Operating Manual

multiWin pro

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

Table of contents

1   Software at a glance

The multiWin prosoftware has been developed by Analytik Jena to control the analyzers for the sum parameter analysis.

The software can be used with the Windows 10/11 operating system.

Software version

The information in this manual is based on version 1.3.0.0.

Supported devices

The software supports device control and data analysis for all current multi N/C models:
- multi N/C 2300
- multi N/C 2300 duo
- multi N/C 2300 N
- multi N/C 3300
- multi N/C 3300 duo
- multi N/C 3300 HS
- multi N/C 4300 UV

The software can also control the latest generation of devices from software version multiWin 4.10:
- multi N/C 2100S (with all models)
- multi N/C 3100 (with all models)
- multi N/C pharma HT
- multi N/C UV HS
- multi N/C pharma UV

Notes on this manual

This manual uses the following typographical marks:
- Software terms are marked in bold.
- Menu items are strung together separated by a vertical line "|", e.g. **Help|Content**.
- Work steps for operating the software are highlighted by a "▶".

1.1   TOCnology made for you

The multiWin pro software allows you to determine the sum parameters TOC and TN_b in liquid and solid samples from the environment and agriculture, from the chemical and pharmaceutical industries.

The software controls the analyzers and their accessories, carries out measurements and automatically evaluates measurement results.

The optional FDA 21 CFR Part 11 Compliance module provides complete data integrity and conforms to the pharmaceutical guidelines 21 CFR Part 11.

Device control

The three fold-out device panels on the left-hand side of the software interface show you the current status of the device and important device information at all times. The buttons in the **Instrument control** panel allow quick access to important menu commands such as initialization or standby.

These and other functions for controlling the device can be found in the **Instrument** menu. Here you can adjust the autosampler or create and edit device configurations.

Methods

The software summarizes measurement settings in methods. You can manage methods and create new methods in the **Method** menu and the corresponding **Methods** window.

Measurements

In the **Sequences** menu, you can create and manage sequences for analyzing samples, calibrations, blanks, and daily factors.

Start the measurement in the corresponding **Add new sequence** window and follow the recording of current measurement results on the screen.

Calibrations

You can manage and edit the calibrations performed in the **Calibrations** menu and the associated **Calibrations** window.

Measurement results

You can manage the measurement results via the **Result details** menu. The **Result tables** window shows an overview of all results tables that you can load.

After loading a result table, the **Result table** window opens, where you can view and edit measurement results. Report and export functions are available here.

Blank values

The blanks of reagents used or sample boats play an important role, particularly in pharmaceutical purity control or in the environmental sector. You can therefore record various blanks within a sequence or enter them manually. The software automatically subtracts the measured blanks from all subsequent measurement results.

Daily factor

The analysis system delivers reproducible results over a long period of time. It is therefore not necessary to repeat calibrations on a daily basis. By measuring daily factors, the software offers you the option of checking calibrations with one or more standard solutions and correcting them within defined limits.

System Suitability Test (SST)

The System Suitability Test (SST) is part of the FDA 21 CFR Part 11 Compliance module and ensures the quality of TOC determinations in the pharmaceutical sector. The SST compares the analysis of a substance that is easy to oxidize and a substance that is difficult to oxidize. The software automatically evaluates the SST and displays the results in the **Result details | SSTs** menu.

User Management

The User Management can be found in the **Program | User management** menu. In the **User management** window, you can manage the created users with their passwords and access rights, which you can assign individually by assigning different user roles.

Audit trail

The audit trail is part of the FDA 21 CFR Part 11 Compliance module and is used for analytical quality assurance. You can find the audit trail in the **Program | Show Audit Trail** menu. In the audit trail, the software logs important events such as commissioning and decommissioning of the device, measurements carried out and errors that have occurred.

2   Installation

2.1   Installing the software

If the analysis system is delivered without a PC, you must install the control and analysis software on an external PC. A minimum of ≥64 GB space on the hard drive is required.

All modules of the program are saved in the program directory during installation. The initialization files (.ini files), the database and the user files are saved in the program files in the folder *C:\ProgramData\Analytik-Jena*. No entries are made to any Windows system files.

Installing the software

▶ Switch on the PC and wait for Windows to start. Log in as a Windows administrator.

▶ Insert the software CD into the CD-ROM drive.

▶ Browse to the *multiWin pro installer* folder. Start the installation by double-clicking on the *multiWinProSetup_win32.exe* file.

    ✓ The software is installed. In addition to the program files in the directory *C:\ProgramData\Analytik-Jena\multiWinPro*, a software icon is created on the desktop, as well as entries in the Windows start menu.

2.2   Access rights for Windows user accounts

If the PC is not just used locally with administrator rights, you will need to change the access rights to the program data for any Windows user accounts that are created after the software has been installed.

▶ As Windows administrator, grant read/write access to the folder *C:\ProgramData\Analytik-Jena* to new Windows users created after multiWin pro has been installed.

2.3   Installing the software with the FDA 21 CFR Part 11 Compliance module

The optional software module protects electronic records and ensures data confidentiality. To do this, the software module uses a central CDM service with a CDM server or a DBMS (database management system) in the company's local, internal network, and CDM clients on the measuring station computers. *CDM* stands for Central Data Management. The CDM service and clients communicate in encrypted form via a RESTful API interface. Alternatively, if there is only one client you can install the CDM server on the local computer.

Installation involves the following steps:
- Install the PostgreSQL 16 database on a server or on a database management system in the company's internal network.
  The database is used to store large volumes of data permanently and error-free and makes the data available as required.
- Install the CDM service and configure it as a Windows service so that the CDM service starts automatically when the server boots up
- Install the multiWin pro software on the client computer

When installing on a server or a virtual PC in the company's internal network, ensure that communication between the database, CDM service and client takes place via the defined ports. The ports can be freely configured by your IT department. Ensure that the ports are enabled on the relevant computers.

2.3.1   Ensuring data integrity

The following measures ensure the data integrity of the CDM service. Implementation of the measures is the responsibility of the user or their information technology (IT) department.

The connection between clients and the CDM service is established using the TCP communication protocol via a single defined port. The secure connection uses its own certificate and encrypts communication via HTTPS. There is a version page for the CDM service that documents all changes when the URL is accessed directly.

Note the following:
- Use your own system for the CDM service. Prevent other computers from accessing the database.
  When installing the CDM service and database on a computer: Prevent other computers from accessing the database port.
- Create a separate database user for the CDM service that only has read/write/modify rights for the **cdmserver** PostgreSQL 16 database. Do not set up an administration account for the server that has all access rights.
- Restrict the logins to the computers of the CDM service and the database management system. Do not create any role accounts in the CDM service or leave any role accounts active.
- Set up a custom database user for maintenance tasks. When assigning rights, please note that a technician does not necessarily have to have write or delete rights.
- Schedule times for maintenance on the system and communicate these to users. The FDA 21 CFR Part 11 Compliance module cannot ensure data integrity in the software without CDM service. The CDM service cannot function without a started and connected database.
- Back up the database regularly and before every update. Test the recovery of data via backups.
- Recommendation: If you outsource individual tables such as the audit trail to separate database areas, known as "TableSpaces", you are protecting them from failure.
- Monitor the free hard disk space for the server or the database management system.

2.3.2   Install database and CDM service

▸ Unpack the *cdm-service-setup-xxxx-complete.zip* zip folder on the installation CD. (*xxxx* is a placeholder for the version.)

▸ Double click on the setup file *cdmServiceSetup.exe* then use the wizard to install the PostgreSQL 16 database.
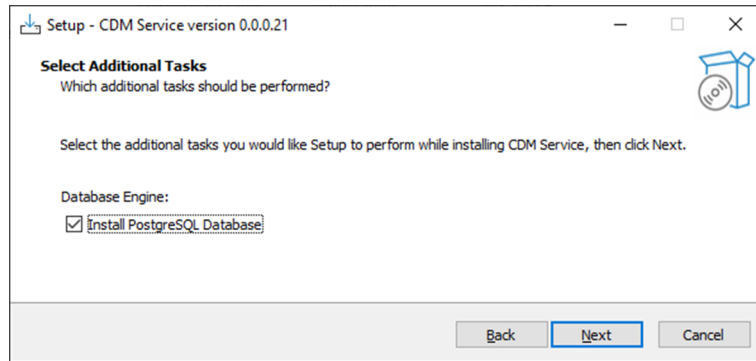
Fig. 1   Install the database using the wizard

▶ Create a database password in the wizard and store it securely.
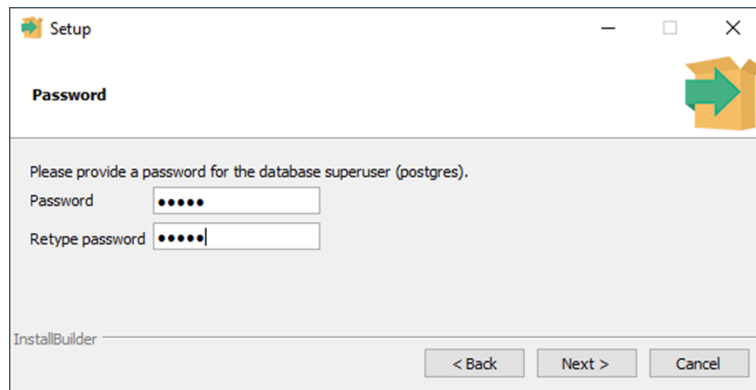
Fig. 2   Set the database password

▶ Enter **Port 5432** as the network address or specify a different port according to your company's network.
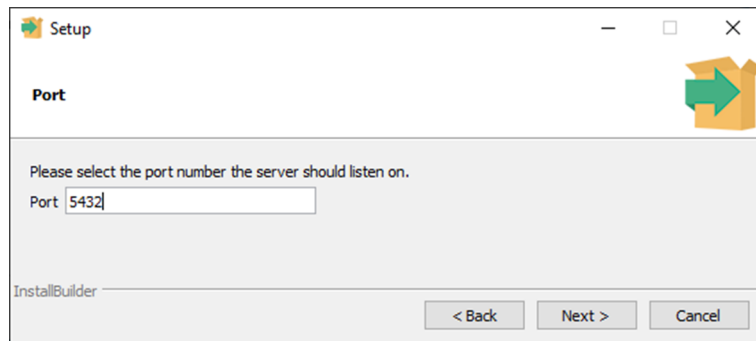
Fig. 3   Enter network address

▶ After the database has been installed, the wizard asks whether "StackBuilder" should be started and configured.
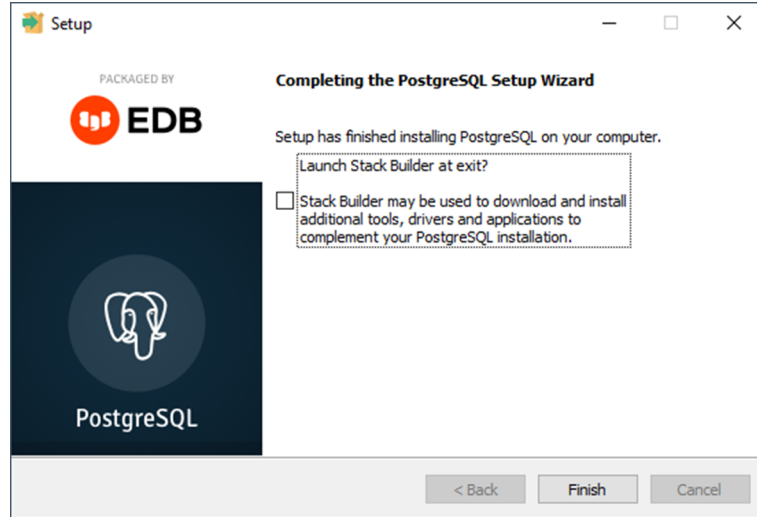
Fig. 4   Remove the checkmark by "StackBuilder"

▸ Remove the checkmark so that this does not happen.

  ✓ The database is installed and configured automatically.

▸ Troubleshooting if the database is not configured automatically: After installing the database, start the pgAdmin 4 software.
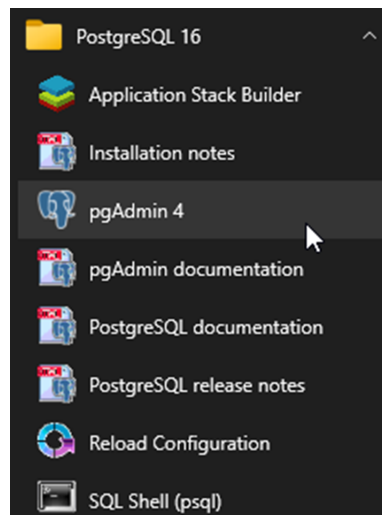
Fig. 5   Start the pgAdmin 4 software

▸ Enter the password you created earlier in the **Connect to Server** window to establish the connection.
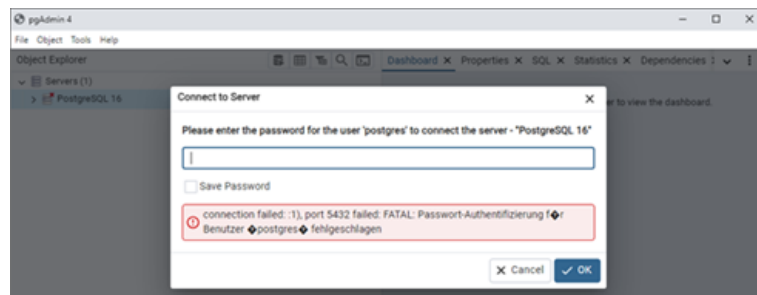
Fig. 6   Enter the database password

▸ Create the **cdmserver** database in the software. To do this, in the Object Explorer go to **PostgreSQL 16 | Database** and select **Create | Database**.
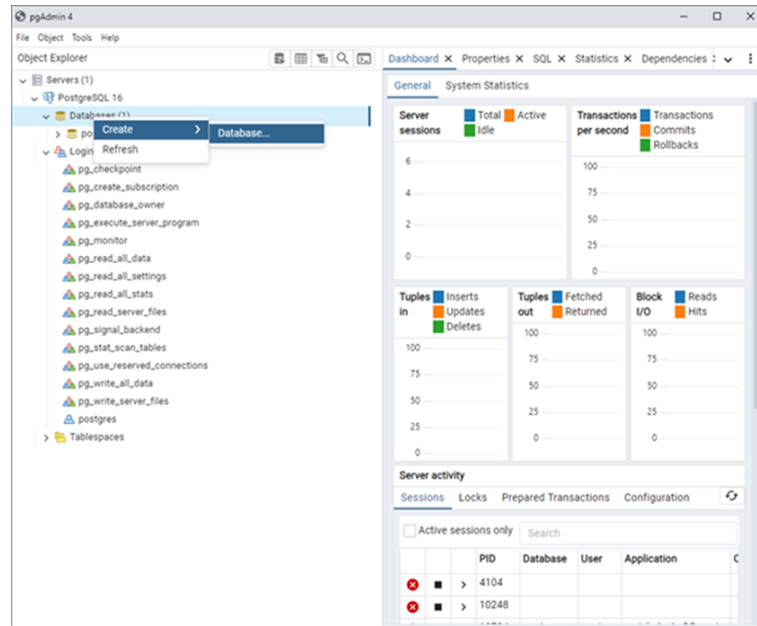
Fig. 7   Create the cdmserver database

▸ In the **Create - Database** window, enter **cdmserver** as the name in the **Database** field.

▸ Save the **cdmserver** database by clicking on the **Save** button.

▸ Close the pgAdmin 4 software.

  ✓ You have created the **cdmserver** PostgreSQL 16 database.

▸ Once the database has been installed, the installation routine unpacks the CDM service and tests it. By default, the installation routine unpacks the CDM service into the directory *C:/ProgramFiles (x86)/CDM Service*.
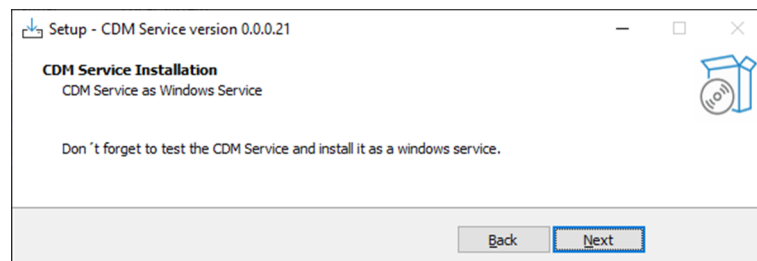
Fig. 8   Installation of the CDM service

2.3.3   Configuring the Windows service

▸ Install the Windows service. To do this, start the **Command Prompt** as an administrator.

▸ Navigate to the CDM directory by entering **cd c:\ProgramFiles (x86)\CDM Service**. **cdmserver-xxx-x86_64.exe** Enter **/install** in the command line. Replace *-xxx-* with the version number.

  ✓ If the installation is successful, the **command prompt** program displays the following text: **Service Part11 CDM installed successfully**.

▸ Type **Services** into the Windows search bar to open the Windows services.
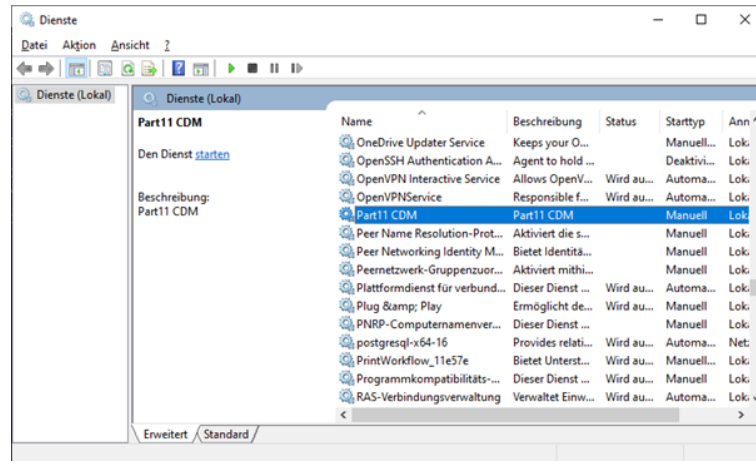
Fig. 9   Configure CDM service as a Windows service

▸ Double-click to open the properties of the **Part11 CDM** service.

▸ After installing the service, change the startup type from **Manual** to **Automatic**. To do this, select **Automatic** from the drop-down menu under **Startup type** on the **General** tab.
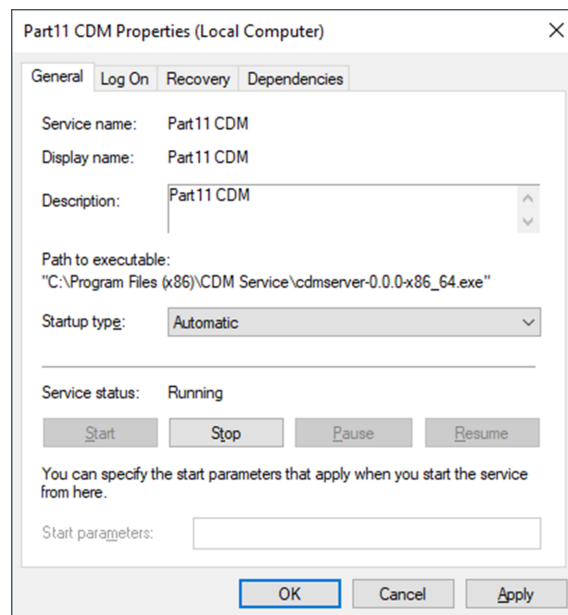
Fig. 10   Properties of the Windows service

▸ Click on **Start** to start the service.

▸ Save changes by clicking on the **Apply**.

  ✓ You have configured the CDM service as a Windows service. The CDM service now starts automatically when the system boots up.

▸ Test the CDM service.

▸ Open the browser and enter the **localhost:8443** address. Change the port if Port 8443 was not selected.

  ✓ When the service is running, the following line is visible: **CDM Service vxxx** (The long sequence of numbers -*xxx* indicates the version of the service).
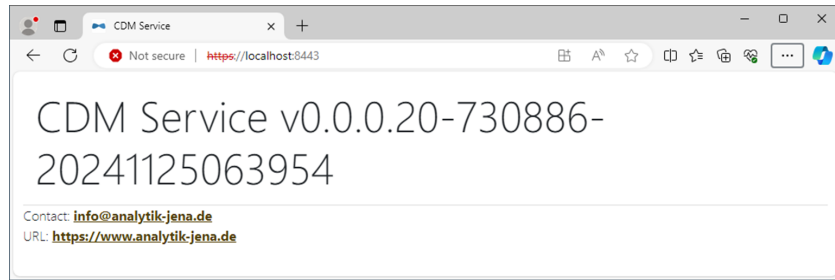
Fig. 11   Browser display when testing the CDM service as a Windows service

2.3.4   Installing the multiWin pro software

You only install the multiWin pro software on the client, not on the server.

Once installed, you need to set up the connection to the CDM service when you start the software for the first time.

Installing the software

▸   Switch on the PC and wait for Windows to start. Log in as a Windows administrator.

▸   Insert the software CD into the CD-ROM drive.

▸   Browse to the *multiWin pro installer* folder. Start the installation by double-clicking on the *multiWinProSetup_win32.exe* file.

   ✓ The software is installed. In addition to the program files in the directory *C:\ProgramData\Analytik-Jena\multiWinPro*, a software icon is created on the desktop, as well as entries in the Windows start menu.

See also

▤ Starting and configuring the software for the first time with the FDA 21 CFR Part 11 Compliance module [▸ 19]

2.4   Updating the software

If there is a software update, contact Analytik Jena Customer Service. Customer Service will provide you with a new installation file.

▸   Double-click on the installation file to start the software update.

   ✓ The new software version is installed. The previous version is automatically uninstalled. The initialization files .ini files), the database, and user files are retained.

▸   If the database schema has changed, the software will guide you through migrating the database when you first start the software:

▸   When prompted, create a backup of the old database.

▸   Migrate the old database according to the instructions.

   ✓ The software displays the result of the data migration.

▸   If you have purchased a new software license with the update, the software will prompt you to enter the new license the first time you start the software. Enter the license.

▸   If the software does not prompt you to enter the new license, enter the old license first.

▸   Open the **Licences** window with the **Help** |**Licence management** menu option.

▸   Enter the new license code in the **Licence code** box.

▶ Check the license by clicking on the **Check** button.

▶ Close the window by clicking on the **Close** button.

▶ Restart the software to apply the new license.

✓ You have performed a software update.

Software updates may also require a firmware update for the analyzer itself. Discuss with Customer Service whether you can carry out the firmware update yourself with the support of Customer Service or whether a service visit is necessary.

3   Starting and exiting the software

3.1   Starting and setting up the software for the first time

After installing the software, you need to license it.

Then log in to the software for the first time. An administrator is preset in the software for this purpose, with the user name and password **Admin**. Change the password after the first time you log in. Administrators only have very limited rights besides user and device management rights. You can set up User Management.

You also define the device configuration when you start the software for the first time. The software adapts the device settings and the selection options for methods and sequences to the device configuration.

You can configure cross-software settings and initialize the device system.

▶ Switch on the PC.

▶ Open the gas supply as described in the operating manual for the analyzer. To do this, open the valve on the pressure reducer of the gas supply in the laboratory.

▶ Switch on the components of the analysis system. Finally, switch on the analyzer at the main switch. When ready for operation, the status LED on the front door lights up green.

▶ Start the software using the Windows start command **Start | multiWinPro** or by double clicking on the software icon on the desktop.

Licensing the software

Fig. 12   Licence management window

▶ When the software starts, enter the serial number and license code in the **Licence management** window to license the software.
The license code is sent to you by e-mail. The device documentation also contains a license data sheet with a license code for the standard software.

▶ Click on **Check**. Check licensed software modules in the table.

▶ Close the window by clicking on the **Close** button.

First login

▸ In the login window enter the user name and password. Click **OK** to confirm the entered data.
User name **Admin** and password **Admin**.

Setting the device configuration

▸ Set the device configuration in the **Instrument configuration** window.

▸ Name the device configuration under **Instrument name**. The default name is: NewDevice_Timestamp

▸ Under **Serial number:**, the software automatically enters the serial number when licensing. Check serial number.

▸ Select the interface to the analyzer in the drop-down menu, under **COM channel:**. If necessary, check the COM port in the Windows device manager.

▸ Select the device model in the drop-down menu under **Instrument type**.

▸ Select autosampler and sample tray for **Sampler type:** and **Rack size:**.

▸ If you have purchased several autosamplers or sample trays: After starting the software for the first time, create additional device configurations, e.g. for solids measurement, or change the existing device configuration under the menu item **Instrument | Instruments**.

▸ Select UV reactor, internal furnace or external furnace from the drop-down menu under **Furnace type:**.

Drop-down menu	Options
Furnace type:	**Internal vertical** option Select for liquid measurements with high-temperature oxidation
	UV reactor option Select for liquid measurements with UV oxidation
	Internal horizontal option Select for solids measurements with internal solids module
	External horizontal option Select for manual or automated solids measurements with external solids module

▸ Select detectors in the **C sensor:** and **N sensor:** drop-down menus.

▸ Select the volume of the sample vials from the **Vial size (mL):** drop-down menu. The software adjusts the dead volume accordingly. Optionally you can adjust the dead volume under **Dead volume (mL):**.

▸ Click on **OK** to save the device configuration.

Setting up User Management

▸ You can continue to use the default administrator. Change the administrator password after the first time you log in under **Program | Change password**.

▸ Set up User Management with **Program | User management**.
Create at least one user who can create methods, perform measurements, and analyze them. The **Lab technician** and **Intermediate user** user roles are suitable for this.

Making cross-software settings

▸ Define cross-software settings such as the language of the software interface under **Program | Settings**.

▸ Define settings for initialization of the analysis system when the software starts and the routine for shutting down the analysis system under **Program | Settings**.

▸ As a user with appropriate access rights, create an initial method in the **Method** menu.

▸ Make the method a default method under **Program | Settings** by clicking on **Select default** in the **Default method** section.

NOTICE

The initialization of the analysis system is only successful if you define a default method.

- Click on **Select default** in the **Software settings** window and choose a default method.

Initializing the analysis system

▶ As a user with the appropriate rights, initialize the analysis system by clicking on the **Initialize instrument** button in the **Instrument control** panel.

  ✓ The software initializes the analysis system and activates the created device configuration as the default configuration.

▶ Wait for the warm-up phase.
  Warm-up phase for device models with high-temperature oxidation: 30 min, for device models with UV oxidation: 15 min

▶ Check the device status in the **Instrument status** panel.

▶ The analysis system is not ready for measurement after the warm-up phase if components in the **Instrument status** panel are displayed in color. If so, start troubleshooting.

▶ For NPOC measurements: Set the NPOC blow-out flow on the analyzer.
  To do this, use the menu option **Instrument|Single control steps|Purge** to activate the purge flow. Set the gas flow at the "NPOC" needle valve. Check the **Purge:** display in the **Instrument status** panel.

▶ Adjust the autosampler before the first measurement and after each changeover. To do this, open the **Sampler alignment** window via the menu command **Instrument| Sampler alignment**.

  ✓ The analysis system is ready for measurement.

See also

📄 Changing the password [▶ 48]

📄 Editing a user [▶ 46]

📄 Configuring software settings [▶ 34]

📄 Adjusting the autosampler [▶ 115]

3.2 Starting and configuring the software for the first time with the FDA 21 CFR Part 11 Compliance module

After installing the software, you need to license it.

You set up the connection to the CDM service. To do this, use the previously created first user with the user name **initialcdmsetupuser** and the password **admin**. The first user has no rights in the software. While you are initializing the connection, set up your first user with administrator rights.

Then log in to the software for the first time with the newly created user. Administrators only have very limited rights besides user and device management rights. Tip: You should therefore use the first time the software starts to configure additional users in the user administration.

You also define the device configuration when you start the software for the first time. The software adapts the device settings and the selection options for methods and sequences to the device configuration.

You can configure cross-software settings and initialize the device system.

▶ Switch on the PC.

▶ Open the gas supply as described in the operating manual for the analyzer. To do this, open the valve on the pressure reducer of the gas supply in the laboratory.

▶ Switch on the components of the analysis system. Finally, switch on the analyzer at the main switch. When ready for operation, the status LED on the front door lights up green.

▶ Start the software using the Windows start command **Start|multiWinPro** or by double clicking on the software icon on the desktop.

Licensing the software

Fig. 13   Licence management window

▶ When the software starts, enter the serial number and license code in the **Licence management** window to license the software.
The license code is sent to you by e-mail. The device documentation also contains a license data sheet with a license code for the standard software.
🛈 NOTICE! Use the license code from the e-mail.

▶ Click on **Check**. Check licensed software modules in the table. The **21 CFR Part 11 Compliance** module must be active.

▶ Close the window by clicking on the **Close** button.

Setting up the connection to the CDM service

▶   The software opens the **Select CDM connection** window.

Fig. 14   Select CDM connection window

▶   Enter the Internet address of the CDM server in the local network in the **CDM connection URL** area.

  –   If the CDM server is installed on the local computer, enter the following address:
     localhost:8443
     If necessary, change the default port.

  –   If using a central CDM server, enter the address of the server on the local network.

▶   Click **Check connection**.

▶   In the **CDM application initialisation** area, enter the previously created initial user with the user name **initialcdmsetupuser** and enter the password **admin**.

▶   Under **First user username:** define a user name for a first user with administrator rights, e.g. Admin.

▶   Click **Initialize application**.

  ✓   The software sets up the connection to the CDM service and automatically assigns an initial password for the first user.

▶   Press **Ctrl + C** to copy the initial password to the clipboard.

▶   Close the window by clicking on the **Close** button.

NOTICE

No software start without initial password

While you are configuring the connection to the CDM service, create your first user. You cannot log in to the multiWin pro software without the initial password.

  ▪   Copy the initial password of your first user to the clipboard using **Ctrl + C** or make a note of it.

First login

▶   In the login window enter the user name and password. Click **OK** to confirm the entered data. Use your first user with their initial password to do this.

▸ When prompted by the software, change the password in the **Change password** window.

Setting the device configuration

▸ Set the device configuration in the **Instrument configuration** window.

▸ Name the device configuration under **Instrument name**. The default name is: NewDevice_Timestamp

▸ Under **Serial number:**, the software automatically enters the serial number when licensing. Check serial number.

▸ Select the interface to the analyzer in the drop-down menu, under **COM channel:**. If necessary, check the COM port in the Windows device manager.

▸ Select the device model in the drop-down menu under **Instrument type**.

▸ Select autosampler and sample tray for **Sampler type:** and **Rack size:**.

▸ If you have purchased several autosamplers or sample trays: After starting the software for the first time, create additional device configurations, e.g. for solids measurement, or change the existing device configuration under the menu item **Instrument | Instruments**.

▸ Select UV reactor, internal furnace or external furnace from the drop-down menu under **Furnace type:**.

Drop-down menu	Options
Furnace type:	**Internal vertical** option Select for liquid measurements with high-temperature oxidation
	UV reactor option Select for liquid measurements with UV oxidation
	Internal horizontal option Select for solids measurements with internal solids module
	External horizontal option Select for manual or automated solids measurements with external solids module

▸ Select detectors in the **C sensor:** and **N sensor:** drop-down menus.

▸ Select the volume of the sample vials from the **Vial size (mL):** drop-down menu. The software adjusts the dead volume accordingly. Optionally you can adjust the dead volume under **Dead volume (mL):**.

▸ Click on **OK** to save the device configuration.

Setting up User Management

▸ Set up User Management with **Program | User management**.
Create at least one user who can create methods, perform measurements, and analyze them. The **Lab technician** and **Intermediate user** user roles are suitable for this.

▸ Select the first user **initialcdmsetupuser** from the **Users** table. Disable the user by clicking on the **Activated** button.

Making cross-software settings

▸ Define cross-software settings such as the language of the software interface under **Program | Settings**.

▸ Define settings for initialization of the analysis system when the software starts and the routine for shutting down the analysis system under **Program | Settings**.

▸ As a user with appropriate access rights, create an initial method in the **Method** menu.

▸ Make the method a default method under **Program | Settings** by clicking on **Select default** in the **Default method** section.

NOTICE

The initialization of the analysis system is only successful if you define a default method.

- Click on **Select default** in the **Software settings** window and choose a default method.

Initializing the analysis system

▶ As a user with the appropriate rights, initialize the analysis system by clicking on the **Initialize instrument** button in the **Instrument control** panel.

  ✓ The software initializes the analysis system and activates the created device configuration as the default configuration.

▶ Wait for the warm-up phase.
  Warm-up phase for device models with high-temperature oxidation: 30 min, for device models with UV oxidation: 15 min

▶ Check the device status in the **Instrument status** panel.

▶ The analysis system is not ready for measurement after the warm-up phase if components in the **Instrument status** panel are displayed in color. If so, start troubleshooting.

▶ For NPOC measurements: Set the NPOC blow-out flow on the analyzer.
  To do this, use the menu option **Instrument|Single control steps|Purge** to activate the purge flow. Set the gas flow at the "NPOC" needle valve. Check the **Purge:** display in the **Instrument status** panel.

▶ Adjust the autosampler before the first measurement and after each changeover. To do this, open the **Sampler alignment** window via the menu command **Instrument| Sampler alignment**.

  ✓ The analysis system is ready for measurement.

See also

- 🗎 User Management in the FDA 21 CFR Part 11 Compliance module [▶ 120]
- 🗎 Configuring software settings [▶ 34]
- 🗎 Adjusting the autosampler [▶ 115]

3.3   Starting the software

▶ Start the software using the Windows start command **Start|multiWinPro** or by double clicking on the software icon on the desktop.

▶ In the login window enter the user name and password. Click **OK** to confirm the entered data.

▶ View and check the device configuration via the menu command **Instrument|Instruments**. Adjust or change the device configuration as necessary. Activate the desired device configuration by clicking on the **Set default** button or by double-clicking.

▶ Initialize the analysis system by clicking on the **Initialize instrument** button in the **Instrument control** panel.
  If you activate the **Auto-Initialization on start** option under **Program|Settings** the software will automatically initialize the analysis system when the software starts.

   ✓ The software initializes the analysis system, switches on the gas flow, and activates the standard configuration. For devices with high-temperature oxidation, the software heats the device to the furnace temperature specified in the default method. (Default method under **Program**|**Settings**|**Default method**)

▶ Wait for the warm-up phase.
Warm-up phase for device models with high-temperature oxidation: 30 min, for device models with UV oxidation: 15 min

▶ The analysis system is not ready for measurement after the warm-up phase if components in the **Instrument status** panel are displayed in color. If so, start troubleshooting.

▶ Adjust the autosampler after each modification. To do this, open the **Sampler alignment** window using the menu option **Instrument**|**Sampler alignment**.

   ✓ The analysis system is ready for measurement.

See also

  📄 Creating a new device configuration [▶ 115]

3.4   Switching the software to standby

Switch the analysis system to standby for measurement breaks of ≥30 min, for example while you are evaluating measurement results or overnight.

In standby mode, the software switches off the gas flow. The software lowers the furnace temperature to the standby temperature for models with high-temperature oxidation. For models with UV oxidation, the software switches off the UV lamp.

▶ Select the **Instrument**|**Standby** menu option.

   ✓ The software stays open. The analysis system will be put in standby mode.

▶ Or: In the **Instrument control** panel click on the **Instrument standby or switch off** button.

   – Select the **Standby** option.
Set standby temperature in (°C) for models with high-temperature oxidation.

   – Tick the **Reverse rinse** checkbox to rinse the sample path before entering standby mode. Observe the instructions for rinsing in the operating manual for the analyzer.

   – Press **OK** to close the dialog box.

   ✓ The software stays open. The analysis system will be put in standby mode.

Further options when the **Close behaviour**|**Always ask** setting is enabled:

▶ Select the **Program**|**Close** menu option. In the **Standby** dialog box, select the **Standby** option.

▶ Or: Shut down the software using the ✕ icon (top right). In the **Standby** dialog box, select the **Standby** option.

See also

  📄 Defining the behavior when closing the software [▶ 36]

3.5   Exiting the software

Switch off the analysis system before long periods of inactivity, e.g. at weekends or during vacations.

The software switches off the gas flow and pumps out the TIC condensate container. For models with UV oxidation, the software switches off the UV lamp. The furnace temperature drops to room temperature in models with high-temperature oxidation.

▶ Select the **Program**|**Close** menu option.

▶ Or: Shut down the software using the ✕ icon (top right).

▶ Or: Select the **Instrument**|**Switch off** menu option.

▶ Or: In the **Instrument control** panel click on the **Instrument standby or switch off** button.

▶ Select the **Switch off** option.

   – Tick the **Reverse rinse** checkbox to rinse the sample path before switching off. Observe the instructions for rinsing in the operating manual for the analyzer.

   – Press **OK** to close the dialog box.

   ✓ The software is closed when options 1 and 2 are selected. If options 3 and 4 are selected, the software remains open.

   ✓ The analysis system shuts down. You can now switch off the components of the analysis system at their main switches.

Standby / switch off at end of measurement

At the end of a sequence, you can automatically shut down the analysis system or put it into standby. For example, they can save gas and energy when measuring overnight.

▶ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▶ Standby: At the end of the sequence use the **Add control step** button to set the **Standby instrument** control step. Set the standby temperature in the **Step properties** panel.

▶ If necessary, use the **Wake up** control step to make the analysis system ready for operation again at the desired time.

▶ Switching off: Set the control step **Turn off instrument** at the end of the sequence.

See also

▤ Defining the behavior when closing the software [▶ 36]

4   Software interface

Tip

The software is optimized for display on a 24 in full HD screen (PC) or 14 in full HD (laptop) with a resolution of 1920 x 1080 px. On smaller screens, it may be that not all menus are displayed.

- If menus are not fully displayed, reduce the screen resolution in the Windows settings.

Element	Description
Menu bar (top)	Menus with menu commands that you can use to access all program functions
Toolbar (top)	Icons with important menu commands ■ A tooltip is displayed when you hover over an icon. ■ If required, customize the toolbar via **View** |**Customize**.
Dialog window (middle)	Dialog window for detailed display and editing of important program functions ■ Open windows via menu commands. The windows are arranged as tabs on the software interface. ■ To undock, hold down the mouse button and drag the tabs or select **Undock** in the context menu. ■ Use the **Rename** and **Close view** commands (in the context menu) to rename or close windows.
Fold-out device panels (left)	Three fold-out panels: ■ **Instrument control** panel for quick access to device control ■ **Instrument status** panel for displaying the device status ■ **Instrument info** panel for displaying further device and software information
Status bar (bottom)	Information displayed: ■ Logged in user ■ Device status ■ Date and time ■ Remaining time until automatic logout after periods of inactivity ■ Amount of data in database in (MiB) or address of the CDM server ■ Software version

Menu commands are active or inactive depending on the user's access rights. You can set access rights under **Program**\|**User management**.

See also

   📄 Customizing the toolbar [▶ 117]

4.1   Menu bar

The menus in the menu bar group together the main program functions. Many menu commands open dialog windows for detailed display and editing of additional functions.

Menu	Menu functions
Program	■ Make system-wide settings such as language ■ Create and manage users ■ Change user or log in again after automatic logout ■ Lock the software to prevent unwanted access ■ Change the password ■ View audit trail and add manual entries to the audit trail (only with FDA 21 CFR Part 11 Compliance module) ■ Exit the software
Method	Manage methods and create new methods
Measurement	■ Create sequences for measuring samples, calibrations, blanks, daily factors, QC standards, and system suitability tests (only with FDA 21 CFR Part 11 Compliance module) and start measurements ■ Manage saved sequences
Calibrations	View and edit calibrations performed
Result details	■ Manage result tables and load selected result tables to view and edit measurement results ■ View results of system suitability tests (SST) (only with FDA 21 CFR Part 11 Compliance module)
Instrument	■ Initialize the device, switch it to standby or switch it off ■ Switch gas flow off and on again during measurement pauses ■ Adjust the autosampler ■ Create and manage device configurations ■ Manually control the device outside the measurement sequence, for example to prepare the device for maintenance ■ After consulting Customer Service, individually control valves and assemblies in the device component test and retrieve sensor-specific data for the detectors.
View	■ Arrange dialog windows ■ Customizing the toolbar ■ Open service mode (password protected)
Help	■ Open the software help ■ Contact Customer Service by email ■ Manage licenses for software modules ■ View software version, copyright information and contact details ■ Open folder with log files for error analysis

4.2   Toolbar

Icons with frequently used menu commands are arranged in the toolbar as extended menu navigation. A tooltip is displayed when you hover over an icon.

Click on an icon to open a dialog window for detailed display and editing of further program functions.

You can customize the toolbar via **View** | **Customize**.

Layout of the toolbar

Icon	Select the menu command	Description
	Sequences	Open **Sequences** window
	Settings	Open **Software settings** window
	Calibrations	Open **Calibrations** window
	started software	For automated solids measurement, move the boat carousel of the solids autosampler to fill the first positions with sample boats.
	Solid sampler next level	Continue moving the boat carousel to fill further positions with solid samples.

4.3   Device panels

You can control the device and view the device status and device information via the three fold-out panels on the left-hand side.
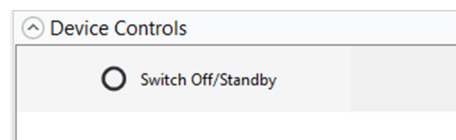
Fig. 15   Instrument control panel

Panel	Description
Instrument control	Control the device via buttons ■ **Initialize instrument**: Initialize the device ■ **Instrument standby or switch off**: Switch the device to standby or switch it off
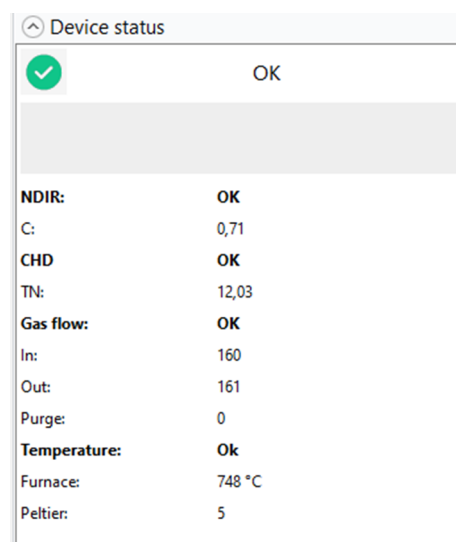
Fig. 16   Instrument status panel

Panel	Description
Instrument status	Detect operational readiness and status errors
	View the current status of individual components: ■ Detection modules (NDIR, CLD, ChD) ■ Gas flow (In, Out, Purge) ■ Temperature (furnace, Peltier cooling) ■ Status of the UV lamp (for devices with UV oxidation)
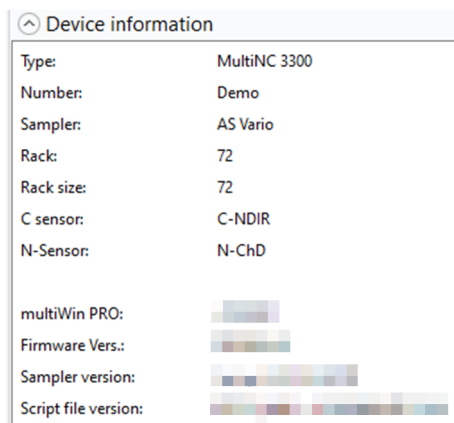
Fig. 17   Instrument info panel

Panel	Description
Instrument info	View information about the device, connected accessories, software and firmware version
	Tip: Have information ready to provide to customer service if servicing is required!

4.4   Dialog window

You open the dialog windows using the menu commands in the menu bar or toolbar. The windows are arranged as tabs on the software interface.

■ To undock, double-click and hold down the mouse button and drag the tabs or select **Undock** in the context menu.

■ Close with **Close view** (in the context menu).

■ Rename windows with **Rename**.
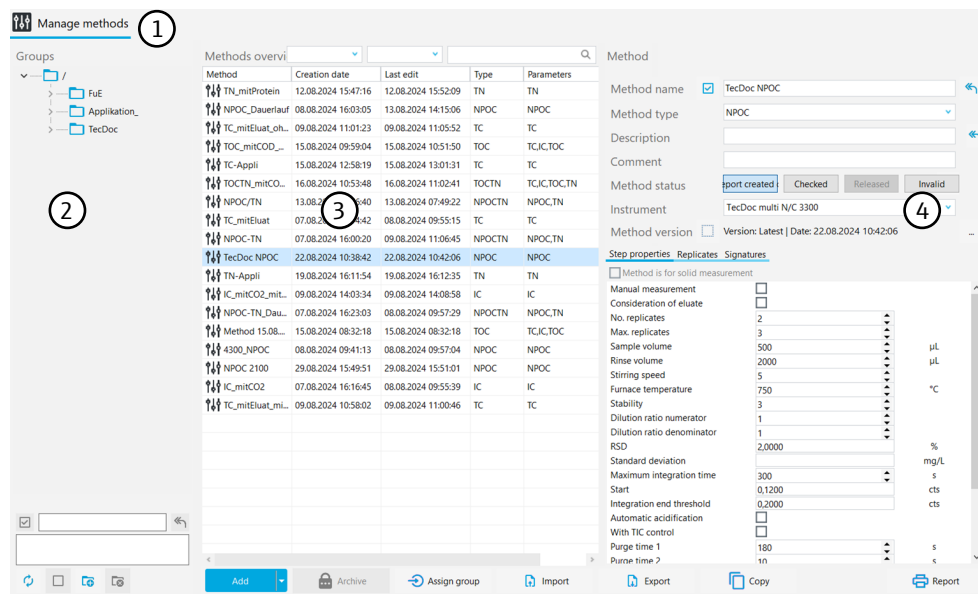
Fig. 18   Methods dialog window

The **Methods**, **Sequences**, **Calibrations**, **Result tables** and **SSTs** windows have a similar structure. These windows are used to manage methods, sequences, calibrations and results tables.

Area	Description
Tab bar (1)	Tabs of the open windows
Group management (2)	Group management with directory structure
Tabular overview (3)	Management of methods, sequences, calibrations and results tables, with search function
Detailed view (4)	Detailed view for selected elements with editing options

You can change the width of areas and columns.

▸   Position the mouse cursor on the boundary so that the ◀▋▶ icon is displayed.

▸   Drag the area or column to the desired width.

Tabular overview

The tabular overview shows all saved elements (methods, sequences, calibrations, results tables).
- If you select a group in the **Groups** area, the tabular overview only shows the elements of the group. By clicking on the ↻ or ☐ icon, you can display all elements, regardless of the directory structure.
- You can search the tabular overview by entering search terms in the search field (with the 🔍 icon).

The tabular overview contains the following information:
- Name of the element (method, sequence, calibration, results table, SST report)
- Date created and last changed
- Further element-specific information, such as the calibrated measurement parameters (TC, NPOC, TN, etc.)

You can create new elements in the tabular overview using the buttons. You can organize elements in groups, import, export or delete them (only in standard software). You cannot edit the elements in the table.

Detailed view

The detailed view shows detailed information for an element selected in the overview. You can edit elements in the detailed view.

Buttons

Button	Description
Add	Add new element
Load	In the windows **Sequences** and **Result tables**
	▪ Load saved sequence for further processing
	▪ Load results table for viewing and editing measurement results
delete	Delete selected element from table (standard software)
Archive	In the future: Archiving of elements in the database (with FDA 21 CFR Part 11 Compliance module), function currently still grayed out
Assign group	Assign selected element to a group via the **Select group** window
Import	Import elements in .XML file format
Export	Export selected element
	Default export folder: *C:/ProgramData/Analytik-Jena/MultiWinPro/export*
	File format: .XML, also for results .CSV
Copy	Copy selected method in the **Methods** window
Report	In the windows **Methods**, **Calibrations** and **SSTs**, generate report for selected elements
▶	Continue loading the elements, e.g. when updating (only with FDA 21 CFR Part 11 Compliance module)
⊗	Cancel loading of the elements (only with FDA 21 CFR Part 11 Compliance module)

See also

- 📄 Methods window [▶ 49]
- 📄 Sequences window [▶ 67]
- 📄 Calibrations window [▶ 93]
- 📄 Result tables window [▶ 98]

4.5   Search and filter

Search

You can search the tabular overview in the dialog windows.

▶ Enter the search term in the search field above the tabular overview.

   ✓ The software limits the display to hits.

▶ Delete the search term to display the full overview.

Filtering

You can filter methods and results according to various criteria.

With the optional FDA 21 CFR Part 11 Compliance module, you can also filter calibrations and System Suitability Tests (SST) according to their signing status.

▶ To filter results, click on the ▽ icon above the tabular overview in the dialog box.

▶ Select filter criteria from the drop-down menus.

▶ In the drop-down menus, specify the desired period in the calendar next to **Filter by Time**.

   ✓ The software limits the display to hits.

▶ Remove individual filters by deleting the filter criteria or selecting **all**.

4.6   Organize in groups

You can organize methods, sequences, calibrations, results tables and SST reports in groups. To do this, you can create a directory structure with groups and subgroups. All windows use the same directory structure.

Deleting groups   You can delete groups in the standard software.

NOTICE

Risk of data loss

When a group is deleted, the standard software deletes all subgroups, methods, sequences, calibrations and measurement results contained in the group.

- The software displays a security warning to protect you from unintentional data loss.
- Check the contents of all windows before deleting a group.

If you don't want to delete data but instead want to archive it, you can create a group called "Archive". Move the data that you no longer need to the "Archive" group.

In the FDA 21 CFR Part 11 Compliance module, data is protected from being deleted. You can therefore only delete empty groups that do not contain any data.

Groups area
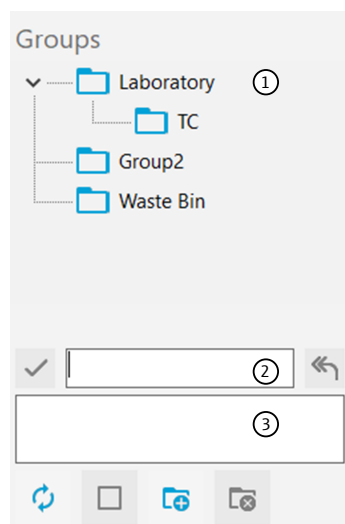
Fig. 19   Groups area

Element	Description
Directory structure (1)	Expand and collapse the directory tree by clicking on the ⌄ icon
Input field for group name (2)	Define a group name
Input field for comment (3)	Enter a comment for a group

Icons

Icon	Description
☑	Save entry
⤺	Reset entry
↻	Refresh the view
☐	Clear group selection Alternatively, click in the gray area to deselect the group.
🗀⊕	Add group
🗀⊗	Delete group with all subgroups and contained elements A confirmation prompt protects you from accidental data loss in the standard software.

Create new group

▸ Create a new main group:

Ensure that no group is preselected. To clear any selection, click on the ☐ icon or click in the gray area.

▸ Create a new subgroup:
Select the main group in the directory structure.

  ✓ The selected group is marked with the 🗀 icon.

▸ Click on the 🗀⊕ icon to create a new group. The default name is: "Group + number".

▸ Change the group name in the input field. Optionally add a comment.

▸ Save the entries by clicking on the ☑ icon.

  ✓ You have created a new group at the desired level of the directory structure.

Organize in groups

You can organize methods, sequences, calibrations, results tables, System Suitability Tests (SST), and device configurations into groups for a better overview.

▸ Before creating a new element, clear the selection in the **Groups** area with the ☐ icon or click in the gray area.
(If a group is preselected, at first you will not be able to see the new element in the overview).

▸ Select an element from the overview table.

▸ Click on **Assign group**.

▸ In the **Select group** window, browse to the desired group in the directory structure.

  ✓ The selected group is marked with an 🗀 icon and displayed in the input field.

▸ Confirm the assignment with **OK**.
  ℹ NOTICE! When assigning an element to a group, the software removes the signing status of the element.

  ✓ The software assigns the element to the selected group.

5   Program menu

You define system-wide settings in the **Program** menu.

In the Program menu

- Use the **Settings** menu command to open the **Software settings** window, where you can define the language, default settings, and export paths.
- Press **User management** to open User Management.
- Press **Change user** to change the user. Avoid changing users while a measurement is running, as the new user will then act as the creator of the measurement.
- Press **Lock user** to lock the program for processing. You must log in again to continue processing.
- Use **Change password** to change your password.
- With the FDA 21 CFR Part 11 Compliance module, use the **Show Audit Trail** menu command to open the audit trail with logging of important events and errors. Press **Manually add audit trail entry** to add manual entries to the audit trail.
- Press **Close** to exit the software.

5.1   Configuring software settings

You can define system-wide settings such as the language in the **Software settings** window.

Open the **Software settings** window via the menu command **Program | Settings**.
- Most system-wide settings are configured on the **General** tab.
- Use the **Units and precision** tab to define dimensions for the results output.
- On the **Storage, Export and Report** tab, you can define export directories for methods, results and sequences. You define data fields for CSV export and CSV import. You activate the automatic export of measurement results and the generation of reports at the end of the measurement.

General tab
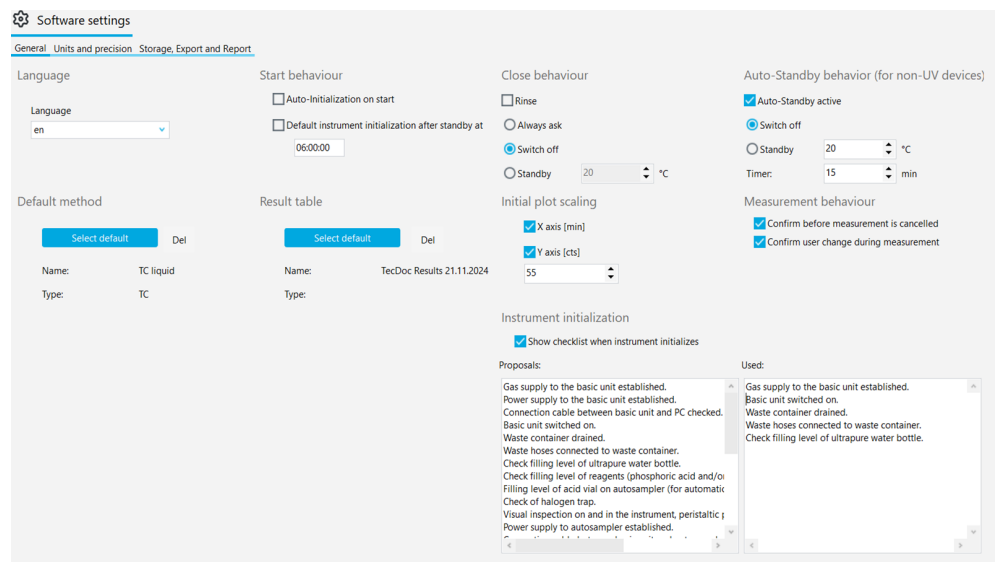
Fig. 20   Software settings window, General tab

Area	Description
Language	Select the language of the software interface from the drop-down menu
	After changing the language, click on **Restart application** to restart the software so that the new language is applied
Start behaviour	Define the behavior of the device when the software starts up
	Auto-Initialization on start Automatically initialize device on software startup and activate default device configuration
	Default instrument initialization after standby at time: Set time of day for automatic device initialization, e.g. 07:00:00 in the morning shortly before starting work. The analysis system must have been in standby beforehand.
Close behaviour	Defining the behavior when closing the software
	Reverse rinse Rinse the sample path as a first step
	Always ask Show prompt when exiting the software
	Switch off Shut down the analysis system when exiting the software
	Standby Switch analysis system to standby when exiting the software Set standby temperature
Auto-Standby behavior (for non-UV devices)	Set a routine for automatic standby or switch-off after periods of inactivity **Auto-Standby active** Enable automatic standby/switch-off
	Switch off Shut down the analysis system when inactive
	Standby Switch analysis system to standby when inactive Set standby temperature
	Timer: Set the duration of inactivity in (min) after which the software automatically switches the analysis system to standby or switches it off
	The software does not count ongoing measurements as a period of inactivity.
Default method	Click on **Select default** and choose a default method that is loaded when the program starts
	Click on **c** (next to button) to clear the preset method
	The software displays the method name and method type under **Name:** and **Type:**.
Result table	Click on **Select default** and choose a default results table
	Click on **c** (next to button) to clear the preset results table
	If you do not select a different results table in the sequence, the software automatically saves measurement results in the default results table.
Initial plot scaling	Set up display of the current measurement curve
	X axis [min] Activate scaling of the X-axis at the start of the measurement

Area	Description
	Y axis [cts] Set the scaling of the Y-axis at the start of the measurement If the value is too small, the software displays the noise of the baseline very large at the start of the measurement. If the value is too high, the signals cannot be detected.
Measurement behaviour	Specify whether the software displays a confirmation prompt if the measurement is aborted or the user changes during the measurement
	Confirm before measurement is cancelled Show confirmation prompt if measurement is canceled
	Confirm user change during measurement Show confirmation prompt if user changes while measurement is running
Instrument initialization	Activate and design checklist with checkpoints for device startup
	Show checklist when instrument initializes Activate checklist whose checkpoints you can process and confirm one after the other when the software starts up
	Proposals: list box List with suggestions
	Used: list box Checklist with checkpoints ■ Transfer checkpoints from the **Proposals:** list box using copy and paste ■ Or: Create your own checkpoints by entering them in the list box ■ Or: Delete checkpoints from the list box

NOTICE

The initialization of the analysis system is only successful if you define a default method.

■ Click on **Select default** in the **Software settings** window and choose a default method.

5.1.1 Defining the behavior when closing the software

Under **Program|Settings** you define how the analysis system behaves when the software is closed. You can choose between the Shutdown or Standby options.

Configuration

▸ Select the **Program|Settings** menu option.

▸ Define the routine for shutting down the analysis system under **Close behaviour**.

▸ Tick the **Reverse rinse** checkbox to rinse the sample path before switching off or standby.

▸ Select an option via the radio buttons:

– **Always ask**: A prompt is displayed when the software is closed.

– **Switch off**: Shut down the analysis system when the software is closed.

– **Standby**: Switch the analysis system to standby when the software is closed. Set standby temperature in (°C) for models with high-temperature oxidation.

▸ Tick the **Auto-Standby active** checkbox under **Auto-Standby behavior (for non-UV devices)** if the analysis system should be automatically switched to standby or shut down after periods of inactivity.

▸ Select an option via the radio buttons:

- **Switch off**: Shut down the analysis system when inactive.

- **Standby**: Switch the analysis system to standby when inactive.
  Set standby temperature in (°C) for models with high-temperature oxidation.

- Set the period of inactivity in (min) under **Timer:**.

  ✓ You have defined routines for shutting down the analysis system, as well as auto standby.

5.1.2 Define units and decimal places for results output

In the **Software settings** window on the **Units and precision** tab, you define the dimensions for the results output.

Option	Description
Concentration	Define units and decimal places for concentrations
Amount	Define units and decimal places for absolute masses and volumes
Standard deviation	Define units and decimal places for standard deviations
by volume	Define specifications for volume-related units and decimal places
by mass	Define specifications for mass-related units and decimal places
by area	Define specifications for area-related units and decimal places, e.g. for the examination of wipes from wipe-down disinfection

In the **Sequence**, **Result details** and **Result overview table** areas, you can configure different default settings for the results output in the sequence, results overview and results table.

Fig. 21   Software settings window, Units and precision tab

▶ Use the menu command **Program|Settings** to open the **Software settings** window, and switch to the **Units and precision** tab.

▶ Define units and decimal places in the **Sequence**, **Result details** and **Result overview table** areas:

- Units and decimal places for concentrations

- Units and decimal places for absolute masses and volumes

- Units and decimal places for standard deviations

Customizing the results output at a later time

You can also adjust the dimensions for the results output in the **Add new sequence** and **Result table** windows:

▸ Right-click to open the context menu outside the sequence table or within the results table.

▸ Select **Select output units** or **Adjust units** from the context menu.

▸ Change the units and decimal places in the **Unit and precision** section.

▸ For the results output in the **Result table** window: On the **Result details** tab, define the units and decimal places for the results table. On the **Result overview table** tab, configure the settings for the detailed view.

▸ Click **OK** to confirm your choices.

▸ Click the **Load default units** button to restore the settings that you previously defined in the **Software settings** window on the **Units and precision** tab.

Customize input units

In the **Add new sequence** window, you can use the **Select input units** command (from the context menu) to customize the units for entering sample information.

▸ Right-click outside the sequence table to open the context menu.

▸ Select the **Select input units** command.

▸ In the **Unit input** window, customize the units and decimal places for the following sample information:
Sample volume
Sample mass
Sample area
Sample density

▸ Confirm the entries by clicking on the **Confirm** button.

5.1.3 Define export and report settings

In the **Software settings** window on the **Storage, Export and Report** tab, define the following settings:

- You can view and customize storage and export directories.
- You define the automatic export of results in the analysis process.
- You define the automatic generation of reports in the analysis process.
- You define data fields for the CSV export of results and the CSV import of sequences.
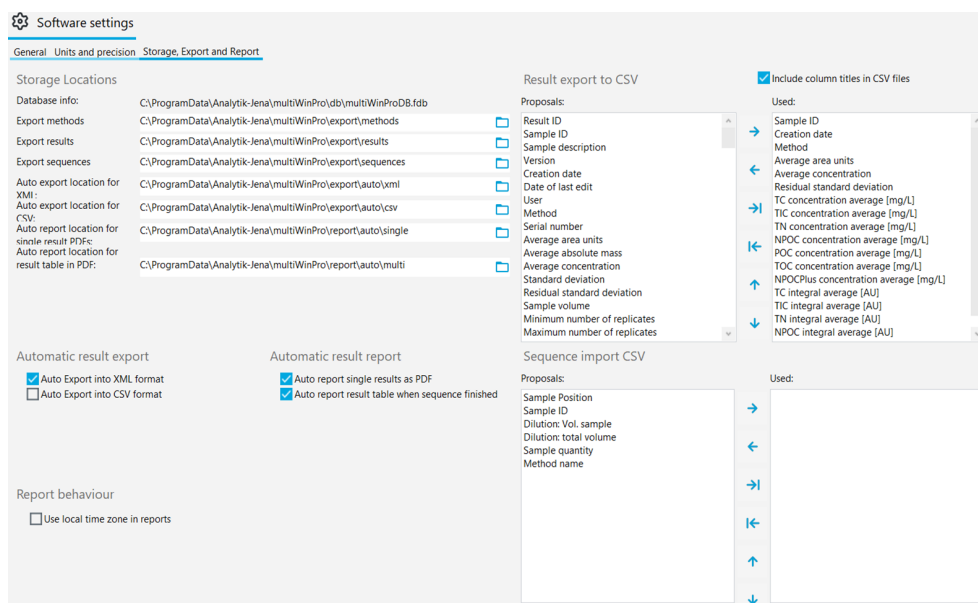
Fig. 22   Software settings window, Storage. Export and Report tab

Area	Description
Storage Locations	**Database info:** View the storage location of the database
	Export methods, **Export results**, **Export sequences** View default export directories for methods, results and sequences and customize them by clicking on 🗀
	Auto export location for XML:, **Auto export location for CSV:** View default export directories for the automatic export of results in XML and CSV format and customize them by clicking on 🗀
	Auto report location for single result PDFs:, **Auto report location for result table in PDF:** View default storage directories for automatically generated result reports for individual measurement steps or for all measurement steps at the end of the sequence and customize them by clicking on 🗀
Result export to CSV	Define data fields for the CSV export of results
	Proposals: list box List with possible data fields
	Used list box List with exported data fields
	The software uses ";" as the separator.
Checkbox **Include column titles in CSV files**	Transfer the name of the data fields to CSV export
Automatic result export	Automatically export results in the analysis process
	Auto Export into XML format Automatically export results in XML format
	Auto Export into CSV format Automatically export results in CSV format
Automatic result report	Automatically generate a results report in PDF format during the analysis process
	Auto report single results as PDF Automatically generate a report for each result after the measurement
	Auto report result table when sequence finished Automatically generate a report for all results after processing the sequence
Sequence import CSV	Define data fields for the CSV import of sequences
Report behaviour	**Use local time zone in reports** Checkbox to output the time of the local time zone in the CSV export and PDF reports

Data fields for CSV export and CSV import

Data field (export/import)	Description
Result ID	ID of the result entry
Sample ID	Sample ID
Sample description	Description
Version	Number of re-processed versions
Creation date	Measuring time
Date of last edit	Time of last editing
User	User logged in during the measurement

Data field (export/import)	Description
Method name	Method name
Method	Measurement method
Serial number	Serial number of the device
Amount	Sample volume or sample initial weight
Average area units	Mean integral in (AU), without blank correction
Average absolute mass	Mean absolute mass in (µg) adjusted for blanks
Average concentration	Mean concentration in (mg/l), adjusted for blanks
Standard deviation	Standard deviation in (mg/l)
Residual standard deviation	Relative standard deviation in (%)
Sample volume	Sample volume
Minimum number of replicates	Minimum number of repeat measurements
Maximum number of replicates	Maximum number of repeat measurements
Number of replicates	Number of prepared repeat measurements or planned measurements
Number of measured replicates	Number of measurements performed
Method type	Method type (TC, NPOC, etc.)
Sample type	Sample type
Sample position	Position on sample tray
Physical state	Aggregate state of the sample
Dilution: Vol. sample	Numerator of the dilution ratio
Dilution: total volume	Denominator of the dilution ratio
Target concentration	Target concentration
Comment	Comments
Results status	Signing status
Measurement status	Display of measurement success
Software version	Software version
Firmware version	Firmware version
TC concentration average [mg/L], etc.	Mean concentrations for the various measurement channels
COD average	COD (Chemical Oxygen Demand) determined for TOC and NPOC methods
BOD5 average	BOD_5 (Biochemical Oxygen Demand) determined for TOC and NPOC methods
Total Protein average	TP (Total Protein) content determined for TN methods
CO2 concentration average [ppm]	Carbon dioxide concentration determined for TIC methods
TC integral average [AU], etc.	Mean integrals for the various measurement channels
TC standard deviation [mg/L], etc.	Standard deviation for the various measurement channels
TC residual standard deviation [%], etc.	Relative standard deviation in (%) for the various measurement channels
TC replicates [mg/L], etc.	Concentrations of the individual determinations for the various measurement channels
	The software summarizes all individual values in one column, separated by |.

Data field (export/import)	Description
TC replicates integrals [AU], etc.	Integrals of the individual provisions
	The software summarizes all individual values in one column, separated by |.
TC concentration replicate 1 [mg/L], etc.	Concentrations for the individual repeat measurements and measurement channels
TC integral replicate 1 [AU], etc.	Raw integrals for the individual repeat measurements and measurement channels

5.1.4 Set up data exchange with an external job management system

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

You can also import sequences manually in CSV format from an external program, such as a LIMS or spreadsheet program.

You define the settings for this in the **Software settings** window on the **Storage, Export and Report** tab.
- Set up the automatic CSV export of results in the analysis process.
- If you want to export results manually, simply define the data fields for the manual CSV export.
- Define data fields for the manual import of sequences.

The software uses the ";" character as a separator for data fields.

With an automatic results export, the software creates the export file immediately after the end of each measurement step. The software generates a separate export file for each measurement step. The software uses the result ID as the file name.

5.1.5 Automatically generate exports and reports

In the **Software settings** window on the **Storage, Export and Report** tab, configure the automatic export of results. You can also specify that results reports are generated automatically during the analysis process.

Configure automatic export

▶ Use the menu command **Program|Settings** to open the **Software settings** window, and switch to the **Storage, Export and Report** tab.

▶ Tick the **Auto Export into XML format** checkbox in the **Automatic result export** area to automatically export results in XML format during the analysis process.

▶ Tick the **Auto Export into CSV format** checkbox to automatically export results in CSV format.

▶ The software saves the export files in the directories displayed under **Auto export location for XML:** and **Auto export location for CSV:**. If required, change the export directories by clicking on the ☐ icon.

▶ In the **Result export to CSV** area, select data fields for the CSV export of results.

▶ Check the data fields in the **Used:** list box. Change the selection if required:

▶ Select the data fields in the **Used:** list box and remove them from the list box by clicking on the ← icon. Click |← to remove all data fields from the list box.

▶ Select the data fields in the **Proposals:** list box and click on → to transfer them to the **Used:** list box. Click on →| to accept all data fields.

▶ Click on ↑ and ↓ to change the order of the data fields in the **Used:** list box.

▶ Check the **Include column titles in CSV files** checkbox so that the name of the data fields is transferred to the CSV export.

▶ Tick the **Use local time zone in reports** checkbox in the **Report behaviour** area to output the time of the local time zone in the CSV export and PDF reports.

  ✓ You have set up the automatic results export and defined data fields for the CSV export. The software uses ";" as the separator.

Generate reports automatically   ▶ Use the menu command **Program | Settings** to open the **Software settings** window, and switch to the **Storage, Export and Report** tab.

▶ Tick the **Auto report single results as PDF** checkbox in the **Automatic result report** area to automatically generate a report in PDF format for each result in the analysis process.

▶ Tick the **Auto report result table when sequence finished** checkbox to automatically generate a PDF report for all results after processing the sequence.

▶ Tick the **Use local time zone in reports** checkbox in the **Report behaviour** area to output the time of the local time zone in the CSV export and PDF reports.

▶ The software saves the reports in the directories displayed under **Auto report location for single result PDFs:** or under **Auto report location for result table in PDF:** If necessary, change the report directories by clicking on the ⬜ icon.

  ✓ You have configured the automatic generation of results reports in the analysis process.

5.1.6   Define data fields for the manual import of sequences

In the **Software settings** window on the **Storage, Export and Report** tab, you can define data fields for the manual CSV import of sequences.

▶ Use the menu command **Program | Settings** to open the **Software settings** window, and switch to the **Storage, Export and Report** tab.

▶ In the **Sequence import CSV** area, select the data fields in the **Proposals:** list box and click on → to transfer them to the **Used:** list box. Click on →| to accept all data fields.

▶ For a successful CSV import, transfer the **Method name** data field.

▶ To correct the selection, select the data fields in the **Used:** list box and remove them from the list box by clicking on the ← icon. Click |← to remove all data fields from the list box.

▶ Click on ↑ and ↓ to change the order of the data fields in the **Used:** list box.

  ✓ You have now configured the data fields for the manual CSV import of sequences. After importing, load the sequence in the **Sequences** window and add further settings for the measurement sequence if required.

Prerequisites for a successful CSV import:
- The name and sequence of the data fields in the CSV file must match the data fields that you have defined under **Software settings**, **Storage, Export and Report** tab.
- The **Method name** data field in the CSV file must be filled with the name of a method already created in the software.

5.2   Managing users

The User Management differs in the standard software and in the FDA 21 CFR Part 11 Compliance module.

See also

▤ User Management in the FDA 21 CFR Part 11 Compliance module [▶ 120]

5.2.1   Users and user roles

First login

An administrator with the following login details is created for the first login after the software installation:
- User: Admin
- Password: Admin

Change the administrator password after the first time you log in under **Program | Change password**.

If the password is lost, the profile cannot be restored by Analytik Jena. Keep the password in a safe place.

User Management

Open User Management with menu command **Program | User management**.

The **User management** window shows an overview of all users and user roles with their access rights.

As an administrator, you can create new users and user roles. You can grant new user roles individual access rights.

Fig. 23   User management window

User

When selecting a user in the **Users** table, you can view and edit the settings of their user profile. To do this, use the input fields, checkboxes and buttons in the **Edit user** area.

Checkbox/field/ button	Description
Name	Specify a user name for logging into the system
Display name	Specify user name that is displayed in the status bar, signature and reports
User expires	▪ Check the checkbox if the user should only be valid for a limited time ▪ Select the last day of validity in the calendar next to **Date** After the user's account has expired, that user can no longer log into the system. An administrator can reactivate the user and set a new expiration date.
Activated /De-activated	When activated, the user can log into software If deactivated, the user profile is locked
User is external	When activated, the user can log in via an external technical system using LDAP (only with FDA 21 CFR Part 11 Compliance module) *LDAP* stands for Lightweight Directory Access Protocol. The protocol allows organizations to store and manage user data.
Add	Add a new user by entering the username, etc. After you clicking on **Add**, the software displays the initial password for the user's first login.
Update	Update existing user after selecting them in the **Users** table and editing the fields
reset password	Reset user's password The software displays a new initial password below the table.
Clear	Delete users after a prompt The software deletes the user, but not their measurement data.

When a user is selected in the **Users** table, the software shows which user role the user is assigned to in the **Roles** table.

A user can have several user roles. The user then has the access rights of all these user roles.

User roles

The **Roles** table shows an overview of the user roles. After selecting a user role, you can view its access rights.

	Description
Checkbox	Tick the checkbox to assign a user role to the selected user

Use the input field and the buttons in the **Edit role** area to edit the user roles.

Field / button	Description
Add	Add new user role after entering a role name
Update	Update custom user role after changing the role name Changes to the rights settings do not need to be saved.
Copy	Copy user role
Clear	Delete user role after a prompt

User roles with tiered access rights are available by default in the software.
- You cannot change the access rights of default user roles.
- You can define individual access rights for new user roles.

User	Access rights
Administrator	■ Administrators can manage users and access rights. ■ Administrators can change the software license. ■ Administrators can view and export the audit trail. ■ Administrators can create groups. They set up data storage and data export. ■ Administrators are not authorized to perform measurements.
Service	■ The service role is reserved for service technicians of Analytik Jena or persons authorized by Analytik Jena. ■ Service is the only role that can access the password-protected service functions via the **View** | **Service desktop** menu item. ■ The service role has extensive access to software functions and can, for example, start measurements, view results and edit them.
Lab manager	Lab managers have extensive access to software functions, with the exception of user management and license management.
Lab technician	Lab technicians rank between lab managers and lab assistants in terms of their rights.
Intermediate user	The rights of lab assistants are limited to the measurement operation.
Basic user	Temporary staff have fewer access rights than lab assistants.
Data auditor	■ Raw data validators have an important role in the optional FDA 21 CFR Part 11 Compliance module. They can view, sign and comment on methods, sequences, calibrations and measurement results. ■ Raw data validators can generate reports, export data and view the audit trail.

See also

▤ Changing the password [▶ 48]

5.2.2 Access Rights

User roles with tiered access rights are available by default in the software.
■ You cannot change the access rights of default user roles.
■ You can define individual access rights for new user roles.

The **Rights** table in the **User management** window allows you to view the access rights assigned to a user role. The **Rights** table controls access to all software functions.

Access rights include creating, editing, importing/exporting, and approving data.
■ Configure software settings
■ Edit device configuration and change software licensing
■ Configure data storage, data import and export
■ Manage users
■ Configure groups to manage data
■ Customize sequence and results table
■ Create and edit methods
■ Create and edit sequences and perform measurements
■ Create and edit calibrations
■ View and edit results
■ Import and export data
■ Approve data using electronic signatures (only with FDA 21 CFR Part 11 Compliance module)
■ Acknowledge error messages
■ View audit trail and add manual entries

You can activate access rights for your own user roles by ticking the checkboxes. Saving is not required. The access rights apply to all users with that user role from the next time they log in to the software.

Read rights only allow read-only access to data. Users can view and use data, but not edit it. Read rights are a prerequisite for editing rights: Editing rights must be assigned together with reading rights.

Some rights restrict access to certain elements, for example **Can only create sequences for the default instrument**.

If a user does not have access rights in menus and dialog windows, the relevant areas are not displayed or are grayed out.

You can quickly change the rights selection using the buttons below the table:

Button	Description
Clear all	Clear rights selection
Select all	Select all rights

5.2.3   Editing a user

Creating a new user role

▸ Log in to the software as an administrator.

▸ Select the menu command **Program** | **User management**.

▸ Enter a new role name under **Edit role**.

▸ In the **Roles** area, click on **Add** to save the user role.

▸ Alternatively, copy an existing user role by clicking on the **Copy** button.

▸ Select access rights for user role in the **Rights** table. Tick the checkboxes for this. Saving is not necessary.

   ✓ You have created a new user role with customized user rights. You can now as-sign the new user role to users.

Creating a new user

▸ Log in to the software as an administrator.

▸ Select the menu command **Program** | **User management**.

▸ In the **Edit user** area, enter the user name in the **Name** input field.

▸ Enter the display name.

▸ Activate the **User expires** option if the user should only be valid for a limited time. Set the date of the last date on which they can log in to the software under **Date**.

▸ In the **Edit user** area, click on **Add** to save the user.

   ✓ The software displays the initial password for the user's first login below the **Users** table.

▸ Select the initial password and copy it to the clipboard with **Ctrl + C** and forward it to the new user.

▸ Select user role for new user in the **Roles** table and activate it via the checkbox.

   ✓ You have created a new user and assigned a user role to the user. The new user is authorized to log in to the system.

A user can have several user roles. The user then has the access rights of all these user roles.

It is recommended that a new user changes their password after logging in for the first time using the menu command **Program** | **Change password**.

Editing user settings

▶ Log in to the software as an administrator.

▶ Select the menu command **Program | User management**.

▶ Select the user in the **Users** table.

▶ Customize user data under **Edit user**.

▶ Save changes by clicking the **Update** button.

▶ If required, assign a new user role to the user. To do this, activate the checkbox in the **Roles** area.

▶ For own user roles: Select a role in the **Roles** area. Change access rights in the **Rights** table.
The access rights of predefined user roles cannot be edited.

✓ You have customized the user settings.

All users assigned to a user role are affected by any changes to access rights.

Deleting users and user roles

You can delete users and your own user roles which are not assigned to any users.

▶ Log in to the software as an administrator.

▶ Select the menu command **Program | User management**.

▶ Select the user in the **Users** table.

▶ Delete a user by clicking on the **delete** button.
The pre-defined administrator cannot be deleted.

▶ Select a user role in the **Roles** area.

▶ Delete a user role by clicking on the **delete** button.

✓ You have deleted selected users or user roles.

Deactivating users

You can deactivate users to deny them access to the software. You can unblock the users again at a later date.

▶ Log in to the software as an administrator.

▶ Select the menu command **Program | User management**.

▶ Select the user in the **Users** table.

▶ Click on the **Activated** toggle switch.

✓ The user is deactivated.

▶ If required, reactivate the user by clicking on the toggle switch again.

Resetting the password

You can reset a user's password, for example if a user has forgotten their password.

▶ Log in to the software as an administrator.

▶ Select the menu command **Program | User management**.

▶ Select the user in the **Users** table.

▶ Click on **reset password**.

✓ The software resets the current password and generates a new initial password for the first login. The software displays the password below the **Users** table.

5.2.4 Configuring password rules and automatic logout

In the **User management** window, you can define criteria for the validity of passwords and configure automatic logout after periods of inactivity.

▶ Log in to the software as an administrator.

▶ Select the menu command **Program | User management**.

▶ Set the password conditions in the **Password rules and auto lock** (see table).

▶ Activate the **Enable** option to automatically log users out when inactive. Set the period of inactivity in (min) under **User locks after [min]**.

   ✓ The new password conditions are valid for all new passwords. Passwords created before the change are still valid.

Criterion	Description
Minimum length	Set the minimum password length (min. 4 characters)
Max length	Set the maximum password length (max. 100 characters)
last passwords checked	Define the number of permitted repetitions for previously used passwords (max. 10 repetitions)
max. input attempts	Define the number of invalid login attempts until the user profile is locked (max. 10 attempts) An administrator can unlock a locked user profile under **User management**.
Password expires [days]	Set the number of days after which the password becomes invalid (1 to 365 days)
User locks after [min]	▪ Activate automatic logout of inactive users via a checkbox ▪ Define the duration of inactivity, default setting: 30 min (1 to 2000 min) The software locks the screen and thus prevents unwanted access to data. Measurements continue to run.
Lower case **Upper case** **Numbers** **Special characters**	Define which characters the password must contain: ▪ Upper and lower case letters ▪ Digits ▪ Special characters
Ban common PW	Use an internal software list to reject trivial passwords

5.3   Changing the password

▶ Open the **Change password** window with the **Program | Change password** menu option.

▶ Enter the old password in the **Password:** input field.

▶ Enter the new password under **New password:**.

▶ Repeat the new password in **Confirm new password:**.

▶ Click **OK** to confirm the entered data.

▶ If the password does not meet the criteria defined under **Program | User management**, the software displays an error message. Adjust the password if necessary.

▶ Click on **OK** to close the window.

   ✓ You have changed your password.

6   Method menu

Define the settings for a procedure in a method. The settings depend on the method type (TC, TOC, TN, etc.).

Create and manage methods in the **Method** menu.

6.1   Methods window

Open the **Methods** window via the menu command **Method**|**Methods**.

In the Methods window

- You can create a new method by clicking on the **Add** button. Select the method type from the drop-down menu.
- You edit method settings on the right-hand side of the window in the **Method** view.
- You delete methods by clicking on the **delete** button.
- The optional FDA 21 CFR Part 11 Compliance module prevents data from being deleted.
- You organize methods into groups by clicking on **Assign group** in the **Select group** window.
- You import and export methods in XML format using the **Import** and **Export** buttons.
- Click on **Copy** to copy a selected method to use it as a template for a new method.
- Click on **Report** to open the print preview. Here, you can print a method report or save it in PDF format.

Layout of the window
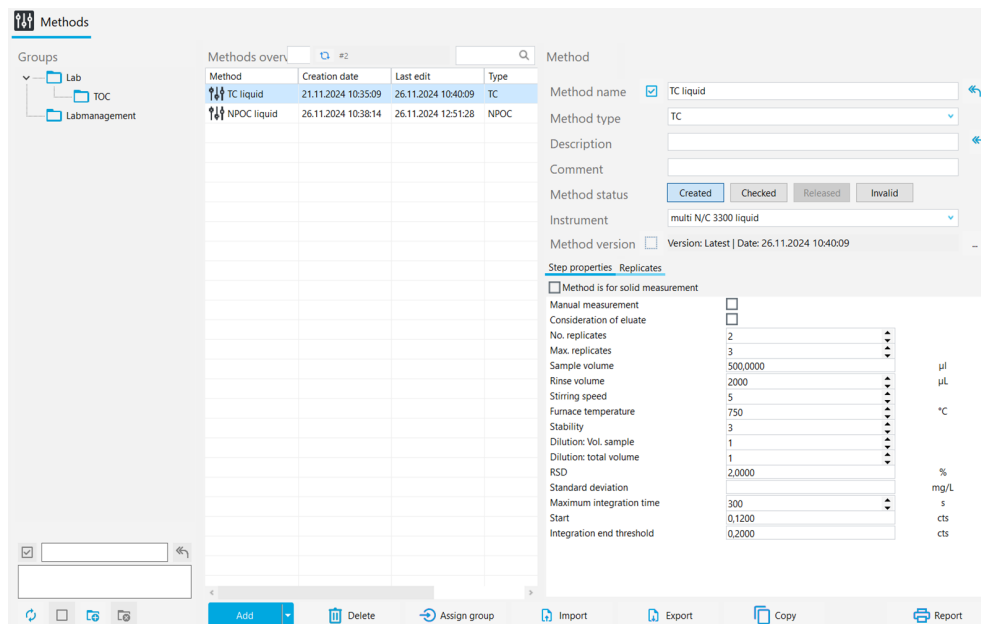
Fig. 24   Methods window

Area	Description
Groups (left)	Manage groups
Methods overview (middle)	Tabular overview of the created methods ■ Method name ■ Date created and last changed ■ Method type and measurement channels, for example: **Type**: NPOCTN, **Parameters**: NPOC, TN **Type**: TOC, **Parameters**: TC, IC, TOC ■ Signing status of the method
Method (right)	Detailed view for selected method with editable method parameters and information on the signing status

Electronic signatures are an important part of the optional FDA 21 CFR Part 11 Compliance module. You can restrict the use of non-approved data with the help of signatures and the corresponding assignment of rights. When signing, it is mandatory to enter a user name and password.

In the standard software, you can set the status of data, e.g. to **Checked**. However, you cannot add an electronic signature to data. The **Signatures** tab remains empty. No restrictions are linked to the status of the data. This means that even blocked data can still be used.

See also

- 📄 Electronic signatures [▶ 130]
- 📄 Organize in groups [▶ 32]

6.2   Editable method parameters

You create and edit methods in the **Methods** window.

In the **Method Details** view, you can adapt the method parameters for a selected method to your measurement task within defined limits. The values preset in the software provide good results for most measurements.

General method settings

You define general method settings in the first rows of the detailed view. Save changes with the ☑ button next to the **Method name** input field.

Parameters	Description
Method name	Define method name
Method type	Change method type ■ TC: To determine the total carbon content of the sample ■ TIC: To determine the total inorganic carbon from carbonates and hydrogen carbonates, as well as the free carbon dioxide ■ TN: To determine the total bound nitrogen in ammonium salts, nitrites/nitrates, amino acids, proteins, etc. ■ NPOC: To determine non-purgeable organic carbon Do not apply this method if the sample contains easily purgeable organic substances, as these substances are purged with the CO_2. ■ NPOC plus: To determine low TOC content in samples with high TIC content or a high portion of free carbon dioxide ■ TOC: To determine total organic carbon contained in the sample, in accordance with the differential method Use the differential method if the sample contains easily

Parameters	Description
	purgeable organic substances such as benzene, cyclohexane, chloroform, etc. Do not use the differential method if the TIC content of the sample is significantly higher than the TOC content.
	▪ POC: To determine the total purgeable organic carbon (not available with all analyzers)
	You can combine the determination of several parameters in methods: TOC-TN, TC-TN, NPOC-TN or NPOC plus-TN.
Description Comment	Enter a description and comment
Method status	▪ View the signing status of the method ▪ Release or block the method incrementally after testing
	Only for FDA 21 CFR Part 11 Compliance module: View detailed information on signatures on the **Signatures** tab.
Instrument	Assign method to a device configuration if required
	The software automatically assigns the method to the active device configuration.
Method version	Version of the method
	Whenever you edit a method, the software creates a new version. ▪ Click on the ⋯ icon, then navigate through the versions ▪ Click on the ☐ icon to return to the last version

Step properties tab

Parameter	Description
Method is for solid measurement	Activate solids measurement for TC and IC methods via the checkbox
	The software adjusts the method parameters accordingly.
Manual measurement	Activate manual sample application via the checkbox
Consideration of eluate	Use the checkbox for eluted samples to specify that the software takes the eluate blank value into account
No. replicates Max. replicates	Set the minimum and maximum number of repeat measurements from the same sample vessel
	If you enter different values for the minimum and maximum number, the software automatically selects outliers according to the criteria specified under relative or absolute standard deviation.
Sample volume	Select sample volume for measuring liquid samples
Rinse volume	Select rinse volume for rinsing the sample path with sample
Stirring speed	Set stirring intensity in stages (only for sample feeding with autosampler)
Furnace temperature	Select furnace temperature (only for analyzers with high-temperature oxidation)

	Recommended temperatures:
	▪ Platinum catalyst $Pt(Al_2O_3)$: 750 °C,
	  for samples with a high salt content: 720 to 750 °C,
	  with salt kit: 680 °C
	▪ Special catalyst (CeO_2): 850 °C
	▪ Solids module HT 1300: 900 to 1300 °C

Parameter	Description
Dilution: Vol. sample	Enter dilution ratio
Dilution: total volume	Specify the dilution ratio: ■ Parts of the primary sample (**Dilution: Vol. sample**) in total parts (**Dilution: total volume**) (e.g. 1 in 10 means 1 ml primary sample in 10 ml total volume) ■ A dilution of 1 in 1 means that the sample is not diluted.
RSD **Standard deviation**	Specify relative or absolute standard deviation as termination criteria for repeat measurements ■ If the specified standard deviation is not reached after the minimum number of determinations, the analyzer will not carry out any further determinations. ■ If the specified value is exceeded, the analyzer carries out further measurements from the same sample vessel until the maximum number of determinations is reached. You can define the criteria separately for each measurement channel.
Stability	Specify the number of measured values to be included in the routine for determining the end of integration The default value is optimized and applies to all method types. ■ If you increase the stability value, this will lead to the correct end of integration with a high degree of certainty, but the analyses will take longer. ■ If you reduce the stability value, this leads to a quicker end of integration, but some of the content may not be identified.
Maximum integration time	Specify the maximum integration time as a criterion for terminating the integration The maximum integration time is the period from the start to the end of the integration. It is used as a termination criterion if none of the other criteria have already ended the integration. The required integration time depends on the carbon and nitrogen content in the samples. ■ Adjust the integration time to the expected concentration. ■ Do not set the integration time too high, otherwise the analysis will take a long time.
Start	Set the distance to the baseline from which the integration starts Integration starts when the measured value exceeds the start value. The default value is optimized. ■ Reduce the start value slightly for low concentrations. Too low a selected value can, however, result in the baseline noise being identified. ■ If the selected values are too high, low measurement peaks may not be detected.
Integration end threshold	Set the distance from the baseline at which integration ends Integration ends when the measured value falls below this value. The default value is optimized. ■ Values that are too low extend the analysis time. ■ Values that are too high end the integration too early. Some of the content may not be identified.

Parameter	Description
Add reagent	Use checkbox to specify that sodium persulfate is dosed into the UV reactor (only for analyzers with UV oxidation)
	Activate option if TOC concentration is >1 mg/l
Automatic acidification	Acidify samples automatically via autosampler (only for NPOC methods)
	If activated, the autosampler takes acid from the acid container on the autosampler and acidifies the samples (not for all autosamplers).
With TIC control	Specify that the TIC is determined as a control immediately after purging (only for NPOC methods)
	The TIC control checks whether TIC has been completely purged. The determined value is not included in the measurement result.
Purge time 1 Purge time 2	Specify how long samples are purged before the first NPOC determination
	The second purge time is between repeat measurements and can only be implemented in manual mode or for non-parallel purging with autosampler.
COD calculation active	For TOC and NPOC methods, activate calculation of the COD (Chemical Oxygen Demand) on the basis of the TOC/NPOC
	Formula: $c(CSB) = A \times c(TOC) + B$
COD conversion factor A COD offset B	Specify slope (A) and intercept (B) for the calculation of COD, default setting: A = 3.000, B = 0.000
BOD_5 calculation active	For TOC and NPOC methods, activate calculation of the BOD_5 (Biochemical Oxygen Demand) on the basis of the TOC/NPOC
	Formula: $c(BOD_5) = A \times c(TOC) + B$
BOD_5 conversion factor C BOD_5 offset D	Specify slope (A) and intercept (B) for the calculation of BOD_5, default setting: A = 3.000, B = 0.000
CO_2 calculation active	For TIC methods for liquid samples, activate calculation of the carbon dioxide concentration based on the TIC
	Formula: $c(CO_2) = 2.833 \times c(TIC)$
Total protein conversion active	For TN methods, activate calculation of the total protein content based on the TN
	Formula: $c(Total\ Protein) = A \times c(TN)$
Total protein conversion factor A	Set the factor for calculating the total protein content between 0 and 10, default setting: A = 6.250 (comparison substance: BSA - bovine serum albumin)

Automated solids analysis

Parameter	Description
Furnace holing position	Hold point in the furnace of the solids module for feeding the boats with autosampler
Holding time	Waiting time at first furnace position
Furnace feed speed	Feed rate for boat feed (after passing **Furnace holing position**)

Integration criteria

The software determines the baseline before each measurement. The following parameters define the integration criteria: **Stability**, **Maximum integration time**, **Start** and **Integration end threshold**. You can define the integration criteria for carbon and nitrogen separately. The default integration criteria are already optimized.

ℹ NOTICE! If you change the integration criteria significantly, you will distort the measurement results.

Replicates tab

Parameters	Description
No. rinse cycles	Specify the number of rinse cycles before sample application
	The autosampler rinses the sample path x times with sample before each repeat measurement.
Purge	For NPOC measurements, activate or deactivate blowing out the sample before a repeat measurement
	An additional second blow-out of the sample is only possible in manual mode or with non-parallel blow-out with autosampler.
Sample mass	Determine sample mass for solids measurements, suitable for solids measurements with the same sample mass as for the adsorption of air pollutants on activated carbon
Sample position	Define sample positions for repeat measurements of solids

6.3 Creating a new method

▸ Open the **Methods** window with the **Method | Methods** menu option.

▸ Click on the arrow next to the **Add** button. Select the method type from the drop-down menu.

   ✓ The software creates a new method. The method has the default name: Method + timestamp.

▸ When you click on **Add**, the software creates a TC method (default setting).

▸ Select the method in the **Methods overview** table.

▸ Edit the method settings in the **Method** area.

▸ If necessary, adjust the method type again under **Method type**.

▸ The software automatically assigns the method to the active device configuration. If necessary, assign the method to a different device configuration via the drop-down menu next to **Instrument**.

▸ Check the **Method is for solid measurement** checkbox for solids methods. The method parameters are adjusted accordingly. Solids methods are possible for TC and TIC.

▸ Change the method name under **Method name**.
   Recommendation: If you create methods for different device configurations, add the abbreviation for the device configuration to the method name.

▸ Optionally, enter a description and comment for the method.

▸ Customize the method parameters for the measurement task within defined limits on the **Step properties** tab. The preconfigured values provide good results for most measurements.

▸ On the **Replicates** tab, specify whether and how often the autosampler rinses the sample path with sample before a repeat measurement.
   For NPOC methods, specify whether the sample is purged again before a repeat measurement. The analysis system can only purge samples again in manual mode or with non-parallel purging with autosampler.

▸ Save the method by clicking the ☑ button.

       ✓ You have created a new method.

6.4   Editing a method

▸ Open the **Methods** window with the **Method** | **Methods** menu option.

▸ Select the method in the **Methods overview** table.

▸ If necessary, change the method type under **Method type**. If you change the method type, the parameter selection is adapted to the method type.

▸ Edit the method settings in the **Method** area.

▸ Save the method by clicking the ☑ button.

    ✓ A new version of the method is created when saving. The edited method is saved with the modification date.

You can browse through the method versions by clicking on the ▦ icon under **Method version**. Click on the ▢ icon to return to the current version.

6.5   Copying a method

You can use methods as a template for developing new methods. To do this, create a copy of the method.

▸ Open the **Methods** window with the **Method** | **Methods** menu option.

▸ Select the method in the **Methods overview** table.

▸ Click on **Copy**.

    ✓ The software copies the method. The new method has the default name: Method + timestamp.

▸ Select the method in the **Methods overview** table.

▸ Change the method name under **Method name**.
Recommendation: If you create methods for different device configurations, add the abbreviation for the device configuration to the method name.

▸ Edit the method settings in the **Method** area.

▸ Save the method by clicking the ☑ button.

    ✓ You have created a new method based on an existing method.

6.6   Importing or exporting a method

Importing a method

Import a method in XML format as follows:

▸ Open the **Methods** window with the **Method** | **Methods** menu option.

▸ Click on the **Import** button.

▸ Select the method in the **Open** window in the Windows file manager.

▸ Click on **Open**.

    ✓ The software imports the method. If a method with the same name already exists, the software prompts you to enter a new name.

Exporting a method

Export a method in XML format as follows:

▶ Open the **Methods** window with the **Method** |**Methods** menu option.

▶ Select the method in the **Methods overview** table.

▶ Click on **Export**.

▶ Select the storage location in the **Save as** window. Default export folder:
C:/ProgramData/Analytik Jena/multiWinPro/export/methods.

▶ Change the file name if required and click on **Save**.

   ✓ The software exports the method.

6.7   Printing and saving the method report

Print report

▶ Open the **Methods** window with the **Method** |**Methods** menu option.

▶ Select the method in the **Methods overview** table.

▶ Click on **Report** to open the print preview.

▶ For a better overview, click on the **Page overview** button to display the navigation area with a page summary to the left of the report. Zoom in or out of the view by clicking on **Zoom in** and **Zoom out**.

▶ Add company logo to the report. Click on the **Load** button in the **Report logo** area, and then select the logo in the Windows file manager and load it into the report with **Open**.

▶ Click on **Printer options** to set up the printer.

▶ Click on **Page setup** to configure page settings such as paper size or orientation. Default: A4, portrait. Apply layout to current page or all report pages.

▶ Click on **Print** to start printing.

Save report

▶ Open the **Methods** window with the **Method** |**Methods** menu option.

▶ Select the method in the **Methods overview** table.

▶ Click on the **Report** button to open the print preview.

▶ Click on **Save** then specify the file name, storage directory and file type in the **Save as** window.

▶ Save the report by clicking on the **Save** button.

You can save reports in the following file formats: PDF (default), RTF, HTML, TXT, FP3.

When you edit a method, the changes are only applied to the report after you save it.

7   Measurement menu

In the **Measurement** menu, you can create and manage sequences for measuring samples, calibrations, daily factors, QC standards, blanks and SST tests. SST tests are only possible with the FDA 21 CFR Part 11 Compliance module.

In the Measurement menu
- Use the **Add new sequence** menu command to open the **Add new sequence** window. Here you create sequences and start the measurement.
- Use the **Measurement** menu command to open the **Sequences** window for managing saved sequences.

7.1   Sample types

You can measure different sample types in the software. To do this, specify the sample type for each measurement step in the sequence.

Selecting a sample type
▶ Use the **Measurement** | **Add new sequence** menu option to create a new sequence.
▶ Create a measurement step in the sequence with **Add by method**. Select the method from the drop-down menu.
  ✓ The software creates a new measurement step with the sample type **Sample**.
▶ Adjust the sample type if required:
  – Select one or more measurement steps in the sequence.
  – Select the sample type from the drop-down menu by **Sample type**.
  – Only select **Calibration** sample type if you want to add or re-measure calibration points subsequently in the calibration.
▶ To create the measurement series for calibration, open the **Calibration wizard** wizard by clicking on the 📈 icon.
▶ To create the measurement series for a system suitability test (SST), open the **Create SST** wizard by clicking on the ✡ icon (only with FDA 21CFR Part 11 Compliance module).
  ✓ You have defined the sample type for individual measurement steps or a measurement series in the sequence.

7.1.1   Sample

Select the sample type **Sample** for the measurement of samples and eluates. The software calculates a concentration as a result.

If you dilute a sample manually before the measurement, enter the dilution under **Step properties** | **Step** | **Dilution: Vol. sample** and **Dilution: total volume**. The software takes the dilution into account when calculating the result.

The software analyzes the sample using the selected method and calculates the results based on the selected calibration.

If you determine or manually specify reagent blanks for H_3PO_4 and $Na_2S_2O_8$ (only for analyzers with UV oxidation), the software takes the blanks into account when calculating the results.

7.1.2 Calibration

In a calibration, you measure a series of calibration standards of known concentration.

You create a calibration within the sequence using the **Calibration wizard** wizard. To do this, click on the 🖊 icon.

Select the calibration type:
- Preferably perform multiple-point calibrations with a constant sample volume and variable standard concentrations. Option: **Fixed volume**
- Alternatively, use a standard of constant concentration and dose different volumes of the standard. Option: **Fixed concentration**

You can re-measure calibration standards at a later time or add standards to a calibration. To do this, select the sample type **Sample type|Calibration** in the sequence.

You can measure the preparation water blank value in the calibration sequence or enter it manually in the wizard. If a reagent is used for the measurement performed, you can measure the reagent blank value or specify it manually. The software adjusts the measured values of the calibration standards by the preparation water blank value and reagent blank value.

See also
- 🗎 Carrying out calibration [▶ 81]

7.1.3 Daily factor

The daily factor is used to check and correct the calibration with a standard solution. The software multiplies all subsequent measurements by the daily factor.

Daily factor = c_{target}/c_{actual}

You can specify the daily factor manually or determine it using a measurement. To do this, select **Sample type|Daily factor**.
- If you carry out a new calibration or add a calibration range, the software calculates with a daily factor = 1.
- The software applies the daily factor to the calculation of the results until you measure or enter a new daily factor.
- Before measuring daily factors for low concentration ranges (< 10 mg/l), determine the current preparation water blank value.
- If a reagent is used for the measurement, the software adjusts the daily factor by the reagent blank value.

You define limits for the daily factor in the sequence. A complete calibration is required if the value falls below or exceeds the limits.

If the measured value is outside the tolerance range, the software adds a note to the results.

When using an autosampler, you can select actions to be taken in the event that the value is outside the limits.

ignore	The software ignores when the value falls below or exceeds limits.
ask	The software displays a prompt. You have the option of stopping the sequence or continuing it.
cancel	The software aborts the sequence.

7.1.4   QC Standard

Select the **QC standard** sample type if you want to measure standards for analytical quality control. The analysis is carried out with the selected method and calibration, which you select in the **Step type properties** panel.

Before measuring a QC standard for low concentration ranges (< 10 mg/l), determine the preparation water blank value.

If a reagent is used for the measurement, the software adjusts the result by the reagent blank value.

Enter the target concentration of the QC standard in the **Step type properties** panel. You can define a tolerance range under **Lower limit** and **Upper limit**.

If the measured value is outside the tolerance range, the software adds a note to the results.

When using an autosampler, you can select actions to be taken in the event that the value is outside the limits.

ignore	The software ignores when the value falls below or exceeds limits.
ask	The software displays a prompt. You have the option of stopping the sequence or continuing it.
cancel	The software aborts the sequence.

7.1.5   Preparation water blank value

The preparation water blank value is the blank value of the water that you use to prepare standards.

The software adjusts all standard measurements (QC standard, daily factor, calibration) by the preparation water blank value. Determine the blank value especially for measuring low concentrations (in the µg/l range).

In the wizard, you can specify for a calibration that the preparation water blank value is measured before the calibration. Provide preparation water for this. The software determines the mean integral for the preparation water. Alternatively, you can determine the blank value separately and enter it in the software.

The blank value can change over time. Determine the preparation water blank value again before measuring standards. Otherwise, the software will use the last blank value.

If a reagent is used for the measurement, the software adjusts the blank value by the reagent blank value.

To monitor the blank value, you can specify boundaries in the sequence under **Step type properties**.

These are specified in area units AU/ml.

If the measured value is outside the tolerance range, the software adds a note to the results.

When using an autosampler, you can select actions to be taken in the event that the value is outside the limits.

ignore	The software ignores when the value falls below or exceeds limits.
ask	The software displays a prompt. You have the option of stopping the sequence or continuing it.
cancel	The software aborts the sequence.

7.1.6   Reagent blank value

The reagent blank value is the blank value of the reagents used:
- Phosphoric acid H_3PO_4 (reagent for TIC branch) − TIC blank value
- Sodium persulfate $Na_2S_2O_8$ (reagent for TC branch, i.e. UV reactor) − TC blank value

The reagent blank for $Na_2S_2O_8$ is only available for analyzers with UV oxidation.

The software adjusts the results of samples and all other blank values by the reagent blank value. Take the reagent blank value into account, especially if you are measuring low concentrations (in the µg/l range).

You can measure the blank value in a sequence. Alternatively, you can determine the blank value separately and enter it in the software.
- The reagent blank values cannot be measured with mixing methods such as TOC.
- The phosphoric acid blank value must be measured using an IC method.
- The blank value of the sodium persulfate solution can be measured using an NPOC or TC method.

The blank value can change over time. You should therefore determine the blank value again at the start of a measurement series. Otherwise, the software will use the last blank value.

To monitor the blank value, you can specify boundaries in the sequence under **Step type properties**.

The injection volume of reagents is constant and independent of the sample volume. The reagent blank value is therefore specified as an absolute value in area units (AU).

If the measured value is outside the tolerance range, the software adds a note to the results.

When using an autosampler, you can select actions to be taken in the event that the value is outside the limits.

ignore	The software ignores when the value falls below or exceeds limits.
ask	The software displays a prompt. You have the option of stopping the sequence or continuing it.
cancel	The software aborts the sequence.

7.1.7   Diluent blank value

The diluent blank value is the blank value of the water that you use to dilute samples.

If you measure a sample with dilution, the software adjusts the result by the diluent blank value. The software takes into account the volume of diluent used.

You can measure the blank value in a sequence. Alternatively, you can determine the blank value separately and enter it in the software.

The blank value can change over time. You should therefore determine the blank value again at the start of a measurement series. Otherwise, the software will use the last blank value.

Definition of the dilution:
- Percentage of primary sample
  (e.g. 1 part in 10 parts), i.e. 1 ml primary sample are diluted with dilution water to a total volume of 10 ml.
- A dilution of 1 in 1 means that the sample is not diluted.

If a reagent is used for the measurement, the software adjusts the blank value by the reagent blank value.

To monitor the blank value, you can specify boundaries in the sequence under **Step type properties**.

These are specified in area units AU/ml.

If the measured value is outside the tolerance range, the software adds a note to the results.

When using an autosampler, you can select actions to be taken in the event that the value is outside the limits.

ignore	The software ignores when the value falls below or exceeds limits.
ask	The software displays a prompt. You have the option of stopping the sequence or continuing it.
cancel	The software aborts the sequence.

7.1.8 Eluate blank value

The eluate blank value is a blank value for samples from cleaning validation or eluate preparation. The blank value corresponds to the TOC content of the ultrapure water used, e.g. for extracting/eluting swabs.

You define the consideration of the eluate blank value in the method. To do this, activate the Consideration of eluate option.

You can measure the blank value in a sequence. Alternatively, you can determine the blank value separately and enter it in the software.

The blank value can change over time. You should therefore determine the blank value again at the start of a measurement series. Otherwise, the software will use the last blank value.

The software adjusts the measurement result for the blank value and takes the injection volume into account. The software does not use the eluate blank value for calibration measurements, as you do not generally elute standards.

If a reagent is used for the measurement, the software adjusts the blank value by the reagent blank value.

To monitor the blank value, you can specify boundaries in the sequence under **Step type properties**.

These are specified as absolute values in area units AU/ml.

If the measured value is outside the tolerance range, the software adds a note to the results.

When using an autosampler, you can select actions to be taken in the event that the value is outside the limits.

ignore	The software ignores when the value falls below or exceeds limits.
ask	The software displays a prompt. You have the option of stopping the sequence or continuing it.
cancel	The software aborts the sequence.

7.1.9 Boat blank value

The boat blank value is the blank value of the boats with which you introduce solid samples into the analyzer.

You determine the boat blank value by inserting an empty boat or a boat with sample additives into the combustion furnace and analyzing it.

You can measure the blank value in a sequence. Alternatively, you can determine the blank value separately and enter it in the software.

The blank value can change over time. You should therefore determine the blank value again at the start of a measurement series. Otherwise, the software will use the last blank value.

To monitor the blank value, you can specify boundaries in the sequence under **Step type properties**.

This is specified as an absolute value in area units AU.

If the measured value is outside the tolerance range, the software adds a note to the results.

When using an autosampler, you can select actions to be taken in the event that the value is outside the limits.

ignore	The software ignores when the value falls below or exceeds limits.
ask	The software displays a prompt. You have the option of stopping the sequence or continuing it.
cancel	The software aborts the sequence.

7.2   Add new sequence window

Open the **Add new sequence** window using the menu command **Measurement** |**Add new sequence**.

You can also get to the window when you load a saved sequence in the **Sequences** window by clicking on the **Load** button or by double-clicking. The window has the name of the saved sequence.

In the Add new sequence window

You create sequences and start the measurement in the **Add new sequence** window.
- In the sequence, use the **Add by method** button to create individual measurement steps and select the method and sample type for each measurement step. You can use the **Add multiple steps** command (in the context menu) to quickly create several measurement steps.
- Click on the ✷ or 📈 button to create the measurement series for system suitability tests (SST) and calibrations using wizards. (System suitability tests only with FDA 21 CFR Part 11 Compliance module)
- In the **Step properties** panel, you can adapt selected method parameters to the measurement task. You select the calibration. You view blank values and edit the blank values if required.
- In the **Step type properties** panel, you can define parameters specific to the sample type, such as target values, limit values, and actions for when limits are exceeded.
- In the **Sequence properties** panel, you can define settings that apply to multiple sequences, such as automatic dilution.
- Use the **Result table** button to select a results table for saving the results.
- After starting the measurement by clicking on the ▶ icon, you can follow the recording of current measurement results in the bottom part of the window. You can view the results of samples that have already been measured in the **Step results** panel.
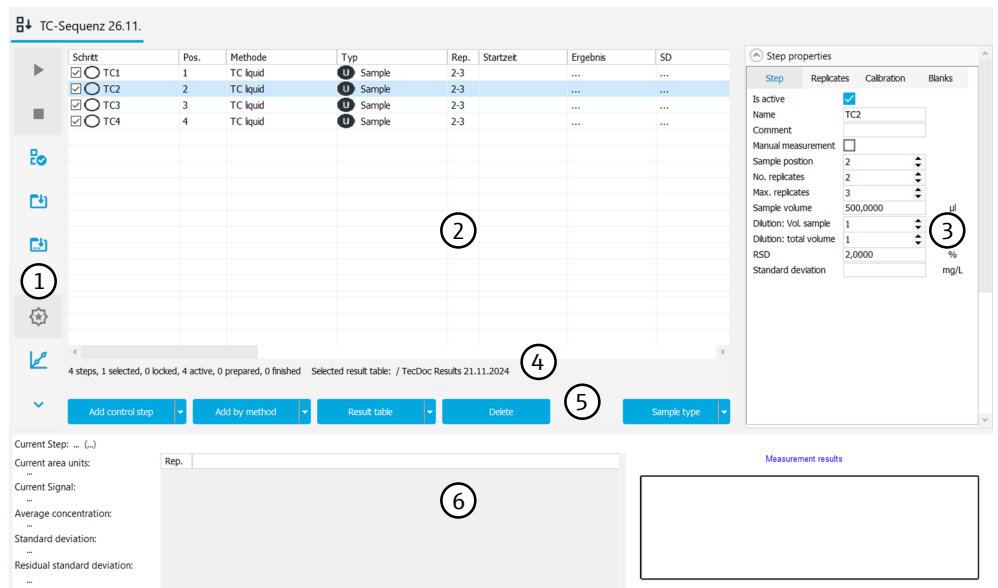
Layout of the window

Fig. 25   Add new sequence window

Element	Description
Toolbar with icons (1)	■ Start measurement of the sequence with the ▶ icon or cancel with ■ After canceling a sequence, you can measure the unprocessed steps by clicking on the ▶ icon. To do this, click on **yes** in the prompt. If you click on **no**, the software does not carry out a measurement. ■ Check sequence for plausibility with ⊟⊘ ■ Save sequence or save as with ⬆/⬇ ■ Assign empty sequence to another device configuration with ⊟∞ ■ Open **Create SST** wizard with ✿ and prepare system suitability test (only with FDA 21 CFR Part 11 Compliance module) ■ Open **Calibration wizard** with ↗ and prepare calibration
Sequence table (2)	View sequence with measurement steps in tabular overview
Fold-out panels (3)	View and edit settings and results for selected steps **Step properties** ■ Assign sample names and define sample positions ■ Adjust method parameters to the measurement task ■ Select calibration ■ Viewing and editing blanks **Step type properties** ■ Define limit values and actions when limits are exceeded ■ For the **Calibration** sample type (only re-measurements) and **Daily factor**, define target values of standards and select the calibration to which the measured value is to be assigned **Step results** ■ View measurement results for selected steps, with integrals, masses and concentrations, relative and absolute standard deviations

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Element	Description
	Sequence properties ■ Activate settings that apply to multiple sequences: Solids measurement, automatic/intelligent dilution, intelligent volume reduction and parallel purge for NPOC methods The software adapts the available settings to the device configuration.
Sequence info row (4)	View summarized information on the sequence and current processing status: ■ Number of total steps as well as selected, blocked and active steps ■ Number of analyses prepared and performed ■ Selected results table ■ Assigned device configuration
Button bar (5)	Edit sequence (see below)
Fold-out results view (6)	■ Track measurement progress and recording of current measurement results in tabular and graphical view ■ Expand/collapse with ⌄ / ⌃

Buttons

Button	Description
Add control step	Insert control steps in sequence **Pause** Pause processing of the sequence, set pause duration in (s) under **Step properties**, continue sequence with or without user confirmation **Rinse** Insert additional rinsing step in sequence **Reverse rinse** Backwash the sample path with ultrapure water (not all analyzers) **Purge** Blow out NPOC samples, specify position on sample tray and blow-out time under **Step properties**. If necessary, enable manual measurement **Turn off instrument** Shut down the device at the end of the sequence **Standby instrument** Put the device in standby. The device lowers the furnace temperature to the temperature selected under **Step properties** and shuts off the gas flow. **Set gasflow** Switch the gas flow on or off ■ Insert **Set gasflow** control step into the sequence to switch off gas flow, for example at the end of the measurement ■ Insert **Set gasflow** control step into the sequence and tick the **GasFlowActive** checkbox in the **Step properties** panel to switch the gas flow back on **Wake up** Initialize the device after standby
Add by method	Add step in sequence, select method from drop-down menu or in the **Select method** window Tip: Add several steps with the **Add multiple steps** command (in the context menu of the sequence table)

Button	Description
Result table	■ Select results table for saving results from the drop-down menu ■ Create new results table
	Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** | **Settings** | **Result table**
	i NOTICE! The sequence cannot be started without a results table.
delete	Delete selected step
Sample type	■ Select sample type from the drop-down menu: Calibration standard, daily factor, QC standard and various blank values ■ Click on the **Sample type** button to change the sample type back to sample

7.2.1   Sequence table

The sequence table is part of the **Add new sequence** window. The sequence table summarizes information on all measurement steps in a tabular overview.

Layout of the sequence table

You can customize the layout of the sequence table using the **Adjust display columns** command (in the context menu).

Column	Description
Step	Checkbox and sample name
	Use the checkboxes to activate or deactivate control steps in the sequence
	The following special characters are not permitted in the sample name: % & ( ) = ` ´ + ~ ' # , ; - _
	You can change the sample name in various ways: ■ Open the **Step step properties** window with a quick double-click on the measurement step. Define the sample name in the window. ■ After a slow double-click, rename the measurement step directly in the sequence table ■ Edit the sample name in the **Step properties** panel under **Name**.
Pos.	Position on sample tray
	Edit the sample position after double-clicking in the **Step step properties** window or in the **Step properties** panel.
Method	Measurement method
Type	Sample type (sample, calibration standard, daily factor, QC standard, blank value)
	Customize the sample type via the **Sample type** button
Rep.	Minimum and maximum number of repeat measurements, specification: min-max
Start time	Start time of the measurement
Result	Measurement result (mean concentration)
SD	Standard deviation of the measurement result
RSD	Relative standard deviation of the measurement result in (%)
c(TC), etc.	Mean concentration for the various measurement channels
SD(TC), etc.	Standard deviation for the results of the various measurement channels

Column	Description
RSD(TC), etc.	Relative standard deviation for the results of the various measurement channels in (%)
Volume	Sample volume
Mass	Sample mass for solids measurements
Info	Individual information
Target concentration	Target concentration
	Specify the target concentration in the **Step type properties** panel
Parameters	Measuring channels
Dil. Water	Dilution ratio for manually or automatically diluted samples
COD	COD (Chemical Oxygen Demand) determined for TOC and NPOC methods
BOD$_5$	BOD$_5$ (Biochemical Oxygen Demand) determined for TOC and NPOC methods
TP	TP (Total Protein) content determined for TN methods
CO$_2$	Carbon dioxide concentration determined for TIC methods

Context menu

Command	Description
Position	Move measurement step in the sequence table
	Move up Move one row up
	Move down Move one row down
	Move to list top Move to top of list
	Move to list bottom Move to bottom of list
	Move to position In the **Move to position** window, select the desired position and move the measuring step by clicking on the **OK** button
Delete selected steps	Delete selected steps
Change step type	Change sample type for selected steps
Assign method	Select new method for selected steps
Measure as next step	Measure selected step next
	The software moves the step to the beginning of the sequence or to the next position for ongoing measurements.
Import sequence	Import sequence in XML or CSV format
Export this sequence	Export sequence in XML format
Add multiple steps	Add several steps to the sequence, which are measured using the same method and named according to a standardized scheme ■ Select a method under **Method of steps to be created:** ■ Define the number of steps under **Count of steps:** ■ Define the root word under **Base name:** ■ Enter the start number in the **Use numbers:** input field to number the samples ■ Transfer the sample series to the sequence by clicking on **Create steps**
Define new columns	Create your own sequence columns with ID and column name

Command	Description
Step properties	Customize the sample name and position on sample tray for a measurement step, add individual information
Adjust display columns	Customize the selection and order of sequence columns
Select output units	Right-click outside the table and select **Select output units** to adjust the units and decimal places for the results display in the **Add new sequence** window
Select input units	Right-click outside the table and select **Select input units** to adjust the units and decimal places for the entry of sample information in the **Add new sequence** window

7.2.2   Customizing the sequence table

You can customize the layout of the sequence table using the **Adjust display columns** command (in the context menu).

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▸ Right-click in the sequence table to open the context menu.

▸ Select the **Define new columns** command to create your own columns.

▸ In the **Define new columns** window, define an ID for the column under **Unique column identifier**. Specify a name under **Column name**. The name is displayed in the table header.

▸ Click **OK** to confirm the entered data.

▸ Select the **Adjust display columns** command.

▸ In the **Configuration view**, customize the display and order of the table columns:

 – Use the → icon to transfer a column from suggestions (left) to the table (right).

 – Use the ← icon to remove a column from the table (right).

 – Use the →| icon to transfer all columns from suggestions (left) to the table (right).

 – Use the |← icon to remove all columns from the table (right).

 – Use the ↓ icon to move a column down or to the right in the sequence table.

 – Use the ↑ icon to move a column up or to the left in the sequence table.

 – Use the ↻ icon to restore the preset column.

▸ Click **OK** to confirm the entered data.

 ✓ You have customized the table columns.

7.3   Sequences window

Open the **Sequences** window using the menu command **Measurement** |**Sequences**.

In the Sequences window

You can manage saved sequences in the **Sequences** window.
▪ You can load saved sequences by double-clicking on the sequence or clicking on the **Load** button. You can then edit the sequence or start the measurement.
▪ You delete sequences by clicking on the **delete** button.

■ The optional FDA 21 CFR Part 11 Compliance module prevents data from being deleted.

■ You organize sequences into groups by clicking on **Assign group** in the **Select group** window.

■ You import and export sequences in XML format using the **Import** and **Export** buttons.
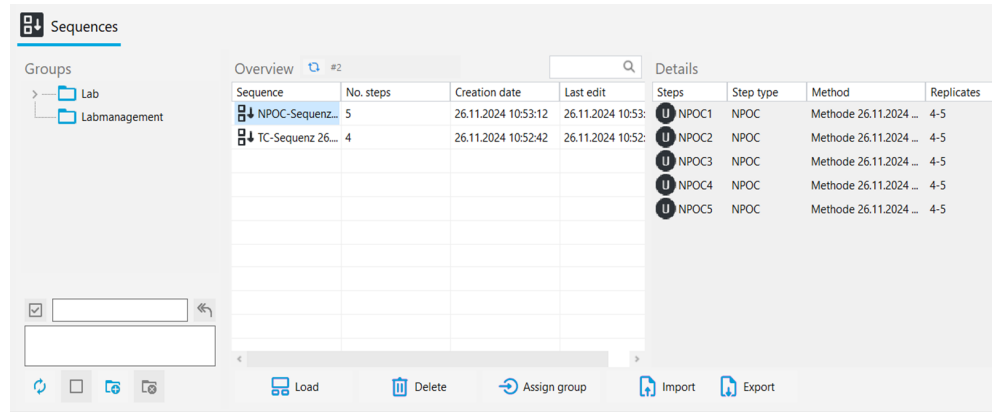
Layout of the window

Fig. 26   Sequences window

Area	Description
Groups (left)	Manage groups
Overview (middle)	Tabular overview of the saved sequences with the details: ■ Sequence name ■ Number of measurement steps ■ Date created and last changed
Details (right)	Detailed view for selected sequence with columns: ■ Measurement step with name ■ Measurement type or control step ■ Method ■ Minimum and maximum number of repeat measurements (min-max)

See also

▤ Organize in groups [▶ 32]

7.4   Calibration wizard

In the **Calibration wizard** you can prepare a calibration.

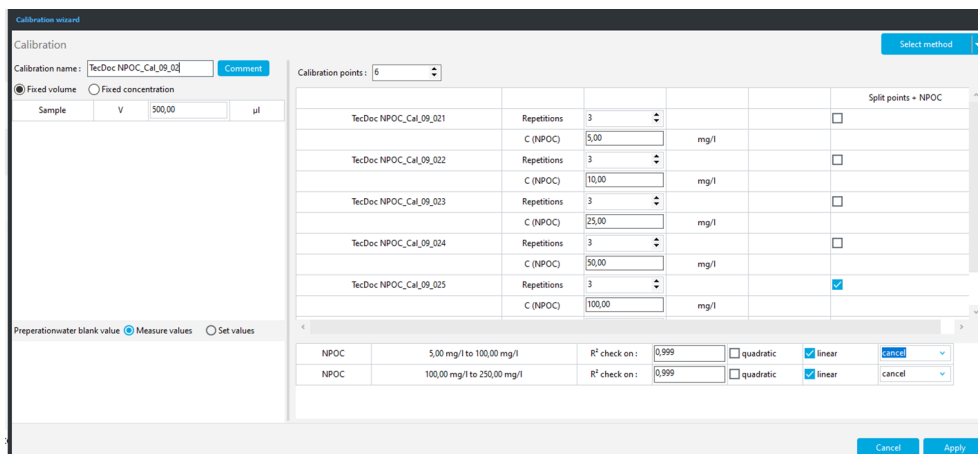Open the wizard via the 🖉 icon in the **Add new sequence** window.

Layout

Fig. 27   Calibration wizard

Element	Description
Button **Select method**	Click on **Select method** then select the method in the **Select method** window
Input field **Calibration**	Assign a name for the calibration The default name is: Methodtype_Cal.
Button **Comment**	Click on **Comment** then enter a comment in the **Comment** window
Radio buttons ▪ **Fixed volume** ▪ **Fixed concentration**	Select option: ▪ Perform multiple-point calibration with constant dosing volume and multiple standards of different concentrations ▪ Alternatively, perform multiple-point calibration with a standard of constant concentration and variable dosing volumes
Input field **Sample**	▪ For calibration with constant volume: The software takes the volume from the method. Optionally adjust the volume. ▪ For calibration with constant concentration: Enter the concentration of the calibration standard.
Preparation water blank: with radio buttons ▪ **Measure values** ▪ **Set values**	Take the preparation water blank value into account: ▪ Measure the preparation water blank value immediately before calibration. The software creates the blank value determination in the sequence. ▪ Alternatively, determine the preparation water blank value separately and enter in (AU/ml) (enter value 0 if the preparation water blank value is not to be taken into account)
Field **Calibration points:**	Specify the number of calibration points
Table with calibration points	▪ The software defines the name for calibration points: Methodtype_Cal_No If necessary, adjust the name in the **Add new sequence** window. ▪ For calibration points, specify the number of repeat measurements under **Replicates**. The software suggests the maximum number of determinations from the method. ▪ Enter the concentration or volume of the standards for calibration points
Split points + measurement channel checkbox	Activate split points for each measurement channel and thus define several calibration ranges that each have a common split point

Element	Description
Table of calibration ranges	■ Define the coefficient of determination R^2 as the limit for each calibration range, default setting 0.999 ■ Select linear or quadratic regression type ■ From the drop-down menu, select the action to be taken if the coefficient of determination fails to reach the limit value, e.g. **cancel**
Button **cancel**	Cancel preparation of the calibration
Button **Apply**	Transfer calibration to the sequence

See also

▤ Carrying out calibration [▶ 81]

7.5 Create sequence and measure with manual sample feed

Preliminary considerations:
■ Blank values change over time. You should therefore decide whether to re-measure blank values at the start of the sequence.
■ If necessary, you can correct the calibration with a daily factor. To do this, measure one or more standard solutions at the beginning of the sequence to determine the daily factor(s). The software automatically transfers the daily factors to the calibration.

▸ Prepare one or more methods for manual sample feed. To do this, activate the **Manual measurement** checkbox in method parameters.
A sequence can contain sample steps with different methods. However, liquids and solids cannot be measured in a sequence.
Deactivate the **Automatic acidification** method parameter for manual measurements.

▸ Alternatively: Wait to activate the **Manual measurement** checkbox until the sequence was created in method parameters.

▸ Use the **Measurement** | **Add new sequence** menu option to create a new sequence.

▸ In the **Sequence properties** panel activate the **Is a solids measurement** checkbox for manual solids measurement.

▸ By default, the software assigns a new sequence to the active device configuration. If necessary, click on the 🖳 icon to assign the empty sequence to a different device configuration.
To do this, select a device configuration in the **Select instrument configuration** window. Confirm the selection by clicking on the **OK** button.

▸ Alternatively, open an already prepared sequence. Open the **Sequences** window using the menu option **Sequences** | **Sequences**. Select prepared sequence from the **Overview** table. Open the sequence by double-click or with **Load**.

▸ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▸ Select the method from the dropdown menu or in the **Add by method** window.

▸ Enter sample name in sequence table by double-click on measurement step or in the **Step properties** panel, Tab **Step**.
The default name is: method type + step number.
Optionally add a comment.

▸ If necessary, create several sample steps using the option **Add multiple steps** (in context menu).

  – Select the method in the window **Add multiple steps to sequence**.

  – Set the number of measurement steps under **Count of steps:**.

  – Choose a common base word for the designation of the steps under **Base name:**. The default name is: sample + method type.

  – Start number in input field Enter **Use numbers:** to number the measurement steps.

  – Transfer the measurement steps to the sequence by clicking on **Create steps**.

▸ In case of manually diluted samples, enter the dilution ratio under **Dilution: Vol. sample** and **Dilution: total volume**: Parts of the primary sample in the total parts. The software takes the dilution into account when calculating the results.

▸ If required, select one or more measurement steps in the sequence table and adjust the method settings in the **Step properties** panel to the measurement task. After selecting a method setting, you can navigate from measurement step to measurement step by clicking on the Enter button.

▸ For each measuring channel, select the calibration for calculating the measurement results from the drop-down menu in the **Step properties** panel, Tab **Calibration**.

▸ View blank values for each measuring channel on the **Blanks** tab. Edit blank values if required.
The software automatically corrects the measurement results for any blank values. Unless you redefine the blank values at the start of the sequence, the software uses the last blank values.

▸ The software creates measurement steps with sample type **Sample**. Select measurement step and after clicking on the **Sample type** button, select other sample type, such as **Daily factor**, from the drop-down menu.

▸ Optionally specify lower and upper limit value for the measurement result in the **Step type properties** panel. Select actions from the dropdown menu if the limit is exceeded, such as **cancel** for measuring stop.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program**|**Settings**|**Result table**
i NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on 🗎. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with 🗎. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Provide samples. For liquid measurements, dip the sample intake cannula into the sample. For NPOC measurements, also insert a purge cannula into the sample.

▸ Before starting the measurement: Check device readiness in the **Instrument status** panel.

▸ Start the measurement by clicking on ▶ . Follow the instructions on the screen. Remain next to the device during repeat measurements so that instructions can be followed and acknowledged.

  ✓ The analysis system processes the sequence. You can add further steps to the sequence during the measurement.

The software displays the current measurement results during recording graphically in the lower window area and in a result table.

In the **Step results** panel you can view the results of already measured samples. When the sequence was processed, you can see the results in the **Results** menu.

See also

▤ Measuring and editing blanks [▶ 80]

▤ Determine daily factor [▶ 85]

7.6 Creating a sequence and measuring with automatic sample feed

Preliminary considerations:
- Blank values change over time. You should therefore decide whether to re-measure blank values at the start of the sequence.
- If necessary, you can correct the calibration with a daily factor. To do this, measure one or more standard solutions at the beginning of the sequence to determine the daily factor(s). The software automatically transfers the daily factors to the calibration.

▸ Prepare one or more methods for the measurement.
  A sequence can contain measurement step with different methods. However, liquids and solids methods cannot be measured in a sequence.

▸ Provide samples on sample tray.

▸ Use the **Measurement** | **Add new sequence** menu option to create a new sequence.

▸ In the **Sequence properties** panel, configure settings that apply to multiple sequences:
  Solids measurement, automatic or intelligent dilution, intelligent reduction of sample volume, and parallel purge for NPOC methods.
  To do so, tick the corresponding checkbox.
  The available options depend on the device configuration.

▸ By default, the software assigns a new sequence to the active device configuration. If necessary, click on the ⬚ icon to assign the empty sequence to a different device configuration.
  To do this, select a device configuration in the **Select instrument configuration** window. Confirm the selection by clicking on the **OK** button.

▸ Alternatively, open an already prepared sequence. Open the **Sequences** window using the menu option **Sequences** | **Sequences**. Select prepared sequence from the **Overview** table. Open the sequence by double-click or with **Load**.

▸ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▸ Select the method from the dropdown menu or in the **Add by method** window.

▸ Enter sample name in sequence table by double-click on measurement step or in the **Step properties** panel, Tab **Step**.
  The default name is: method type + step number.
  Optionally add a comment.

▸ If necessary, create several sample steps using the option **Add multiple steps** (in context menu).

  – Select the method in the window **Add multiple steps to sequence**.

  – Set the number of measurement steps under **Count of steps:**.

- Choose a common base word for the designation of the steps under **Base name:**. The default name is: sample + method type.

- Start number in input field Enter **Use numbers:** to number the measurement steps.

- Transfer the measurement steps to the sequence by clicking on **Create steps**.

▸ The software creates measurement steps with sample type **Sample**. Select measurement step and after clicking on the **Sample type** button, select other sample type, such as **Daily factor**, from the drop-down menu.

▸ Determine position on sample tray under **Step properties** | Tab **Step** under **Sample position**.
You can occupy positions on the autosampler tray more than once in a sequence.

▸ If required, select one or more measurement steps in the sequence table and adjust the method settings in the **Step properties** panel to the measurement task.
After selecting a method setting, you can navigate from measurement step to measurement step by clicking on the Enter button.

▸ In case of manually diluted samples, enter the dilution ratio under **Dilution: Vol. sample** and **Dilution: total volume**: Parts of the primary sample in the total parts. The software takes the dilution into account when calculating the results.

▸ For each measuring channel, select the calibration for calculating the measurement results from the drop-down menu in the **Step properties** panel, Tab **Calibration**.

▸ View blank values for each measuring channel on the **Blanks** tab. Edit blank values if required.
The software automatically corrects the measurement results for any blank values. Unless you redefine the blank values at the start of the sequence, the software uses the last blank values.

▸ Optionally specify lower and upper limit value for the measurement result in the **Step type properties** panel. Select actions from the dropdown menu if the limit is exceeded, such as **cancel** for measuring stop.

▸ Click on the **Add control step** button to add control steps such as pauses or additional rinsing steps to the sequence.

▸ Add the control steps **Reverse rinse**, **Standby** or **Turn off instrument** at the end of the sequence in order to shut the analysis system down after sequence processing.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** | **Settings** | **Result table**
ℹ NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ⬛✅. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with ⬛. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Before starting the measurement: Check device readiness in the **Instrument status** panel.

▸ Start the measurement by clicking on ▸ .

✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

The software displays the current measurement results during recording graphically in the lower window area and in a result table.

In the **Step results** panel you can view the results of already measured samples. When the sequence was processed, you can see the results in the **Results** menu.

See also

- 🖹 Measuring and editing blanks [▶ 80]
- 🖹 Determine daily factor [▶ 85]
- 🖹 Intelligent reduction of the sample volume [▶ 92]
- 🖹 Diluting samples automatically or intelligently [▶ 87]

7.7   Importing and exporting sample data

In the **Sequences** window, you can import and export sequences in XML format.

Import sequence

- ▶ Open the **Sequences** window using the menu option **Sequences**|**Sequences**.
- ▶ Click on the **Import** button.
- ▶ Select a sequence in the **Open** window in the Windows file manager.
- ▶ Click on **Open**.
  - ✓ The software imports the sequence. If a sequence with the same name already exists, the software prompts you to enter a new name.

Export sequence

- ▶ Open the **Sequences** window using the menu option **Sequences**|**Sequences**.
- ▶ Select the sequence from the **Overview** overview.
- ▶ Click **Export**.
- ▶ Select the storage location in the **Save as** window. Default export folder: *C:/ProgramData/Analytik-Jena/multiWinPro/export/sequences*.
- ▶ Change the file name if required and click on **Save**.
  - ✓ The software exports the sequence.

The exported sequence contains sample data. If you have already measured the sequence, the measurement results are only stored in the results table, but not in the sequence.

Alternatively, you can import or export sequences in the **Add new sequence** window. To do this, use the commands **Import sequence** and **Export this sequence** in the sequence table context menu. You can also import sequences in CSV format here.

Import sequence in CSV format

- ▶ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.
- ▶ Right-click in the sequence table to open the context menu.
- ▶ Select the **Import sequence**|**Import from file** menu option.
- ▶ In the **Open** window, select the **CSV file** type.
- ▶ Select the CSV file in Windows File Manager.
- ▶ Import the CSV file by clicking the **Open** button.
  - ✓ The software imports the CSV file into the **Add new sequence** window. You can now expand the sequence table and start the measurement.

Prerequisites for a successful CSV import:
- ▪ The name and sequence of the data fields in the CSV file must match the data fields that you have defined under **Software settings**, **Storage, Export and Report** tab.

■ The **Method name** data field in the CSV file must be filled with the name of a method already created in the software.

Import sequence from clip-board

▸ Create a sequence as an Excel spreadsheet.

▸ Copy the spreadsheet.

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▸ Right-click in the sequence table to open the context menu.

▸ Select the **Import sequence**|**Import from clipboard** menu option.

   ✓ The software imports the sequence from the clipboard.

7.8 Customizing method settings in the sequence

In the **Add new sequence** window, you can view and edit selected method settings for each measurement step in the **Step properties** panel. To do this, select one or more measurement steps in the sequence table.

If you select multiple measurement steps in the sequence table, you can change the method settings for multiple measurement steps. The software highlights different method settings in color.

The optional FDA 21 CFR Part 11 Compliance module strictly limits the editing of ap-proved methods. You can customize only a few method settings, such as sample volume in the sequence.

Step tab

Parameter	Description
Is active	Activate or deactivate measurement step.
Name	Sample name
Comment	Comments
Sample position	Position on sample tray
Manual measurement	Activate manual sample application via the checkbox
No. replicates **Max. replicates**	Set the minimum and maximum number of repeat measurements from the same sample vessel If you enter different values for the minimum and max-imum number, the software automatically selects out-liers according to the criteria specified under relative or absolute standard deviation.
Sample volume	Select sample volume for measuring liquid samples
Rinse volume	Select rinse volume for rinsing the sample path with sample
Dilution: Vol. sample	Enter dilution ratio
Dilution: total volume	Specify the dilution ratio: ■ Parts of the primary sample (**Dilution: Vol. sam-ple**) in total parts (**Dilution: total volume**) (e.g. 1 in 10 means 1 ml primary sample in 10 ml total volume) ■ A dilution of 1 in 1 means that the sample is not diluted.

Parameter	Description
RSD **Standard deviation**	Specify relative or absolute standard deviation as termination criteria for repeat measurements ■ If the specified standard deviation is not reached after the minimum number of determinations, the analyzer will not carry out any further determinations. ■ If the specified value is exceeded, the analyzer carries out further measurements from the same sample vessel until the maximum number of determinations is reached. You can define the criteria separately for each measurement channel.
Automatic acidification	Acidify samples automatically via autosampler (only for NPOC methods) If activated, the autosampler takes acid from the acid container on the autosampler and acidifies the samples (not for all autosamplers).
Purge time 1 **Purge time 2**	Specify how long samples are purged before the first NPOC determination The second purge time is between repeat measurements and can only be implemented in manual mode or for non-parallel purging with autosampler.
Add reagent	Use checkbox to specify that sodium persulfate is dosed into the UV reactor (only for analyzers with UV oxidation) Activate option if TOC concentration is >1 mg/l
COD calculation active	For TOC and NPOC methods, activate calculation of the COD (Chemical Oxygen Demand) on the basis of the TOC/NPOC Formula: $c(CSB) = A \times c(TOC) + B$
COD conversion factor A **COD offset B**	Specify slope (A) and intercept (B) for the calculation of COD, default setting: A = 3.000, B = 0.000
BOD₅ calculation active	For TOC and NPOC methods, activate calculation of the BOD_5 (Biochemical Oxygen Demand) on the basis of the TOC/NPOC Formula: $c(BOD_5) = A \times c(TOC) + B$
BOD₅ conversion factor C **BOD₅ offset D**	Specify slope (A) and intercept (B) for the calculation of BOD_5, default setting: A = 3.000, B = 0.000
CO₂ calculation active	For TIC methods for liquid samples, activate calculation of the carbon dioxide concentration based on the TIC Formula: $c(CO_2) = 2.833 \times c(TIC)$
Total protein conversion active	For TN methods, activate calculation of the total protein content based on the TN Formula: $c(Total\ Protein) = A \times c(TN)$
Total protein conversion factor A	Set the factor for calculating the total protein content between 0 and 10, default setting: A = 6.250 (comparison substance: BSA - bovine serum albumin)

Replicates tab

Parameters	Description
No. rinse cycles	Specify the number of rinse cycles before sample application
	The autosampler rinses the sample path x times with sample before each repeat measurement.
Purge	For NPOC measurements, activate or deactivate blowing out the sample before a repeat measurement
	An additional second blow-out of the sample is only possible in manual mode or with non-parallel blow-out with autosampler.
Sample mass	Determine sample mass for solids measurements, suitable for solids measurements with the same sample mass as for the adsorption of air pollutants on activated carbon
Sample position	Define sample positions for repeat measurements of solids

Calibration tab

On the **Calibration** tab, select the calibration for calculating the measurement results for each measurement channel from the corresponding drop-down menu. The software shows the calibration parameters under the drop-down menu.

Blanks tab

The **Blanks** tab shows the blank values stored in the software for each measurement channel. If you have the appropriate permissions, you can edit blank values manually.

If you create the measurement of a blank in the sequence, the software automatically takes the new blank into account when calculating all subsequent measurement results.

7.9   Editing a saved sequence

You can load saved sequences at a later time and start the measurement. You can edit saved sequences or use them as a template for new sequences.

▶ Open the **Sequences** window using the menu option **Sequences│Sequences**.

▶ Select the sequence from the **Overview** overview.

▶ Check sequence settings in the **Details** view.

▶ Load the selected sequence by double-clicking or clicking on the **Load** button.

▶ View and edit the measurement steps of the sequence.

▶ If necessary, save the edited sequence with the same name by clicking on the 📥 icon or save it with a new name by clicking on the 📥 icon.

▶ If you have used the saved sequence as a template for a new sequence, save the new sequence under a new name.

　✓ You have edited a saved sequence or used it as a template for a new sequence.

7.10   Performing a NPOC measurement

In the NPOC analysis, you determine the total non-purgeable organic carbon. After acidifying the sample, purge the carbon dioxide formed manually or on the autosampler. The analyzer then determines the remaining organic carbon in the sample.

Analyzers with flow injection technology can aspirate a sample and purge a second sample on the autosampler at the same time. Some autosamplers can acidify samples automatically. This gives the process a high degree of automation.

▸ Set the NPOC purge flow.
  The purge flow is preset, but can be adapted to the measuring task.

  – Activate purge flow via the **Instrument**|**Single control steps**|**Purge** menu command.
    Set the gas flow at the "NPOC" needle valve.

▸ Prepare the NPOC method.

▸ In method settings, define the purge time under **Purge time 1**.

▸ In manual mode or with non-parallel purging on the autosampler, you can purge samples again between multiple determinations.

  – To do this, set a second purge time under **Purge time 2**.

  – On the **Replicates** tab, select the repeat measurements before which samples are to be purged again. To do this, tick the checkbox under **Purge**.

▸ Stir samples on the autosampler for efficient purging. Specify the stirring intensity under **Stirring speed**.

▸ Check the **With TIC control** checkbox as required. The software then uses TIC measurement to check whether TIC has been completely purged. The value determined is only a check value and is not included in the measurement result.

▸ For automatic acidification of the samples, check the **Automatic acidification** checkbox in the method settings.

  – AS 60: Place the acid container in acid position.

  – AS vario: Place the acid container at the acid position of the sample tray:
    The acid position is blocked in the sequence for NPOC methods and cannot be used for samples.
    Tip: If the acid position is unknown, use the menu command **Instrument**|**Sampler alignment**|**Acid position** to move to the acid position on the sample tray.

Sample tray	Acid position
47 (dilut)	28
52	42
72	55
100	85
146	131

  – EPA sampler: Place the acid container at the 54 acid position of the sample tray.

▸ Alternatively, acidify samples to pH <2 outside the autosampler.

▸ Provide samples on sample tray.

▸ For manual sample application, dip the sample and purge cannula into the acidified sample.

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▸ For parallel sample purging, select the **Parallel purge** option in the **Sequence properties** panel.

▸ Use the **Add by method** button to create measurement steps with the NPOC method in a sequence.

▸ To carry out further non-NPOC measurements after NPOC measurements, leave one position free on the sample tray between measurements.

    –   The software issues a corresponding message. When the samples are correctly positioned on the sample tray, confirm the message with **OK**. The software continues the measurement.

    –   Otherwise acknowledge the message with **cancel**. Position samples correctly.

    Continue the sequence by clicking on the ▶ icon.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program | Settings | Result table**
ℹ NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ▣⊘. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with ⬓. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Instead of creating a new sequence, it is also possible to use a saved sequence. Select the saved sequence in the **Sequences** window and load it by double-clicking. For parallel sample purging, select the **Parallel purge** option in the **Sequence properties** panel.

▸ Start the measurement by clicking on ▶ .

    ✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

NPOC analysis according to the NPOC plus method

This method was developed especially for the detection of low TOC content in samples with high TIC content or a high level of dissolved CO_2. The NPOC method is generally recommended for the analysis of such samples. For high and, in particular, unknown TIC content, very long time periods (t > 10 min) may, however, be required for complete purging of the CO_2. This is why the inorganic bound carbon is purged externally with this method.

The NPOC plus method process is a combination of the NPOC and the differential method.
- Acidify the sample outside the analyzer (pH <2).
- Purge most of the carbon dioxide formed externally immediately before analyzing.
- Prepare an NPOC plus method and analyze the samples.
- The analyzer determines the TC and TIC content of the prepared samples and calculates the NPOC content from the difference.

Since you have purged most of the inorganically bound carbon externally, the TIC value determined using this method is only a calculated value and has no analytical relevance.

Highly volatile organic substances are also purged during the sample preparation and not detected for this reason.

The device models multi N/C 3300 and multi N/C 3100 can perform automatic and intelligent dilution of samples.

ℹ NOTICE! Automatic acidification in NPOC mode and automatic or intelligent dilution usually cannot be performed at the same time.

7.11   Measuring and editing blanks

You define the determination of blanks in the sequence. The software automatically adopts the measurement results for all subsequent measurements until you determine new blanks.

Measuring blanks

▸ Provide blank samples.

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▸ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▸ Select the method from the drop-down menu or in the **Add by method** window. The software requires a suitable method to measure a blank. However, the software stores blanks independently of methods for the corresponding measurement channel (TC, IC, NPOC, TN).

▸ Click on **Sample type**, then select the sample type from the drop-down menu:

   – **Preparation water blank (PB)**: Blank of the preparation water for standards (QC standards, daily factors, calibrations)

   – **H₃PO₄ reagent blank (RB)** and **Na₂S₂O₈ blank (RB)**: Blanks for the reagents phosphoric acid and sodium persulfate ($Na_2S_2O_8$). The procedure is defined in the software: The reagents for the blank determination are taken from the reagent bottles.
   ℹ NOTICE! Reagent blanks cannot be measured with differential methods.

   – **Dilution blank (DB)**: Blank for the diluent water. Prepare a sample vessel with ultrapure water on the sample tray to determine the blank value.

   – **Eluate blank (EB)**: Blank of the water that you use to elute swabs

   – **Boat blank (BB)**: Blank of the boats with which you introduce solid samples into the analyzer

▸ Define limit values for the blank in the **Step type properties** panel.

▸ Select the action to be taken if the limit is exceeded from the drop-down menu next to **Action:**, e.g. **cancel** to abort the sequence.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** |**Settings** |**Result table**
ℹ NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ▣✓. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with ▣. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Start the measurement by clicking on ▸ .

   ✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

Viewing and editing blanks

The software saves blanks regardless of the method. You can view the blanks saved in the software in the sequence. If you have the appropriate permissions, you can edit the blanks in the sequence. The changes only apply to the sequence.

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▶ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▶ Select the method from the dropdown menu or in the **Add by method** window.

▶ Select one or more measurement steps from the sequence table.

▶ View saved blanks in the **Step properties** panel, on the **Blanks** tab for each measurement channel.

▶ Edit blank values manually as required. The changes apply to the current sequence.

▶ If necessary, save the sequence with ⊞. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▶ Start the measurement by clicking on ▶ .

✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

The software takes the blanks into account when calculating the result.

Alternatively, you can also view the blanks used for the calculation in the measurement results and edit them there.

Viewing and editing blanks in the device configuration

The software saves blanks regardless of the method. You can view the blanks saved in the software in the **Instruments** window. If you have the appropriate permissions, you can edit the blanks in the device configuration. The changes apply across all software.

▶ Open the **Instruments** window with the **Instrument** |**Instruments** menu option.

▶ Select the device configuration in the **Instrument overview** table.

▶ Right-click to open the context menu and select **Blank values**.

▶ View blanks on the different tabs in the **Blank values** window.

▶ If necessary, edit blanks by clicking on the ✏ icon.

▶ Confirm the changes by clicking on the **OK** button.

✓ The changed blanks apply across all software.

See also

▤ Reagent blank value [▶ 60]

▤ Diluent blank value [▶ 60]

▤ Eluate blank value [▶ 61]

▤ Boat blank value [▶ 61]

7.12 Carrying out calibration

To enable the software to calculate measurement results, you must carry out a calibration for each measurement channel using the prepared method.

▶ Prepare the method in the **Methods** window.

▶ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▶ Click on the 🖉 icon to open the **Calibration wizard** wizard.

▶ In the **Calibration wizard** wizard, click on **Select method** to open the **Select method** window. Select prepared method from the **Overview** table. Click **OK** to confirm your choice.

▶ Define a name for the calibration under **Calibration**. The default name is: Method-type_Cal.

▶ Optionally: Click on **Comment** then enter a comment. Confirm the comment with **Apply**.

▶ Select calibration type. Preferably, perform multiple-point calibrations with a constant sample volume and variable standard concentrations. To do this, select the **Fixed volume** option.

▶ For a calibration with constant volume: The software automatically uses the sample volume set in the method. Only change the volume if the standard volume is to deviate from the volume set in the method.

▶ For a calibration with a constant concentration, select the **Fixed concentration** option. Enter the concentration of the standard in the table.

▶ Select how the preparation water blank is to be determined by **Preparation water blank:**.

    – If you select **Measure values**, the software measures the content of the preparation water immediately before calibration. To do this, prepare a container with preparation water on the autosampler. If you enter the sample manually, the software prompts you to provide the preparation water.

    – If you select **Set values**, determine the content of the preparation water separately and enter it in (AU/ml) in the input fields for each parameter.

    – If the software should not take the preparation water blank into account, enter the value "0" in the input field.

▶ Specify the number of calibration points under **Calibration points:**.
You can create a maximum of 50 calibration points in one calibration.

▶ Fill out the calibration table.

    – The software defines the name for the calibration points. If necessary, adjust the name in the **Add new sequence** window.

    – For **Replicates**, the software enters the maximum number of repeat measurements specified in the method. Change the number as required.

    – For calibration with constant volume: Enter the concentration of the prepared standards for each measuring channel (TC, TN, etc.) in the input fields.

    – For calibration with constant concentration: Enter the volumes of the standards for each measuring channel in the input fields.

▶ Activate split points for each measurement channel using the checkboxes in the **Split points** column. This allows you to define multiple calibration ranges.

▶ If required, define the minimum coefficient of determination R^2 and regression type for each measurement channel and calibration range.

▶ Select an action from the drop-down menu if the calibration does not reach the coefficient of determination, e.g. **cancel** to abort the calibration.

▶ Include the prepared calibration in the sequence with **Apply**.

    ✓ The software transfers the calibration steps to the sequence. To check the coefficient of determination, the software defines a "QA..." step (quality assurance) in the sequence. No measurement takes place here.

▶ The software automatically suggests the first free spaces on the sample tray for calibration steps. If necessary, select a step and change the position under **Step properties|Step|Sample position**.

▶ View method settings under **Step properties** and adjust if necessary.

▶ If necessary, add further measurement steps to the sequence. In addition to the calibration, you can perform further measurements in the same sequence.

▶ To calculate the measurement results, select the created calibration , from the drop-down menu in the **Step properties** panel, **Calibration** tab.

▶ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** | **Settings** | **Result table**
ⓘ NOTICE! It is not possible to start a measurement without a results table.

▶ Check the finished sequence for plausibility by clicking on 🗹. The software checks whether the created measuring steps can be measured.

▶ If necessary, save the sequence with 🖫. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▶ Start the sequence with the ▶ icon.
    ✓ The analysis system processes the sequence.

The software displays the current measurement results during recording graphically in the lower window area and in a result table.

In the **Step results** panel you can view the results of already measured samples. When the sequence was processed, you can see the results in the **Results** menu.

You can view and edit calibrations in the **Calibrations** window.

See also

▤ Calibration [▶ 58]

▤ Preparation water blank value [▶ 59]

▤ Calibration menu [▶ 93]

7.13   Performing a solids calibration

▶ Prepare device configuration for solids measurement in the **Instruments** window.

   – In the **Instrument configuration** area for manual or automatic solids measurement with an external solids module, from the **Furnace type:** drop-down menu, select the **External horizontal** option.

   – For work with an internal solids module, select the **Internal horizontal** option.

   – For automated solids analysis, select the FPG 48 autosampler by **Sampler type:**.

   – Save the device configuration with the ☑ save button and activate by clicking on the **Set default** button.

▶ Prepare TC method for solids measurement.

   – In the method settings, check the **Method is for solid measurement** checkbox on the **Step properties** tab.

   – For manual sample feeding: Tick the **Manual measurement** method parameters checkbox.

   – Set the furnace temperature according to the specifications in the operating instructions for the analyzer.

   – For automatic sample feeding: Specify the method parameters **Furnace holing position**, **Holding time** and **Furnace feed speed**.

▸ Use the **Measurement |Add new sequence** menu option to create a new sequence.

▸ In the **Sequence properties** panel, check the **Is a solids measurement** checkbox.

▸ Click on the ✎ icon to open the **Calibration wizard** wizard.

▸ In the **Calibration wizard** wizard, click on **Select method** to open the **Select method** window. Select prepared method from the **Overview** table. Click **OK** to confirm your choice.

▸ Activate the **Fixed concentration** option.

▸ Enter the carbon content in mg/kg of the solid standard in the wizard.

▸ Measure the boat blank value at the start of the calibration sequence or determine it separately and enter it in the wizard.

▸ Specify the number of calibration points under **Calibration points:** .

▸ Weigh in different masses of the solid standard in boats.

▸ Fill out the calibration table. Enter the weights in (µg) in the table.

▸ Include the prepared calibration in the sequence with **Apply**.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program |Settings |Result table**
ℹ NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ⊡⊘. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with ⊡⤓. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Start the measurement by clicking on ▶ .

   ✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

For information on how to carry out manual and automated solids measurements, see the user manual for the HT 1300 solids module.

7.14   Re-measure or add calibration standards

You can subsequently repeat the measurement of calibration points or add further calibration points to a calibration.

Individual calibration points are measured by selecting the **Calibration** sample type in the sequence. The software automatically transfers the calibration points to the selected calibration.

Measuring calibration points

▸ Use the **Measurement |Add new sequence** menu option to create a new sequence.

▸ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▸ Select the method from the drop-down menu or in the **Select method** window.
ℹ NOTICE! Use the method that served as the basis for the calibration.

▸ Click on the **Sample type** button, then select the **Calibration** sample type from the drop-down menu.

▶ In the **Step properties** panel, browse to the desired measuring channel in the **Calibration** tab. Select the calibration from the drop-down menu.

▶ In the **Step type properties** panel, enter the concentration of the standard under **Target concentration**.

▶ Select the calibration from the drop-down menu in the **Step type properties** panel for which you want to re-measure or add standards. Alternatively, select the calibration by clicking on ⬚ in the **Select calibration** window.

▶ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** | **Settings** | **Result table**
ℹ NOTICE! It is not possible to start a measurement without a results table.

▶ Check the finished sequence for plausibility by clicking on ▣✓. The software checks whether the created measuring steps can be measured.

▶ If necessary, save the sequence with ▣. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▶ Start the measurement by clicking on ▶ .

✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

The software subtracts the preparation water blank value from the measurement results. For the preparation water blank value, see the **Step properties** panel, **Blanks** tab, **Water** field.

| Manually including calibration points in a calibration | In the **Result tables** window, you can alternatively include calibration points in a calibration manually. |

▶ Open the **Result tables** window with the **Result details** | **Result tables** menu option.

▶ Select the results table with new calibration points from the **Overview** table.

▶ Open the results table by double-clicking or using the **Load** button.

▶ Select the desired measurement in the **Result table** window in the **Overview** table.

▶ Click on the **Add to calibration** button then assign the calibration point to the calibration in the **Select calibration** window.

▶ Click **OK** to confirm your choice.

✓ You have added a new calibration point to a calibration.

7.15   Determine daily factor

You can use daily factors to check and correct a calibration. To determine daily factors, select the **Daily factor** sample type in the sequence and measure one or more standard solutions.

If the daily factor is within the specified limits, the software automatically adopts the daily factor into the selected calibration.

The software multiplies the results of all subsequent measurements by the daily factor. The software uses the daily factor until you send a new daily factor to the calibration.

You can only use one calibration range for quadratic regressions. The software automatically assigns the daily factor to the appropriate calibration range. The daily factor applies only to this calibration range.

Measuring the daily factor

▸ Provide one or more standard solutions.

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▸ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▸ Select the method from the dropdown menu or in the **Add by method** window.

▸ Click on **Sample type**, then select the **Daily factor** sample type from the drop-down menu.

▸ In the **Step type properties** panel, enter the concentration of the standard under **Target concentration**.

▸ Specify limits for the daily factor in (mg/l) under **Lower limit** and **Upper limit**. Recommendation: Lower limit 0.8 x c(standard) and upper limit 1.2 x c(standard)

▸ Select actions from the drop-down menu in the event that the limit is exceeded. Recommendation: If limits are exceeded, cancel the sequence and recalibrate.

▸ Select the calibration from the drop-down menu in the **Step type properties** panel for which the daily factor should be applicable. Alternatively, select the calibration by clicking on ▄ in the **Select calibration** window.

▸ For each measuring channel, select the calibration for calculating the measurement results from the drop-down menu in the **Step properties** panel, Tab **Calibration**.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program**|**Settings**|**Result table**
ℹ NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ▣. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with ▣. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Start the measurement by clicking on ▶ .

  ✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

Viewing daily factors

▸ View the calculated daily factor in the results in the **Result table** window.

▸ Open the **Calibrations** window with the **Calibrations** |**Calibrations** menu option.

▸ Select the calibration in the **Overview** table. Before that, update the calibration overview by clicking on the icon ⟳ (above the table).

▸ View calibration data in the **Details** view on the **Details** tab.

▸ Check the daily factor in the table of calibration coefficients under **Daily factor** and change if necessary.

See also

▤ Daily factor [▸ 58]

7.16   Diluting samples automatically or intelligently

The software can automatically and intelligently dilute samples on the following au-
tosamplers if you are using multi N/C 3300 or multi N/C 3100:

Autosampler	Sample tray	Automatic dilution	Intelligent dilution	Automatic acidification
AS vario	47 (dilut)	Yes	No	No
	72	Yes	Yes	Yes (intelligent dilution)
				No (auto dilution)
	100	Yes	Yes	Yes (intelligent dilution)
				No (auto dilution)
AS 21hp	10 (dilut)	Yes	Yes	No
AS 10e (without stirring function)	10 (dilut)	Yes	Yes	No

In the case of automatic and intelligent dilution, the option for automatic acidification of
a sample is disabled in the software by default.
- For NPOC methods, you must therefore manually acidify the original samples.
- For automatic dilution, you can alternatively pipette acid into the empty sample ves-
  sels into which the autosampler dilutes the samples.
- In both cases check if the pH value of the samples is <2. Only then can the autosam-
  pler completely remove the inorganic carbon compounds (TIC) as CO_2 during purg-
  ing.

An exception is intelligent dilution when using the AS vario autosampler and the 72 or
100 sample tray. In this case, automatic acidification is possible. The following positions
must be kept free for the acid vessel:
- Position 55 (72 sample tray)
- Position 85 (100 sample tray)

7.16.1 Automatic dilution

Use automatic dilution when measuring samples with very high TC or TN_b content or
with an unknown highly loaded sample matrix. You specify the dilution ratio in the soft-
ware.

Dilution provides the following advantages:
- You increase the service life of the reactor.
- You save working time through automation.
- No extra calibration is required for high concentration ranges.

▸ Use autosampler with a suitable sample tray, for example AS vario autosampler with
  72 tray. Install a suitable cannula holder on the AS vario autosampler.

Create and activate device con-
figuration
▸ Create device configuration for automatic dilution. Open the **Instruments** window via
  the menu command **Instrument|Instruments**.

▸ Under **Instrument type:** select multi N/C 3300 or multi N/C 3100.

▸ Under **Sampler type:** and **Rack size:**, select autosampler and sample tray, for exam-
  ple AS vario and 72. Under **Vial size (mL):**, select 50 ml.
  When selecting 100 for **Vial size (mL):** select 20 ml.
  When selecting 47 (dilut) for **Vial size (mL):** select 50 ml.

▸ If displayed by the software, tick the **Automatic dilution** checkbox.

▸ Save the device configuration by clicking the ☑ button.

▸ Select the device configuration from the **Instrument overview** table and activate as the default configuration by clicking on **Set default**. Alternatively, double-click to activate the device configuration.

Load the 72 sample tray

▸ Load the sample tray with empty sample vessels at positions 1 to 36 (50 ml).

▸ Fill the original samples into sample vessels (50 ml). Load the sample tray with samples at positions 37 to 72.

▸ Place samples that are not to be diluted in any of the positions 1 to 36.

▸ Fill ultrapure water into the ultrapure water bottle.

Load the 100 sample tray

▸ Load the sample tray with empty sample vessels at positions 1 to 50 (20 ml).

▸ Fill the original samples into sample vessels (20 ml). Load the sample tray with samples at positions 51 to 100.

▸ Place samples that are not to be diluted in any of the positions 1 to 50.

▸ Fill ultrapure water into the ultrapure water bottle.

Load the 47 (dilut) sample tray

▸ Equip the sample tray with empty sample vessels (50 ml).

▸ Fill the original samples into sample vessels (12 ml). Equip the sample tray with the samples.

▸ Fill samples that are not to be diluted into sample vessels (50 ml) and place them in the outer row of the tray.
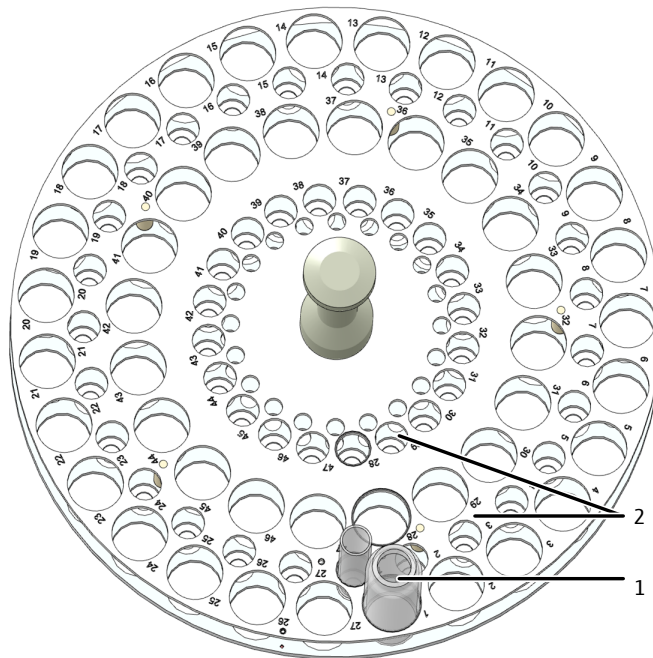
▸ Fill ultrapure water into the ultrapure water bottle.

Fig. 28   Dilution tray

  1 Position 1 to 47 for 50 ml vessels   2 Position 1 to 47 for 12 ml vessels

Adjusting the AS vario autosampler

▸ Open the **Sampler alignment** window with the **Instrument | Sampler alignment** menu option.

▸ Align the sample intake cannula with the sample tray. To do this, select **Position 1** in the **Sampler position** table.

     ✓ If using the 47 (dilut) tray, the autosampler arm moves over position 1 in the outer row.

▸ Adjust position 1 in a sample vessel (50 ml). For the 100 tray, use sample vessel (20 ml).

▸ Adjust the immersion depth in steps with **- higher / + lower**.

▸ After each change, click on the **Move** button to move to the position and check.

▸ Save the adjusted position with **Confirm**.

▸ If using the 47 (dilut) tray, then check position 1 in a small sample vessel (12 ml). To do this, select Position 1 in the **Move to position** area and click on the **Move** button. If the **Dilution position** checkbox is activated, the autosampler moves to position 1 in the inner row.

Create a method and a sequence

▸ Prepare the method. Edit method settings in the **Method** view:

▸ Select the dilution ratio by **Dilution: Vol. sample** and **Dilution: total volume**.

▸ Use the **Measurement** | **Add new sequence** menu option to create a new sequence.

▸ In the **Sequence properties** panel activate the checkbox **Automatic dilution**.

▸ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▸ Select the method from the dropdown menu or in the **Add by method** window.

▸ Click on **Sample type**, then select the **Dilution blank (DB)** option to determine the dilution blank value. Prepare a sample vessel with ultrapure water on the sample tray to determine the blank value.

▸ Optionally adjust the dilution ratio for individual measurement steps in the method settings in the sequence. To do this, edit the entries under **Dilution: Vol. sample** and **Dilution: total volume** in the **Step properties** panel on the **Step** tab.

▸ For samples that are not to be diluted, enter **1** under both **Dilution: Vol. sample** and **Dilution: total volume**.

▸ For each measuring channel, select the calibration for calculating the measurement results from the drop-down menu in the **Step properties** panel, Tab **Calibration**.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** | **Settings** | **Result table**
  ℹ NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ⬚✅. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with ⬚. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Start the measurement by clicking on ▶ .

     ✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

Dilution with AS 21hp and AS 10e autosamplers

▪ Use the 10 (dilut) tray.
▪ Fill the samples into the sample containers in 50 ml.
▪ Position the undiluted original samples at positions 11 to 20.
▪ Provide empty 50 ml sample vessels for dilution at positions 1 to 10. The sample at position 11 is diluted into the sample vessel at position 1, and so on.

- Place samples that are not to be diluted in any of the positions 1 to 10. Enter **1** under both **Dilution: Vol. sample** and **Dilution: total volume**.
- Adjust the autosampler before starting measurements as described in the operating instructions for the analyzer.

Observe the following for automatic dilution:
- The autosampler dilutes the original samples into the provided sample vessels at the selected dilution ratio.
- When working in NPOC mode, the samples are each diluted in a complete series and then analyzed. The autosampler purges the diluted samples.
- The number of possible multiple determinations is the result of the selected method, the injection volume and the number of flushing cycles.
- The software displays the area integrals for the diluted samples and automatically calculates the concentration of the undiluted primary samples from these values.

7.16.2 Intelligent dilution

Intelligent dilution is particularly helpful for samples of unknown TC or TN_b concentration or samples in an unknown sample matrix.

With intelligent dilution, the analyzer first measures the original sample. After the first determination, the software uses the TC or TN_b content to decide whether to automatically dilute the sample or continue with the repeat measurements. The software determines the dilution ratio itself.

▸ Use autosampler with a suitable sample tray, for example AS vario autosampler with 72 tray. Install a suitable cannula holder on the AS vario autosampler.

Create and activate device configuration

▸ Create device configuration for intelligent dilution. Open the **Instruments** window via the menu command **Instrument|Instruments**.

▸ Under **Instrument type:** select multi N/C 3300 or multi N/C 3100.

▸ Under **Sampler type:** and **Rack size:**, select autosampler and sample tray, for example AS vario and 72. Under **Vial size (mL):**, select 50 ml.
When selecting 100 for **Vial size (mL):** select 20 ml.
When selecting 47 (dilut) for **Vial size (mL):** select 50 ml.

▸ Save the device configuration by clicking the ☑ button.

▸ Select the device configuration from the **Instrument overview** table and activate as the default configuration by clicking on **Set default**. Alternatively, double-click to activate the device configuration.

Load the 72 sample tray

▸ Fill the original samples into sample vessels (50 ml). Place the samples in positions 1 to 36 on the sample tray.

▸ Load the sample tray with empty sample vessels at position 37 to 72 (50 ml). The sample at position 1 is diluted into the sample vessel at position 37, and so on.

▸ Do not place samples in position 19 and 55 if the **Automatic acidification** option is activated in NPOC methods. Place acid vessel at position 55.

▸ Fill ultrapure water into the ultrapure water bottle.

Load the 100 sample tray

▸ Fill the original samples into sample vessels (20 ml). Place the samples in positions 1 to 50 on the sample tray.

▸ Load the sample tray with empty sample vessels at position 51 to 100 (20 ml). The sample at position 1 is diluted into the sample vessel at position 51, and so on.

▸ Do not place samples in position 35 and 85 if the **Automatic acidification** option is activated in NPOC methods. Place acid vessel at position 85.

▶ Fill ultrapure water into the ultrapure water bottle.

Adjusting the AS vario autosampler

▶ Open the **Sampler alignment** window with the **Instrument** | **Sampler alignment** menu option.

▶ Align the sample intake cannula with the sample tray. To do this, select **Position 1** in the **Sampler position** table.

    ✓ The autosampler arm moves over position 1.

▶ Adjust position 1 in a sample vessel (50 ml). For the 100 tray, use sample vessel (20 ml).

▶ Adjust the immersion depth in steps with **- higher / + lower**.

▶ After each change, click on the **Move** button to move to the position and check.

▶ Save the adjusted position with **Confirm**.

Prepare a method and a sequence

▶ Prepare the method. Edit method parameters in the **Method** view. The entries by **Dilution: Vol. sample** and **Dilution: total volume** have no effect on intelligent dilution.

▶ Use the **Measurement** | **Add new sequence** menu option to create a new sequence.

▶ In the **Sequence properties** panel activate the checkbox **Intelligent dilution**.

▶ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▶ Select the method from the dropdown menu or in the **Add by method** window.

▶ Click on **Sample type**, then select the **Dilution blank (DB)** option to determine the dilution blank value. Prepare a sample vessel with ultrapure water on the sample tray to determine the blank value.

▶ For each measuring channel, select the calibration for calculating the measurement results from the drop-down menu in the **Step properties** panel, Tab **Calibration**.

▶ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** | **Settings** | **Result table**
🛈 NOTICE! It is not possible to start a measurement without a results table.

▶ Check the finished sequence for plausibility by clicking on 📋✅. The software checks whether the created measuring steps can be measured.

▶ If necessary, save the sequence with 💾. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▶ Start the measurement by clicking on ▶ .

    ✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

Dilution with AS 21hp and AS 10e autosamplers

▪ Use the 10 (dilut) tray.
▪ Fill the samples into the sample containers in 50 ml.
▪ Position the undiluted original samples at positions 1 to 10.
▪ Provide empty 50 ml sample vessels for dilution at positions 11 to 20. The sample at position 1 is diluted into the sample vessel at position 11, and so on.
▪ Adjust the autosampler before starting measurements as described in the operating instructions for the analyzer.

Observe the following for intelligent dilution:
▪ The number of possible multiple determinations is the result of the selected method, the injection volume and the number of flushing cycles.

- The software displays the area integrals for the diluted samples and automatically calculates the concentration of the undiluted primary samples from these values.
- The diluted sample appears immediately after the original sample in the results table. The software marks diluted samples.

7.17 Intelligent reduction of the sample volume

The software can automatically reduce the injection volume for highly concentrated samples so that the results are within the calibrated range. This option is only available for the analyzers multi N/C 2300 and multi N/C 3300.

- The software starts the intelligent volume reduction when the sample concentration is outside the calibration range.
- The software can reduce the sample volume down to the minimum injection volume, see technical data of the analyzer.

▸ Use the **Measurement** | **Add new sequence** menu option to create a new sequence.

▸ In the **Sequence properties** panel activate the checkbox **Intelligent volume reduction**.

▸ Create measurement steps in sequence with **Add by method**. Ensure that the method settings, such as the sample volume, match the device configuration.

▸ Select the method from the dropdown menu or in the **Add by method** window.

▸ For each measuring channel, select the calibration for calculating the measurement results from the drop-down menu in the **Step properties** panel, Tab **Calibration**.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program** | **Settings** | **Result table**
🛈 NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ▣✓. The software checks whether the created measuring steps can be measured.

▸ If necessary, save the sequence with ⬇. Set the name for the sequence in the **Save as** window and confirm with **OK**. The software names the window accordingly.

▸ Start the measurement by clicking on ▶ .

   ✓ The analysis system processes the sequence. You can add further measurement or control steps to the sequence during the measurement.

The analyzer first measures the original sample. After the first determination, the software uses the content to decide whether to reduce the sample volume or continue with the repeat measurements.

For the measurement with reduced sample volume, the software automatically creates a new measurement step in the sequence. For the results table, the software calculates the concentration of the sample taking into account the reduced injection volume.

You can view the results of both measurement steps in the results table:
- Original sample with original sample volume
- Original sample with reduced sample volume

If you select automatic volume reduction and intelligent dilution in the sequence settings under **Sequence properties**, the software prefers to perform the volume reduction. The software only performs intelligent dilution if the volume reduction is not sufficient to reach the calibration range.

8   Calibration menu

You can manage the calibrations performed in the **Calibrations** menu. You view and edit calibration data.

Note:
- If you want to prepare and measure a calibration, select the **Sequences** menu.
- If you want to view the measurement curves for individual calibration points or manually add further calibration points to a calibration, select the **Result details** menu.

See also

📄 Carrying out calibration [▷ 81]

📄 Viewing results [▷ 105]

8.1   Calibrations window

Open the **Calibrations** window via the menu command **Calibrations|Calibrations**.

In the Calibrations window
- You can view calibration details such as calibration points, calibration diagrams or process characteristics in the **Details** view. If you have the appropriate permissions, you can edit calibrations.
- Click on the **Add** button to create an empty calibration to which you can add calibration points using the **Add to calibration** button in the **Result table** window.
- You delete calibrations by clicking on the **delete** button.
- The optional FDA 21 CFR Part 11 Compliance module prevents data from being deleted.
- You organize calibrations into groups by clicking on **Assign group** in the **Select group** window.
- You import and export calibrations in XML format using the **Import** and **Export** buttons.
- Click on **Report** to view the calibration report. You can print the report or save it in PDF format.
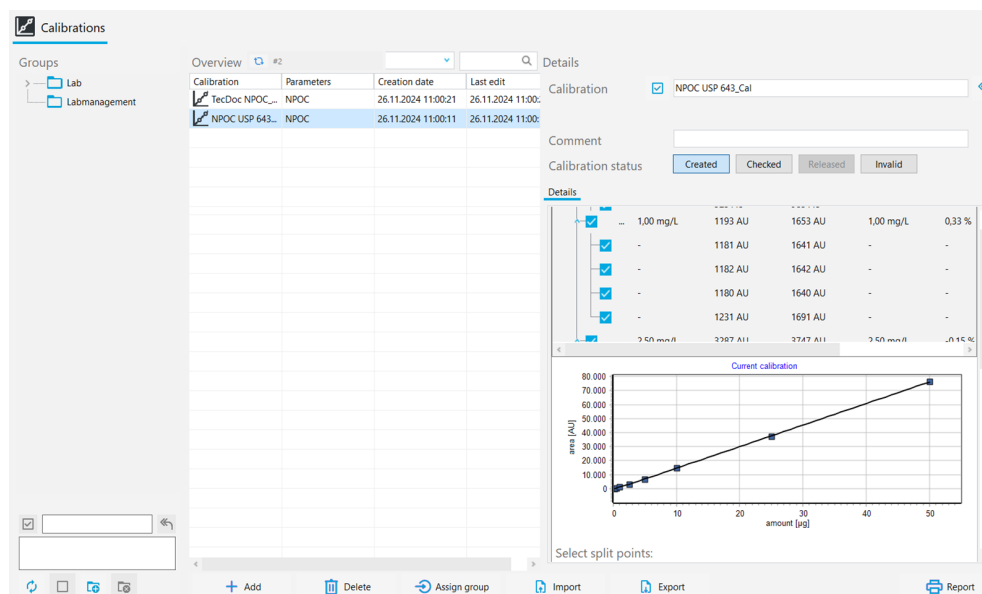
Layout of the window

Fig. 29   Calibrations window

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Area	Description
Groups (left)	Manage groups
Overview (middle)	Tabular overview of the saved calibrations with: ■ Name of the calibration and calibrated measuring parameters ■ Date created and last changed
Details (right)	Detailed view for the selected calibration: ■ General information: Name of calibration, description, comment and release status ■ **Details** tab, **Details** panel with calibration details ■ **Details** tab, **Method** panel with method parameters ■ **Signatures** tab with information in signatures (only with FDA 21 CFR Part 11 Compliance module)

Electronic signatures are an important part of the optional FDA 21 CFR Part 11 Compliance module. You can restrict the use of non-approved data with the help of signatures and the corresponding assignment of rights. When signing, it is mandatory to enter a user name and password.

In the standard software, you can set the status of data, e.g. to **Checked**. However, you cannot add an electronic signature to data. The **Signatures** tab remains empty. No restrictions are linked to the status of the data. This means that even blocked data can still be used.

Details panel

You can view the results of the calibration in the **Details** panel.

Area	Description
Preparation water blank value	Preparation water blank value If required, edit the preparation water blank value and save with the **Confirm** button
Results table	Display for measuring channels, calibration points and individual repeat measurements: ■ Target concentration ■ Mean value of the area integrals (specification of gross integrals and net integrals, adjusted by the preparation water blank) ■ Mean concentration ■ Percentage deviation of the calculated concentration from the target concentration ■ Preparation water blank value ■ Sample volume Expand and collapse the display for measuring channels, calibration points and repeat measurements with ∨ / ∧ Select or deselect measurement data by ticking or clearing the checkboxes
Calibration graph	Regression graph with x-axis: Content in (amount [µg]) y-axis: Area integral in (AU) ■ If you activate or deactivate measurements in the results table, the software adjusts the graphical display. ■ To zoom in: Place the mouse pointer in the diagram and drag the desired section from left to right. ■ To zoom out: Drag the enlarged section from right to left.
Area **Select split points:**	Specify cut-off points and therefore several calibration ranges for each measuring channel (TC, TN, etc.) via the checkboxes

Area	Description
Range with radio buttons ■ **Default: linear** ■ **Default: quadratic**	For all calibration ranges, define the calculation of the regression equation on the basis of a linear or quadratic regression The software displays the calibration coefficients for the selected regression type.
Table with process characteristics	■ Regression type If required, select the regression type for each calibration range individually ■ Calibration coefficients k_0, k_1, k_2 (k_2 only with quadratic regression) ■ Lower and upper limit of the calibration range ■ Daily factor ■ Coefficient of determination R^2 ■ Limit of detection and limit of quantification (only for linear regression) The software calculates the process characteristics based on DIN 32645 (calibration function) with a significance level of $P = 95\%$. The software defines the limit of quantification for a relative results uncertainty of 33.3 % (with $k = 3$ factor).

See also

▤ Electronic signatures [▶ 130]

▤ Organize in groups [▶ 32]

8.2   View calibration

In the **Calibrations** window, you can view calibrations with calibration diagram, process characteristics and the results for individual measuring channels, calibration points and repeat measurements.

▸   Open the **Calibrations** window with the **Calibrations** | **Calibrations** menu option.

▸   Select the calibration in the **Overview** table. Before that, update the calibration overview by clicking on the icon ↻ (above the table).

▸   View calibration data in the **Details** view on the **Details** tab:

  –   Editable preparation water blank value

  –   Fold-out result display for various measuring channels, calibration points and repeat measurements

  –   Calibration graph

  –   Cut-off points that can be activated for several calibration ranges

  –   Process characteristics: selectable regression type, calibration coefficients, lower and upper limits of the calibration range, editable daily factor, coefficient of determination and limit of detection as well as limit of quantification

▸   View method settings in the **Method** panel.

▸   Enter an optional comment under **Comment**.

▸   After making changes, save the calibration by clicking the ☑ button.

8.3 Editing calibration

Users with the appropriate permissions can edit calibrations in the **Calibrations** window:
- You can activate and deactivate calibration points and repeat measurements in the results table using the checkboxes.
- You can select either linear or quadratic regression.
- You can define cut-off points for several calibration ranges.
- You can view and edit the preparation water blank value and daily factor.

You can specify several calibration ranges for different concentration ranges. Two consecutive calibration ranges must have a common cut-off point.

After each change, the software recalculates the calibration coefficients, process characteristics and regression graph.

▸ Open the **Calibrations** window with the **Calibrations** |**Calibrations** menu option.

▸ Select the calibration in the **Overview** table. Before that, update the calibration overview by clicking on the icon ⟳ (above the table).

▸ View calibration data in the **Details** view on the **Details** tab.

▸ If necessary, make the following changes:

  – Check the preparation water blank value. Enter the new preparation water blank value in the **Preparation water blank value** field. Accept the value with **Confirm**.

  – In the results table, expand the results display for measuring channels, calibration points and repeat measurements one after the other with ⌄ . If required, deactivate individual calibration points or repeat measurements via checkboxes.

  – Define cut-off points for several linear calibration ranges in the **Select split points:** area.

▸ Select regression type (linear or quadratic) for all calibration ranges by **Range**.

  – Optionally, define the regression type individually for each calibration range in the table with process characteristics.

  – View and edit the daily factor in the table with process characteristics.

▸ Save changes by clicking the ☑ button.

8.4 Printing and saving the calibration report

Print calibration report

▸ Open the **Calibrations** window with the **Calibrations** |**Calibrations** menu option.

▸ Select the calibration in the **Overview** table. Before that, update the calibration overview by clicking on the icon ⟳ (above the table).

▸ Click on **Report** to open the print preview.

▸ For a better overview, click on the **Page overview** button to display the navigation area with a page summary to the left of the report. Zoom in or out of the view by clicking on **Zoom in** and **Zoom out**.

▸ Add company logo to the report. Click on the **Load** button in the **Report logo** area, and then select the logo in the Windows file manager and load it into the report with **Open**.

▸ Click on **Printer options** to set up the printer.

▶ Click on **Page setup** to configure page settings such as paper size or orientation. Default: A4, portrait. Apply layout to current page or all report pages.

▶ Click on **Print** to start printing.

  ✓ You have printed a calibration report.

Save calibration report

▶ Open the **Calibrations** window with the **Calibrations** |**Calibrations** menu option.

▶ Select the calibration in the **Overview** table. Before that, update the calibration overview by clicking on the icon ⟳ (above the table).

▶ Click on **Report** to open the print preview.

▶ Click on **Save** then specify the file name, storage directory and file type in the **Save as** window.

▶ Save the report by clicking on the **Save** button.

You can save reports in the following file formats: PDF (default), RTF, HTML, TXT, FP3.

When you edit a calibration, the changes are only applied to the report after you save it.

9   Result details menu

The software saves measurement results in results tables. Results tables can contain re-
sults from various measurements: Samples, calibration standards, system suitability
tests (SST), QC standards and blank values. In the **Result details** menu, you manage the
result tables and the measurement results saved in them.

In the Result details menu
- Use the **Result tables** menu command to open the **Result tables** window. Here, you
  can manage result tables and load selected result tables to view and edit measure-
  ment results.
- Use the **SSTs** menu command to open the **SSTs** window with the results in system
  suitability tests (SST). SSTs are only possible with the FDA 21 CFR Part 11 Compli-
  ance module.

See also

📄 System Suitability Test (SST) [▶ 131]

9.1   Result tables window

Open the **Result tables** window via the menu command **Result details | Result tables**.

In the Result tables window
You manage results tables in the **Result tables** window.
- Double-click or click on the **Load** button to open a selected results table in order to
  view and edit measurement results in the **Result table** window.
- Click on the **Add** button to create a new results table for future measurements.
- Click on **delete** to delete a results table with all the measurement results saved in it.
- The optional FDA 21 CFR Part 11 Compliance module prevents data from being
  deleted.
- You organize results tables into groups by clicking on **Assign group** in the **Select
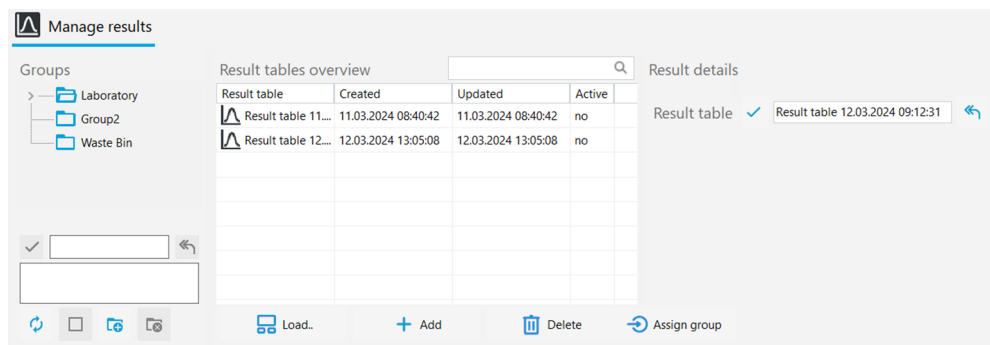 group** window.

Layout of the window

Fig. 30   Result tables window

Area	Description
Groups (left)	Manage groups
Overview (middle)	Tabular overview of the results tables with: - Name of the results table - Date created and last changed - Status of the results table (**yes**: yes / **no**)
Result details (right)	Selected result table with name

See also

9.2   Result table window

You can view the measurement results saved in a results table in the **Result table** window. Users with the appropriate permissions can edit results manually.

Open the **Result table** window by loading a selected result table by clicking on the **Load** button in the **Result tables** window. Alternatively, you can open the window by double-clicking on the desired results table.
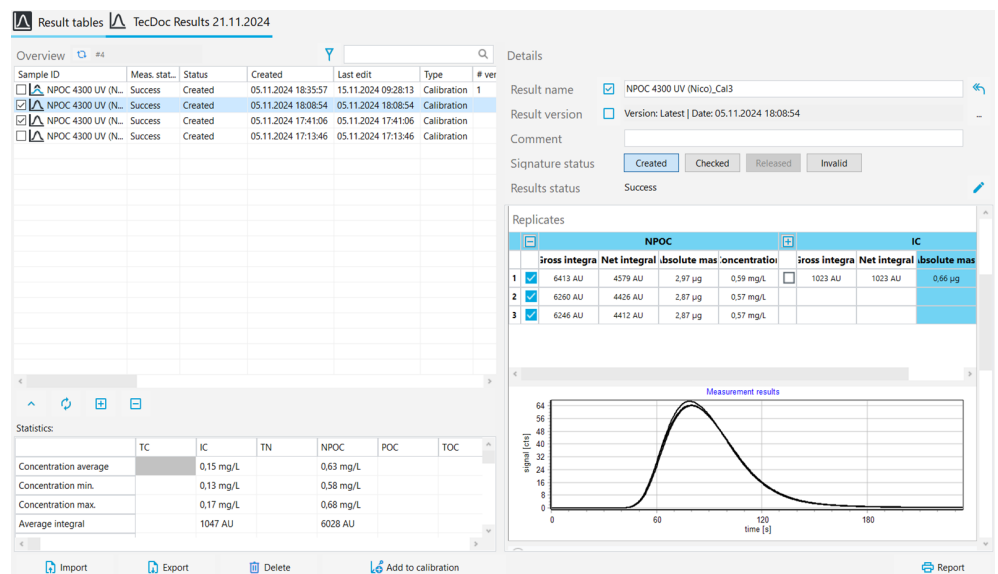
Layout of the window

Fig. 31   Result table window

Element	Description
Overview table (left)	■ View results for each measurement step in a tabular overview ■ If required, customize the table using the **Adjust display columns** command in the context menu
Details overview with fold-out panels (right)	■ View details for individual measurement results and edit them by clicking on the ✏ icon ■ Release results after verification by clicking on one of the buttons in the **Signature status** area
Icon and button bar (bottom)	■ Expand and collapse the **Statistics:** area with ⌄ / ⌃ ■ Select all results in the **Overview** table with ⊞ ■ Deselect all results in the table with ⊟ ■ Use **Import** to import results in XML format ■ Use **Export** to export results in XML format, default export folder: *C:/ProgramData/Analytik-Jena/multiWinPro/export/results* ■ Use **Add to calibration** to add calibration points to a calibration ■ Use **Go to SST** to select measurement results of a System Suitability Test in the table (only with FDA 21 CFR Part 11 Compliance module) ■ Use **Sign all checked results** to sign several results at once ■ Use **Report** to open print preview, print or save a report Select results before further processing by ticking the checkboxes

Element	Description
Fold-out **Statistics:** area (bottom)	■ Expand and collapse the **Statistics:** area with ⌄ / ⌃ ■ Calculate and display mean integral and mean concentration for selected measurements. The selected measurements are recorded by the software as repeat measurements. ■ Select measurement results by ticking the checkboxes in the **Overview** table

9.2.1   Overview table

The **Overview** table is part of the **Result table** window. The tabular overview shows all measurement results that are saved in a results table.

You can customize the layout of the table using the **Adjust display columns** command (in the context menu).

Column	Description
Sample ID with checkbox	Sample ID with checkbox ■ Tick the checkbox to select results for mean value calculation, import/export or report
Meas. status	Measurement success
Status	Signing status
Created	Measuring time
Last edit	Time of the last update
Type	Sample type (sample, calibration standard, blank, daily factor, QC standard, SST sample)
Version	Number of result versions Whenever you edit results, the software creates a new version of the results.
c(actual)	Mean concentration The software determines the mean concentration from the results of the repeat measurements and adjusts it for the blanks.
SD	Standard deviation of the measurement result
RSD	Relative standard deviation of the measurement result in (%)
Method	Measurement method
Procedure	Method type (**TC**, **NPOC**, etc.)
Replicates	Number of repeat measurements ■ Specification: Number of measurements carried out, minimum and maximum number of repeat measurements in brackets (min-max)
Volume	Sample volume
Dil. Water	Dilution ratio for manually or automatically diluted samples
Parameters	Measuring channels
Target concentration	Target concentration defined in the sequence table
Comment	Individual information as comment
Density	Density of liquid samples
Pos.	Position on sample tray
COD	COD (Chemical Oxygen Demand) determined for TOC and NPOC methods

Column	Description
BOD$_5$	BOD$_5$ (Biochemical Oxygen Demand) determined for TOC and NPOC methods
Total protein	TP (Total Protein) content determined for TN methods
CO$_2$	Carbon dioxide concentration determined for TIC methods
User	User logged in during the measurement

9.2.2   Customize Overview

The **Overview** table is part of the **Result table** window. The tabular overview shows all measurement results that are saved in a results table.

You can customize the layout of the table using the **Adjust display columns** command (in the context menu).

▸ Open the **Result tables** window with the **Result details | Result tables** menu option.

▸ Select the result table in the **Overview** table. Load the selected results table by double-clicking or clicking on the **Load** button.

▸ Right-click in **Overview** to open the context menu. Select the **Adjust display columns** command.

▸ In the **Configuration view** window, adjust the table columns:

   – Use the $\rightarrow$ icon to transfer a column from suggestions (left) to the table (right).

   – Use the $\leftarrow$ icon to remove a column from the table (right).

   – Use the $\rightarrow\!|$ icon to transfer all columns from suggestions (left) to the table (right).

   – Use the $|\!\leftarrow$ icon to remove all columns from the table (right).

   – Use the $\downarrow$ icon to move a column down or to the right in the **Overview**.

   – Use the $\uparrow$ icon to move a column up or to the left in the **Overview**.

   – Use the $\circlearrowleft$ icon to restore the software's preset columns.

▸ Click **OK** to confirm the entered data.

   ✓ You have customized the table columns.

You can customize the units and decimal places for the displayed results in the **Result table** window.

▸ Select **Select output units** or **Adjust units** from the context menu.

▸ Change the units and decimal places in the **Unit and precision** section.

▸ For the results output in the **Result table** window: On the **Result details** tab, define the units and decimal places for the results table. On the **Result overview table** tab, configure the settings for the detailed view.

▸ Click **OK** to confirm your choices.

▸ Click the **Load default units** button to restore the settings that you previously defined in the **Software settings** window on the **Units and precision** tab.

9.2.3   Details

The **Details** view is part of the **Result table** window. The overview shows details of individual measurement results.

If you have the permission to edit results manually, you can edit measurement results by clicking on the ✏ icon.

General specifications

Displayed parameter	Description
Result name	Editable sample ID
Result version	Version of the result
	Whenever you edit results, the software creates a new version of the results.
	▪ Click on the ⸬ icon, then navigate through the result versions
	▪ Click on the ☐ icon to return to the last version
Comment	Enter individual information
Signature status	▪ View the signing status of the results
	▪ Release or block results after testing
Results status	Display of measurement success

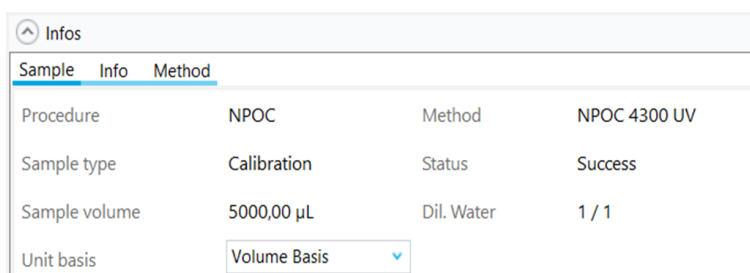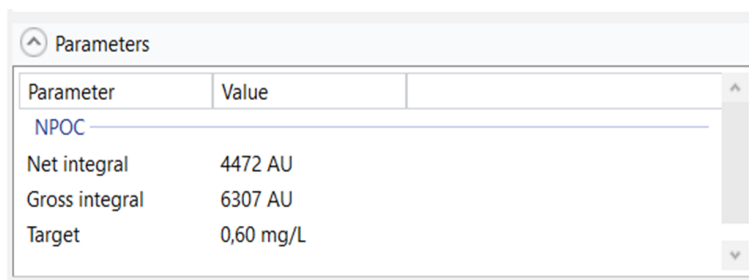You can view detailed information on the measurement results in four fold-out panels.

Infos panel

Fig. 32   Infos panel

Area	Description
Tab **Sample**	▪ Method type and method
	▪ Sample type
	▪ Measurement success
	▪ Sample volume in (µl)
	▪ Dilution ratio of manually or automatically diluted samples
	▪ Drop-down menu by **Unit basis** for selecting the unit reference for the results in the **Parameters** and **Replicates** panels (volume-based, mass-based or area-based)
Tab **Info**	▪ Device type and serial number
	▪ Software and firmware version
	▪ User logged in at the time of measurement
Tab **Method**	Method parameters with settings
Tab **Signatures**	Detailed information on the signing status (only with FDA 21 CFR Part 11 Compliance module)

Electronic signatures are an important part of the optional FDA 21 CFR Part 11 Compliance module. You can restrict the use of non-approved data with the help of signatures and the corresponding assignment of rights. When signing, it is mandatory to enter a user name and password.

In the standard software, you can set the status of data, e.g. to **Checked**. However, you cannot add an electronic signature to data. The **Signatures** tab remains empty. No restrictions are linked to the status of the data. This means that even blocked data can still be used.

Parameters panel

Fig. 33   Parameters panel

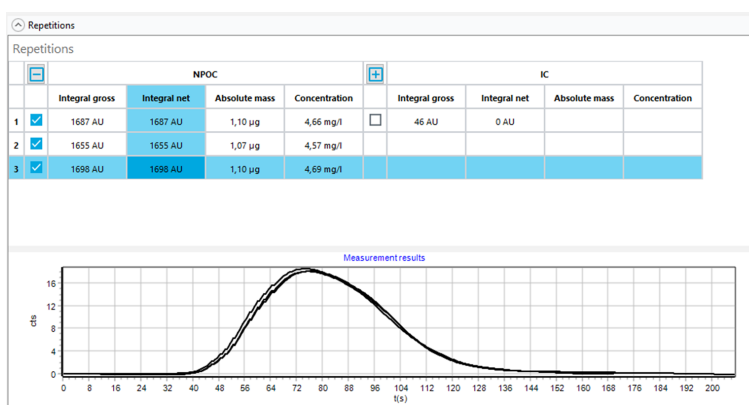| Area	Description
Measurement channels with results	Display of the determined results and process characteristics for each measurement channel: ■ Mean raw integral in (AU) and net integral, adjusted for blanks ■ Mean mass in (µg) and mean concentration in (mg/l), adjusted for blanks ■ Standard deviation in (mg/l) ■ Relative standard deviation in (%)

Replicates panel

Fig. 34   Replicates panel

Area	Description
Table with results of repeat measurements	Result display for each measurement channel and each repeat measurement: ■ Measured raw integral in (AU) and net integral, adjusted for blanks ■ Calculated absolute mass ■ Calculated concentration The software adjusts the absolute mass and concentration for the existing blanks. The software detects outliers and highlights the corresponding table rows in gray. ■ You can activate or deactivate repeat measurements using the checkboxes. The software does not take deactivated measurements into account when calculating results.
Graphical presentation of the measurement curves	Graphical presentation of the measurement curve for each measurement channel and each repeat measurement (x-axis: time in (s), y-axis: measurement signal in (cts)) When measuring several measurement channels, the software displays the measurement curves in different colors.

Area	Description
	■ If you activate or deactivate measurement channels or repeat measurements in the table, the software adjusts the graphical display.
	■ To zoom in: Place the mouse pointer in the curve and drag the desired section from left to right.
	■ To zoom out: Drag the enlarged section from right to left.
	■ Hold the mouse button down and move the section.

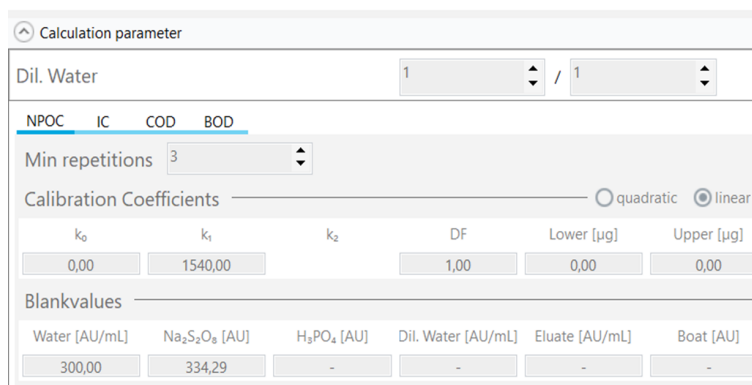Calculation parameter panel

Fig. 35   Calculation parameter panel

In the **Calculation parameter** panel, you can use the tabs to switch between the results for the various measurement parameters.

Area	Description
Field **Dil. Water**	Dilution ratio taken into account for the calculation, editable
Field **No. replicates**	Editable number of repeat measurements used for the result calculation
Area **Calibration coefficients**	■ Radio buttons for selecting the regression type (**quadratic** or **linear**) ■ Editable calibration coefficients k_0, k_1, k_2 (k_2 only with quadratic regression) ■ Editable daily factor ■ Lower and upper limit of the calibration range
Area **Blank values**	Editable blank values
Area **COD / BOD / Total Protein conversion parameters**	Editable slope and intercept for calculating COD, BOD_5 and total protein content, which can be viewed on the tabs **COD**, **BOD₅** and **Total protein**

See also

📄 Electronic signatures [▶ 130]

9.3   Create new results table

The software saves measurement results in results tables.

▸ Open the **Result tables** window with the **Result details** | **Result tables** menu option.

▸ Click on **Add** and create a new results table. The default name is: Result table + time-stamp.

▸ If necessary, change the name in the **Result table** field in the **Result details** view. Save changes by clicking the ☑ button.

Alternatively: Create a new result table in the **Add new sequence** window.

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▸ Open drop-down menu on the **Result table** button.

▸ Use **Create new result table** to create a new results table.

    ✓ The software creates a new results table with the name Result table + timestamp in the **Result tables** window.

9.4   Viewing results

You can view the measurement results saved in a results table in the **Result table** window. Users with the appropriate permissions can edit results manually.

▸ Open the **Result tables** window with the **Result details** |**Result tables** menu option.

▸ Select the result table in the **Overview** table. Load the selected results table by double-clicking or clicking on the **Load** button.

▸ View measurement results in the **Overview** table. If required, search results or filter them by clicking on ▽ .

▸ Select measurement in the **Overview** table and view results in the **Details** view:

▸ **Infos** panel
Sample tab: Method type and method, sample type and sample volume, etc.
Info tab: Background information such as device type or software version
Method tab: Method parameters
Signatures tab: Detailed information on the signing status, only available with FDA 21 CFR Part 11 Compliance module

▸ **Parameters** panel: Results of the individual measurement channels with mean raw integrals and net integrals, mean absolute masses, mean concentrations, and statistical data

▸ **Replicates** panel: Results of the individual repeat measurements with measurement curves and the option to select outliers

▸ **Calculation parameter** panel: Dilution ratio, number of repeat measurements used for the calculation, calibration parameters, daily factors and blanks, with the option of manual post-processing

▸ Optionally enter a comment under **Comment**.

▸ After making changes, save the result by clicking the ☑ button.

Calculation and display of results

- The software calculates the raw integral in (AU) for each measurement curve.
- The software detects outliers and highlights them in the results. The software excludes outliers from the calculation of the mean integrals.
- The software calculates the mean concentrations on the basis of the mean integrals.
- The software adjusts the mean integrals and mean concentrations for the existing blanks.
- The software takes into account daily factors stored in the calibration.
- The software flags results that lie outside the calibrated range.
- With the appropriate settings in the sequence parameters, the analysis system dilutes highly concentrated samples automatically or intelligently. The software calculates the concentration of the undiluted primary sample for the results. However, the integrals displayed are the integrals that were measured for the diluted sample.

■　With the appropriate settings in the sequence parameters, the analysis system auto-
matically reduces the sample volume of highly concentrated samples. The software
displays the results for the measurement with original sample volume and reduced
volume one below the other in the **Overview** table.

■　The software marks results that you have edited manually.

9.5　Editing results

If you have the appropriate permissions, you can edit results in the **Result table** window.

▸　Open the **Result tables** window with the **Result details** | **Result tables** menu option.

▸　Select the result table in the **Overview** table. Load the selected results table by dou-
ble-clicking or clicking on the **Load** button.

▸　Edit results in the **Details** view. To do this, click on the ✎ icon.

▸　If required, activate or deactivate repeat measurements in the **Replicates** panel in
the tabular overview using the checkbox in order to subsequently select outliers.

▸　Check the following parameters in the **Calculation parameter** panel and change
them if necessary:

–　Dilution ratio

–　Number of minimum determinations used to calculate the mean values

–　Regression type and calibration coefficients

–　Daily factor

–　Blank values

–　Slope and intercept for calculating COD, BOD_5 and total protein content

▸　After making changes, save the result by clicking the ☑ button.

✓　You have edited a result manually. The software marks edited results.

Whenever a result is edited, the software creates a new version of the results. The origi-
nal data is retained. Click on ▦ then navigate to the result versions in the **Select version**
window.

9.6　Navigating versions of edited results

When you edit results in the **Result table** window, the software creates a new version of
the results. The original data is retained. By default, the software displays the last ver-
sion of the results.

▸　Open the **Result tables** window with the **Result details** | **Result tables** menu option.

▸　Select the result table in the **Overview** table. Load the selected results table by dou-
ble-clicking or clicking on the **Load** button.

▸　Select result in the **Overview** table.

▸　In the **Details** view, click ▦ icon to open the **Select version** window.

▸　Select the version in the **Versions:** table.

▸　Open the version with **OK**.

✓　The software shows an older version of the edited results. Version see field: **Re-
sult version**.

▶ Load the current version of the results by clicking on the ☐ icon.

9.7   Calculating the mean value for selected results

You can calculate the mean value and standard deviation for selected results in the **Result table** window. You can use this option to combine individual determinations into one result for solids measurements.

▶ Open the **Result tables** window with the **Result details | Result tables** menu option.

▶ Select the result table in the **Overview** table. Load the selected results table by double-clicking or clicking on the **Load** button.

▶ Activate the desired measurements in the **Overview** tabular overview using the checkboxes.

▶ Click in ˅ to expand the **Statistics:** area.

✓ The software calculates the mean integral and mean, minimum and maximum concentration for the selected measurements. The software displays the results in the **Statistics:** area.

9.8   Importing and exporting results

Importing results

Import results in XML format as follows:

▶ Open the **Result tables** window with the **Result details | Result tables** menu option.

▶ Select the result table in the **Overview** table. Load the selected results table by double-clicking or clicking on the **Load** button.

▶ Click **Import**.

▶ Select a results file in XML format in the **Open** window in the Windows file manager.

▶ Click on **Open**.

✓ The software imports the results into the open results table.

Export results

Export results in XML or CSV format as follows:

▶ For CSV export: Check the export scope in the **Software settings** window, **Storage, Export and Report** tab and adjust if necessary.

– Open the **Software settings** window, **Storage, Export and Report** tab using the menu command **Program | Settings**.

– Restrict the export scope if required. To do this, remove entries from the **Used:** list box by clicking the ← icon.

– Extend the export scope. To do this, copy entries from the **Proposals:** list box to the **Used:** list box by clicking the → icon.

▶ Open the **Result tables** window with the **Result details | Result tables** menu option.

▶ Select the result table in the **Overview** table. Load the selected results table by double-clicking or clicking on the **Load** button.

▶ Activate the desired measurements in the **Overview** tabular overview using the checkboxes.

▶ Click **Export**.

▶ Select the storage location in the **Save as** window. Default export folder:
   C:/ProgramData/Analytik-Jena/multiWinPro/export/results.

▶ Change the file name if required.

▶ Select export format under **file type**: XML or CSV.

▶ Click **Save**.

   ✓ The software exports the selected results and summarizes them in an XML or CSV
     file.

See also

 ▤ Define export and report settings [▷ 38]

9.9   Printing and saving the results report

Print report

▶ Open the **Result tables** window with the **Result details** | **Result tables** menu option.

▶ Select the result table in the **Overview** table. Load the selected results table by dou-
   ble-clicking or clicking on the **Load** button.

▶ Activate the desired measurements in the **Overview** tabular overview using the
   checkboxes.

▶ Click on **Report** to open the print preview.

▶ For a better overview, click on the **Page overview** button to display the navigation
   area with a page summary to the left of the report. Zoom in or out of the view by
   clicking on **Zoom in** and **Zoom out**.

▶ Specify the scope of printing via checkboxes in the **Report** window:

   – **Summary** (shortened form)
     Print overview table of all measurement results at the beginning of the report

   – **Measurement results**
     Display overview table with sample ID, measurement method and sample volume
     When the checkbox is activated, the software activates the following three check-
     boxes.

   – **Meta data**
     Show metadata for individual measurements

   – **Parameter data**
     Show the results (means) of the individual measurement parameters

   – **Replicates**
     Show the measurement results of the individual repeat measurements

   – **Diagrams**
     Add graphical representation of the measurement curves for all measurements,
     measurement channels, and repeat measurements
     The software only activates the checkbox if the **Parameter data** checkbox is acti-
     vated.

▶ Add company logo to the report. Click on the **Load** button in the **Report logo** area,
   and then select the logo in the Windows file manager and load it into the report with
   Open.

▶ Click on **Printer options** to set up the printer.

▶ Click on **Page setup** to configure page settings such as paper size or orientation. De-
   fault: A4, portrait. Apply layout to current page or all report pages.

▸ Click on **Print** to start printing.

Save report

▸ Open the results table.

▸ Activate the desired measurements in the **Overview** tabular overview using the checkboxes.

▸ Click on **Report** to open the print preview.

▸ Define the print scope and logo.

▸ Click on **Save** then specify the file name, storage directory and file type in the **Save as** window.

▸ Save the report by clicking on the **Save** button.

You can save reports in the following file formats: PDF (default), RTF, HTML, TXT, FP3.

When you edit a result, the changes are only applied to the report after you save it.

10   Instrument menu

You can use the **Instrument** menu to control the analysis system outside the measurement process and to manage the device configuration.

In the Instrument menu

- Use **Initialize** to initialize the analysis system. You can switch the analysis system to standby or shut it down using the **Standby** and **Switch off** menu commands.
- You can switch the gas flow off and on again during measurement pauses using the **Gas flow off** and **Gas flow on** menu commands.
- Click on **Sampler alignment** then adjust the autosampler in the **Sampler alignment** window.
- Click on **Instruments** then create new device configurations, change and manage them in the **Instruments** window. In addition, you can access the blanks stored in the software for the device configuration via the context menu.
- Click on **Single control steps** then prepare the analysis system for maintenance or rinse it in the **Single control steps** window.
- After consulting Customer Service, click on **Instrument component test** to be able to control valves and assemblies individually and retrieve sensor-specific data for the detectors in the **Instrument component test** window.

10.1   Sampler alignment window

Open the window using the menu command **Instrument | Sampler alignment**.

In the **Sampler alignment** window, you adjust the autosampler so that it can correctly approach the various positions on the autosampler or the sample feed system of the analyzer.

NOTICE

Risk of device damage

When the autosampler is maladjusted or not adjusted at all, the autosampling tool can hit a hard surface during operation. This can destroy the autosampling tool and the drive.

- Adjust the autosampler before it is used for the first time and after each modification as well as after transporting or storing it for a longer period of time.
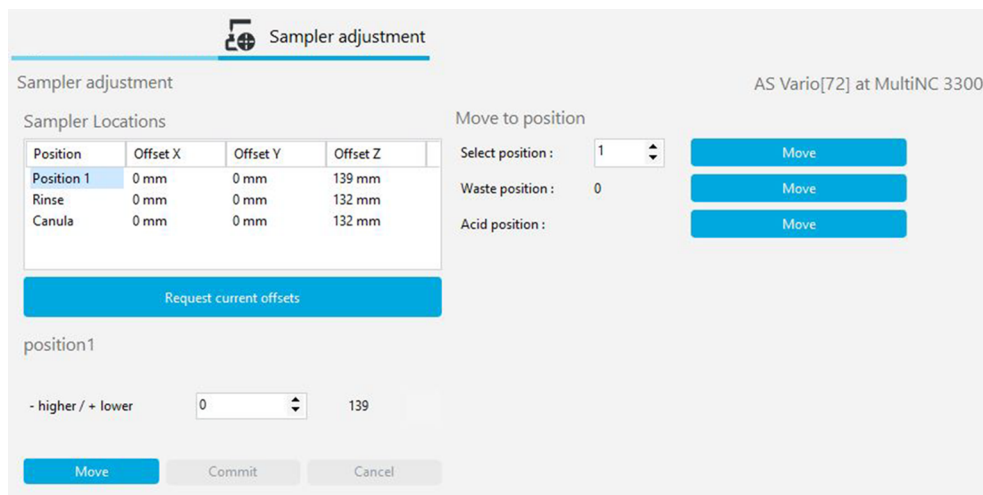

Layout of the window

Fig. 36   Sampler alignment window

Area	Description
Sampler alignment (top left)	List box with adjustment positions and offset values in X, Y, Z direction. ▪ Select adjustment position from the list box ▪ Click the **Request current values** button to query current offset values
Area for step-by-step adjustment (bottom left)	▪ Use **- backwards / + forwards** to move the autosampler arm forwards or backwards (not with all autosamplers) ▪ Use **- left / + right** to move the autosampler arm left or right (not with all autosamplers) ▪ Use **- higher / + lower** to move the autosampler arm or piston up or down ▪ Use the **Move** button to move to a position after changes ▪ Use the **Confirm** button to save the adjusted position ▪ Use the **cancel** button to cancel adjustment and reset to the starting values You adjust the position to which the autosampler arm moves. For a piston, adjust the distance by which the piston is moved. The piston adjustment cannot be canceled with **cancel**.
Move to position area (right)	Select positions to check the adjustment by moving to them ▪ Use the **Move** button to move to a position to check it

See also

▤ Adjusting the autosampler [▶ 115]

10.2   Instruments window

Open the **Instruments** window using the menu command **Instrument|Instruments**.

You manage device configurations in the **Instruments** window.

In the Instruments window

▪ Click on **Add** to create a new device configuration, for example for liquid or solid measurements.
▪ Click on **Set default** to activate a device configuration as the default configuration. The software adapts the selection options for methods and sequences to the active configuration.
▪ Use **delete** to delete a selected device configuration.

■ The optional FDA 21 CFR Part 11 Compliance module prevents data from being deleted.

■ Use **Assign group** to organize device configurations into groups in the **Select group** window.

■ Use the **Blank values** menu command (in the context menu) to open the **Blank values** window. Here you can view and globally change stored blanks for the device configuration.
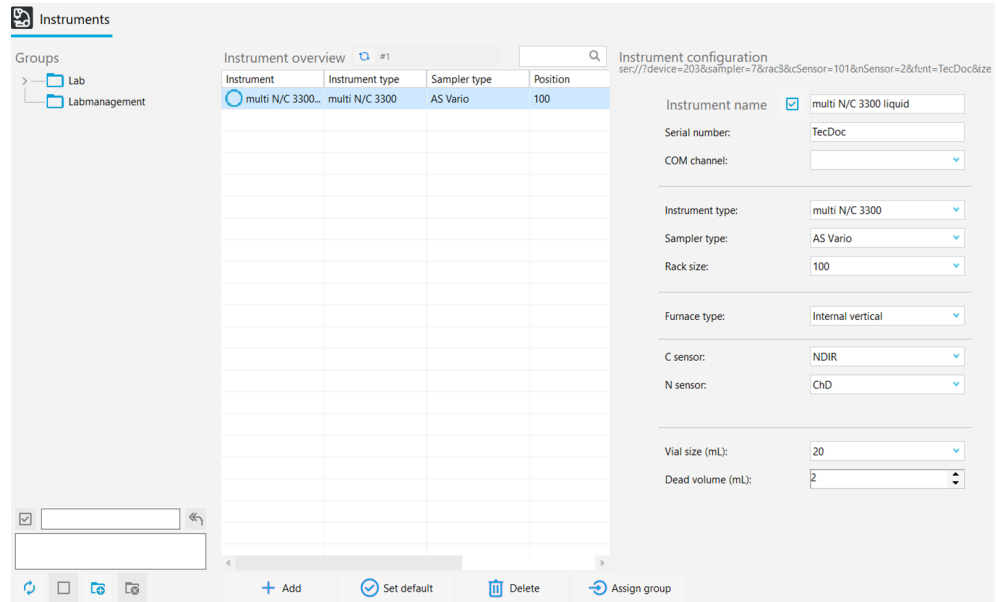
Layout of the window

Fig. 37 Instruments window

Area	Description
Groups (left)	Manage groups
Instrument overview (middle)	Tabular overview with details: ■ Designation of the device ■ Device type ■ Autosampler ■ Sample tray ■ Detectors The active device configuration is highlighted.
Instrument configuration (right)	Detailed view for selected device configuration with editable settings

Instrument configuration detailed view

You can view and edit device configurations in the detailed view.

Option	Description
Instrument name	Define name for device configuration The default name is: NewDevice_Timestamp.
Serial number:	Serial number of the analyzer The software automatically copies the serial number into the field during licensing. The serial number cannot be changed.
COM channel:	Select the interface of the PC to the analyzer from the drop-down menu If required, view COM port in the Windows device manager
Instrument type	Select device model from the drop-down menu

Option	Description
Sampler type:	Select autosampler from the drop-down menu
Rack size:	Select sample tray from the drop-down menu
Furnace type:	**Internal vertical** option Select for liquid measurements with high-temperature oxidation **UV reactor** option Select for liquid measurements with UV oxidation **Internal horizontal** option Select for solids measurements with internal solids module **External horizontal** option Select for manual or automated solids measurements with external solids module
C sensor:	Select carbon detector from the drop-down menu
N sensor:	Select nitrogen detector from the drop-down menu: ■ **ChD** for electrochemical detection with internal ChD ■ **CLD** for chemiluminescence detection with external CLD
Vial size (mL):	Select the volume of the sample vessels from the drop-down menu
Dead volume (mL):	View the preset dead volume of the sample vessels and adjust if necessary
Checkbox **Automatic dilution**	Activate automatic dilution option (only displayed if an autosampler with dilution tray is selected)

See also

▤ Creating a new device configuration [▶ 115]

10.3   Single control steps window

Open the **Single control steps** window via the menu command **Instrument|Single control steps**.
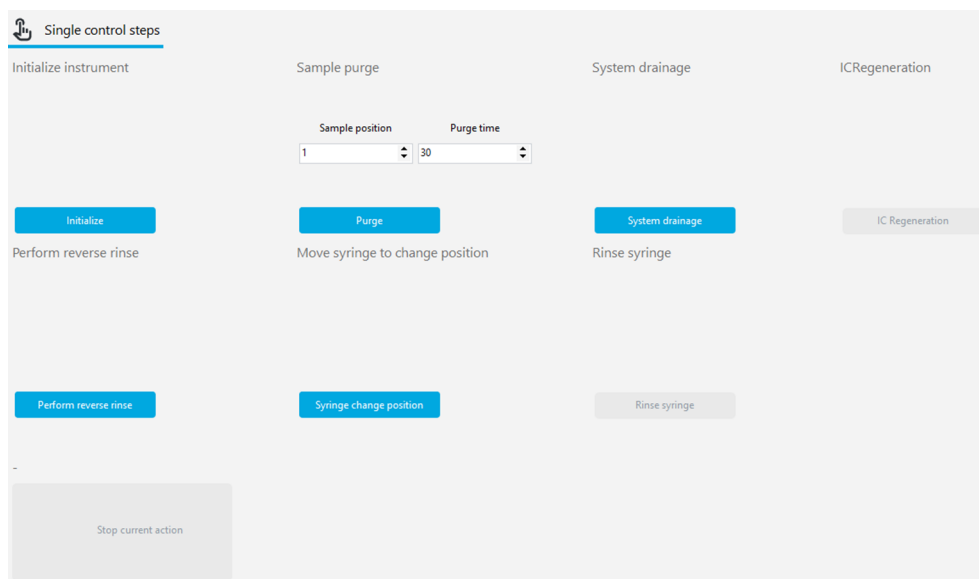

Fig. 38   Single control steps window

In the **Single control steps** window, you can control the analysis system outside the measurement sequence and prepare it for maintenance.

Area	Description
Initialize instrument	Initialize the device by clicking on **Initialize**
	The TIC condensate container is pumped out and refilled.
Sample purge	Activate NPOC purge, e.g. to set the NPOC purge flow rate
	■ In autosampler mode, select the sample position at **Sample position**
	■ Set the purge time at **Purge time**
	■ Click on **Purge** to start purging
System drainage	Click on **System drainage** to pump off the TIC condensate container and set the syringe pump to the initial state
Reactor regeneration	Click on **Reactor regeneration** to rinse the TIC condensate container with phosphoric acid and purge with carrier gas (for analyzers with direct injection)
Perform reverse rinse	Click on **Perform reverse rinse** to backwash the tubes of the sample feed system with high-purity water, to backwash the rinsing liquid into the rinsing vessel of the autosampler or into the waste vessel (for analyzers with flow injection)
Move syringe to change position	Click on **Syringe change position** to empty the syringe pump of the analyzer completely and move the piston to the change position (for analyzers with flow injection)
Rinse syringe	Click on **Rinse syringe** to rinse the dosing syringe of the autosampler and empty into the waste position (for analyzers with direct injection)
Stop current action	Click on **Stop current action** to cancel the current action

10.4   Instrument component test window

Open the **Instrument component test** window using the menu command **Instrument|Instrument component test**.

In the **Instrument component test** window you can control valves and assemblies individually and retrieve sensor-specific data for the detectors.
■ Only use the functions after consulting Customer Service.
■ Provide the retrieved data and test results to Customer Service for assessment.

Layout of the window

Area	Description
Valves (left)	Individual control of valves and assemblies
	■ Click on the **Start** button to activate the area. Click on **Stop** to deactivate the area again.
	■ After consulting with Customer Service, select valve or assembly and activate or deactivate with **On/Off** toggle switch.
Optical bench (middle)	To check the status of the carbon detector, retrieve analog values and calculate sensor-specific data
	■ Click on the **Start** button to start data retrieval in the **Analog** area. Start data calculation in the **Calculated parameters** area.
	■ Click on **Stop** to end data retrieval or data calculation.
	■ Click on the **Zero Point Adjustment** button to remeasure the baseline.
CLD (right)	Retrieve sensor-specific data to check the status of the nitrogen detector
	■ Click on the **Start** button to start data retrieval.
	■ Click on **Stop** to end data retrieval.

When you close the **Instrument component test** window, the software automatically stops all running component tests.

While a component test is running, the software does not update the displays in the **Instrument status** panel.

10.5 Adjusting the autosampler

NOTICE

Risk of device damage

When the autosampler is maladjusted or not adjusted at all, the autosampling tool can hit a hard surface during operation. This can destroy the autosampling tool and the drive.

- Adjust the autosampler before it is used for the first time and after each modification as well as after transporting or storing it for a longer period of time.

▶ Open the **Sampler alignment** window with the **Instrument** | **Sampler alignment** menu option.

▶ Select adjustment position from the list box in the **Sampler position** area.

▶ View detailed information on adjustment and adjustment positions in the operating manual for the analyzer.

▶ Click the **Request current values** button to query current offset values.

▶ Adjust offset values for **- backwards / + forwards** , **- left / + right** and **- higher / + lower** in steps.

▶ After each change, click on the **Move** button to move to the position and check.

▶ Save the adjusted position with **Confirm**.

▶ Finally, check the adjustment of the autosampler:

  – Select the position in the **Move to position** area.

▶ Check adjusted positions and other positions such as acid position.

  – Move to positions by clicking on **Move**.

▶ If necessary, adjust the adjustment again and save.

  ✓ You have adjusted the autosampler and can start the first measurements.

10.6 Creating a new device configuration

You can create device configurations in the **Instruments** window, e.g. for liquid or solid measurements.

You can set a device configuration as the default configuration. The software adapts the selection options for methods and sequences to the active device configuration.

▶ Open the **Instruments** window with the **Instrument** | **Instruments** menu option.

▶ Click on **Add** to create a new device configuration.

▶ Name the device configuration under **Instrument name**. The default name is: NewDevice_Timestamp

▶ Under **Serial number:**, the software automatically enters the serial number when licensing. Check serial number.

▶ Select the interface to the analyzer in the drop-down menu, under **COM channel:**. If necessary, check the COM port in the Windows device manager.

▶ Select the device model in the drop-down menu under **Instrument type**.

▶ Select autosampler and sample tray for **Sampler type:** and **Rack size:**.

▶ Select UV reactor, internal furnace or external furnace from the drop-down menu under **Furnace type:**.

Drop-down menu	Options
Furnace type:	**Internal vertical** option Select for liquid measurements with high-temperature oxidation
	UV reactor option Select for liquid measurements with UV oxidation
	Internal horizontal option Select for solids measurements with internal solids module
	External horizontal option Select for manual or automated solids measurements with external solids module

▶ Select detectors in the **C sensor:** and **N sensor:** drop-down menus.

▶ Select the volume of the sample vials from the **Vial size (mL):** drop-down menu. The software adjusts the dead volume accordingly. Optionally you can adjust the dead volume under **Dead volume (mL):**.

▶ Save the device configuration by clicking the ☑ button.

▶ Select the device configuration from the **Instrument overview** table and activate as the default configuration by clicking on **Set default**. Alternatively, double-click to activate the device configuration.

▶ Restart the software after every change to device configurations.

  ✓ You have defined and activated a new device configuration.

10.7   Changing blanks in the device configuration

The software saves blanks regardless of the method. You can view the blanks saved in the software in the **Instruments** window. If you have the appropriate permissions, you can edit the blanks in the device configuration. The changes apply across all software.

▶ Open the **Instruments** window with the **Instrument |Instruments** menu option.

▶ Select the device configuration in the **Instrument overview** table.

▶ Right-click to open the context menu and select **Blank values**.

▶ View blanks on the different tabs in the **Blank values** window.

▶ If necessary, edit blanks by clicking on the ✏ icon.

▶ Confirm the changes by clicking on the **OK** button.

  ✓ The changed blanks apply across all software.

11   View menu

You can customize the view of the program interface using the **View** menu. Customer Service can access the password-protected service mode here.

In the View menu

- You can use the **Window** menu command to arrange undocked dialog windows in the foreground.
- Click on **Customize** to customize the menu bar and toolbar in the **Customize** window.
- Click on **Service desktop** to allow Customer Service open the password-protected service mode with diagnostic and maintenance functions.

11.1   Customizing the toolbar

You can customize the view of the toolbar using the **Customize** menu.
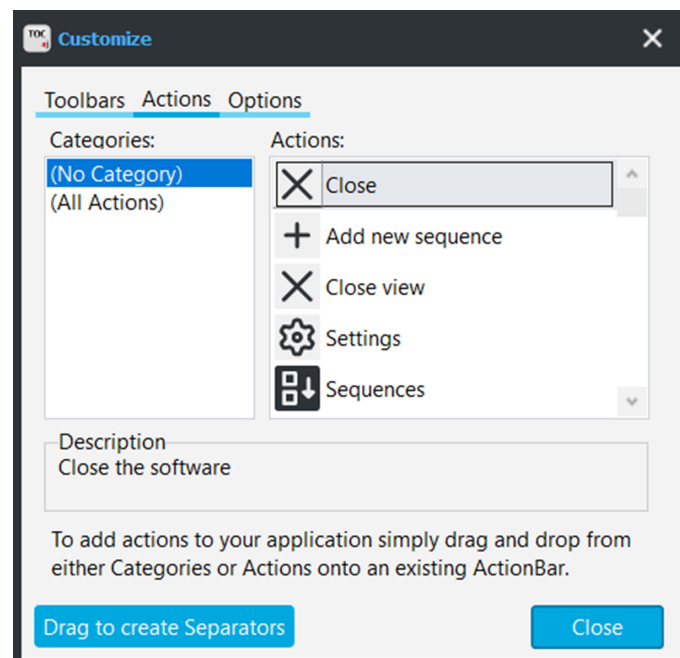
Fig. 39   Customize window

‣ Open the **Customize** window with the **View** |**Customize** menu option.

‣ On the **Toolbars** tab, show or hide the toolbar using the checkbox.

‣ Use the drop-down menu in the **Toolbar Options** area next to each icon to show or hide the menu command.

‣ Select icons to be displayed in the toolbar on the **Actions** tab. Select the icon from the **Actions** list box and drag it to the toolbar while holding down the mouse button.

‣ If required, click on **Drag to create separators** and drag separators to the desired position in the toolbar by holding down the mouse button.

‣ On the **Options** tab, check the **Menu shows recently used items first** checkbox to arrange the most recently used menus first in the menu bar.

‣ In the **Other** area, enlarge icons as required. Show or hide tooltips and shortcut keys. Personalize the menu animation.

▶ To remove entries from the toolbar:
With the **Customize** window open, hold down the mouse button and drag the icon or menu command from the toolbar.

▶ To remove separators:

– Click on the separator. The separator is selected when it is highlighted by a rectangle.

– Hold down the mouse button and drag the separator from the toolbar.

▶ Click **Close** to close the **Customize** window.

✓ You have customized the menu bar and toolbar.

12   Help menu

In the **Help** menu you will find help with operating problems and errors. You can access information about the software and license new software modules.
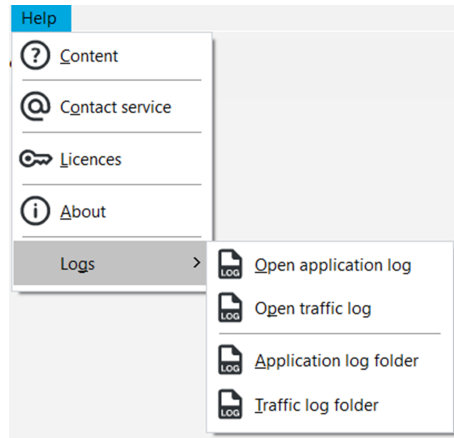
Fig. 40   Help menu

In the Help menu

- Use the **Content** menu command to open the software help.
- Click on **Contact service** for the software to automatically create an e-mail template that you can use to contact Customer Service in the event of a fault.
- Click on **Licences** to view the software licensing in the **Licence management** window. License additional software modules if required. You will receive the required license codes when you purchase the modules.
- Use the **About** menu command to view information about the software such as software version, copyrights, licenses or contact details.
- Use the menu commands **Help**|**Logs**|**Application log folder** and |**Traffic log folder** to open the folders with the log files. Attach the current log files to your e-mail for error analysis by Customer Service.

13   FDA 21 CFR Part 11 Compliance module

The optional FDA 21 CFR Part 11 Compliance module provides complete data integrity and conforms to the pharmaceutical guidelines 21 CFR Part 11.

Protection of electronic records

The optional software module protects electronic records and ensures data confidentiality. To do this, the software module uses a central CDM service with a CDM server or a DBMS (database management system) in the company's local, internal network, and CDM clients on the measuring station computers. *CDM* stands for Central Data Management. The CDM service and clients communicate in encrypted form via a RESTful API interface. Alternatively, if there is only one client you can install the CDM server on the local computer.

User Management

The software module applies User Management to limit access to the software and selected software functions to authorized persons. User Management is centralized; any changes affect all clients.

Audit trail

The software generates audit trails that document every access and every change to the system with a timestamp.

Electronic signatures

In the software module, a multi-stage check and approval of data (methods, calibrations, results) is mandatory. Electronic signatures allow signatories to be identified beyond doubt.

System Suitability Test (SST)

The system suitability test (SST) is intended for quality assurance for TOC or NPOC determination in the pharmaceutical sector and is only possible with the FDA 21 CFR Part 11 Compliance module. The test checks the suitability of the device for measuring organic substances that are difficult to oxidize (*p*-benzoquinone) in comparison to sucrose. In the work according to JP 17 2.59 you investigate the oxidizability of sodium dodecyl benzenesulfonate in comparison to potassium hydrogen phthalate.

See also

📄 Viewing, printing or exporting the audit trail [▶ 126]

13.1   User Management in the FDA 21 CFR Part 11 Compliance module

13.1.1 Users and user roles

First login

The first time you log in after installing the software, you set up the connection to the CDM server. In doing so, you create a user with administrator rights and an initial password. After logging in, a dialog appears in which you must change the initial password.

The administrator can set up additional users in User Management.

Recommendation: In User Management, set up a user with the **Administrator Recovery** role. Use this user to restore the administrator profile in the event the password is lost. Profiles cannot be restored by Analytik Jena.

User Management

Open User Management with menu command **Program**|**User management**.

The **User management** window shows an overview of all users and user roles with their access rights.

As an administrator, you can create new users and user roles. You can grant new user roles individual access rights.
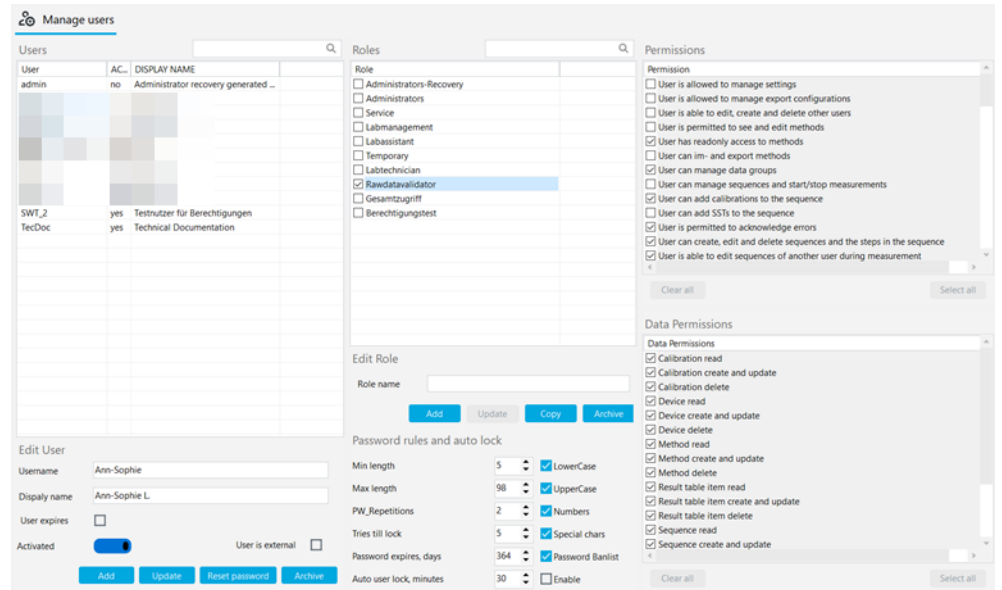

Fig. 41   User management window

User

When selecting a user in the **Users** table, you can view and edit the settings of their user profile. To do this, use the input fields, checkboxes and buttons in the **Edit user** area.

Checkbox/field/ button	Description
Name	Specify a user name for logging into the system
Display name	Specify user name that is displayed in the status bar, signature and reports
User expires	▪ Check the checkbox if the user should only be valid for a limited time ▪ Select the last day of validity in the calendar next to **Date** After the user's account has expired, that user can no longer log into the system. An administrator can reactivate the user and set a new expiration date.
Activated /De- activated	When activated, the user can log into software If deactivated, the user profile is locked
User is external	When activated, the user can log in via an external technical system using LDAP (only with FDA 21 CFR Part 11 Compliance module) *LDAP* stands for Lightweight Directory Access Protocol. The protocol allows organizations to store and manage user data.
Add	Add a new user by entering the username, etc. After you clicking on **Add**, the software displays the initial password for the user's first login.
Update	Update existing user after selecting them in the **Users** table and editing the fields
reset password	Reset user's password The software displays a new initial password below the table.

When a user is selected in the **Users** table, the software shows which user role the user is assigned to in the **Roles** table.

A user can have several user roles. The user then has the access rights of all these user roles.

User roles

The **Roles** table shows an overview of the user roles. After selecting a user role, you can view its access rights.

	Description
Checkbox	Tick the checkbox to assign a user role to the selected user

Use the input field and the buttons in the **Edit role** area to edit the user roles.

Field / button	Description
Add	Add new user role after entering a role name
Update	Update custom user role after changing the role name
	Changes to the rights settings do not need to be saved.
Copy	Copy user role
Archive	Archive selected user role after confirmation prompt
	Archived user roles cannot be restored.
	Archiving is only possible for user roles to which no user is assigned.

User roles with tiered access rights are available by default in the software.
- You cannot change the access rights of default user roles.
- You can define individual access rights for new user roles.

User	Access rights
Administrator	▪ Administrators can manage users and access rights. ▪ Administrators can change the software license. ▪ Administrators can view and export the audit trail. ▪ Administrators can create groups. They set up data storage and data export. ▪ Administrators are not authorized to perform measurements.
Service	▪ The service role is reserved for service technicians of Analytik Jena or persons authorized by Analytik Jena. ▪ Service is the only role that can access the password-protected service functions via the **View** |**Service desktop** menu item. ▪ The service role has extensive access to software functions and can, for example, start measurements, view results and edit them.
Lab manager	Lab managers have extensive access to software functions, with the exception of user management and license management.
Lab technician	Lab technicians rank between lab managers and lab assistants in terms of their rights.
Intermediate user	The rights of lab assistants are limited to the measurement operation.
Basic user	Temporary staff have fewer access rights than lab assistants.
Data auditor	▪ Raw data validators have an important role in the optional FDA 21 CFR Part 11 Compliance module. They can view, sign and comment on methods, sequences, calibrations and measurement results. ▪ Raw data validators can generate reports, export data and view the audit trail.

See also

☷ Installing the software with the FDA 21 CFR Part 11 Compliance module [▶ 9]

13.1.2 Access rights

User roles with tiered access rights are available by default in the software.
- You cannot change the access rights of default user roles.
- You can define individual access rights for new user roles.

The **Rights** and **Data Permissions** tables in the **User management** window allow you to view the access rights assigned to a user role.

The **Data Permissions** table governs the fundamental right to view, create, update and delete data on the central CDM service.

The **Rights** table controls access to various software functions in detail. For example, you can assign rights for data release individually using the **Checked** and **Released** signatures. Furthermore, you can authorize user roles to use data before it is released.

You can use the tables to define the following access rights:
- Configure software settings
- Edit device configuration and change software licensing
- Configure data storage, data import and export
- Manage users
- Configure groups to manage data
- Customize sequence and results table
- Create and edit methods
- Create and edit sequences and perform measurements
- Create and edit calibrations
- View and edit results
- Import and export data
- Approve data using electronic signatures (only with FDA 21 CFR Part 11 Compliance module)
- Acknowledge error messages
- View audit trail and add manual entries

You can activate access rights for your own user roles by ticking the checkboxes. Saving is not required. The access rights apply to all users with that user role from the next time they log in to the software.

Read rights only allow read-only access to data. Users can view and use data, but not edit it. Read rights are a prerequisite for editing rights: Editing rights must be assigned together with reading rights.

Some rights restrict access to certain elements, for example **Can only create sequences for the default instrument**.

If a user does not have access rights in menus and dialog windows, the relevant areas are not displayed or are grayed out.

You can quickly change the rights selection using the buttons below the table:

Button	Description
Clear all	Clear rights selection
Select all	Select all rights

13.1.3 Editing a user

Creating a new user role

▶ Log in to the software as an administrator.

▶ Select the menu command **Program | User management**.

▶ Enter a new role name under **Edit role**.

▶ In the **Roles** area, click on **Add** to save the user role.

▸ Alternatively, copy an existing user role by clicking on the **Copy** button.

▸ Select access rights for user role in the **Data Permissions** and **Rights** table. Tick the checkboxes for this. Saving is not necessary.

    – The **Data Permissions** table governs the fundamental right to view, create, update and archive data on the central CDM service.

    – The **Rights** table controls access to various software functions in detail.

    ✓ You have created a new user role with customized user rights. You can now assign the new user role to users.

Creating a new user

▸ Log in to the software as an administrator.

▸ Select the menu command **Program | User management**.

▸ In the **Edit user** area, enter the user name in the **Name** input field.

▸ Enter the display name.

▸ Activate the **User expires** option if the user should only be valid for a limited time. Set the date of the last date on which they can log in to the software under **Date**.

▸ In the **Edit user** area, click on **Add** to save the user.

    ✓ The software displays the initial password for the user's first login below the **Users** table.

▸ Select the initial password and copy it to the clipboard with **Ctrl + C** and forward it to the new user.

▸ Select user role for new user in the **Roles** table and activate it via the checkbox.

    ✓ You have created a new user and assigned a user role to the user. The new user is authorized to log in to the system.

A user can have several user roles. The user then has the access rights of all these user roles.

The software opens the **Change password** window the first time you log in, where a new user must change their password.

Editing user settings

▸ Log in to the software as an administrator.

▸ Select the menu command **Program | User management**.

▸ Select the user in the **Users** table.

▸ Customize user data under **Edit user**.

▸ Save changes by clicking the **Update** button.

▸ If required, assign a new user role to the user. To do this, activate the checkbox in the **Roles** area.

▸ For own user roles: Select a role in the **Roles** area. Change access rights in the **Data Permissions** and **Rights** table.
The access rights of predefined user roles cannot be edited.

    ✓ You have customized the user settings.

All users assigned to a user role are affected by any changes to access rights.

Archive user roles

You can archive users and your own user roles which are not assigned to any users. Users and user roles cannot be deleted.

▸ Log in to the software as an administrator.

▸ Select the menu command **Program | User management**.

▸ To do this, select a user role you have created in the **Roles** area and click on the **Archive** button. Confirm confirmation request.

✓ You have archived a user role. You cannot restore archived users and user roles at a later date.

Deactivating users

You can deactivate users to deny them access to the software. You can unblock the users again at a later date.

▶ Log in to the software as an administrator.

▶ Select the menu command **Program** | **User management**.

▶ Select the user in the **Users** table.

▶ Click on the **Activated** toggle switch.

✓ The user is deactivated.

▶ If required, reactivate the user by clicking on the toggle switch again.

Resetting the password

You can reset a user's password, for example if a user has forgotten their password.

▶ Log in to the software as an administrator.

▶ Select the menu command **Program** | **User management**.

▶ Select the user in the **Users** table.

▶ Click on **reset password**.

✓ The software resets the current password and generates a new initial password for the first login. The software displays the password below the **Users** table.

13.1.4 Configuring password rules and automatic logout

In the **User management** window, you can define criteria for the validity of passwords and configure automatic logout after periods of inactivity.

▶ Log in to the software as an administrator.

▶ Select the menu command **Program** | **User management**.

▶ Set the password conditions in the **Password rules and auto lock** (see table).

▶ Activate the **Enable** option to automatically log users out when inactive. Set the period of inactivity in (min) under **User locks after [min]**.

✓ The new password conditions are valid for all new passwords. Passwords created before the change are still valid.

Criterion	Description
Minimum length	Set the minimum password length (min. 4 characters)
Max length	Set the maximum password length (max. 100 characters)
last passwords checked	Define the number of permitted repetitions for previously used passwords (max. 10 repetitions)
max. input attempts	Define the number of invalid login attempts until the user profile is locked (max. 10 attempts) An administrator can unlock a locked user profile under **User management**.
Password expires [days]	Set the number of days after which the password becomes invalid (1 to 365 days)
User locks after [min]	▪ Activate automatic logout of inactive users via a checkbox ▪ Define the duration of inactivity, default setting: 30 min (1 to 2000 min) The software locks the screen and thus prevents unwanted access to data. Measurements continue to run.

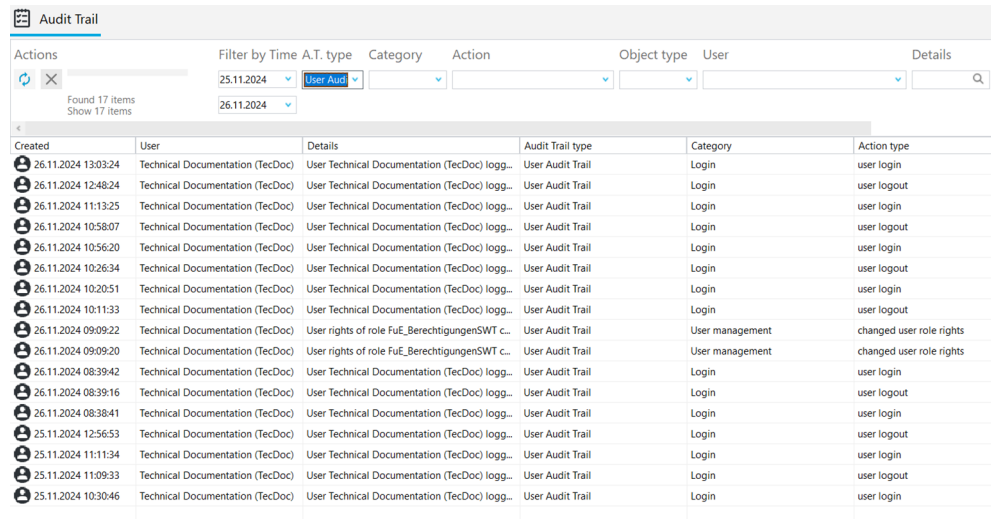| Criterion	Description
Lower case	Define which characters the password must contain:
Upper case	■ Upper and lower case letters
Numbers	■ Digits
Special characters	■ Special characters
Ban common PW	Use an internal software list to reject trivial passwords

13.1.5 Recover administrator if password is lost

Recommendation: In User Management, set up a user with the **Administrator Recovery** role. Use this user to restore the administrator profile in the event the password is lost. Profiles cannot be restored by Analytik Jena.

▶ If the administrator password is lost: Log in to the software as a user with the role of **Administrator Recovery**.

▶ Open User Management. Select administrator from the **Users** table.

▶ If necessary, reactivate the administrator by clicking on the **Deactivated** button.

▶ Reset the administrator password by clicking on the **reset password** button.

▶ Copy the new initial password to the clipboard using **Ctrl + C** and provide it to the administrator so they can log into the software.

13.2 Viewing, printing or exporting the audit trail

You can view the audit trail under **Program|Show Audit Trail**. To do this, select the desired period under **Filter by Time** and click on the ⟳ icon.

Fig. 42   Audit Trail window

Logged events   The software logs the following events in the audit trail:

■ Start and exit of the software
■ Login and logout of users
■ Initialization, standby and shutdown of the analysis system
■ Creation and editing of a method
■ Errors that have occurred with error messages
■ Manual editing of results
■ Changes in user management such as creating a new user
■ Data release and data import

- Start, end and manual termination of a measurement
- Performing and editing a calibration
- Measurement or input of blanks
- Recording of daily factors
- Carrying out system suitability tests

- Software updates
- Creating or changing a device configuration
- Changing cross-software settings

Structure of the audit trail

The software displays the audit trail in a tabular overview. The software sorts the logged events into categories, which you can use to filter the audit trail. The time and logged-in user are recorded for each event.

Column	Description
Created	Date and time of the event
User	User who was logged in during the event
Details	Logged event (detailed description)
Audit Trail type	Type of logged events: **User Audit Trail** Changes in user management **Run Audit Trail** Documentation of the measurement process **Method Audit Trail** Creating or changing methods **Device Audit Trail** Documentation of device control, including changes to device configuration **Error** Error message
Category	Category of logged event
Action type	Logged event (code)
Type of changed object	Type of software element affected
Changed Object	Affected software element
Instrument	Device model
Serial number	Serial number of the device
App. class	Type of software (TOC)
App. type	Software name
App. instance	Client in the network

You can sort the logged events in ascending order. To do this, click on the header of the column you want to sort.

Filtering

You can filter the audit trail according to the columns in the tabular overview to reduce the number of events displayed.

▸ Select entries from one or more drop-down menus to apply filters.

▸ Next to **Filter by Time**, select the start and end of the time window in the calendar.

▸ Under **Details**, enter free text in the search field to filter the entries in the   Details column.

▸ Click on the ✕ icon to pause the running update.

▸ To delete a filter, select the empty row at the top of the drop-down menu.

Displaying and printing the audit trail

▸ Open the audit trail with the menu command **Program | Show Audit Trail** and click on the ↻ icon.

▸ If required, set filters for certain events or define time windows:
  – Select entries from one or more drop-down menus.
  – Set a time window: Select the start and end date in the displayed calendars.

▸ Sort the events contained in the table in ascending order. To do this, click on the header of the column you want to sort.

▸ Click on **Report** to open the print preview.

▸ For a better overview, click on the **Page overview** button to display the navigation area with a page summary to the left of the report. Zoom in or out of the view by clicking on **Zoom in** and **Zoom out**.

▸ Click on **Printer options** to set up the printer.

▸ Click on **Page setup** to configure page settings such as paper size or orientation. Default: A4, portrait. Apply layout to current page or all report pages.

▸ Add company logo to the report. Click on the **Load** button in the **Report logo** area, and then select the logo in the Windows file manager and load it into the report with **Open**.

▸ Click on **Print** to start printing.

▸ Save the report by clicking on the **Save** button.

The audit trail usually contains a large number of entries. It is therefore advisable to filter the audit trail for relevant entries.

You can save reports in the following file formats: PDF (default), RTF, HTML, TXT, FP3.

13.2.1 Customizing the audit trail

You can customize the layout of the table using the **Adjust display columns** command (in the context menu).

▸ Open the audit trail with the menu command **Program | Show Audit Trail**.

▸ Right-click in the table to open the context menu.

▸ Select the **Adjust display columns** command.

▸ In the **Configuration view**, customize the display and order of the table columns:
  – Use the → icon to transfer a column from suggestions (left) to the table (right).
  – Use the ← icon to remove a column from the table (right).
  – Use the →| icon to transfer all columns from suggestions (left) to the table (right).
  – Use the |← icon to remove all columns from the table (right).
  – Use the ↓ icon to move a column down or to the right in the sequence table.
  – Use the ↑ icon to move a column up or to the left in the sequence table.
  – Use the ↩ icon to restore the preset column.

▸ Click **OK** to confirm the entered data.
  ✓ You have customized the table columns.

13.3   Adding manual entries to the audit trail

You can manually add certain entries to the audit trail, such as a firmware update or maintenance work that has been carried out.

▶ Open the **Manual Audit Trail entry** window with the **Program** | **Manually add audit trail entry** menu option.

▶ Select an entry in the drop-down menu under **Entry type:**.

  ✓ The software displays further drop-down menus to categorize the event.

▶ Use the drop-down menus that appear to store the device configuration and other information such as the type of maintenance in the audit trail.

▶ Add free text about the event in the input field next to **Comment**.

▶ Click on the **Add** to add the manual entry to the audit trail.

  ✓ The software enters the manual entry into the audit trail. The software records the time and the user who logged the event in the audit trail.

Option	Description
Entry type:	**Device Qualification failed** option The device qualification, e.g. as part of an IQ/OQ, has failed.
	Device Qualification successful option The device qualification was successful.
	firmware update option The service has performed a firmware update.
	Installation qualification (IQ) failed option Installation qualification (IQ) has failed.
	Installation qualification (IQ) successful option IQ was successful.
	maintenance option Maintenance work has been carried out.
	Operational Qualification failed option Operational qualification (OQ) failed.
	Operational Qualification successful option OQ was successful.
Instrument	Select device configuration
Old firmware version:	Enter the old firmware version for firmware updates
New firmware version:	Enter the new firmware version for firmware updates
Maintenance type:	Select the type of maintenance:
	maintenance option Planned, regular maintenance work
	Repair option Maintenance work carried out after the occurrence of a device error or analytical problem
Comment	Add further information as a comment

13.4   Electronic signatures

In addition to user administration, signatures are an important component for ensuring data validity pursuant to 21 CFR Part 11.

With the FDA 21 CFR Part 11 Compliance module, it is mandatory to sign data. This means that you can only use released, unblocked methods and calibrations for the measurement. Unless you are explicitly authorized via User Management to use data before it is released.

Signing is carried out according to the dual control principle:
- The user who creates the data automatically signs with **Created**.
- Checking and signing with **Checked** must be carried out by another user.
- Every user with the permission to sign data as released can issue the **Released** signing status.

The software provides for the following signature statuses in succession: **Created**, **Checked** and **Released**. Lock outdated or invalid data by clicking on **Invalid**.

Signature	Description
Created	The signature is added automatically by the user logged in at the time the data is created.
	Authorized users can continue to process the data. The software documents changes in the audit trail.
Checked	The release process begins with the assignment of the **Checked** signature. From that point on, you will no longer be able to edit the data.
	The signing user validates the data. In accordance with the dual control principle, the validator must be different from the creator.
Released	The signing user releases the data for use.
	You can now use methods and calibrations for the measurement. In general, you may use and communicate both released measurement results and SSTs to third parties.
Invalid	The signing user locks the data. You can no longer use the data.
	You can edit locked data again after changing the signature status.

The software provides signing for the following data:
- Methods
- Calibrations
- Measurement results
- System Suitability Tests (SST)

Signing data   You sign data in the **Methods**, **Calibrations**, **Result table** and **SSTs** windows.

▸ Open the window.

▸ Select the method, calibration, measurement result or SST report from the overview table.

▸ Sign data by clicking on the **Checked** and **Released** buttons.

▸ Enter the user name and password when prompted by the software.

▸ Enter a comment and confirm with **OK**.

▸ Lock outdated or invalid data by clicking on **Invalid**.

▸ In the **Result table** window, select several results by ticking the checkbox. Click on the **Sign all checked results** button to sign multiple results at once.

   ✓ The data is signed. The highlighted button shows the current signature status.

▸ View detailed information on the signature such as date, time and the user that signed the data on the **Signatures** tab.

i NOTICE! If you record daily factors in a sequence, the software automatically transfers the daily factors to the calibration. The signing status of the calibration changes to **Created**. You must approve the calibration again to be able to carry out further measurements in the sequence.

The software logs the signing of data in the audit trail.

Signing data is optional in the standard software. No entries are made on the **Signatures** tab.

13.5 Data management

The software protects data against intentional and unintentional data manipulation.

The software stores all data centrally on the CDM server:
- User Management
- Audit trail
- Methods
- Sequences
- Calibrations
- Results
- System Suitability Tests
- Device configuration

If users have the appropriate access rights, they can view and edit data in the software. The software logs all changes in the audit trail. No user has the right to delete data.

13.6 System Suitability Test (SST)

The system suitability test (SST) is intended for quality assurance for TOC or NPOC determination in the pharmaceutical sector and is only possible with the FDA 21 CFR Part 11 Compliance module. The test checks the suitability of the device for measuring organic substances that are difficult to oxidize (*p*-benzoquinone) in comparison to sucrose. In the work according to JP 17 2.59 you investigate the oxidizability of sodium dodecyl benzenesulfonate in comparison to potassium hydrogen phthalate.
- As part of the SST, you measure TOC water, a sucrose standard and *p*-benzoquinone standard using a TOC or NPOC method.
- The software calculates the TOC values: $TOC_{Net} = TOC_{Standard} - TOC_{Water}$
- The software forms the quotient $TOC_{Net}(p$-benzoquinone$) / TOC_{Net}($sucrose$)$.
- The software outputs the results in the **Results|SSTs** window and in the SST report.

The SST is deemed a pass if the SST quotient is 0.85 to 1.15.

In the case of JP 17 2.59, the SST is considered passed if the measured TOC concentration of the sodium dodecyl sulfonate solution is at least 0.450 mg/l.

The use of SST standards with different concentrations or different substances is possible in accordance with the following pharmacopoeia:
- USP SST. Bulk Water (USP 643)
- USP SST. Sterile Water (USP 643)
- EP SST (EP 2.2.44)
- JP-SST (JP 17 2.59)

The software adjusts the substances and target concentrations accordingly.

13.6.1 Performing a System Suitability Test (SST)

▸ Use the **Measurement** |**Add new sequence** menu option to create a new sequence.

▸ Click on the ✿ icon to open the **Create SST** wizard.

▸ Assign a title for the SST in the wizard. The default name is: SST + timestamp. Optionally add a comment.

▸ Select the pharmacopoeia according to which the SST should be carried out:
  USP SST, Bulk Water
  USP SST, Sterile Water
  EP SST
  JP-SST

▸ Click the **Method** button, then select the NPOC or TOC method in the **Select method** window.

▸ Click on the **Calibration** button, then select the calibration in the **Select calibration** window.

▸ If necessary, adjust the target concentration under **Target concentration**. The target concentrations should only be changed if there are changes in the pharmacopoeia.

▸ Confirm the entries in the wizard by clicking on **OK**.

  ✓ The software transfers the SST measurements to the sequence.

▸ Select result table from drop-down menu after clicking on **Result table**. Or: Create a new result table with **Create new result table**.
  Unless you select a result table, the software saves the results in the default result table. For default setting see: **Program**|**Settings**|**Result table**
  ℹ NOTICE! It is not possible to start a measurement without a results table.

▸ Check the finished sequence for plausibility by clicking on ▱✓. The software checks whether the created measuring steps can be measured.

▸ Provide SST samples (TOC water, standards for sucrose and *p*-benzoquinone).

▸ Start the measurement by clicking on ▶ .

▸ If samples are fed manually, follow the software prompts and feed samples one after the other. Acknowledge the measurement of the samples.

  ✓ The software automatically evaluates the SST and outputs the result in the SST report.

You can view SST reports under **Result details**|**SSTs**.

13.6.2 Create SST

Use the **Create SST** wizard to prepare a system suitability test (SST) for TOC and NPOC measurements.

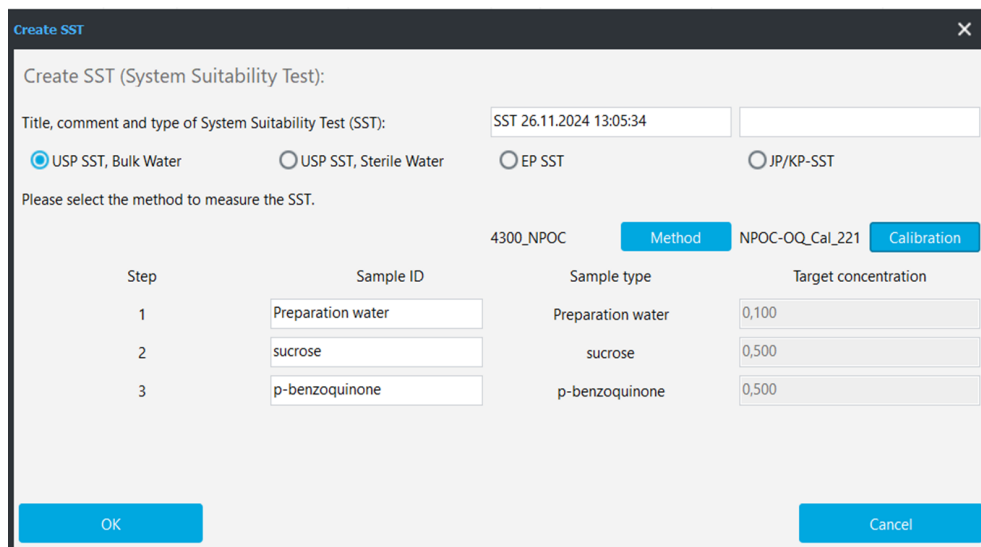Open the wizard via the ✿ icon in the **Add new sequence** window.

Layout

Fig. 43   Create SST

Element	Description
Input fields **Title, comment and type of System Suitability Test (SST):**	▪ Assign name for the SST The default name is: SST + timestamp. ▪ Optionally enter a comment
Radio buttons ▪ **USP SST, Bulk Water** ▪ **USP SST, Sterile Water** ▪ **EP SST** ▪ **JP-SST**	Select SST according to pharmacopoeia: ▪ SST test for ultrapure water according to USP 643 "Bulk Water" ▪ SST test according to USP 643 "Sterile Water" ▪ SST test according to EP 2.2.44 ▪ SST test according to JP 17 2.59 The software adjusts the target concentrations accordingly.
Button **Method**	Click on the **Method** button then select NPOC or TOC method in the **Select method** window
Button **Calibration**	Click on the **Calibration** button then select the calibration in the **Select calibration** window
Table with previous SST samples	**Step** Step number 1 to 3 **Sample ID** Type of SST sample: TOC water, sucrose, *p*-benzoquinone or TOC water, potassium hydrogen phthalate and sodium dodecyl benzenesulfonate (according to JP 17 2.59) **Sample type** Selected SST type **Target concentration** Target concentration The software specifies the target concentration according to the selected pharmacopoeia. Adjust the concentration as required.
Button **OK**	Transfer SST to the sequence
Button **cancel**	Cancel preparation of the SST

13.6.3 View results of System Suitability Tests in the SSTs window

The software automatically evaluates system suitability tests and displays the results in the **SSTs** window. Open the **SSTs** window using the menu command **Results|SSTs**.

In the SSTs window
- You manage the results of SSTs in the **Overview** table.
- You organize SSTs into groups by clicking on **Assign group** in the **Select group** window.
- Clicking on **Go to Result** to load the results table with the results of the SST measurements.
- Click on **Export** to export the results of selected SSTs in XML format, default export folder:
  C:/ProgramData/Analytik-Jena/multiWinPro/export/results.
- Click on **Report** to open the print preview and print or save the report in PDF format.

Layout of the window
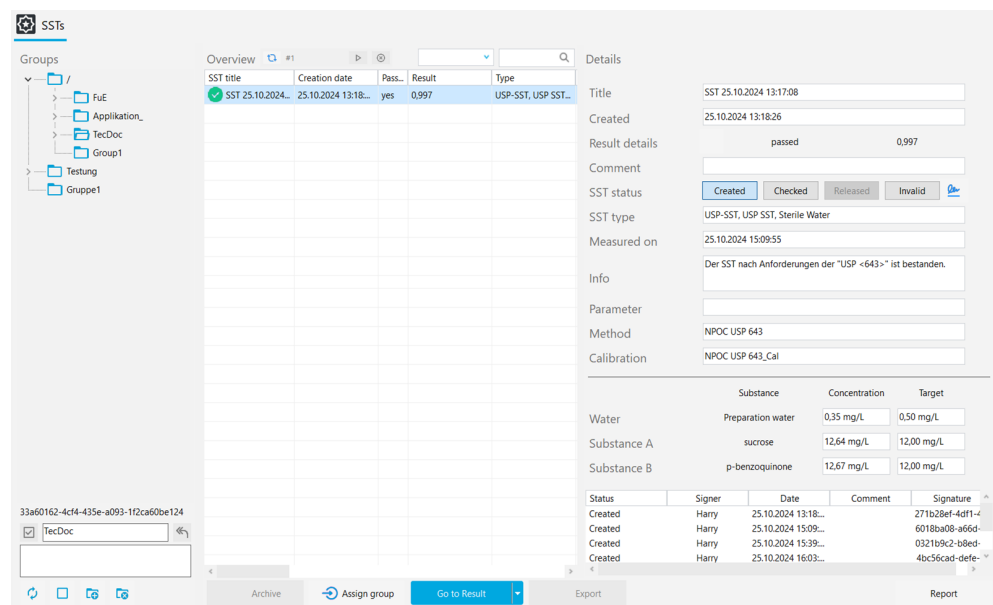
Fig. 44   SSTs window

Area	Description
Groups (left)	Manage groups
Overview (middle)	Tabular overview of the recorded SSTs with results and background information such as measurement success, measurement method and calibration
Details (right)	Detailed view with results of a selected SST with option to sign test and add comments

13.6.4 Overview table

The **Overview** table is part of the **SSTs** window. The tabular overview shows the results of the recorded system suitability tests (SST).

Column	Description
SST title	Name of the SST
Report created on	Measuring time
passed	Test success with display **passed** - **yes**/**no**

Column	Description
	The SST is passed if the SST quotient is 0.85 to 1.15. For JP 17 2.59, the measured TOC concentration of the sodium dodecyl sulfonate solution must be greater than 0.450 mg/l.
Result	Calculated SST quotient according to: TOC_{Net}(p-benzoquinone) / TOC_{Net}(sucrose)
Type	Perform the SST according to the following pharmacopoeia: - SST test for ultrapure water according to USP 643 "Bulk Water" - SST test according to USP 643 "Sterile Water" - SST test according to EP 2.2.44 - SST test according to JP 17 2.59
Start	Start of measurement
End	End of measurement
Info	Individual information
Water Substance A Substance B	Type of SST sample: TOC water, sucrose, p-benzoquinone or TOC water, potassium hydrogen phthalate and sodium dodecyl sulfonate (according to JP 17 2.59)
c(target, Water) c(target, A) c(target, B)	Target concentration of the SST samples (according to pharmacopoeia)
c(Water) c(A) c(B)	Measured concentration of the SST samples
Status	Signature
Comment	Individual information as comment
Method	Measurement method
Calibration	Calibration
Parameter	Measurement channel (NPOC or TOC)
Measured	Measurement success with display Measured - yes/no

13.6.5 Details detailed view

The **Details** table is part of the **SSTs** window. It shows detailed information on selected SSTs.

Displayed parameter	Description
Title	Editable name of the SST
Created	Time of preparation of SST
Result details	- Display **passed**/**NOT passed** - Display of the calculated SST quotient The software calculates the quotient according to: TOC_{Net}(p-benzoquinone) / TOC_{Net}(sucrose). The SST is passed if the SST quotient is 0.85 to 1.15. For JP 17 2.59, the measured TOC concentration of the sodium dodecyl sulfonate solution must be greater than 0.450 mg/l.
Comment	Individual information
SST status	- View the signing status of the SST - Release or block SST after testing

Displayed parameter	Description
SST type	Perform the SST according to the following pharmacopoeia: - SST test for ultrapure water according to USP 643 "Bulk Water" - SST test according to USP 643 "Sterile Water" - SST test according to EP 2.2.44 - SST test according to JP 17 2.59
Measured on	Measuring time
Info	Evaluation of the measurement success
Parameter	Measurement channel (NPOC or TOC)
Method	Measurement method
Calibration	Calibration
Results table	Tabular overview with measured concentrations and target concentrations for: - TOC water - Sucrose - p-benzoquinone According to JP 17 2.59: - TOC water - Potassium hydrogen phthalate - Sodium dodecyl sulfonate
Table of signatures	Detailed information on signatures

13.6.6 Viewing, printing and saving SST reports

Viewing the SST report

- Open the **SSTs** window with the **Result details|SSTs** menu option.
- Select the SST in the **Overview** table and view results in the **Details** view.
- Optionally add a comment under **Comment**.
- Release results after checking using the **Checked** and **Released** buttons.

Print report

- Click on **Report** to open the print preview.
- For a better overview, click on the **Page overview** button to display the navigation area with a page summary to the left of the report. Zoom in or out of the view by clicking on **Zoom in** and **Zoom out**.
- Add company logo to the report. Click on the **Load** button in the **Report logo** area, and then select the logo in the Windows file manager and load it into the report with **Open**.
- Click on **Printer options** to set up the printer.
- Click on **Page setup** to configure page settings such as paper size or orientation. Default: A4, portrait. Apply layout to current page or all report pages.
- Click on **Print** to start printing.

Save report

- Save the report by clicking on the **Save** button.
- Click on **Save** then specify the file name, storage directory and file type in the **Save as** window.

You can save reports in the following file formats: PDF (default), RTF, HTML, TXT, FP3.

List of figures