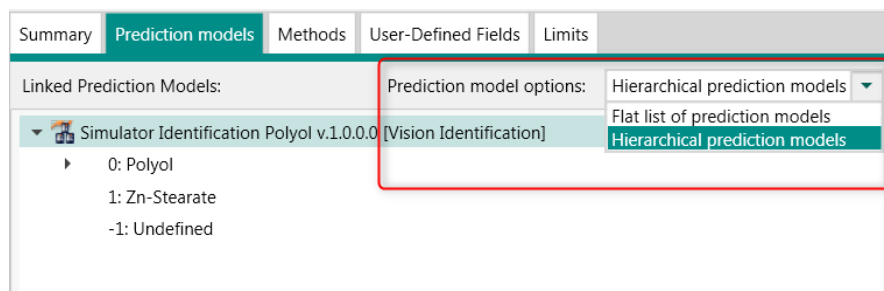
The selected type determines the list of icons. Any icon can be selected if the **Show all icons** check box is activated.

An icon can be selected with the **Icon** drop-down list. The selected icons are displayed in Vision Air Routine.

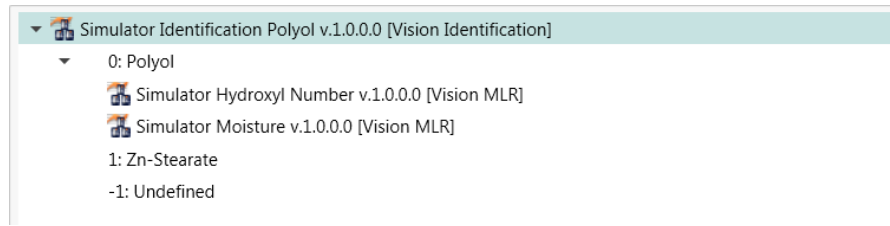
By default, all new operating procedures are active. The check box **Active** is checked. When the user deactivates an operating procedure, the operating procedure is no longer displayed in Vision Air Routine.

Prediction models

Prediction models can be linked to operating procedures. The hierarchical prediction model view allows to link prediction models with products or other prediction models.



In the displayed example, on the first level, a sample identification is conducted. On the second level, if identified as a polyol, Vision Air conducts a quantification of the hydroxyl number and the moisture.



In order to link individual prediction models or products, select the prediction model or product you want to link with another prediction model. Click on **[Add]** or right-click on the prediction model or product. This function allows to configure workflows. For example, a quantification is only performed in Vision Air Routine if the product has been identified correctly.

Methods

Methods can be linked to operating procedures. Multiple methods can only be linked with 1 operating procedure when using the XDS analyzer series. We do not recommend using multiple methods within the same operating procedure in Vision Air Local.

User-defined fields

User-defined fields can be linked to operating procedures.

Limits

Warning limits and intervention limits can be set for operating procedures.

There are 3 types of operating procedure limits:

- Absolute
- Relative
- Differential

The figure below illustrates the difference between the types:

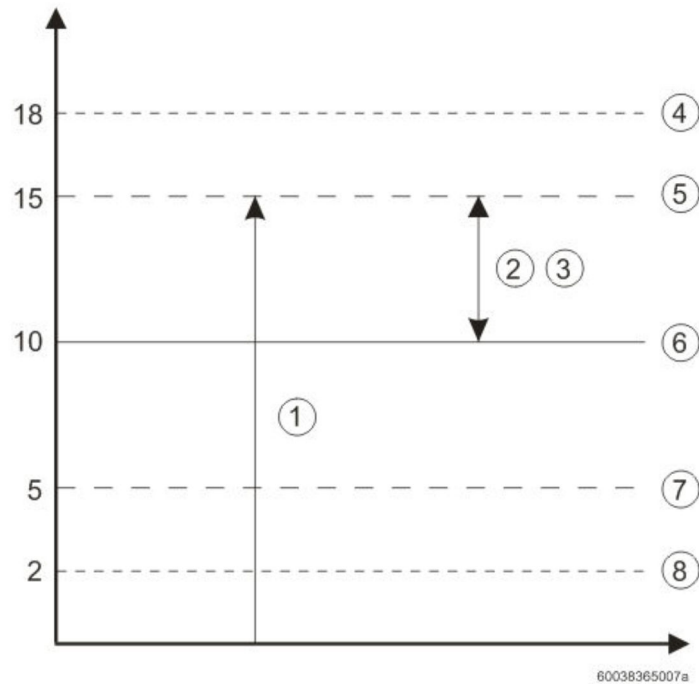


Table 3

1	Absolute upper warning limit = 15
2	Relative upper warning limit = 50%
3	Differential upper warning limit = 5
4	Upper intervention
5	Upper warning
6	Target
7	Lower warning
8	Lower intervention

The target value is always absolute. The differential limit is essentially a distance between corresponding absolute limit and target.

- Absolute Upper Action = Target + Differential Upper Action
- Absolute Upper Warning = Target + Differential Upper Warning
- Absolute Lower Action = Target - Differential Lower Action
- Absolute Lower Warning = Target - Differential Lower Warning

A target value needs to be defined for a relative limit. When using check samples and a check sample definition, the target value is defined by the value of the check sample definition ([see "Check samples", chapter 3.3.4, page 62](#)).

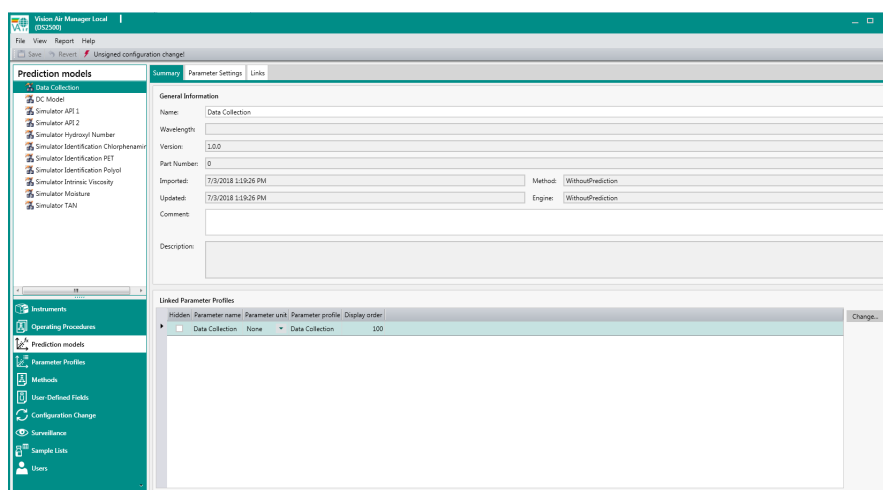
Example of relative limits:

Prediction Model	Parameter Profile	Type	Lower Action	Lower Warning	Target	Upper Warning	Upper Action
lacfruc	Lactose Content	Relative	9.00	6.00	10.00	6.00	9.00

- Lower Action Level: $10-9\% = 10-(0.09 \times 10) = 9.1$
- Lower Warning Level: $10-6\% = 10-(0.06 \times 10) = 9.4$
- Upper Warning Level: $10+6\% = 10+(0.06 \times 10) = 10.6$
- Upper Action Level: $10+9\% = 10+(0.09 \times 10) = 10.9$

Limits of prediction models can be imported/exported as .csv files. Highlight a prediction model and press **[Import...]** and **[Export...]** to open the browser window.

3.1.4 Prediction models section



Prediction models are algorithms correlating NIR spectra to properties of the sample, for example water concentration.

Each prediction model is linked to 1 parameter profile.

4 different prediction model types can be created by right-clicking on the data window screen.

- Imported prediction models
Imported prediction models are standard prediction models for routine analysis that were created in Vision, PLS_Toolbox or The Unscrambler.
- Calculated prediction models
Calculated prediction models allow automatic post processing of values that were evaluated with imported prediction models. Calculated prediction models can also use values from user-entered prediction models (*see "Calculated prediction models", chapter 3.3.6, page 65*).
- User-entered prediction models
User-entered prediction models are values that routine users enter during measurements. These values can be further used with calculated prediction models. A typical user-entered prediction model is a temperature value (*see "User-defined prediction model ", chapter 3.3.7, page 69*).

- Placeholder prediction models
Placeholder prediction models are only used to collect data and are therefore not predicting any result.

The **Prediction models** section contains the following work window tabs.

The tabs that are displayed in the **Prediction models** section depend on the type of selected prediction model.

Summary

The Summary tab contains general information and settings of the prediction models.

The **General information** field shows the following parameters.

- Name of the selected prediction model.
- The standardization group setting is only available for imported prediction models and user-entered prediction models.
A standardization group is a logical group of instruments with linked standardization files. The standardization group defines a standardization file for each instrument that belongs to the group. This function is not needed for the current Metrohm product line.
- The wavelength range of the system is displayed for imported quantitative prediction models. This is for example 400 - 2499.5 nm for a reflection XDS or DS system.
- The version number is automatically updated when an existing prediction model is imported again and updated.
- The part number displays a serial number for protected prediction models.
- The imported and updated dates display the date when the prediction model was imported and updated. If no update has been conducted yet, the imported and updated date are identical.
- Method displays which algorithm was used to create the prediction model.
- Engine displays which software was used to create the prediction model.

The **Linked parameter profiles** area shows a list of the linked parameter profiles.

The link to a parameter can be changed by clicking on **[Change...]** and selecting another parameter profile in the pop-up window.

When the check box in the column **Hidden** is checked, Vision Air Routine does not show the parameter information.

Click on **Parameter unit** to display a list of all available Vision Air units.

In order to select a new unit, an appropriate parameter profile that uses the new unit must be selected by clicking on **[Change]**. Changing the unit

does not affect prediction values or samples that were already analyzed with this parameter (unit is just a parameter attribute displayed with the prediction value).

Parameter settings

Quantitative prediction models

For quantitative prediction models, the **Parameter settings** work section allows to define which data points should be taken into account for slope corrections and intercept corrections.

The moment when a slope correction and intercept correction should be applied can be defined.

To conduct a slope correction or intercept correction, create a sample list in the **Sample lists** section. Perform the correction in the **Sample lists** section or in the **Prediction models** section in the **Slope / Intercept** tab (see "Slope/intercept calculations", chapter 3.3.8, page 69).

Identification prediction models

A list of all products and the according parameter output is displayed in the **Output values option**. The output can be renamed in the section.

Define the warning threshold in Vision Air Routine in **Qualification options**. Here, you can also define whether the actual distance of the sample is displayed or not.

Qualification prediction models

Define the parameter output in the **Output values option**. Define the parameter output for the 3 categories good, warning and bad. Select the warning threshold in **Qualification options**.

Links

The link section provides an overview over all operating procedures that use the selected prediction model. If the selected prediction model has been copied, a list of all existing copies can be displayed.

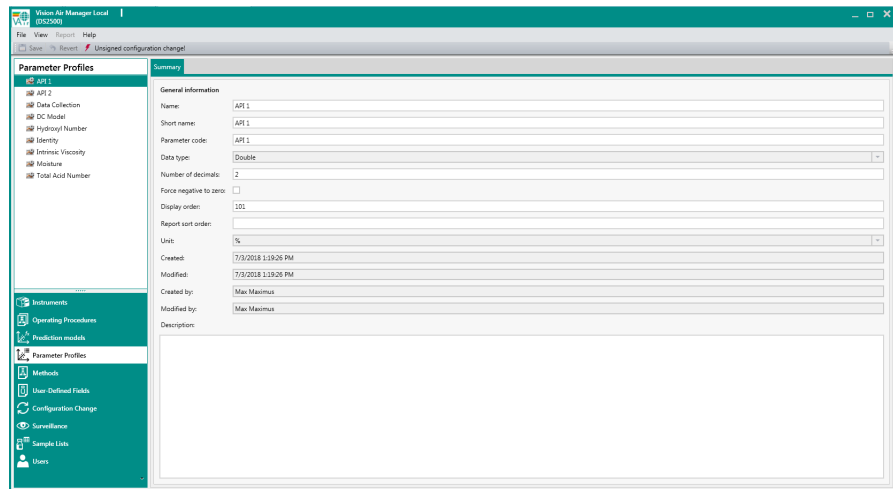
Moisture compensation

Activate or deactivate moisture compensation. This functionality is not used with the current Metrohm product line.

Slope/intercept

Apply a slope and/or intercept correction to a quantitative prediction model (see "Slope/intercept calculations", chapter 3.3.8, page 69).

3.1.5 Parameter profiles section



Parameter profiles define the parameter to be analyzed in accordance with the linked prediction model. For example, a parameter profile for a prediction model to quantify water content is water in %.

The **Parameter profiles** section contains the following work window tab:

Summary

The summary tab contains general information and settings of the parameter profiles. The **General information** field shows the following parameters:

- The name is displayed in Vision Air Manager.
- The short name is displayed during result display in Vision Air Routine.
- The parameter code is used to import reference values with .csv files in Vision Air Routine (*see "Importing reference values with a .csv file", chapter 3.3.3, page 61*).

In Vision Air Manager for DS2500, only methods for DS2500 can be created.

Methods are added by right-clicking on the  icon of the individual module or instrument and selecting **[Add method]**.

The **Methods** tab contains the following work window tabs:

Summary

- Definition of the method name.
- Definition of the sample vessel in the drop-down menu sample handling.

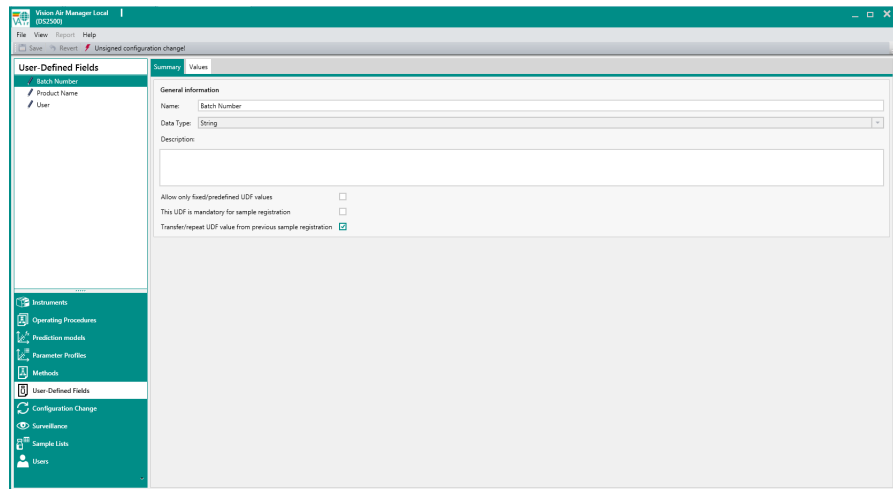
Settings

The Setting tab contains detailed settings of the method with respect to the selected sample vessel.

The following settings are available.

- **Analysis**
The user can define whether the instrument should perform an autolignearization (x-axis correction) before each scan. We suggest to keep this setting active.
The number of reference subscans can be defined. The default value is 32. The frequency of a reference scan (y-axis correction) can be defined. The default value is 0. 0 represents a reference scan before each measurement. Warm-up time refers to the time period when Vision Air Routine is started first. The user can modify the length of the warm-up time (only available with XDS). The default value is 120 minutes. During warm-up time, a reference scan is conducted before each measurement by default.
- **Automatic start control** (only available for DS2500 Liquid Analyzer)
If the checkbox **Automatic start** is checked, the measurement starts automatically after closing the lid of the DS2500 Liquid Analyzer.
- **Display options**
The user can define which information is displayed about the sample vessel and outliers during a routine analysis. Comment fields can be activated or deactivated during sample registration. Comment fields can be set as mandatory.
- **Liquid setup** (only available for DS2500 Liquid Analyzer)
If the checkbox **Check sample vessel type** is enabled, the system checks whether the inserted sample vessel matches with the sample vessel defined in the method.
Defines options regarding the temperature of the sample holder and the sample (*see "Heating and cooling the sample", page 77*).
Defines whether there is a delay before a scan starts and the length of the delay. With a delay before a scan, you can ensure that the sample has the same temperature as the sample holder.

3.1.7 User-defined fields section



The **User-defined fields** section contains the following work window tabs:

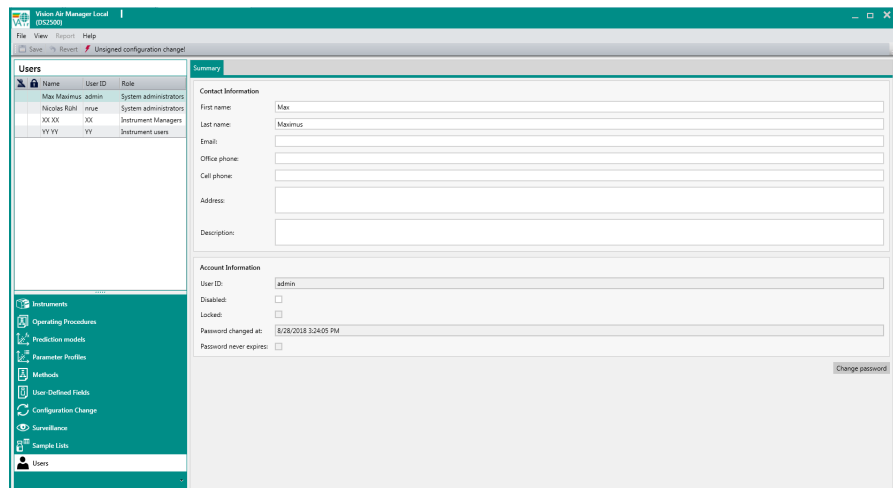
Summary

- The name of the user-defined field.
- Settings that affect the behavior of the user-defined field during sample registration.

Values

Creating, deleting and editing values of user-defined information.

3.1.8 Users section



The **Users** section lists all users.

Users can be created, disabled and edited.

The **Users** section contains the following work window tabs:

<i>Automatic Lock</i>	If a user tries to log in more than 3 times (default) with an incorrect password, the account will be locked and the check box Locked will be activated by the system. To unlock the account, a System Administrator/ Instrument Manager should deactivate the check box Locked and click on [Save]  in the Toolbar.
<i>Password information</i>	The date and time when the user's password was last changed is shown in the Password changed at: field.
<i>No password expiration for specific users</i>	By activating the check box Password never expires in the contact information of a specific user, the user will never be asked to change the password. This checkbox is not activated in pharma mode.
<i>Change password of a specific user</i>	To change the password of an account click on [Change password] . Fill out the Password and the Confirm password field and click on [OK] .
<i>Creating a new user</i>	To access the user creation functions, right-click in the structure window and click on [New System Administrator] or [New Instrument Manager] or [New Instrument User] to create the respective user. All 3 user types can only be created by System Administrators. Instrument Managers can only create Instrument Users.

Login Properties - Options and Description

To access the login properties, right-click in the structure window and click on **[Login properties]**.

Login Options

<i>Password expiration (days)</i>	After this time, the user has to define a new password.
<i>Warn about password expiration (days)</i>	Defines a reminder before expiration. In days before expiration takes place.
<i>Allowed login attempts</i>	Defines how many login attempts with an incorrect password are permitted until the user will be locked.

Logout options

<i>Automatic logout</i>	If the automatic logoff is activated, the user will automatically be logged off after the pre-defined time without any user interaction.
<i>Automatic logout timeout (minutes)</i>	Time in minutes until an automatic logoff takes place.

Password complexity

Password minimum length

A minimum password length can be defined here.

Prevent reuse of recent passwords

The number of recent passwords that are not permitted.

Use numbers and letters

If activated, the password must contain numbers and letters.

Use upper and lower
case letters

If activated, the password must contain upper and lower case letters.

User permissions

To access the user permissions, right-click in the structure window and click on 1 of the 3 menu items **[Instrument User permissions]**, **[Instrument Manager permissions]**, **[System Administrator permissions]**.

Signature permissions

Permissions for configuration changes

Defines which signature options for configuration changes are permitted with this user role.

Permissions for samples

Defines which signature options for samples are permitted with this user role.

Permissions for instrument diagnostics

Defines which signature options for diagnostic tests are permitted with this user role.

Instrument permissions

Routine operation

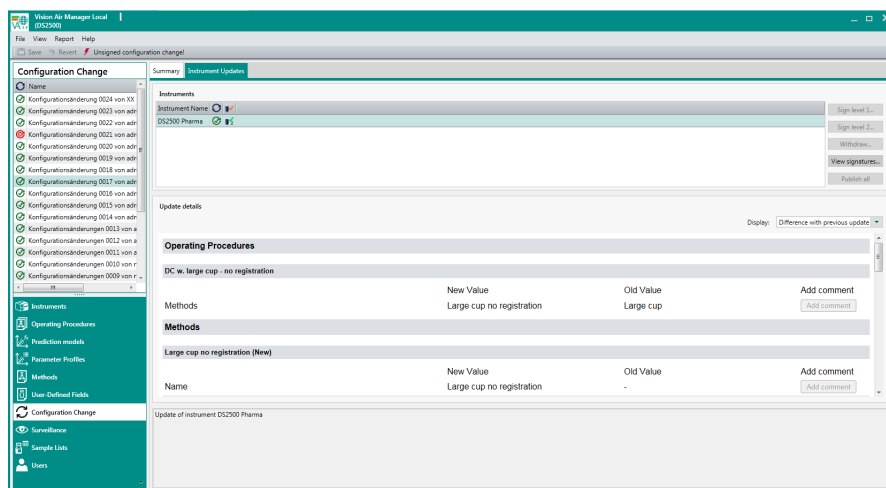
Defines if the user role is allowed to make measurements or not.

Protected tools view options

Defines if advanced features within the **Tools** section in Vision Air Routine are available for this user role or not.

3.1.9 Configuration change section

The **Configuration Change** section lists all the existing configuration changes. A configuration change describes all the settings which affect measurement. All changes (for example changing the name of an operating procedure) are listed and can be compared with an earlier state of the configuration.



A configuration change needs to be signed prior to actively publishing it. Please see ([see "Signing a configuration change", chapter 5.9, page 105](#)) for a workflow description and how to sign configuration changes.

Symbol	Description
	Pending
	Canceled
	Failed
	Completed

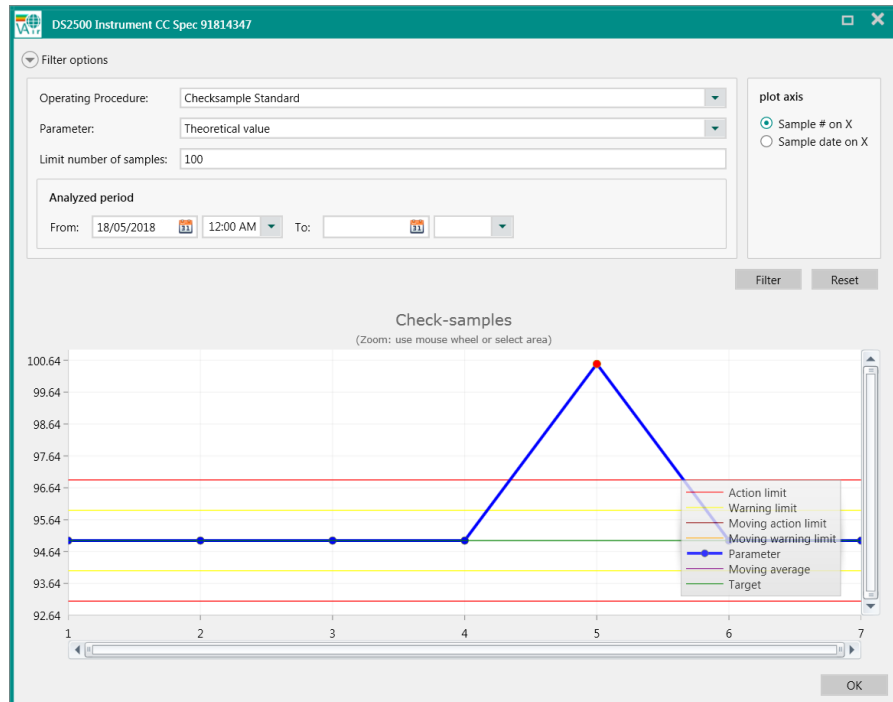
The Configuration Change section contains the following work window tabs:

Summary

Information about the selected configuration change is displayed.

Instrument Updates

- In this tab the content of the configurations changes is displayed.
- The signing process for unsigned configuration changes takes also place here.



It contains the following work window tabs:

Samples

In the **Samples** tab, the user is given an overview over all measured samples within the set filter settings.

Depending on the situation, status symbols can be shown in the raw data (🖨️), reference data (📋), events (⚡), outlier (🔍) and operating procedure limit (🛑) columns. These symbols are summarized in the **Status symbols** section.

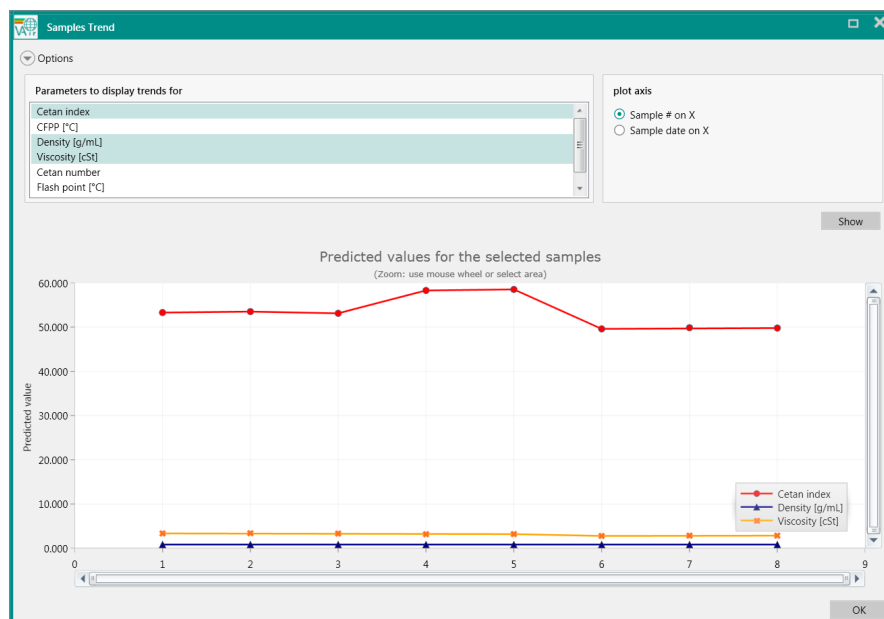
Samples for which outlier limits and/or operating procedure limits are exceeded are colored yellow (warning limits) or red (intervention limits).

i Filtering is not case-sensitive, e.g. 'A' and 'a' are treated equally.

i Always click **[Save]** after changing a sample number and before initiating a new filter search.

By activating the check box **Show sample information**, extra information such as used method and user-defined fields input is immediately displayed in the sample list. By activating the check box **Show secondary parameters**, parameters such as distance for identification and qualification predictions are displayed in the list.

By clicking **[Edit]** in the **Advanced filters** area, up to 5 different advanced filters can be added.



 It is possible to view more than 1 sample in the Samples trend window. To do this, press the **[CTRL]** key and select a number of samples in the sample list. Then click the **[Samples trend...]** button.

Sample details

By double-clicking on a sample in the sample list, the **Sample details** window appears. Alternatively, the **Sample details** window is accessible by right-clicking on the sample and selecting **[Details]**. The upper section of the window shows general information and sample information values.

The **Sample details** window contains the following tabs.

- Predicted values**

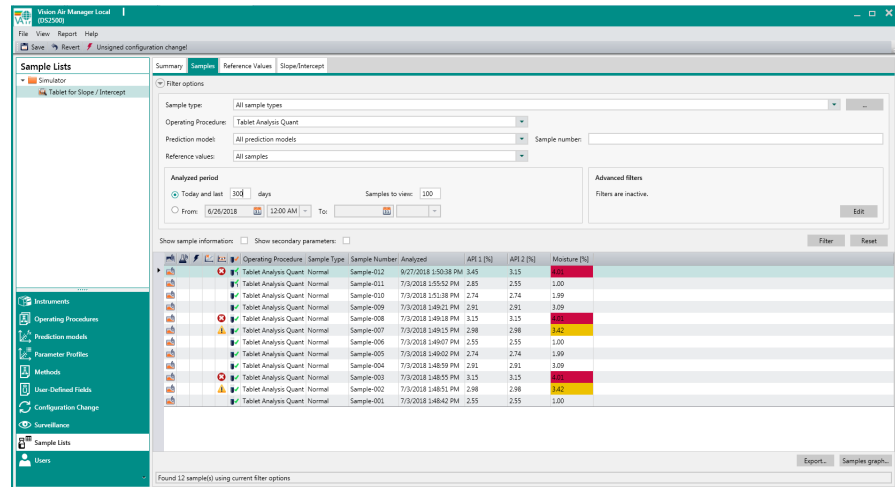
This tab lists the predicted values of the sample including subsamples, if relevant. The list indicates the quality () of the sample and if the sample is an outlier () and/or outside operating procedure limits (). Results for secondary parameters are also listed in this view.

Entity			Lactose Content [%-%]	t-statistics	Comment
SubSample 1			-102.20		
SubSample 2			-101.76		
SubSample 3			-105.49		
SubSample 4			-101.29		
SubSample 5			-105.68		
SubSample 6			-101.79		
SubSample 7			-102.74		
Raw Result			-102.99		
Reported Result			-102.99	-5.35	
Standard Deviation			1.626		
Min			-105.675		
Max			-101.292		

The result in the **Raw result** row is the predicted value of the mean spectrum (depending on the type of instrument and settings) before post-processing i.e. Moisture compensation and Slope/intercept. The **Reported result** is the main result that is also displayed on the **Result** display in Vision Air Routine.

- Software specific
For example new instrument configuration is created.

3.1.11 Sample lists section



The **Sample lists** section allows managing large data sets by using dynamic sample lists and static sample lists. Updates of quantitative prediction models are conducted with slope corrections and intercept corrections by using dynamic sample lists and static sample lists.

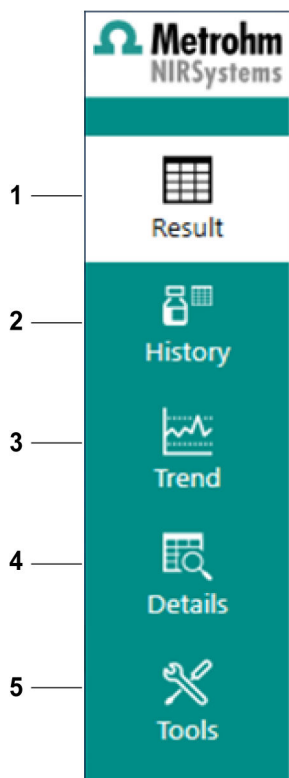
By right-clicking on the structure window, a new sample list group can be defined. The new sample list group is used as a folder for dynamic sample lists and static sample lists. A new sample list is dynamic by default. A new sample list is created within this sample list group by right-clicking on the folder.

Summary

- Name of the sample list.
- Information on when the sample list has been created and modified. If no modification has been conducted, the time stamp for modification and creation are identical.
- By activating the **Static** check box, the sample list is modified to a static sample list. A static sample list cannot be reverted to a dynamic sample list. The sample lists that match the filter settings are fixed. Afterwards, the filter settings are not available anymore for this static sample list.

Samples

Surveillance view with different filter settings. The set filter settings are stored within the sample list. The results are updated automatically. For static sample lists, only the previously defined spectra are displayed.



- | | |
|---|--|
| <p>1 Result
Displays the most recently calculated result with respect to the selected operating procedure.</p> | <p>2 History
Displays all collected results with respect to the selected operating procedure.</p> |
| <p>3 Trend
Graphical display of results over time with respect to the selected operating procedure.</p> | <p>4 Details
Extended sample information, for example spectra display.</p> |
| <p>5 Tools
Section for report creation, instrument tests and general settings.</p> | |

System Events

The system event indicator flashes yellow (🟡) when 1 or more system warnings in the list are waiting for a user action. If the list also contains errors, the system event indicator flashes red (🔴) and the **[Start]** button becomes inactive.

To open the system events list, click on the system event indicator (🔴🟡) in the top right corner of the screen.

Sample event

! Too much light - Sample too light
Check the sample cup

Code

1

Result value

Primary parameter value (predicted value) is followed by possible secondary parameters (depending on prediction model settings). If a parameter cannot be predicted for some reason, the field contains a "-" (minus) sign.

In the case that the selected operating procedure contains an identification prediction model or qualification prediction model, a primary value is displayed as a text string, e.g. lactose or different mesh sizes. If enabled, secondary parameters are displayed, e.g. **Confidence** or **Max. distance**.

Result	
Parameter	Result
Polyethylen conc. [%]	49.05

- Confidence ranges from 1 down to 0. Good confidence is close to 1.
- Max. distance shows the highest allowed normalized distance from unknown sample to best match sample group.

3.2.3 History section

History	
Samples	
Operating procedure	Time
Sample number	Intrinsic Viscosity
Total Acid Number	Moisture [%]
PET Analysis Quant	26/09/2018 3:58 PM
Sample-017	2.91
20.74	3.09
PET Analysis Quant	26/09/2018 3:58 PM
Sample-016	3.15
24.41	4.01
PET Analysis Quant	26/09/2018 3:57 PM
Sample-015	3.15
24.41	4.01
PET Analysis Quant	13/06/2018 6:11 PM
Sample-0014	3.15
24.41	4.01
PET Analysis Quant	13/06/2018 6:11 PM
Sample-0013	2.98
21.76	3.42
PET Analysis Quant	13/06/2018 6:11 PM
Sample-0012	2.55
16.04	1.00
PET Analysis Quant	13/06/2018 6:11 PM
Sample-0011	2.74
18.69	1.99
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0010	2.91
20.74	3.09
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0009	3.15
24.41	4.01
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0008	2.98
21.76	3.42
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0007	2.55
16.04	1.00
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0006	2.74
18.69	1.99
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0005	2.91
20.74	3.09
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0004	3.15
24.41	4.01
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0003	2.98
21.76	3.42
PET Analysis Quant	13/06/2018 6:10 PM
Sample-0002	2.55
16.04	1.00
PET Analysis Quant	13/06/2018 6:07 PM
Sample-0001	2.74
18.69	1.99

History section

The **History** view shows a list of sample results that were measured with the selected operating procedure.

Operating procedure	Time	Sample number	ID_Polymer	Polyethylen Conc. [%]
---------------------	------	---------------	------------	-----------------------

Sample event icons and further information in the data window:

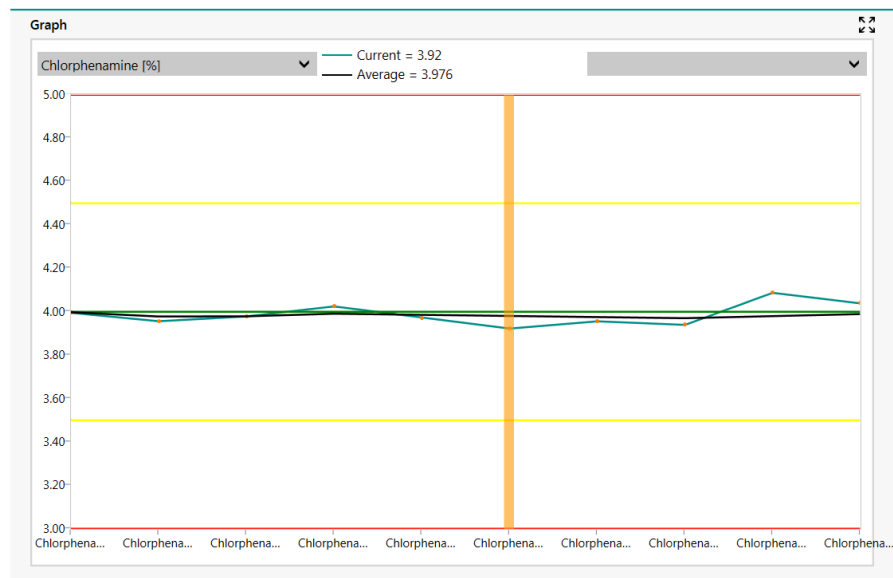
- Raw data status: The type of icon indicates what kind of data has been stored to the database. When extra data is attached to the sample result, a data type icon is displayed in the left column: Sensor and pre-processed data (📷), Pre-processed data (📄, default data type).



Figure 1 Main graph

The trend graph can show 1 or 2 parameter plots. Parameters are selected by using the "Green Plot" and "Orange Plot" drop-down lists on top of the graph. The lists contain all the parameters that were investigated with the currently selected operating procedure.

If only 1 graph is displayed, a graph for the running average can be displayed. If upper and lower warning limits, intervention limits and a target value have been defined in Vision Air Manager, they are also shown, so that up to 5 horizontal lines are displayed.



If a measured value is selected in the graph, a vertical orange line is displayed that highlights the selection. The upper middle part of the window shows the quantitative result(s) of the selected measurement.

Trend settings

The settings field contains the **[Trend settings]** button that gives access to the **Trend settings** dialog window.

Graph view settings ?

Parameter graph options:

☒ Show moving average curves

Number of samples for average calculation:

X-axis options

☒ Use an equally spaced scale

☐ Use a true time scale

Max. samples:

The following trend settings are available:

- **Parameter graph options**
 Show moving average curves: This defines if a moving average should be calculated and displayed as well as the number of recent samples to include in the calculation.
 Number of samples for average calculation: The running average calculation is based on the defined number of samples.
- **X-axis options**
 Use an equally spaced scale, i.e. the x-axis distance between samples must be equal.
 Use a true time scale, i.e. the x-axis distance between samples is proportional to the time between the measurements.
 Max. samples, i.e. the graph shows "max." sample results, from the most recent samples.
- **Set default**
 By clicking the **[Set default]** button, the last graphical settings are saved and used thereafter.

3.2.5 Details section

Information tab

In the **Information** tab, extended information is available for a specific sample. It is also possible to edit or add additional information (depending on the operating procedure settings).

- **Sample registration**
Fixed information of the selected sample.
 - Sample signature
A signature/checksum for the sample that is created at the time of analysis.
 - Database ID
An internal ID in the Vision Air database.
- **Details**
Sample registration information that can be edited.

Click on the **[Save]** button after every change.

Protocol tab

Category	Parameter	Value	Action
General Information (NIRS DS2500)	Cup type	2501 (Small cup)	
Generic absorbance calculation 2 (Si4x6.5mm)	Intensity correction	IntensityCorrection (270)	Export
Generic absorbance calculation 2 (Pb54x10mm)	Intensity correction	IntensityCorrection (281)	Export
Local Vision Air settings (Vision Air)	Automatic printing enabled	Yes	
	Automatic reports enabled	Yes	
	Automatic reports path	USB:\Metrohm\AutomaticReports	
	CSV export enabled	Yes	
	Automatic CSV and Excel export path	USB:\Metrohm\DirectExport	
	Manual CSV and Excel export path	USB:\Metrohm\DirectExport	
	Manual reports path	USB:\Metrohm\ManualReports	
	Printer name		
Analysis (NIRS DS2500 Base)	Autolinearisation enabled	No	
	Number of reference subsans	32	
Compatibility (NIRS DS2500 Base)	NIRS 6500/5000 compatibility mode	No	
RFID (NIRS DS2500 Base)	Cup serial number	0	
	Cup type check	Yes	

The **Protocol** tab gives an overview of measurement settings for the analyzed sample.

Some settings are relevant to the instrument (or a specific part of the instrument) while other settings are related to parameters. The relevant instrument part name or parameter name is shown in brackets.

3.2.6 Tools section

The accessibility to functions for the Instrument User is reduced by default. To modify the accessibility, see [\(see "Users section", chapter 3.1.8, page 31\)](#).

The following functions are accessible in the **Tools** section.

- Export samples
The **[Export samples]** button allows to export collected measurements. A folder with an .xml file is created in the selected destination.
- Data maintenance (not accessible for the Instrument User by default)
The **[Data maintenance]** button allows to start a backup of the database, to restore an existing database or to delete samples for a defined time period.
- Instrument information
The **[Instrument information]** button opens the **Instrument information** window. The **Instrument information** window displays information on the Vision Air version used, the analyzer name that is defined in Vision Air Manager and some computer specific information, for example the IP address.
- Temperature correction (only available for DS2500 Liquid Analyzer)
The **[Temperature correction]** button allows to correct the temperature difference between the sample holder and the sample.
- Settings (not accessible for the Instrument User by default)
The **[Settings]** button grants access to different settings.
 - Import
In the **Import** section, the user can import configuration files or directly access Vision Air Manager.
 - Export
In the **Export** section, the user can define the storage locations for reports and results and allow an automatic export set in Vision Air Manager.
 - Print
In the **Print** section, automatic print can be activated. Automatic print is set in Vision Air Manager. Additionally, the print template and the printer itself can be selected.
 - Protocol
In the **Protocol** section, the user can select a storage location for information that is displayed in the **Protocol** section, in the **Details** section of Vision Air Routine.
 - Backup
In the **Backup** section, the user can set an automatic backup plan and define the storage location.
 - Instrument
In the **Instrument** section, the user can modify a global counter that can be used during automatic sample numbering.
- Photometric test definition (not accessible for the Instrument User by default, only available for XDS instruments and DS2500 Solid Analyzer)
The **[Photometric test definition]** button allows to define reference values for the photometric test by using external standards.

Automatic sample numbering

If the automatic sample numbering option is selected, the sample number is generated automatically during measurement using the defined mask. The mask should be entered into the text field and may contain the following formatting codes, which are substituted by real data:

- [INSTRUMENTNAME] – name of the current instrument
- [PRODUCTNAME] – name of the current operating procedure
- [PRODUCTCODE] – code of the current operating procedure (numeric value)
- [HH] – hours in 24 hour format
- [HHHH] – hours in 12 hour format (AM/PM)
- [MM] – minutes
- [SS] – seconds
- [YY] – year (13)
- [YYYY] – year (2013)
- [Y] – year (3) #-##### – consecutive sample counter. Number can have 1(#) to 6 (#####) digits. Number starts with 0...01 and increments on every measurement.

Truncation:

It is possible to truncate strings in [PRODUCTNAME], [PRODUCTCODE] and [INSTRUMENTNAME] by appending the %n sign, e.g. [INSTRUMENTNAME %3]. If the string is longer than the defined number, it is truncated to the corresponding length (3 in the example) otherwise it is padded with spaces.

Example:

"[PRODUCTNAME%10] Sample-### [HH]:[MM]"

Mask creation rules

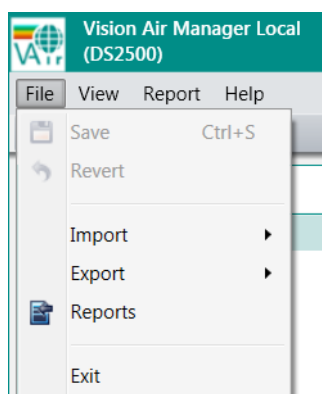
- All formatting codes, except number sequence, must be written in square brackets [].
- All formatting codes must be upper case.
- It is allowed to have only 1 number sequence (###) in the mask.
- It is allowed to not have any number sequence in the mask at all.

- Instrument detail
This report is available when **Instruments** is selected in the navigation window.
- Prediction model list
This report is available when **Prediction models** is selected in the navigation window.
- Prediction model list with details
This report is available when **Prediction models** is selected in the navigation window.
- Instrument slope/intercept 30 days
This report is available when **Surveillance** is selected in the navigation window.
- Instrument status
This report is available when **Surveillance** is selected in the navigation window.
- Flags log
This report is available when **Surveillance** is selected in the navigation window.
- Instrument check samples 5 days
This report is available when **Surveillance** is selected in the navigation window.
- Instrument group events 30 days
This report is available when **Surveillance** is selected in the navigation window.
- Instrument group audit events 30 days
This report is available when **Surveillance** is selected in the navigation window.
- Sample list
This report is available when a sample is selected in the sample work window of the **Surveillance** navigation window.
- Sample list (landscape mode)
This report is available when a sample is selected in the sample work window of the **Surveillance** navigation window. The report will be displayed in landscape format.
- Sample detail
This report is available when **Surveillance** is selected in the navigation window.
- Simple single sample
This report is available when a sample is selected in the sample work window of the **Surveillance** navigation window.
- Instrument diagnostics
This report is available when **Surveillance** is selected in the navigation window and a self test is selected on the **Diagnostics** tab.
- Low flux test
This report is available when **Surveillance** is selected in the navigation window and Low flux test is selected on the **Diagnostics** tab.

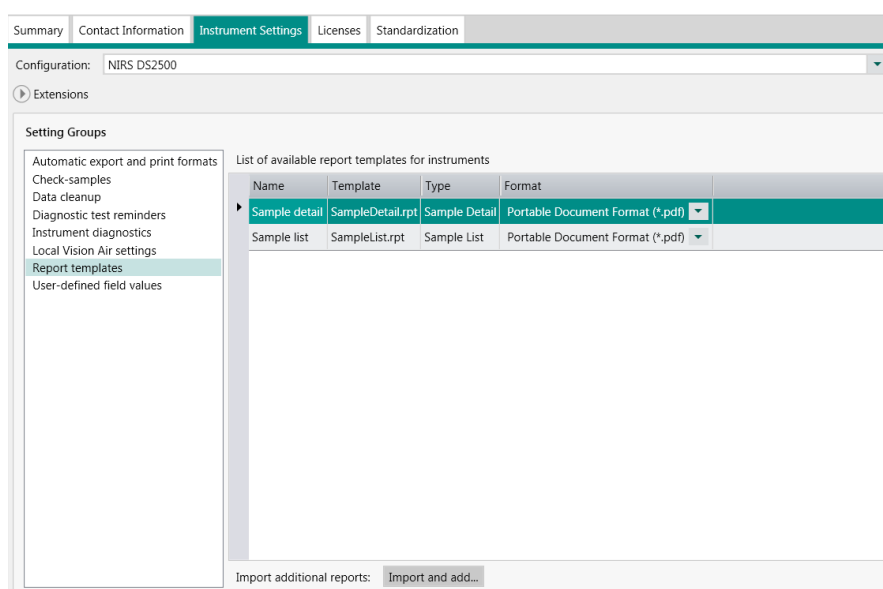
- Wavelength certification test (only available for XDS instruments and DS2500 Solid Analyzer)
This report is available when **Surveillance** is selected in the navigation window and Wavelength certification test is selected on the **Diagnos-tics** tab.
- Instrument events - Selected period
This report is available when **Surveillance** is selected in the navigation window and the work window events.

New report templates can be added with Vision Air Manager. Depending on the part of Vision Air (Routine or Manager), in which the report template should be available, different sections need to be used for the import.

For Vision Air Manager, report templates are imported under **File ► Reports**.



For Vision Air Routine, report templates are imported under **Instruments** ► **Instrument settings** ► **Report templates**.



For automatic export in Vision Air Routine, report templates must be imported under **Instruments ► Instrument settings ► Automatic export and print formats**.

Configuration: NIRS DS2500

Extensions

Setting Groups

Automatic export and print formats

Check-samples
Common hardware selftest limits
Data cleanup
Diagnostic test limits
Diagnostic test parameters
Diagnostic test reminders
Hardware self test limits
Hardware sensor limits
Instrument calibration settings
Instrument diagnostics
Local Vision Air settings
Report templates
Stability test limits (PbS)
Stability test limits (Si)
Stability test parameters
Subscan settings
User-defined field values
Wavelength test limits (PbS)
Wavelength test limits (Si)
Wavelength test parameters

In Method settings automatic export and printing after each measurement can be enabled. The actual options are defined here at instrument level.

Automatic printing options

☒ No printing
☐ Print using report template

Sample detail

Automatic export options

Export file names format: [PRODUCTNAME]_[REPORTNAME_]YYYY-MM-DD[HH]-[MM]-[SS]

☒ No export
☐ Native CSV export
☐ Native CSV export including secondary parameters
☐ Export using report template

Sample detail CSV

Additional spectral export: No spectral export

Import additional reports: Import...

3.3.3 Importing reference values with a .csv file

Reference data can be imported from a .csv file that matches the structure of the displayed reference table.

	A	B	C	D
1	Sample Number	<i>Parametercode 1</i>	<i>Parametercode 2</i>	...
2	Sample name 1	10.1	0.5	...
3	Sample name 2	22.5	0.7	...
4	Sample name 3	40.3	1.1	...
5	Sample name 4	50.3	2.3	...

The list separator follows the PC's regional setting e.g. semicolon, comma, dot.

In the heading of the table, the sample number and the parameter code for reference values are defined.

The bold string **Sample number** is fixed and does not need to be modified.

For the strings **Parameter code x**, enter the appropriate parameter code that is defined in Vision Air Manager.

Sample names must be identical to the sample names that were used during sample registration. Sample names must not be listed in the same order as they were measured.

1 Open Vision Air Routine.

Check Sample ☐

Check Sample
(Definition)

3 Set the check mark to run a definition in order to create your reference value for the following check sample analysis.

4 Place the check sample in the sample compartment.

To analyze a check sample, proceed as follows:

2 Position your check sample. Click on **[Start]**.

- 3 If the check sample passes, the lid opens and you can remove the check sample and run a check sample measurement. If the check sample test fails, follow the instructions on the screen and try again. If the problem persists, run an instrument diagnostic test and check if your check sample has changed. If the problem still persists, contact your local Metrohm representative.

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3.3.5 Exporting samples for prediction model development

Measurements that were carried out in Vision Air Routine can be used to create and update prediction models that were created in Vision, The Unscrambler or PLS_Toolbox.

To export samples, go to the **Surveillance** section in the **Samples** tab and click on **[Export...]**. For the export, select the .xml file.



Select Options for Sample Export

X

Select export options

Select file format XML Samples Files (*.xml)

General options

Include subsamples

☐

Include samples with no spectra

☐

.XML options

Include protocols

☐

Include complete raw data

☐

Export to one sample file and separate rawdata files

☐

.NIR and .CAL options

Trim spectral range

400 - 2500 nm

Custom range (nm)

400

-

2500

Trim spectral resolution

0.5 nm

Apply ISI standardization to raw data

☐

Standardization group

Also create ANL files

☐

Excel and .CSV options

Include secondary parameters

☐

OK

Cancel

Check **Include protocols** to export additional information, e.g. which method has been used (optional). The advantage of including protocols for the export is that data collection methods are automatically created in Vision during a sample import.

 If you import the .xml file in Vision, the products in Vision are named according to the operating procedure used in Vision Air. If a product already exists in Vision, the user has to select whether the spectra has to be included in the product or a new product name has to be created.

3.3.6 Calculated prediction models

Calculated prediction models are defined formulas that allows you to postprocess results and to decide which result is presented to the user.

Creating a calculated prediction model

The **Create calculated prediction model** editor is used to create a formula. The editor can be accessed when creating a new calculated prediction model. To access the editor, right-click in the structure window of the **Prediction models** section and select **Create calculated prediction model**. A formula can be added in the **Prediction models** section on the **Formula** tab.

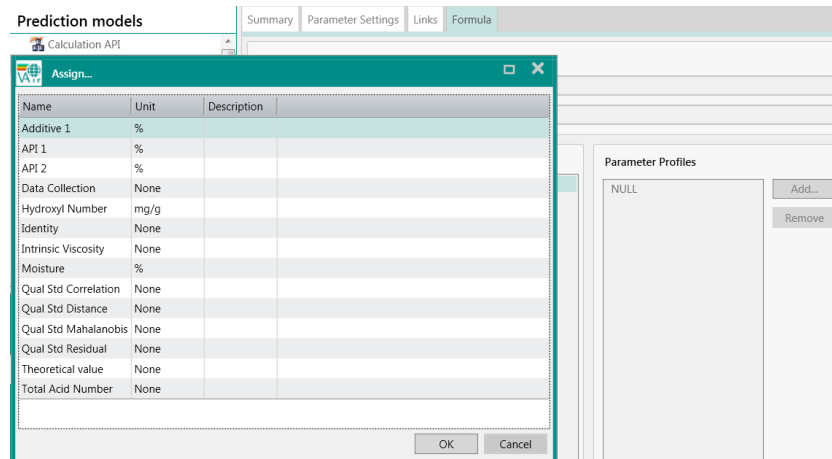
Adding a formula

i It is important that the operating procedure for the calculated prediction model also contains prediction models that include the parameters referenced in the calculated prediction model formula. Otherwise, an error message is displayed at synchronization.

Example 1

The example describes how to postprocess a predicted value of a prediction model.

- 1 Add the parameter profile of the prediction model that you want to postprocess by clicking on **[Add]** in the **Formula** tab.



- Remove the entries in the **Expression** field.
- Enter the formula, e.g. if the result of a prediction should be divided by 2, double-click on the corresponding parameter profile, add the operator **/** and the number **2**.

Expression

[Additive 1] / 2

Parsing results: Formula is valid.

- 4 Save the calculated prediction model. Add the calculated prediction model to the operating procedure that you want to use for postprocessing.

Make sure that the operating procedure includes the prediction model for which the postprocessing should be conducted. If the result of the prediction model should not be displayed, select the prediction model, go to the **Summary** tab and check **Hidden** in the **Linked parameter profiles** window.

Prediction models				
Calculation API				
Calculation API - Demo				
Data Collection				
Qual WL Standard Mahal				
Qual WL Standard ResV				
Qual WL Standard Wavecorr				
Qual WL Standard Wavedist				
Quant WL Standard				
Simulator API 1				
Simulator API 2				
Simulator Hydroxyl Number				
Simulator Identification Chlorophena				

Summary				
General Information				
Name:	Calculation API			
Wavelength:				
Version:	1.0.6			
Part Number:	0			
Imported:	18/06/2018 9:46:56 PM	Method:	CALC	
Updated:	18/06/2018 9:46:56 PM	Engine:	Calculator	
Comment:				
Description:				

Linked Parameter Profiles				
Hidden	Parameter name	Parameter unit	Parameter profile	Display order
☒	Calculation	%	API	101

Example 2

The example describes how to use calculated prediction models for automatic selection of the optimal prediction model and result display during routine analysis. This scenario is important, e.g. if a broad concentration range should be predicted. Typically, instead of using 1 prediction model for the whole concentration range, multiple prediction models are used. This increases the accuracy of the prediction. For this case, If-Then-Else-formulas are used.

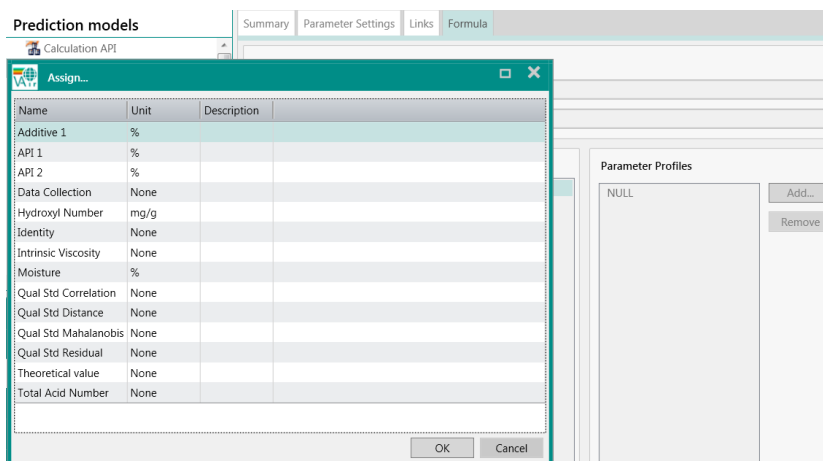
In the following example, a user has 3 prediction models.

- API Full
Parameter profile for the prediction model that is predicting a concentration of API from 0 - 30%.
- API 1
Parameter profile for the prediction model that is predicting a concentration of API from 0 - 10%.
- API 2
Parameter profile for the prediction model that is predicting a concentration of API from 10.01 - 30%.

Only 1 result is displayed where the software chooses whether it displays the API 1 result or the API 2 result.

To start a prediction model, proceed as follows:

- 1 Add the parameter profile of the prediction model that you want to postprocess by clicking on **[Add]** in the **Formula** tab.



- 2 Enter the formula. The following screenshots show the syntax for the example.

Expression

if ([API Full] > 10 ; [API 2] ; [API 1])

Parsing results: Formula is valid.

if ([API Full] > 10 ; [API 2] ; [API 1])

Parameter 1 Then Parameter 2 Else Parameter 3

"If" expressions are put in brackets, the parameter profile names are written in brackets and "then" and "else" expressions are written with ";".

- 3 Save the calculated prediction model. Add the calculated prediction model to the operating procedure that you want to use for postprocessing.

Make sure that the operating procedure includes the prediction model for which the postprocessing should be conducted. If the result of the prediction model shall not be displayed, select the prediction model, go to the **Summary** tab and check **Hidden** in the **Linked parameter profiles** window.

i Make sure that the **Parsing results** field indicates that the entered formula is valid. If the formula is not valid, the prediction model cannot be saved.

3.3.7 User-defined prediction model

i An operating procedure can never consist of user-defined prediction models only.

It is possible to manually add sample parameter data that is measured with other instruments.

User-defined prediction models can be created by right-clicking on an element in the structure Window and selecting **[Create User-defined Prediction Model...]**.

If you create an operating procedure with 2 user-defined prediction models, the sample results include positions for both user-defined prediction models.

During a measurement, a dialog window pops up and the user can type in the values.

3.3.8 Slope/intercept calculations

Slope/intercept data can be displayed for quantitative prediction models in the **Prediction models** section, **Slope/intercept** tab.

Values for slope and intercept can be changed manually in the **Prediction models** section on the **Slope/intercept** tab.

Calculate slope/intercept values

Apply	Instrument	Parameter	IS	New IS	II	New II	Bias	Correlation	RMSEP	RSD	SEP
-------	------------	-----------	----	--------	----	--------	------	-------------	-------	-----	-----

To calculate the slope/intercept correction, a sample list is needed.

The samples that are used for slope/intercept calculation need a reference value for the parameter that should be corrected.

 Make sure that at least 10 samples are available for the calculation of the slope/intercept value.

Using the filter settings in the sample work tab allows you to find matching samples.

Sample Lists

- Simulator
 - Polymer w reference
 - Polymer w/o reference

Summary
Samples
Reference Values
Slope/Intercept

Filter options

Sample type: All sample types

Operating Procedure: PET Analysis Quant

Prediction model: All prediction models

Reference values: With Reference Values

Analyzed period

☒ Today and last 300 days

Samples to view: 100

☐ From: 6/06/2018 12:00 AM To:

Show sample information: ☐

Show secondary parameters: ☐

	Operating Procedure	Sample T	Sample Number	Analyzed	Intrinsic Viscosity	Total Acid Number	
		PET Analysis Quant	Normal	Sample-0012	13/06/20...	2.55	16.04
		PET Analysis Quant	Normal	Sample-0011	13/06/20...	2.74	18.69
		PET Analysis Quant	Normal	Sample-0010	13/06/20...	2.91	20.74
		PET Analysis Quant	Normal	Sample-0007	13/06/20...	2.55	16.04
		PET Analysis Quant	Normal	Sample-0006	13/06/20...	2.74	18.69
		PET Analysis Quant	Normal	Sample-0005	13/06/20...	2.91	20.74
		PET Analysis Quant	Normal	Sample-0002	13/06/20...	2.55	16.04
		PET Analysis Quant	Normal	Sample-0001	13/06/20...	2.74	18.69

In the **Sample lists** section on the **Reference values** tab, reference values can be added or adjusted.

In the **Sample lists** section on the **Slope/intercept** tab, the correction for the individual parameters can be conducted. 3 parameters are available in the presented example.

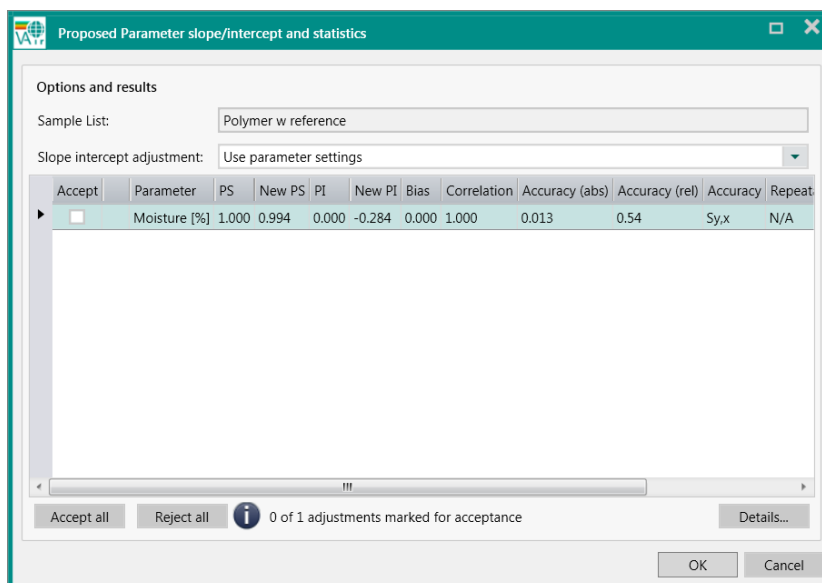
Summary	Samples	Reference Values	Slope/Intercept			
Parameter Slope/Intercept						
				Calculate S/I for other prediction models: ☐		
	Parameter	Prediction model	Version	Slope	Intercept	
▶	Intrinsic Viscosity	Simulator Intrinsic Viscosity	1.0.0.0	1.000	0.000	
	Moisture	Simulator Moisture	1.0.0.0	1.000	0.000	
	Total Acid Number	Simulator TAN	1.0.0.0	1.000	0.000	

The procedure for the correction is explained for the parameter moisture.

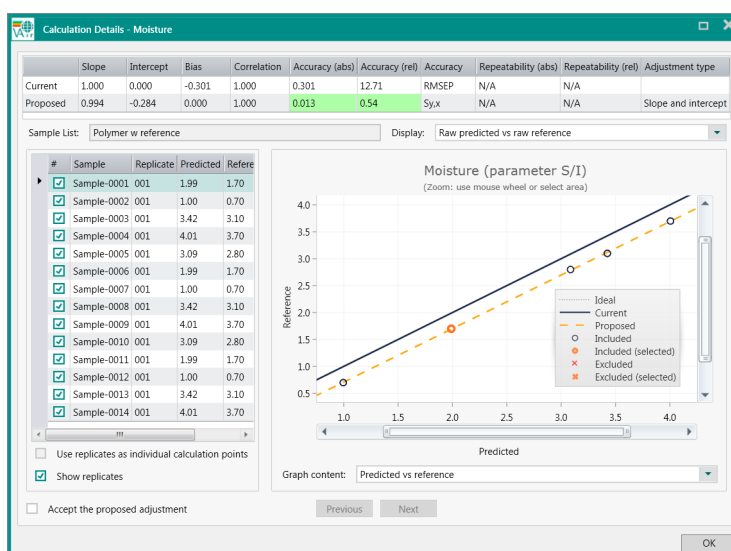
To start a parameter correction, proceed as follows:

- 1 Select the parameter you want to correct and click on **[Calculate slope/intercept]**.

A window with suggested adjustments is displayed.



- 2 Click on **[Details...]** to see the current correlation plot and the new correlation proposal.



The trend section displays the samples as dark blue dots on the gray reference lines. The plot gives an overview of the correlation, the bias, the slope and the presence of outliers.

In this example, predicted values are biased by -0.301. Correction of the slope and mainly the intercept correct for this deviation between predicted values and reference values.

The table in the upper part of the window indicates the improvement of the absolute accuracy and the relative accuracy as a result of the correction.

Zoom in by pointing in the graph area and rolling the mouse wheel. A zoomed in graph can be moved around by using click and drag. Pointing on a sample in the list displays the sample in orange in the graph. Remove a sample from the calculation by unticking the sample in the # column of the list.

- 3 Check **Accept the proposed adjustment** to accept the changes.

3.3.9 Signing

Several objects can or need to be signed in Vision Air Pharma. In principle, each object can be signed on 2 levels. Objects which can be signed are configurations, samples, and diagnostic reports. Each signature needs a pre-defined reason. This can be defined in Vision Air Manager under **File ► Signatures**.

Signatures

Electronic signature options

Sign each sample separately at Instrument: ☐

Sign each sample separately in Vision Air Manager: ☐

Electronic signature reasons

Level: Configuration signature level 1 reasons

Reason	Comment
▶ Approved	☐
Configuration reviewed	☐
Validated	☐
Validation reviewed	☐

Add reason

Remove reason

OK Cancel Apply

In the **Electronic signature options**, signing of multiple samples in one step can be activated or deactivated.

Sign each sample separately at instrument:

If activated, a multiple selection of samples with **[CTRL + SHIFT]** cannot be signed in one step at the instrument (Vision Air Routine).

Sign each sample separately in Vision Air Manager:

If activated, a multiple selection of samples with **[CTRL + SHIFT]** cannot be signed in one step in Vision Air Manager.

Samples or diagnostic tests are signed by right-clicking on the individual sample or diagnostic test and selecting **Sign level 1**.

Operating Procedure	Sample Type	Sample Number	Analyzed	API 1 [%]
Tablet Analysis Quant	Normal	Sample-012	9/27/2018 1:50:38 PM	3.45
Tablet Analysis Quant	Normal	Sample-011	7/3/2018 1:55:52 PM	2.85
Tablet Analysis Quant	Normal	Sample-010	7/3/2018 1:51:38 PM	2.74
Tablet Analysis Quant	Normal	Sample-009	7/3/2018 1:49:21 PM	2.91
Tablet Analysis Quant	Normal	Sample-008	7/3/2018 1:49:18 PM	3.15
Tablet Analysis Quant	Normal	Sample-007	7/3/2018 1:49:15 PM	2.98
Tablet Analysis Quant	Normal	Sample-006	7/3/2018 1:49:07 PM	2.55
Tablet Analysis Quant	Normal	Sample-005	7/3/2018 1:49:02 PM	2.74
Tablet Analysis Quant	Normal	Sample-004	7/3/2018 1:48:59 PM	2.91
Tablet Analysis Quant	Normal	Sample-003	7/3/2018 1:48:55 PM	3.15
Tablet Analysis Quant	Normal	Sample-002	7/3/2018 1:48:51 PM	2.98
Tablet Analysis Quant	Normal	Sample-001	7/3/2018 1:48:42 PM	2.55

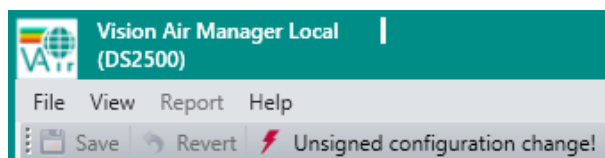
Samples, diagnostic tests, and configurations can be signed multiple times on level 1. Each signature must be done with a different user ID.

After a successful signature, the sample, diagnostic test, or configuration is marked with the number '1'.

Signature Level 1		Tablet Analysis Quant
No Signature		Tablet Analysis Quant

Samples, diagnostic tests and configurations can only be signed on level 2 after being signed on level 1.

Configurations have to be signed when changed. The signing is conducted in the section configuration change. A configuration change is triggered after any change in Vision Air Manager and displayed with a red lightning symbol below the task bar:



Configuration changes need to be signed prior to actively publishing them (see *"Signing a configuration change"*, chapter 5.9, page 105).

3.3.10 Specific functions for DS2500 Solid Analyzer

With the DS2500 Solid Analyzer, the average result of multiple sample cups (cups per sample) and multiple positions within the sample (number of subsamples) can be calculated.

To analyze multiple positions and cups, proceed as follows:

- 1 Go to the **Methods** section.
- 2 Select the method for which you want to configure the number of cups and positions.
- 3 Go to the **Summary** tab. Select a sample vessel type that supports this functionality.

Table 4

Sample vessel type	Intended purpose
Large cup	Subsample Multiple cups per sample
Small cup moving	Subsample Multiple cups per sample
Small cup	Multiple cups per sample
Slurry cup	Subsample Multiple cups per sample
No cup	Multiple cups per sample
Multisample cup	None

Setting Groups

Analysis

Angles

Automatic export and print

Check-sample product

Compatibility

Display options

Repetitions

RFID

Sample numbering

Storage options



Scanning settings for the selected cup

Cups per sample:

1

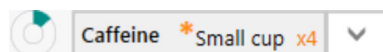
Number of subsamples:

8

Number of subs cans:

4

During the analysis, the expected number of cups is displayed in Vision Air Routine:



When starting the analysis in Vision Air, the sample registration view is displayed as usual but the user is prompted for the next cup. Finally, the mean result for the cups is displayed.

Multisample Cup

The Multisample Cup is supported with Vision Air 2.0.2.25.

To select trays in Vision Air Manager, proceed as follows:

- 1 Go to the **Methods** section.
- 2 Select the method for which you want to configure the tray.
- 3 Go to the **Summary** tab in the data window and make sure that the **Sample vessel** field has the value: **Tray**.
- 4 Go to the **Settings** tab in the data window and select the menu item **Tray configuration**.
- 5 Select a pre-defined tray from the drop-down list.
If a customized tray has been ordered together with Vision Air, a configuration file is provided by Metrohm. Import this configuration file by using the **Custom tray configuration** import.
- 6 Click on **[Save]** in the toolbar.

Calibrating the instrument in Vision Air Routine

2 different processes for instrument calibration are available. One process uses the internal built-in wavelength filter. The other process uses the external wavelength filter. For intensity corrections, the DS2500 Solid Analyzer uses the external reflection standard as reference standard. Only external wavelength filters can be certified.

The instrument must be running for 2 hours before starting the instrument calibration. For external instrument calibration, have the corresponding external wavelength filters ready.

- 1 In Vision Air Routine, go to the **Tools** section.
- 2 Click on **[Instrument calibration]**.

A window opens that prompts the user to enter the PIN code.

[illegible]

- 3** In non-pharma versions of Vision Air, enter your PIN code. The default PIN code is 1234. Click on **[OK]**.

In pharma versions of Vision Air, the user rights define whether a user has access to instrument calibration. No PIN code is required.

The **Instrument calibration** window opens.

Instrument calibration

☒ Use internal wavelength filter

☐ Use external wavelength filter

[Calibrate](#) [Close](#)

- 4** Select whether to use the internal wavelength filter or the external wavelength filter.

Click on **[Continue]** to proceed.

- 5 Click on **[Calibrate]**.

The instrument is calibrated.

A message confirms the successful calibration. The instrument is ready to measure samples.

3.3.11 Specific functions for DS2500 Liquid Analyzer

With the DS2500 Liquid Analyzer, multiple sample vessels are available to address different sample absorbance levels and to enable a convenient operation of the instrument.

To analyze multiple sample vessels and positions, proceed as follows:

- 1** Go to the **Methods** section.

- 2 In the **Method** structure window, select the method for which you want to configure the number of sample vessels and positions.

- 3 Go to the **Summary** tab.

Select a sample vessel type that supports the desired functionality from the **Sample vessel** drop-down list.

Table 5

Sample vessel type	Intended purpose
Disposable vials	One-time use No sample vessel cleaning
Cuvettes	High precision measurements
Flow cell cuvette	Automatization
Transmission wavelength standard	External calibration of the instrument

Heating and cooling the sample

The DS2500 Liquid Analyzer supports a temperature range between 25 °C and 80 °C. The minimum temperature that can be set must be 10 °C above the ambient temperature $T_{\min} = T_{\text{ambient}} + 10\text{ °C}$

To achieve a temperature of 25 °C, the ambient temperature must be 15 °C. As the ambient temperature in most laboratories is approx. 25 °C, Metrohm recommends to set the temperature to a minimum of 35 °C.

To define the target temperature during an analysis, go to the **Methods** section in Vision Air Manager. Go to **Settings ► Liquid setup**. Enable **Temperature control**. Enter the desired temperature in **Equilibrium Temp (°C)**.

A delay before starting a scan ensures that the sample has the same temperature as the sample holder. To define a delay before each scan, go to the **Methods** section in Vision Air Manager. Go to **Settings ► Liquid setup**. Enter the desired length of the delay in **Delay before scanning (seconds)**.

Temperature correction

If you set a sample temperature, the sample holder is heated or cooled to this temperature. There may be slight differences between the temperature of the sample holder and the temperature of the sample.

To correct the sample temperature, proceed as follows:

[illegible]

Temperature control must be enabled for the method that is linked to the operating procedure in use.

- 1 Go to the **Tools** section. Click on **[Temperature correction]**.
A window opens that prompts the user to enter the PIN code.
- 2 Enter your PIN code. The default PIN code is 1234. Click on **[OK]**.
The **Temperature correction** wizard opens.
- 3 Click on **[Start]** to proceed.
- 4 Follow the instructions on the appearing window.
Then click on **[Next]** to proceed.
- 5 Enter the desired sample temperature. Click on **[Save]**.
A confirmation window appears.
- 6 Click on **[Close]** to exit the wizard.
Temperature correction is applied to the sample.

Measurement with open lid

It is possible to measure a sample while the lid of the DS2500 Liquid Analyzer is open.

Automatic start

If **Automatic start** is enabled, then the measurement starts automatically as soon as the lid is closed.

- 1 In Vision Air Manager, go to the **Methods** section.
 - 2 Go to the **Settings** tab.
 - 3 Open the setting group **Automatic start control**.
 - 4 Enable **Automatic start**.
- The measurement starts as soon as the lid is closed.
After the measurement, the lid opens automatically.

Calibrating the instrument in Vision Air Routine

The DS2500 Liquid Analyzer is calibrated with an external wavelength standard (*see "Calibrating the instrument with an external wavelength calibration standard", page 79*) and with an internal wavelength stand-

ard (see "Calibrating the instrument with an internal wavelength standard", page 80).

The external calibration is usually carried out by a regional Metrohm service representative during the start-up of the instrument. If necessary, the external standard can also be obtained separately (article number 6.7494.000). The user can repeat the external calibration if needed. Only external wavelength filters can be certified.

The internal calibration uses the internal built-in wavelength filter. Carry out the internal calibration once a different type of sample vessel to the one used in the previous measurement is inserted. The path length is relevant. Carry out an internal calibration after a DS2500 Holder for 2 mm disposable vials was replaced with a DS2500 Holder for 8 mm disposable vials, for example.

For intensity corrections, the DS2500 Liquid Analyzer uses air as reference standard.



WARNING

Hot surface

Danger of burning due to hot components. The sample holder can be heated to a maximum of 80 °C. After operation, the sample compartment, the sample holder and the sample vessel are very hot.

- Wear protective gloves when handling sample holders and samples.

Calibrating the instrument with an external wavelength calibration standard

Accessories

- DS2500 liquid wavelength calibration standard (6.7494.000)

Precondition

- The instrument must be running for 2 hours before starting the instrument calibration. For external instrument calibration, have the corresponding external wavelength filters ready.

1 Using the wavelength calibration standard

- Place the wavelength calibration standard in the sample compartment.
- Optionally place the cover plate on the sample compartment. If the sample holder is heated, the cover plate protects the user from the heat that is generated.
- Tighten the screw.

2 Calibrating the instrument

- In Vision Air Routine, go to the **Tools** section.
- Click on **[Instrument calibration]**.
A window opens that prompts the user to enter the PIN code.
- Enter your PIN code. The default PIN code is 1234. Click on **[OK]**.
The **Instrument calibration** window opens.

Instrument calibration

☐

 Use internal wavelength filter

☒

 Use external wavelength filter

Calibrate

Close

- Select **Use external wavelength filter**.
- Click on **[Calibrate]**.
- Follow the instructions on the appearing window.
The wavelength filter is heated up to 50 °C automatically.

The instrument is calibrated.

A message confirms the successful calibration. The instrument is ready to measure samples.

Calibrating the instrument with an internal wavelength standard

Accessories

- Sample holder

Precondition

- The instrument must be running for 2 hours before starting the instrument calibration. For external instrument calibration, have the corresponding external wavelength filters ready.

1 Inserting the sample vessel

- Define with which sample vessel the next measurement is to be carried out.
- Insert the selected sample vessel.

 If an incorrect sample vessel was inserted for the calibration with the internal wavelength standard, the error **auto linearization failed** may be displayed during the routine analysis.

2

- ### Instrument calibration

☒

 Use internal wavelength filter

☐

 Use external wavelength filter

Calibrate

Close

- The instrument is calibrated.

3

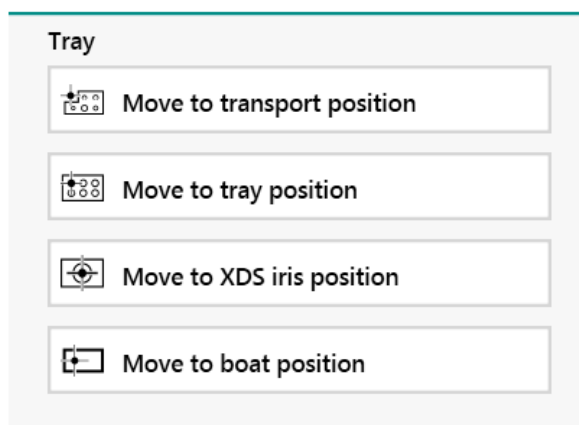
3.3.12

To start up Vision Air Routine, choose between **Reflectance mode** or **Transmission mode**.

In Vision Air Routine, the tray can be moved to different positions.

- 1

- 2



To select trays in Vision Air Manager, proceed as follows:

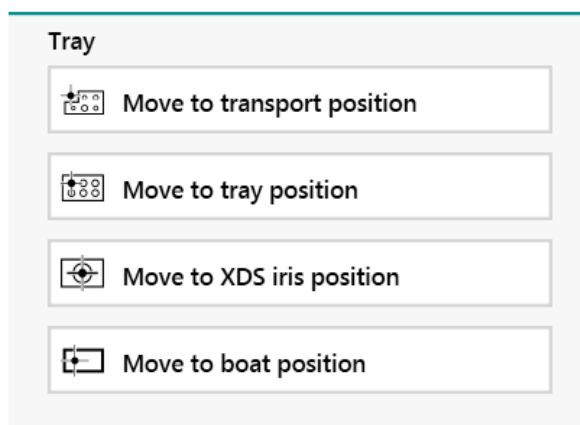
- 1 Go to the **Methods** section.
- 2 Select the method for which you want to configure the tray.
- 3 Go to the **Summary** tab in the data window and make sure that the **Sample vessel** field has the value: **Tray**.
- 4 Go to the **Settings** tab in the data window and select the menu item **Tray configuration**.
- 5 Select a pre-defined tray from the drop-down list.
If a customized tray has been ordered together with Vision Air, a configuration file is provided by Metrohm. Import this configuration file by using the **Custom tray configuration** import.
- 6 Click on **[Save]** in the toolbar.

3.3.13 Specific functions for XDS MultiVial

To move trays manually in Vision Air Routine, proceed as follows:

In Vision Air Routine, the tray can be moved to different positions.

- 1 Go to the **Tools** section.
- 2 Select 1 of the following options to move the tray manually.



To select trays in Vision Air Manager, proceed as follows:

- 1 Go to the **Methods** section.
- 2 Select the method for which you want to configure the tray.
- 3 Go to the **Summary** tab in the data window and make sure that the **Sample vessel** field has the value: **Tray**.
- 4 Go to the **Settings** tab in the data window and select the menu item **Tray configuration**.
- 5 Select a pre-defined tray from the drop-down list.
If a customized tray has been ordered together with Vision Air, a configuration file is provided by Metrohm. Import this configuration file by using the **Custom tray configuration** import.
- 6 Click on **[Save]** in the toolbar.

3.3.14 Specific functions for XDS RapidLiquid

The RapidLiquid Analyzer supports a software controlled heating functionality.

To define temperature control and blank correction, proceed as follows:

- 1 Go to the **Methods** section.
- 2 Select the method to configure the temperature control.
- 3 Go to the **Settings** tab in the data window and select **Liquid setup**.

- 4** Define your settings for temperature control and blank correction.
- If blank correction is activated, the user is guided through the process of blank correction in Vision Air Routine.

 Blank correction, correcting the effect of the used sample holder, has to be conducted once before the first measurement.

3.3.15 Specific functions for XDS SmartProbe and XDS Interactance Probe

Reference scan

Reference measurements with the XDS SmartProbe and the XDS Interactance Probe are conducted by placing the probe into the respective position of the instrument. Whenever a reference measurement is needed, the user is informed in the information field of Vision Air Routine.

Probe

Reference measurement !

Place the probe in the reference position and pull the trigger.

The time period between individual reference scans can be set in Vision Air Manager. The maximal time period is 60 minutes.

 A permanent installation of the probe into a system is not suggested due to maximum validity of a reference scan of 60 minutes.

4 Installation

4.1 System requirements

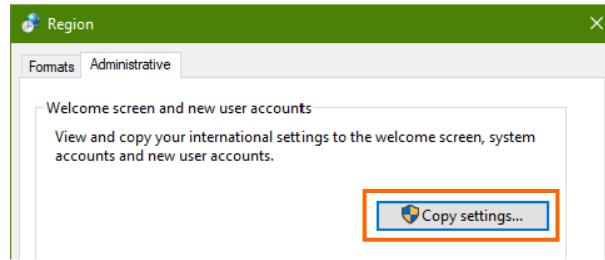
Table 6 Vision Air

Operating system	Windows 7 SP1 (64 bit) Windows 10 (64 bit) Operating System Language must be English (during installation only)
CPU	Dual core 2.8 GHz processor
Memory (RAM)	4 GB
HDD	20 GB free disk space NTFS file system
Display	1024x768 resolution, 32 bit color display (1280x1024 recommended)
NIC	1x 100 Mbit Ethernet
Drives	DVD drive 1 free USB drive
Additional software and requirements	PDF Reader software Support for IP protocol version 4 .NET 4.8 Framework Extended (included) Crystal Reports 13.01 runtime (included)

Firewall

Configure all firewalls and VPN clients to allow UDP broadcasts on port 61525 on the interface that is connected to the instrument. Otherwise, Vision Air might be unable to connect to the instrument.

-  You must be logged in on the PC as an administrator when you install Vision Air.
-  Power options in the PC should not be set to automatic sleep mode or hibernation. If the PC goes into sleep mode or hibernation mode, it will lose connection to the instrument and a restart of both, Vision Air and the instrument, is then required.
-  Vision Air supports all XDS instruments and DS2500 instruments.



- 5 Copy the current settings to the system accounts by activating the check box **Welcome screen and system accounts**.



Confirm with **[OK]**. A Windows restart is required: **[Restart now]**.

4.3 Installation of Vision Air

To install Vision Air, shut down all other programs on the computer.
Make sure that you are logged into the PC with administrator rights.

 There are 3 different installers:

- Installer for XDS instruments
- Installer for DS2500 Solid Analyzer
- Installer for DS2500 Liquid Analyzer

Choose the installer according to the instrument you are connecting.

Proceed as follows:

- 1 Insert the installation medium with the Vision Air installer and double-click on the installer for DS2500 Solid Analyzer, DS2500 Liquid Analyzer or XDS instruments.

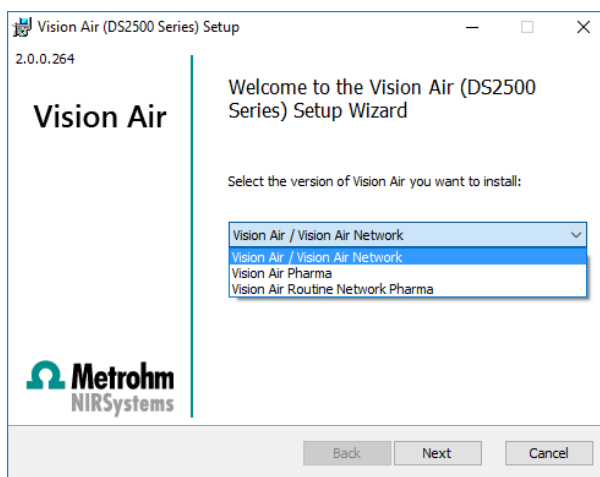
- 2 Before Vision Air is installed, the program checks whether there are any necessary software components missing on the PC.

The first time Vision Air is installed on a PC, all these software components are installed one after the other. Follow the on-screen instructions and click on **[OK]** when prompted. When re-installing Vision Air at a later stage (for example when upgrading to later versions), most of these components needed are already installed and these steps are skipped automatically during the installation.

- 3 Click on **[Install]**.

- 4** Select the version of Vision Air you want to install according to the following table.

Regulated environment?		
Yes		No
Client/server setup?		
Yes	No	
Vision Air Routine Network Pharma	Vision Air Pharma	Vision Air / Vision Air Network
A client installation with pharma features. Installation of Vision Air Routine.	A local installation with pharma features. Installation of Vision Air Routine and Vision Air Manager Local.	A local or client version without pharma features. Installation of Vision Air Routine and Vision Air Manager Local.
The Vision Air Server and the Vision Air Manager Network must be installed separately. Refer to the Vision Air Network and Server Pharma tutorial (8.105.8038EN).	Refer to the Vision Air Local Pharma tutorial (8.105.8034EN).	For the local version, refer to the Vision Air Local tutorial (8.105.8032EN). For the client/server version, the Vision Air Server and the Vision Air Manager Network must be installed separately. Refer to the Vision Air Network and Server tutorial (8.105.8036EN).



After selecting the version, click on **[Next]**.

 A license file is required later to activate the software after installation.

 "Vision Air Complete" is a bundle version of Vision and Vision Air; Vision needs to be installed with the separate installer.

5 Read and accept the license agreement. Click on **[Next]**.

6 For the DS2500 series, there is the option to install Vision Air with an instrument simulator. Select **[Install Vision Air for use with a physical instrument]** and click on **[Install]**.

 The selection **Install Vision Air with an instrument simulator** is only for software demonstration and training purposes and should not be installed on customer PCs.

7 Click on **[Install]** to begin the the installation.

8 A text confirms the successful installation. Click on **[Finish]**.

Installation log files can be found in the temp folder of your operating system. Open Windows Explorer and type in **[%temp%]**. In this folder you will find a file named 'Vision_Air_DATE_TIME.txt'.

9 After the installation, 2 new icons are created on the desktop.

- Vision Air Routine for access to the routine application part of Vision Air.
- Vision Air Manager for access to the managing part of Vision Air.

10 If desired, the Windows language can be changed again.

4.4 Installation of the Unscrambler Prediction Classification Engine

The Unscrambler Prediction Classification Engine is a plug-in that allows to use the third-party software Unscrambler in Vision Air.

Proceed as follows to install the Unscrambler Prediction Classification Engine:

Vision Air must already be installed on your computer.

1 Double-click on the file **setup.exe**.

2 Click on **[Execute]**.

The installation wizard opens.

- 3 Follow the instructions of the installation wizard.
- 4 In the **Personal Information** window, enter the following information.
 - Name
 - Company
 - Activation Key for Prediction Engine
 - Activation Key for Classification Engine

Unscrambler® X Engine 10.4.1 Setup

Personal Information

Please specify your name and the company, then click Next.

Name:
Katja Sahli

Company:
Metrohm

Activation Key for Prediction Engine:
MLLPKCPFLM

Activation Key for Classification Engine:
MSBFNTFMBA

Back Next Cancel

The scope of delivery for Vision Air includes a license CD. Find your activation keys in the **License Certificate.pdf** file on the license CD.

The wizard continues.

- 5 After installing the Unscrambler Prediction Classification Engine, go to **C ► CAMO Software ► Unscrambler X Engine 10.4.1**.

Copy the following files:

- camoengine.dll
- olucx.sys
- olupx.sys

- 6 Go to **C ► Program Files (x86) ► Metrohm ► Vision Air (DS2500 Series) or Vision Air (XDS Series)**. Depending on your installation, you have either the folder Vision Air (DS2500 Series), Vision Air (XDS Series) or both.

Insert the files that you copied in step 5 in your Vision Air folder.

The installation is complete.

5 Start-up

5.1 Configuration

6 configuration steps need to be conducted before using Vision Air for quality control.

1. Calibration of the instrument.
2. Connecting the instrument to Vision Air Routine.
3. Activating the user **Admin**.
4. Import of Vision Air licenses.
5. Importing or creating operating procedures.
6. Signing a configuration change.

5.2 Calibration of the instrument

XDS instruments

Make sure your instrument is calibrated according to *Vision Tutorial – Instrument Calibration (81058054EN)*. Use either Vision or Vision Air Setup for the instrument calibration. Vision Air Setup can be found on the Vision Air installation DVD and needs to be installed manually.

DS2500 instruments

Calibrate the instrument with Vision Air instrument calibration.

To calibrate the DS2500 Solid Analyzer, see *Calibrating the instrument in Vision Air Routine, page 75*.

To calibrate the DS2500 Liquid Analyzer, see *Calibrating the instrument in Vision Air Routine, page 78*.

Before starting the instrument calibration, connect the instrument to Vision Air Routine (*see "Connecting the instrument to Vision Air Routine", chapter 5.3, page 93*).

5.3 Connecting the instrument to Vision Air Routine

To establish a connection between the instrument and Vision Air Routine proceed as follows:

- 1 Connect Vision Air Routine with the analyzer. Make sure that your instrument has no active connection with Vision or another Vision Air installation.

Double-click on the Vision Air Routine program icon.

- 2 Enter the serial number of the analyzer. The serial number can be found on the type plate of your analyzer. For the Metrohm DS2500 Analyzer, it consists of 8 digits, starting with "917xxxxx"; for the XDS Analyzers, it consists of 8 digits in the format "xxxx-xxxx".

- i** To log into Vision Air Routine, Vision Air Routine will ask for a User ID and password after a successful connection with the instrument. During the first start after installation a User ID and password needs to be defined via the Vision Air Manager ([see "Users section", chapter 3.1.8, page 31](#)).

5.4 Activating the user Admin in Vision Air Manager

- 1 Start Vision Air Manager. A login window will request you to log in.
- 2 Enter 'admin' as the user id. The default password is 'a'.
- 3 You will be notified that your password has expired. Enter a new password with at least 5 characters. The password can be modified in the user section in Vision Air Manager.

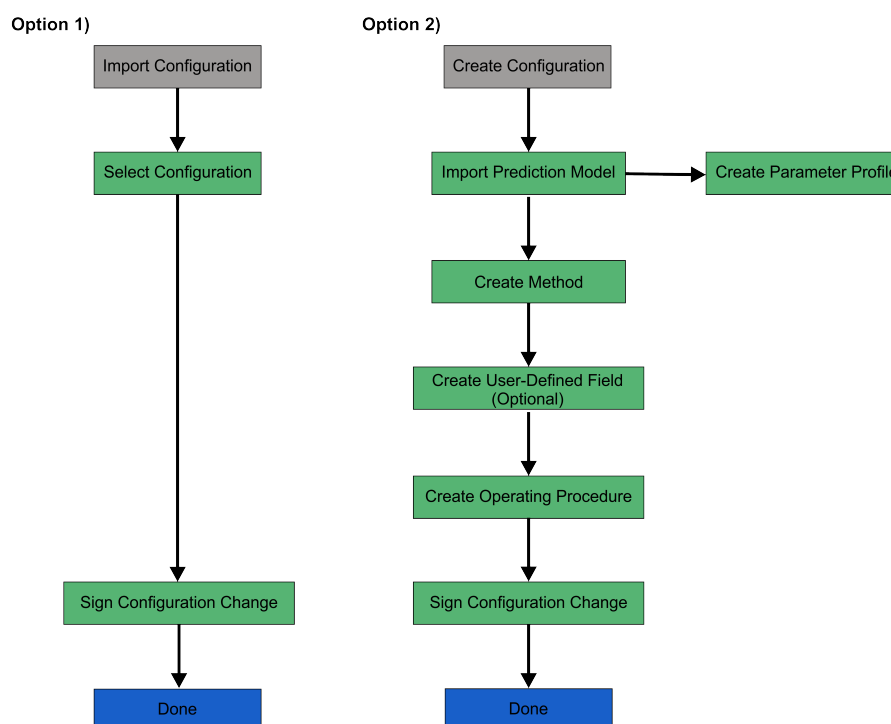


Figure 4 Workflow description for operating procedures

5.7 Importing a complete configuration of operating procedures

Complete operating procedures that were created in Vision can be imported into Vision Air Manager. A complete configuration from a different Vision Air installation that includes all operating procedures of the system can also be imported.

To import a complete configuration of operating procedures, proceed as follows:

- 1 Click on **File ► Import ► Configuration....**

A context menu opens.

- 2 Select the files for import and click on **[Open]**.

The import takes place. A message confirms a successful import.

5.8 Creating a complete configuration of operating procedures

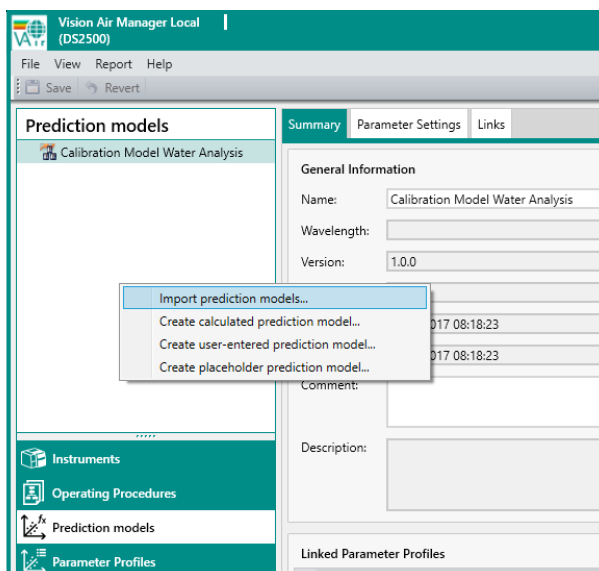
Carry out the following actions to create a complete configuration of operating procedures.

1. Import prediction models (*see "Importing prediction models", chapter 5.8.1, page 96*).
2. Create methods (*see "Creating methods", chapter 5.8.2, page 98*).
3. Create user-defined fields (*see "Creating user-defined fields", chapter 5.8.3, page 99*).
4. Create and configure operating procedures (*see "Creating and configuring operating procedures", chapter 5.8.4, page 100*).

5.8.1 Importing prediction models

Prediction models that were created in Vision, The Unscrambler or PLS_Toolbox can be imported into Vision Air Manager as follows:

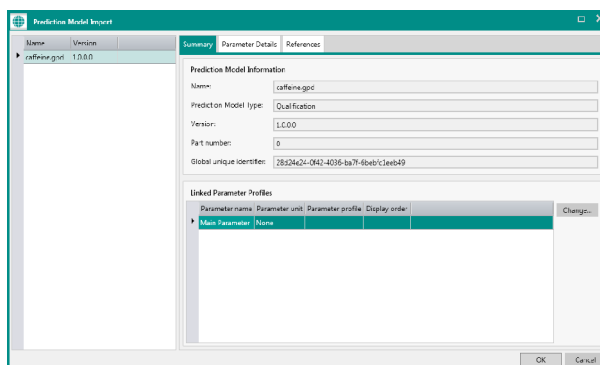
- 1 Click on **[Prediction models]** in the navigation window.
- 2 Select the instrument type where you want to add a prediction model.
- 3 Right-click in the data window on the instrument type (NIRS DS2500 Liquid, NIRS DS2500 Solid or XDS) and select **[Import prediction models]**.



- 4** Select prediction model(s) to import and click on **[OK]**.

The **Import prediction models** window opens.

- 5 Link the imported prediction(s) with parameter profile(s) by clicking on **[Change]**.



The **Link parameter profile to parameter** window opens.

- 6 Select a parameter profile from the list and confirm with **[OK]** or create a new parameter profile by clicking on **[New]**.

If you selected a parameter profile, the import is complete.

If you clicked on **[New]**, proceed with step 7.

- 7 Only perform this step if you want to create a new parameter profile.

Define a new parameter profile name, short name, parameter code and unit. The unit can only be defined with quantitative prediction models.

Summary	
General information	
Name:	new parameter profile
Short name:	parameter
Parameter code:	parameter
Data type:	Double
Number of decimals:	2
Force negative to zero:	☐
Display order:	100
Report sort order:	
Unit:	None
Created:	7/2/2015 9:34:30 AM
Modified:	7/2/2015 9:34:30 AM
Created by:	Oliver Leprnitz
Modified by:	Oliver Leprnitz
Description:	

Go to the **Prediction models** section for a detailed description of the individual functions (*see "Prediction models section", chapter 3.1.4, page 24*).

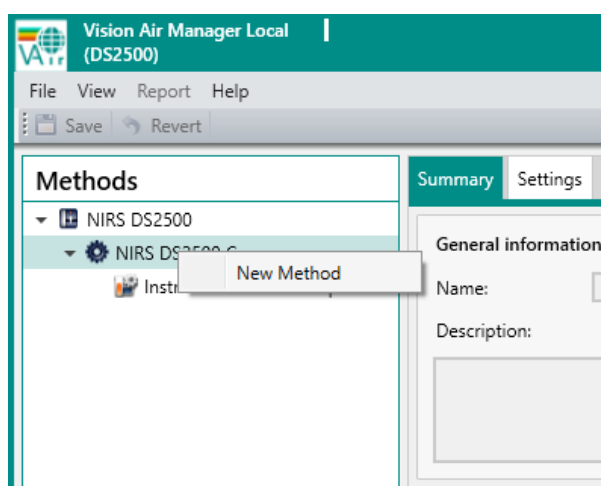
Go to the **Parameter profiles** section for a detailed description of the individual functions (*see "Parameter profiles section", chapter 3.1.5, page 27*).

5.8.2 Creating methods

 The method **Instrument calibration profile** is created automatically for DS2500 instruments when Vision Air is installed in local mode. The instrument calibration profile is currently not used.

To create a new method, proceed as follows:

- 1 Go to the **Methods** section.
- 2 In the structure window, right-click on the icon of the instrument type to which you want to add the method.



- 3 In the **Summary** tab, enter the name and optionally a description.

Summary

Settings

General information

Name:

Sample handling:



Description:

4 Choose a suitable sample vessel that you want to use for your analysis.

5 Save the settings with the **[Save]** button in the toolbar.

Additional settings that are available for methods are described in the methods section ([see "Methods section", chapter 3.1.6, page 28](#)).

5.8.3 Creating user-defined fields

User-defined fields provide additional information on samples and can be added optionally.

To create user-defined fields, proceed as follows:

1 Go to the **User-defined fields** section.

2 Right-click in the structure window and select **New user-defined field**.

The new user-defined field is displayed in the data window.

3

Switch to the **Summary** tab and enter the name and a description.

The following settings are available:

When activating the check box **Allow only fixed/predefined UDF values** (defined on the **Values** tab), only predefined values can be selected during sample registration in Vision Air Routine.

If the check box **This UDF is mandatory for sample registration** is checked, the user is not allowed to do a sample registration without filling out this user-defined field.

By checking **Transfer/repeat UDF value from previous sample registration**, the last user-defined field entry that was made during sample registration in Vision Air Routine is reselected automatically for the next sample registration. The user-defined field entry can always be changed.

3

4

To link prediction models, proceed as follows:

1

2

3

 Multiple items can be selected by keeping the **[CTRL]** key pressed down.

Summary		Prediction models	Methods	User-defined fields	Limits	
Linked Prediction Models:			Prediction model options:		Flat list of prediction models ▾	
	Prediction model	Type	Part number	Version	Imported	Description
▶	 caffeine	User-Entered Prediction...	0	1.0.0	30.05.2018 08:11:43	
	 gasoline	User-Entered Prediction...	0	1.0.0	30.05.2018 08:11:43	
	 lactose	User-Entered Prediction...	0	1.0.0	30.05.2018 08:11:43	

The prediction models are displayed in the work window.

- 4** Save the settings with the **[Save]** button.

To link methods, proceed as follows:

1

Summary

Prediction models

Methods

User-defined fields

Limits

Linked Methods:

Name	Configuration	Description

Add...

Remove

Switch to the **Methods** tab.

- 2 Click on **[Add...]**.

The **Link methods to operating procedure** window opens.

- 3** Select the desired method and link it with **[OK]**.

Summary

Prediction models

Methods

User-defined fields

Limits

Linked Methods:

Name	Configuration	Description	
Small Cup	NIRS DS2500 Common		Add... Remove

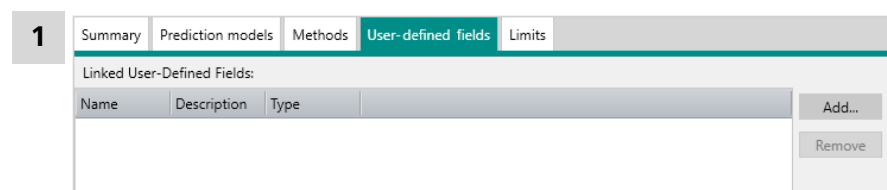
The method is displayed in the work window.

- 4** Save the settings with the **[Save]** button.

Additional settings that are available for operating procedures are described in the operating procedures section (*see "Operating procedures section", chapter 3.1.3, page 20*).

Linking user-defined fields is optional.

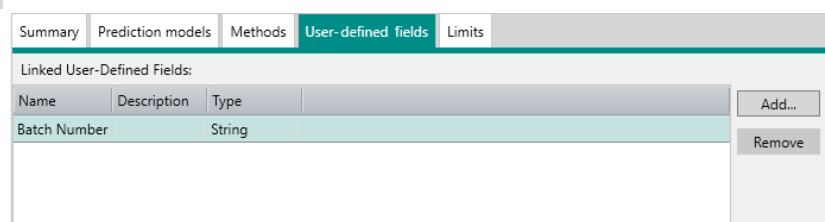
To link user-defined fields, proceed as follows:



Switch to the **User-defined fields** tab.

- 2** Click on **[Add...]**.
- The **Link user-defined field to operating procedure** window opens.

- 3** Select a user-defined field and link it with **[OK]**.



The user-defined field is displayed in the work window.

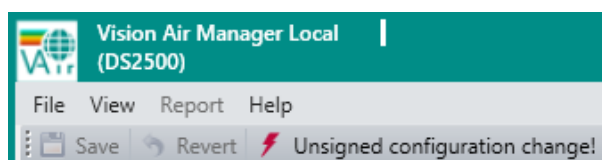
To define limits for operating procedures, proceed as follows:

- 1** Open the **Operating procedures** section.

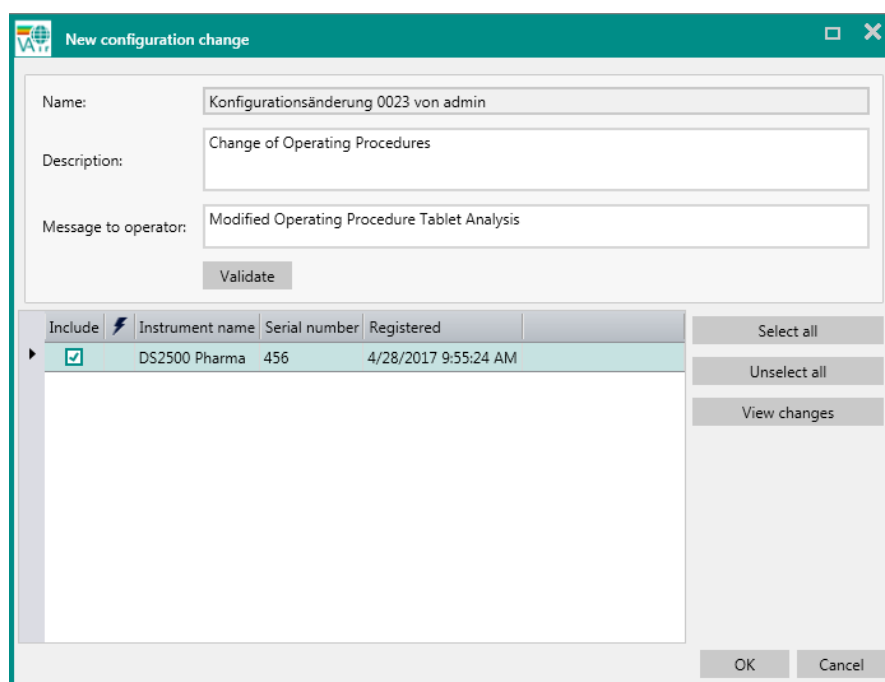
5.9 Signing a configuration change

Any change in the configuration of the system (e.g. changing the name of an operating procedure) will trigger a signing of the new configuration in the Vision Air Manager. Until then, the measurement in the Vision Air Routine will be deactivated.

A **Unsigned configuration change** warning is displayed in the toolbar.



- 1 Click on the warning display **Unsigned configuration change!** to open the window to create the configuration change. Click on the **OK** button to create the configuration change.



- 2 Go to the **Configuration change** section.
- 3 Right-click anywhere in the structure window and select **[Update instrument...]**

A dialog window opens.

Select the configuration change just created and change to the instrument updates work tab.

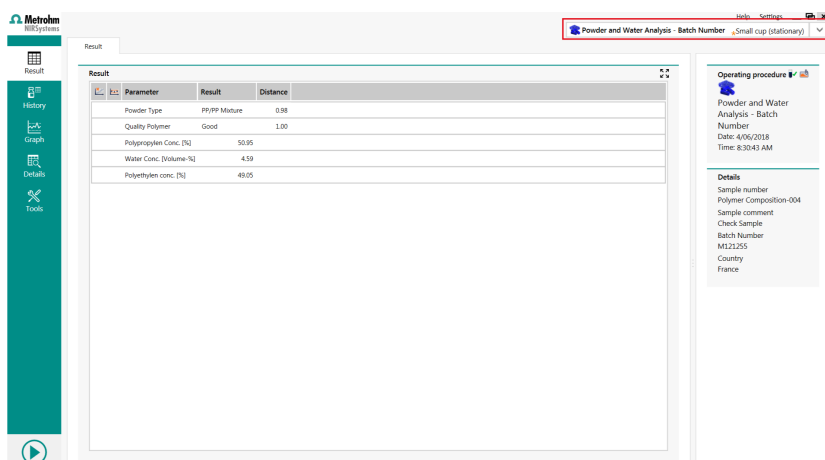
6 Operation and control

6.1 Data acquisition

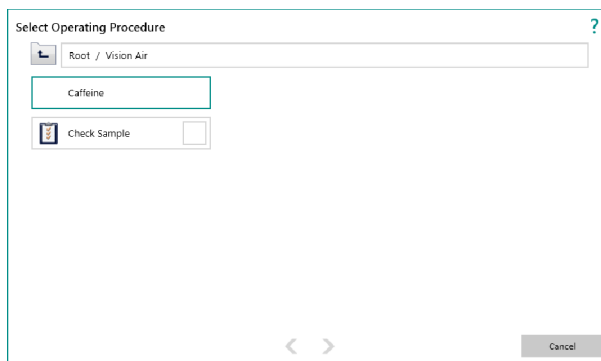
6.1.1 Selecting an operating procedure

To select an operating procedure, proceed as follows:

- 1 Open Vision Air Routine.
- 2 Click on the **[Operating procedure]** drop-down list.



- 3 Select the desired operating procedure.



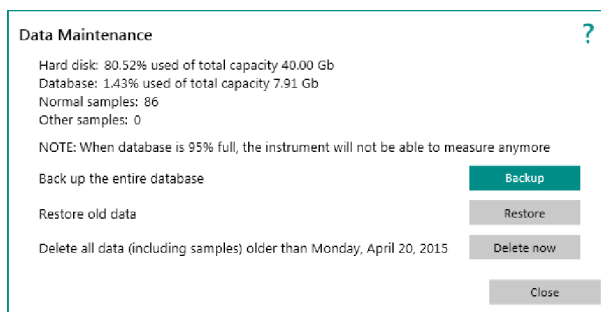
 The  button is available if operating procedure groups were defined in Vision Air Manager.

6.3 Data maintenance

Data can be backed up, restored and deleted. In addition, the capacity of the hard disk and the database as well as the total number of measured samples can be displayed.

To back up data, proceed as follows:

- 1 Click on **[Data maintenance]**.



The top of the dialog box displays the system memory status.

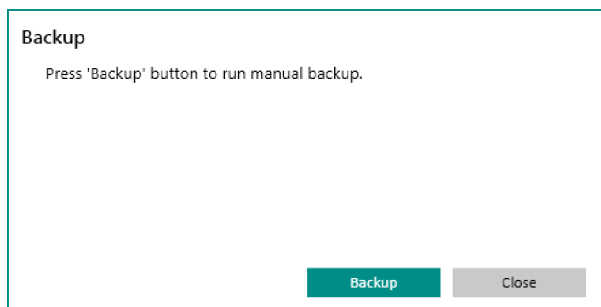
Hard disk: Memory size left for all applications on the PC.

Database: Memory size left in the database for Vision Air data.

Normal samples: Number of analyzed samples.

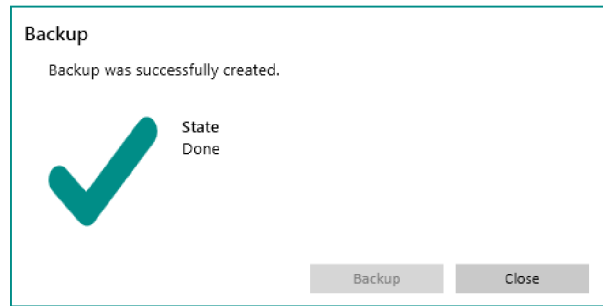
Other samples: Number of analyzed samples that do not belong to the normal type e.g. check sample, check sample operating procedures.

- 2 Click on **[Backup]**.



The **Backup** window opens.

- 3 Click on **[Backup]**.



The backup is created.

- 4** Click on **[Close]** after the backup has been completed.

The storage location is defined under **Tools ► Settings ► Export** in Vision Air Routine (see "Tools section", chapter 3.2.6, page 53).

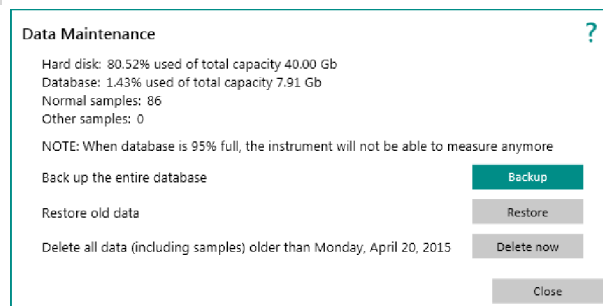
Backup files can be restored in Vision Air. Be aware that database restoration overwrites the existing database. Be careful not to overwrite valuable information.

To restore data, proceed as follows:

Preconditions:

- You are logged in on the PC as an administrator.
- Windows User Account Control (UAC) is turned off.

- 1 Click on **[Data maintenance]**.



- 2** Click on **[Restore]**.

- Click on **[Browse]** and select the backup file that should be restored.

- 4** Click on **[Data restore]** to open the backup file that should be restored.

If a power loss occurs during database restoration, proceed as follows:

Preconditions:

- You are logged in on the PC as an administrator.
- Windows User Account Control (UAC) is turned off.

- 1 Open the installation folder. This is typically **C: ► Program Files (x86) ► Metrohm ► <instrument name>**.
- 2 Start **ServiceRoutinesExecutor**.
The **Restore** dialog window opens.
- 3 In the **Restore** dialog window, click on **[Browse]** to select the database backup.
- 4 Click on **Restore** to start database restoring.

6.4 Data management

6.4.1 Surveillance

To monitor sample data, proceed as follows:

- 1 Go to the **Surveillance** section in Vision Air Manager or Vision Air Manager Network.
- 2 Go to the **Samples** tab.
- 3 Define the filter options, e.g. only show samples that were measured with a specific operating procedure.
- 4 Define the time period of the data.
- 5 Click on **[Filter]**.
- 6 If needed, right-click on a sample and click on **[Details...]** to display detailed sample data.

To monitor diagnostics, proceed as follows:

- 1 Go to the **Surveillance** section in Vision Air Manager.
- 2 Go to the **Diagnostics** tab.
- 3 Click on **[Filter]**.
- 4 Double-click on a start-up test.

- 5** Select the wavelength test. Click on data to view the results.

To monitor instrument events and user related events (login, logout, locking of users etc.), proceed as follows:

- 1 Go to the **Surveillance** section in Vision Air Manager.
- 2 Go to the **Events** tab.
- 3 Define the filter options, e.g. only show errors.
- 4 Define the time period of the data.
- 5 Click on **[Filter]**.

6.4.2 Sample lists

To create sample lists and sample list groups, proceed as follows:

- 1 Select the **Sample lists** section in the navigation window.
- 2 Right-click in the structure window and select **[New sample list group]**.
- 3 Right-click on the new sample list group and click on **[Sample list]** to create a sample list.
- 4 Select the **Samples** tab and add filter settings to filter measurements accordingly.

 Multiple sample lists can be created with different filter settings to conveniently manage large data sets and track conducted measurements.

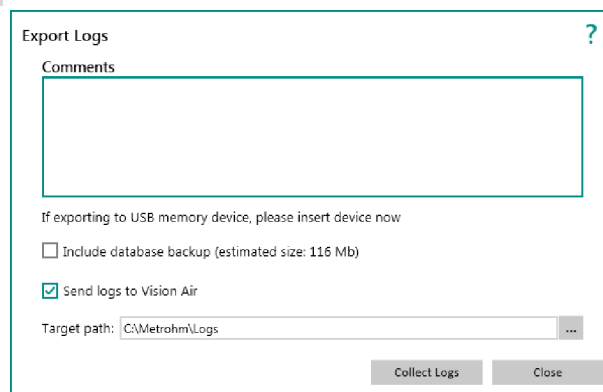
Sample lists are also used for slope/intercept correction (*see "Slope/intercept calculations", chapter 3.3.8, page 69*).

7 Malfunctions and troubleshooting

7.1 Exporting log files

To export log files, proceed as follows:

- 1 Open Vision Air Routine.
- 2 Go to the **Tools** section.
- 3 Click on the **[Export logs]** menu item.



Export Logs

Comments

If exporting to USB memory device, please insert device now

☐ Include database backup (estimated size: 116 Mb)

☒ Send logs to Vision Air

Target path: C:\Metrohm\Logs

Collect Logs Close

The **Export logs** window opens.

- 4 If desired, enter comments regarding the export in the **Comments** field and select the option **Include database backup**. The **Send logs to Vision Air** option is only needed in a client/server setup. Please refer to the tutorials for Vision Air Network Tutorials for details.
- 5 Specify the target path and click on **[Collect logs]**.

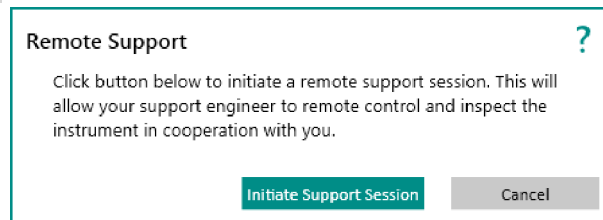
7.2 Remote support

With the **Remote support** functionality, a remote access can be set up with an external program. This remote access enables Metrohm employees to access the instrument in case of an error or for maintenance.

 To use this functionality, a full version of the TeamViewer software needs to be installed on the computer.

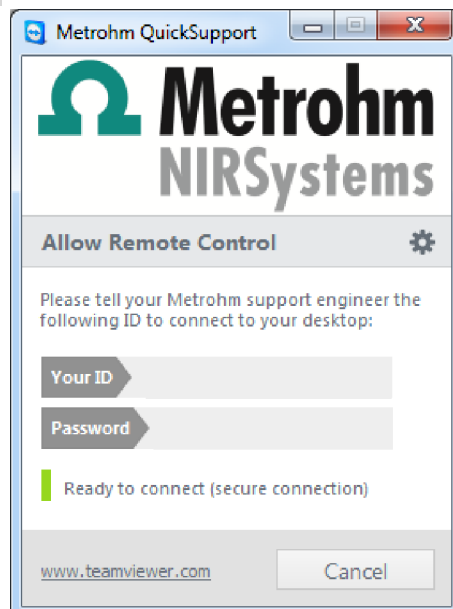
To set up the remote support, proceed as follows:

- 1 Open Vision Air Routine.
- 2 Go to the **Tools** section.
- 3 Click on the **[Remote support]** menu item.



The **Remote Support** window opens.

- 4 Click on **[Initiate support session]**.



The **TeamViewer** software is started and the **Metrohm QuickSupport** window opens.

- 5 Tell the Metrohm employee the displayed ID and the password.

The Metrohm employee can now access your computer and will perform the remote support.

7.3 Troubleshooting

The following table helps with troubleshooting for Vision Air Routine and Vision Air Manager Local.

Problem	Cause	Remedy
Vision Air does not start.	On the Vision Air Routine PC, the Windows language is not set to English.	Set the Windows language to English (<i>see "Pre-installation", chapter 4.2, page 86</i>).
	Vision Air Services are not started after restarting the PC.	Restart the Vision Air Services manually, e.g. as follows: In the Windows search box on the taskbar, type services, and then select Services. 2 services must be started, the respective names may begin with: ▪ Vision Air (XDS Series)... ▪ Vision Air (DS2500 Series)... ▪ Vision Air (DS2500 L Series)... If the Start and Stop commands are grayed out, proceed as follows: ▪ Disable the Vision Air services via context menu ► Properties. ▪ Restart the computer. ▪ Backup the SQL database. ▪ Uninstall Vision Air. ▪ Uninstall the Microsoft SQL Server. ▪ Log on to the PC with full administrator rights and install Vision Air.
	During installation, no database (XDS , DS2500 or DS2500L) was created in the SQL Server Express instance.	Make sure that no SQL Server 2019 is on the PC. Make sure you have full administrator rights during the installation.

Problem	Cause	Remedy
	If a Turkish operating system is used, the collation settings defined during the SQL Server installation will not fit the requirements.	2 remedies are available: - Uninstall the Microsoft SQL Server. Install the same Microsoft SQL Server version manually and change the collation settings to English during the installation process. - Alternatively, change the Windows language to English (<i>see "Pre-installation", chapter 4.2, page 86</i>).
It takes a long time to update the instrument settings during the startup of Vision Air Routine.	VPN client	Uninstall CheckPoint EndPointSecurity that is part of the VPN client.

8 Accessories

Up-to-date information on the scope of delivery and on optional accessories can be found on the Metrohm website. Download this information as follows:

Downloading the accessories list

- 1 Go to <https://www.metrohm.com>.
 - 2 Enter the article number of the product (e.g. **2.1001.0010**) into the search field.
The search result is displayed.
 - 3 Click on the product.
Detailed information regarding the product is shown on various tabs.
 - 4 On the **Included parts** tab, click the link to download the PDF.
The PDF file with the accessories data is loaded.
-  Metrohm recommends downloading the accessories list from the Internet and keeping it for reference purposes.