



OPERATING MANUAL

TitriSoft

SOFTWARE

Version 3.4.0/3.4.0 P

SI Analytics

a xylem brand

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1 System requirements

1.1 Hardware requirements

Processor	Min. Dual core, 2 MHz or comparable
RAM	Min. 4 GB
Disc space	Min 20 GB
Operating system	Windows 7 or higher
Miscellaneous	Microsoft .NET Framework 4.7 or higher
Interfaces	1 x RS 232 or 1 x USB

1.2 Compatibility

TitriSoft databases from version 3.3.0 on can be further used under Titrisoft 3.4.0.

Note: When opening a Titrisoft 3.3.x database for the first time, at least one user profile must be created, assigned to the users and then Titrisoft must be restarted. Once a database has been opened with Titrisoft 3.4, it can no longer be used under Titrisoft 3.3.x. Databases from versions older than TitriSoft 3.3.0 are not compatible.

2 Setup and installation

2.1 Setup und installation

Titrisoft is supplied on a USB stick which contains all necessary files and drivers.

For installation, the **Titrisoft_3.4_Setup** file is executed on the USB stick and the requested settings are made. The file path **C:\Xylem Analytics** is preset for the installation of Titrisoft.

After installation, this folder contains, among other things, 2 databases: an empty database **Titrisoft34.mdb** and a database with sample methods, **Titrisoft34_examples.mdb**. The pharmaceutical version of TitriSoft is additionally delivered with a **Titrisoft34_P.mdb** resp. **Titrisoft34_P_examples.mdb**.

After installation, the database can also be stored in a different location (e.g. a network drive). Full read and write rights must be available here.

2.2 First start of TitriSoft

Titrisoft is started by executing the Titrisoft.exe. This is located in the installation folder or is executed via the link on the desktop.



A login window opens. When TitriSoft is started for the first time no database is selected yet. Clicking on opens an Explorer window with which a database can be selected.

Login TitriSoft 3.4.0

Database C:\Daten\Titrisoft\Softwareversionen\TitriSoft 3.4\2020-0

User name

Password

ok cancel

The selection of the database is only available here at the first start. Afterwards the database can be selected via the system settings in TitriSoft.

In the supplied databases 3 users are preset.

user name	Password	Level
ad	ad	Administrator
ad1	ad1	Administrator
op	op	Level 1

The first login is executed with one of the administrators **ad** or **ad1** with password **ad** respectively **ad1**.

Login TitriSoft 3.4.0

Database C:\Xylem Analytics\TitriSoft 3.4\TitriSoft34.mdb

User name ad


Password ••

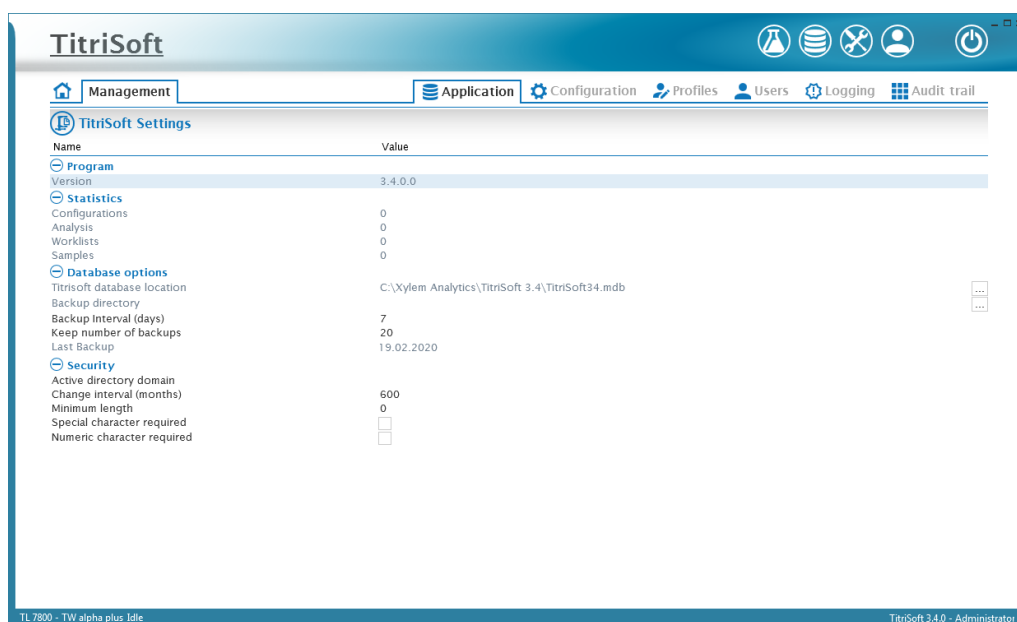
ok cancel

3 Settings Center

3.1 Management - Settings

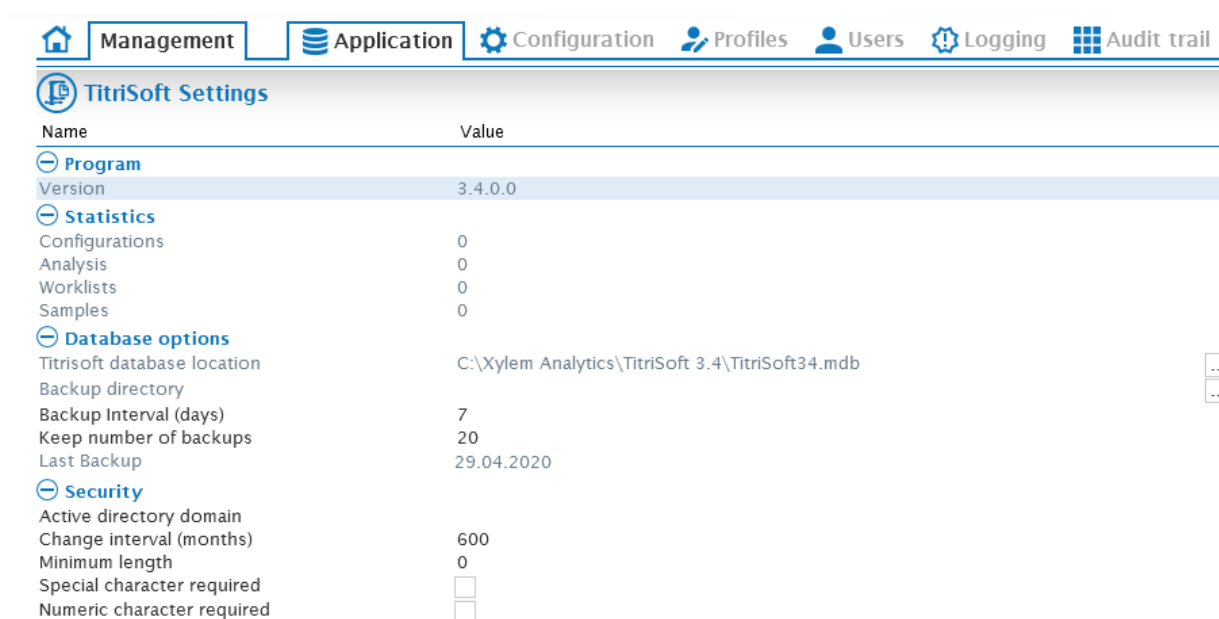
All system related settings for TitriSoft are done in the Settings Center. When TitriSoft is installed it is connected here with the instruments used, new users can be created or new databases can be selected.

The settings center can be reached by clicking on the  button.



3.2 Application

In the menu **Application** information about the current TitriSoft version, the database used as well as statistical information can be found.






Version	Shows the currently installed TitriSoft version
Statistics	Statistical data about the number of used configurations, methods, worklists and stored samples.
TitriSoft database location	A new database can be selected. See also Chapter 3.2.1 Selecting a database
Backup - directory	Location of the backup files.
Backup Interval (days)	Specifies the frequency of performed backups.

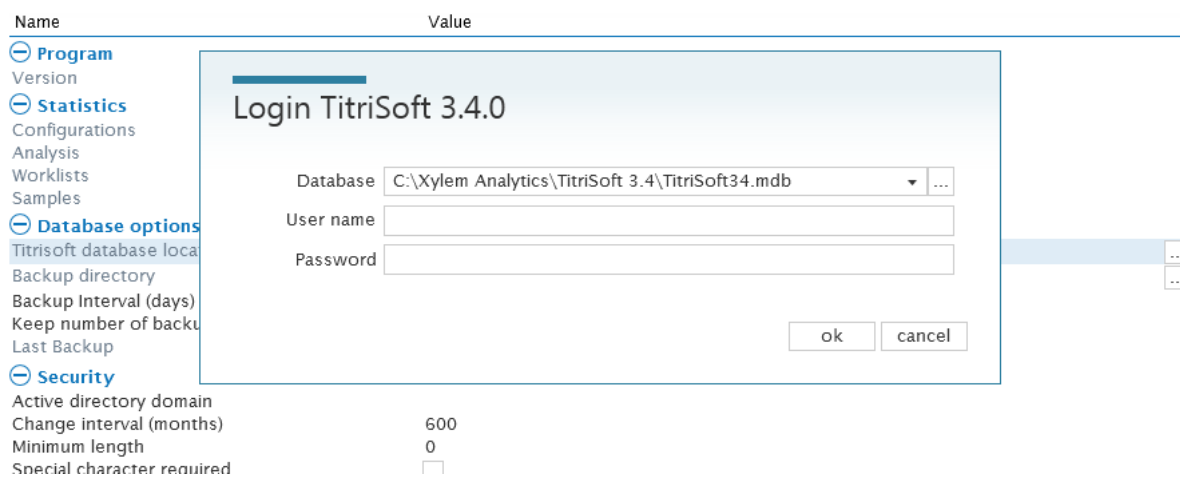
Keep number of backups	Defines the number of previously saved backup files. Files in excess of this number are automatically deleted.
Last Backup	Shows, when the last backup was performed.
Active directory domain	In preparation
Change interval (months)	Sets the time frame for a user to change the password. The new password should not be identical with the last two passwords used.
Minimum length	Defines the minimum length for a password.
Special character required	Defines if special characters are required for the password.
Numeric character required	Defines if numeric characters are required for the password.

3.2.1 Selecting a database

TitriSoft database location shows the file location where the current database is located.

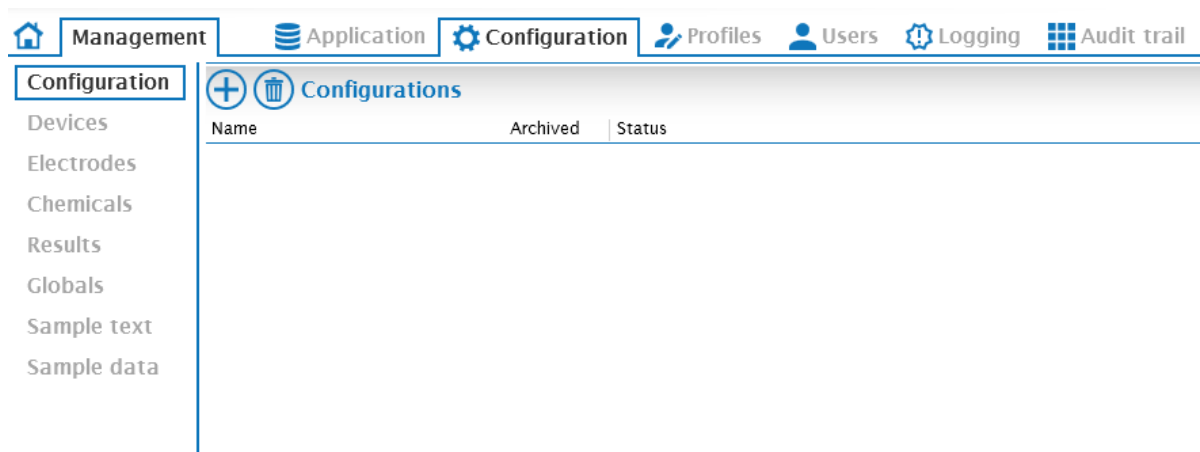


By clicking on  a new database can be selected. The normal startup window is shown after clicking. Here a dropdown menu  can be used to show the last used databases. By clicking on  an Explorer windows opens to select a new path and database.




3.3 Configuration

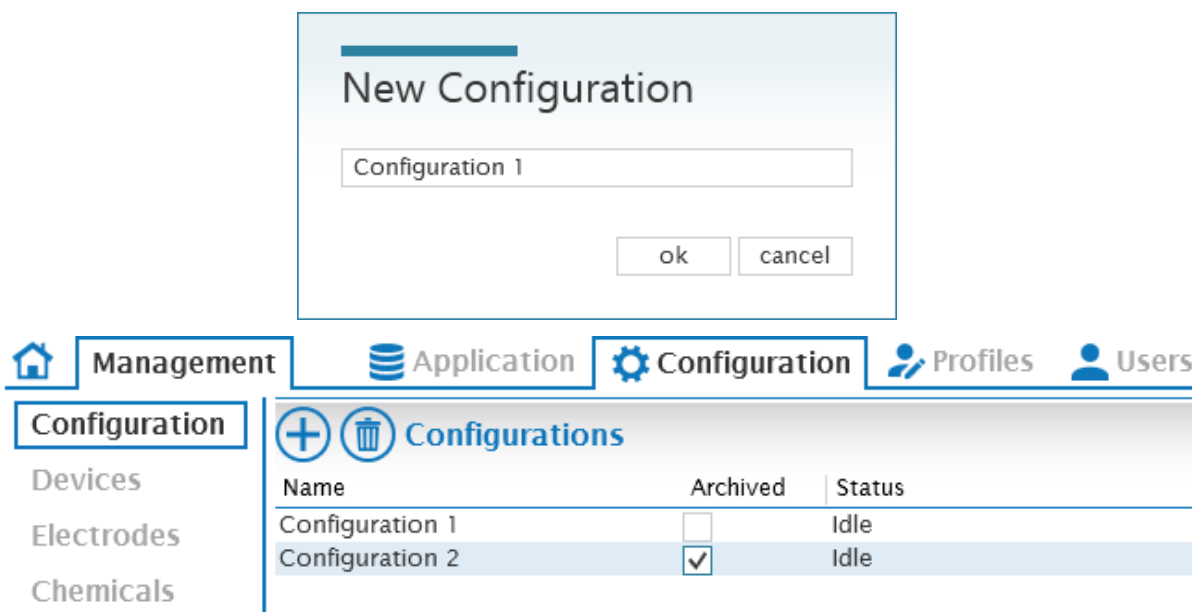
At **Configuration** configurations, serial ports, devices, electrodes, reagents as well as diverse variables are managed.



3.3.1 Configuration

A configuration is virtual combination of several devices. Within one configuration one Worklist can be active at the same time (see also chapter 4. **Titration Center**). If parallel Titrations shall be performed one configuration for each analysis executed at the same time is required.

With  a new configuration can be created. The name for the configuration is freely assignable.



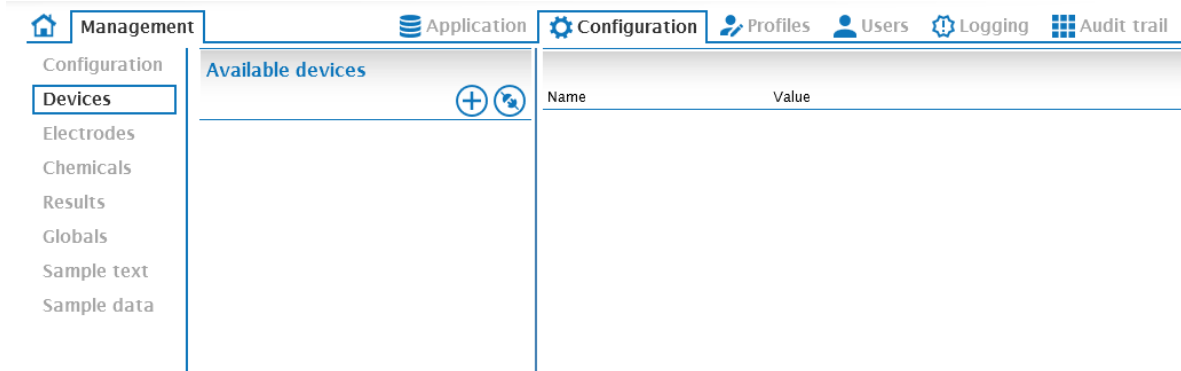
The new configuration is automatically available in the Titration Center.


A new configuration can be archived by marking the corresponding check box (for example Configuration 2). The archived Configuration is no longer available in the Titration Center. Archived Configurations can be reactivated by unmarking the checkbox at any time.

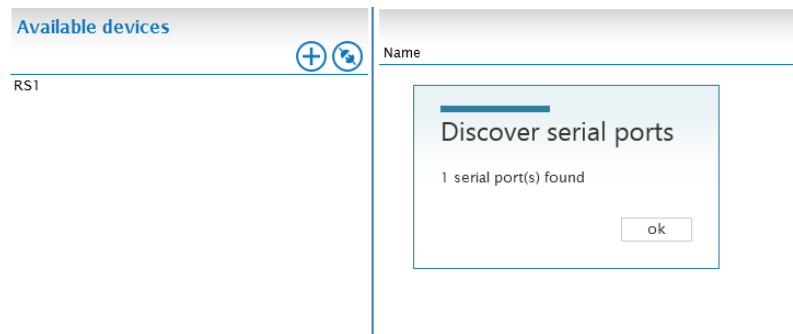
Note: Deleting a configuration automatically deletes all related data created with this configuration!

3.3.2 Devices

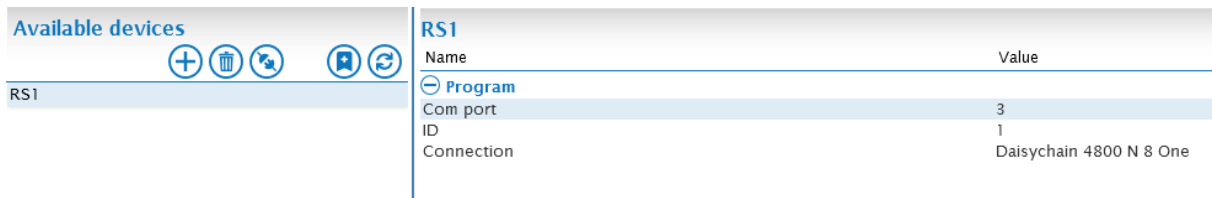
In the **Devices** section it is possible to scan for RS-Ports and devices connected to the COM – Port assigned to the RS.



By clicking on  all available serial ports are detected.



Hereby **RS1** refers to an internal port. In the right part of the window the properties of that internal port are shown and can be set.




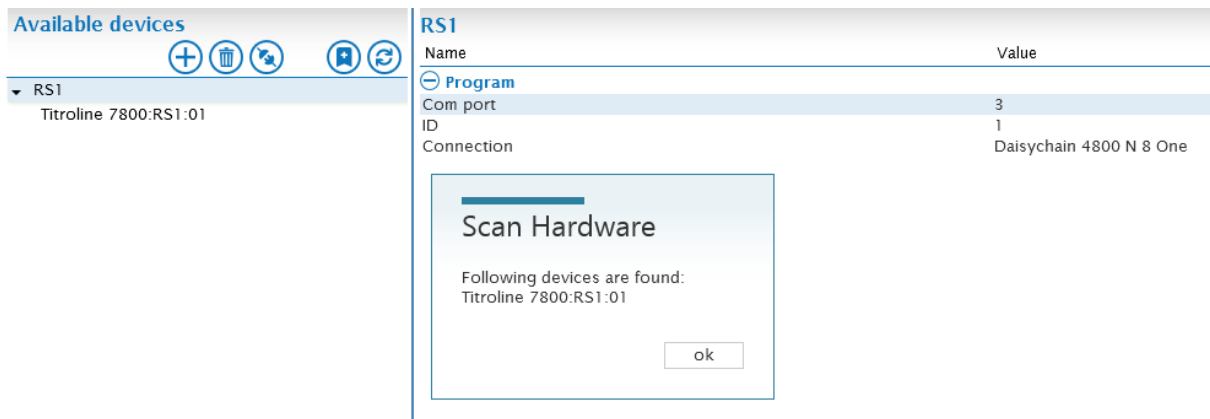
COM-Port is the computer address of the port to which the devices are connected.

ID is the internal RS address of the port (herer 1).

Connection defines the communication parameter of the port. **4800 N 8 one** is preset and appropriate for all latest titration devices. These correspond to the following parameters.


Baudrate	4800
Parity	No
Data Bits	8
Stop Bits	1

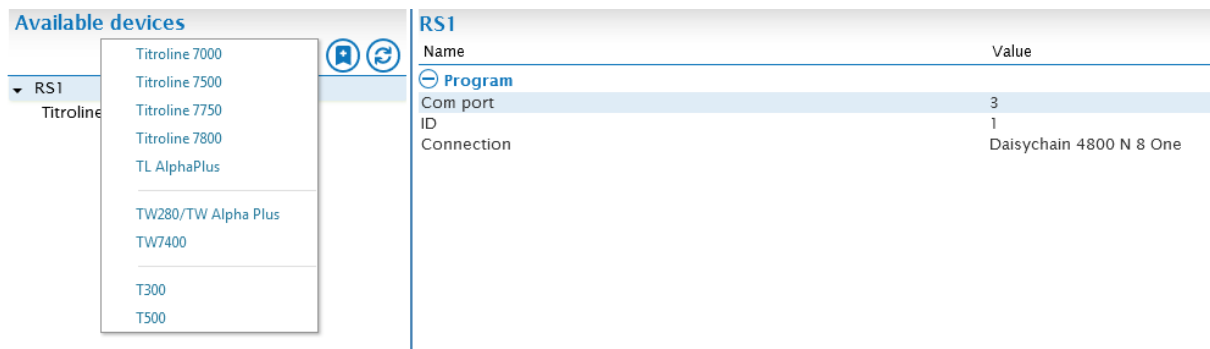
With  it is possible to scan for the devices connected to the COM port.



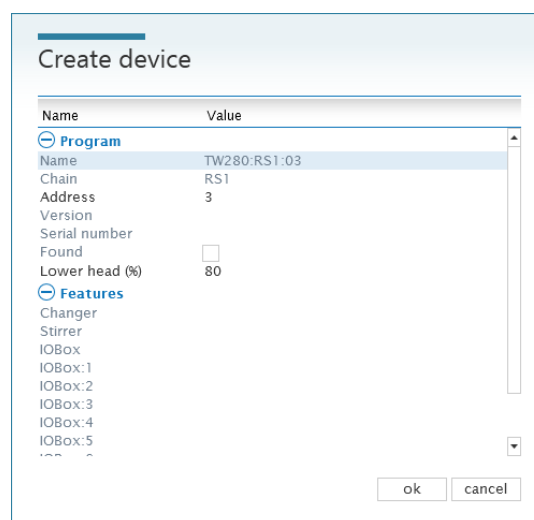
A popup window shows all devices found. The devices are automatically added to the RS port.


Note: RS1 also displays devices that were found during a previous scan or added manually. Devices with the same address are replaced.

Use  to manually add devices that are not connected but should be used. This is used, for example, to prepare methods and worklists.



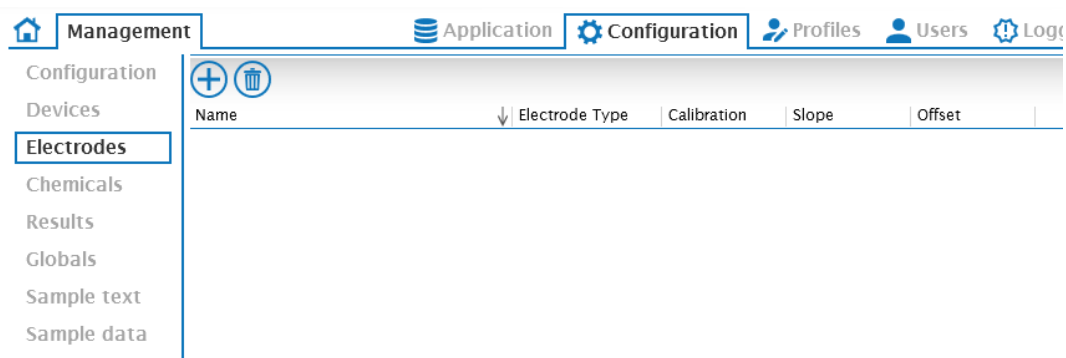
After selecting the desired device, it is listed under the RS port. The device address 0 is preset and must be adapted. In the following example a sample changer TW280 / TW alpha plus with address 3 was added.




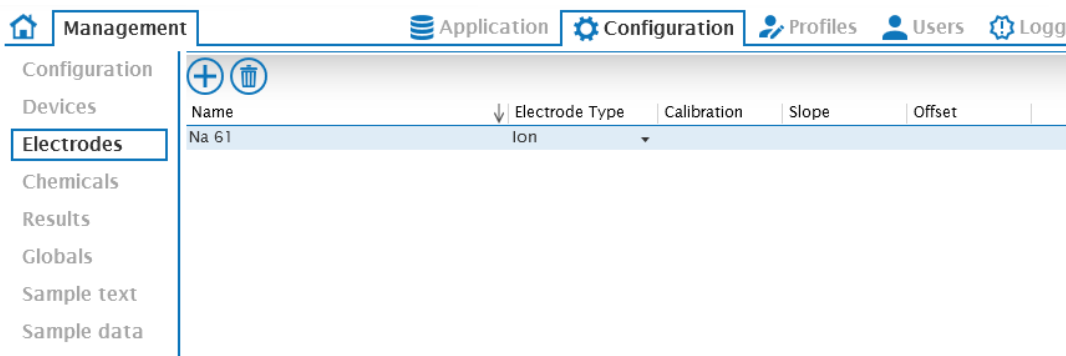
The button  is used to remove devices.

3.3.3 Electrodes

Electrodes used for ISE measurements are placed under **Electrodes**. Recorded calibration data can be viewed here.



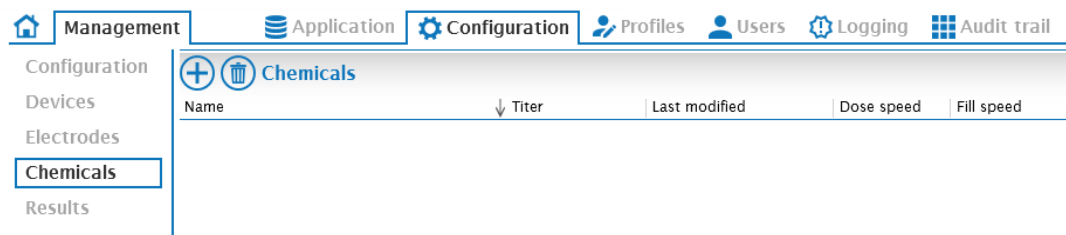
Use  to add a new electrode. The name is freely assignable (here **Na 61**).




An electrode here created is available in the Analysis Center for ISE measurements. Calibration data are automatically stored and can be seen in this section.

3.3.4 Chemicals

Created reagents are managed in the **Chemicals** section.



Use  to add a new reagent.

  Chemicals				
Name	Titer	Last modified	Dose speed	Fill speed
NaOH	0,1	04.05.2020 13:25	0	0

The name is freely assignable, the concentration value is editable.

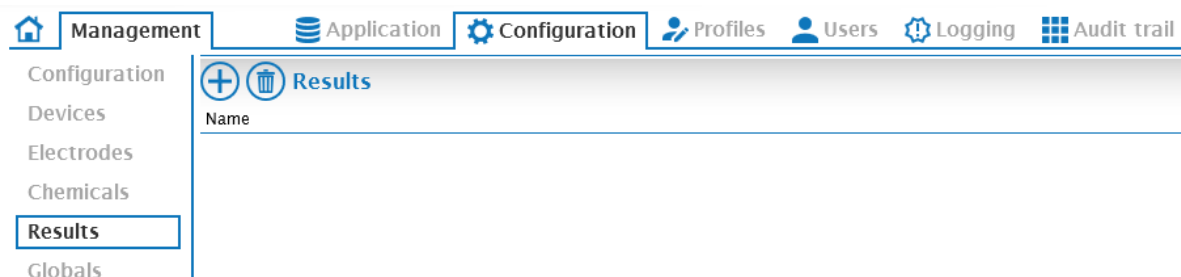
In case of an identical reagent name in TitriSoft and on the exchangeable head of the titrator/burette TitriSoft automatically reads the stored concentration and stores it in the database. Also if the name is identical, the concentration determined during a titer determination is transferred to the exchangeable head and saved.


Usually a new reagent is created in the Analysis Center. Reagents created there can also be found in this Chemical section.

A chemical that has already been used in a method can no longer be deleted.

3.3.5 Results

All available result variables are displayed in the **Results** section.



Press  to add a new result. The name is freely assignable. It is recommendable to use a description of the result together with its unit.



A result variable here created is available in the Analysis Center for calculations.

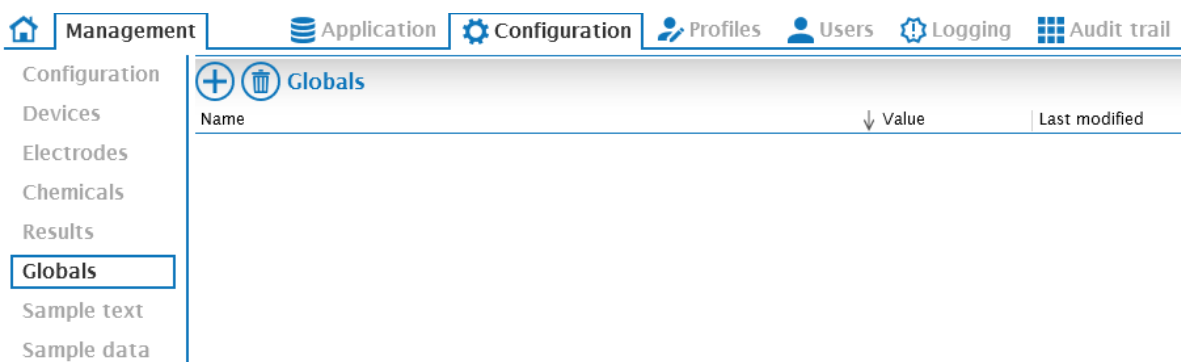
Usually a new result variable is created in the Analysis Center. Reagents created there can also be found in this result section.


A result variable that has already been used in a method can no longer be deleted.

3.3.6 Global Variables

All available global variables are displayed in the **Globals** section.

Global variables are variables that are available for calculations across methods. Global variables are used, for example, for blank values.



Press  to add a new global. The name is freely assignable. The value of the global variable is editable but usually determined by an analysis (for example titration of a blank value).

+ 🗑️ Globals		
Name	↓ Value	Last modified
Balnk value	0,735	04.05.2020 13:29

3.3.7 Sample text

All available Sample text variables are shown in the **Sample text** section.

Sample text variables are used to add additional information to a specific sample. One example for this could be the samples origin. When a sample text is used an additional editable text field is available in the Worklist, comparable to the comment field.

Press **+** to add a new Sample text variable. The name is freely assignable. The name assigned is the name of the editable column in the Worklist.

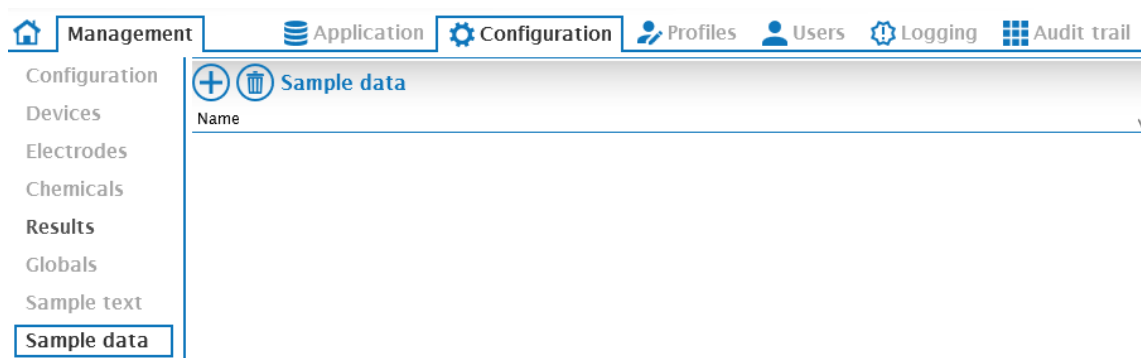
+ 🗑️ Sample data	
Name	↓
sample origin	


The sample text variables thus created are available in the Titration Center.

3.3.8 Sample data

All available Sample data variables are shown in the **Sample data** section.

Sample data variables are used to add additional numeric information to a specific sample. When a sample data variable is used an additional editable numeric field is available in the Worklist, comparable to the amount field.



Press  to add a new Sample data variable. The name is freely assignable. The name assigned is the name of the editable column in the Worklist.



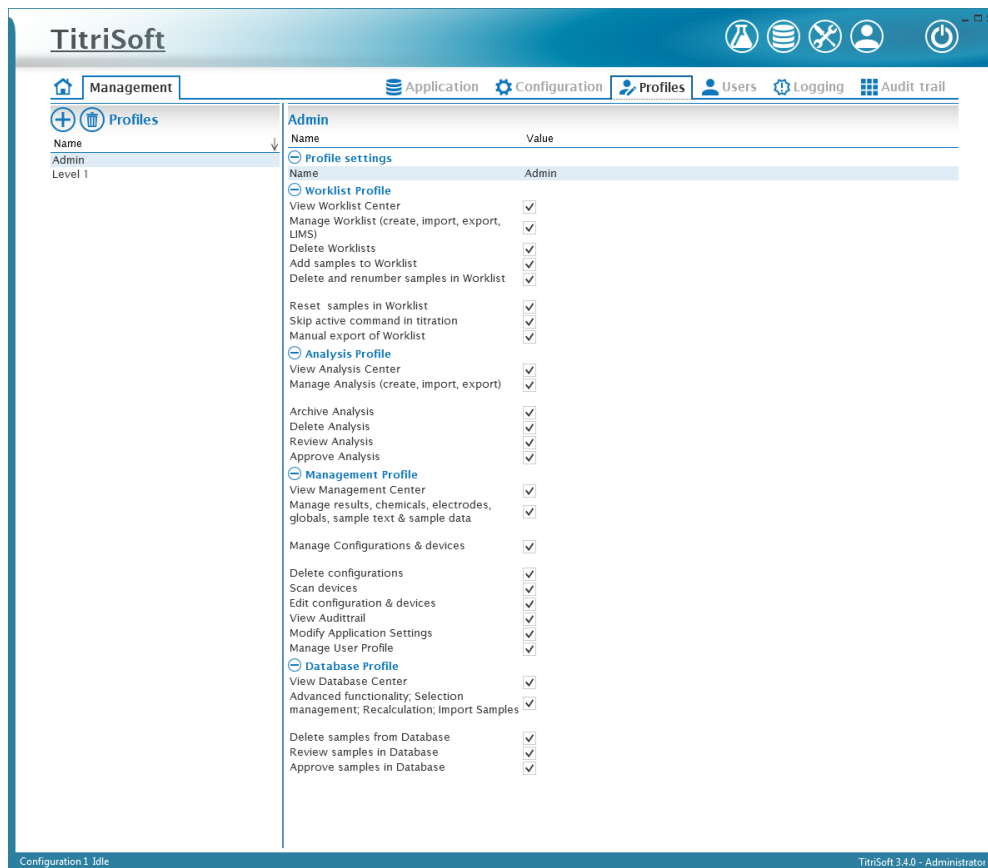
The sample text variables thus created are available in the Titration and Analysis Center.

3.4 Profiles

User profiles are set up and managed in the **Profiles** section.

Note: At least one profile with full administrator rights must be available and assigned to a user!

The profiles Admin (full user rights) and Level 1 (limited user rights) are preset.



3.4.1 Creating a user profile

Press  to add a new User profile. The name is freely assignable.

Enter user name

ok

cancel

The desired rights can be assigned in the **Profile Settings**.

Critical areas in the **Management Center** (everything except **View Management Center** and **Scan Devices**) and **Database Profile** (**Delete samples from database**) should be reserved for administrators.

Name	Value
Profile settings	
Name	Admin
Worklist Profile	
View Worklist Center	<input checked="" type="checkbox"/>
Manage Worklist (create, import, export, LIMS)	<input checked="" type="checkbox"/>
Delete Worklists	<input checked="" type="checkbox"/>
Add samples to Worklist	<input checked="" type="checkbox"/>
Delete and renumber samples in Worklist	<input checked="" type="checkbox"/>
Reset samples in Worklist	<input checked="" type="checkbox"/>
Skip active command in titration	<input checked="" type="checkbox"/>
Manual export of Worklist	<input checked="" type="checkbox"/>
Analysis Profile	
View Analysis Center	<input checked="" type="checkbox"/>
Manage Analysis (create, import, export)	<input checked="" type="checkbox"/>
Archive Analysis	<input checked="" type="checkbox"/>
Delete Analysis	<input checked="" type="checkbox"/>
Review Analysis	<input checked="" type="checkbox"/>
Approve Analysis	<input checked="" type="checkbox"/>
Management Profile	
View Management Center	<input checked="" type="checkbox"/>
Manage results, chemicals, electrodes, globals, sample text & sample data	<input checked="" type="checkbox"/>
Manage Configurations & devices	<input checked="" type="checkbox"/>
Delete configurations	<input checked="" type="checkbox"/>
Scan devices	<input checked="" type="checkbox"/>
Edit configuration & devices	<input checked="" type="checkbox"/>
View Audittrail	<input checked="" type="checkbox"/>
Modify Application Settings	<input checked="" type="checkbox"/>
Manage User Profile	<input checked="" type="checkbox"/>
Database Profile	
View Database Center	<input checked="" type="checkbox"/>
Advanced functionality; Selection management; Recalculation; Import Samples	<input checked="" type="checkbox"/>
Delete samples from Database	<input checked="" type="checkbox"/>
Review samples in Database	<input checked="" type="checkbox"/>
Approve samples in Database	<input checked="" type="checkbox"/>




All user profiles are available in the section **Users** and can there be assigned individually to single users.

3.5 Users

All created users are managed in the **Users** section.

Management					Application	Configuration	Profiles	Users	Logging	Audit trail
Users										
Name	↓ FullName	Profile	Last Login	Status						
ad	Administrator	Admin	04.05.2020	Active						
ad1	Administrator 1	Admin		Active						
op	Operator	Level 1		Active						

3.5.1 Functional overview

	Add a new user
	Reset Account
	Deactivate Account


3.5.2 Preset Users

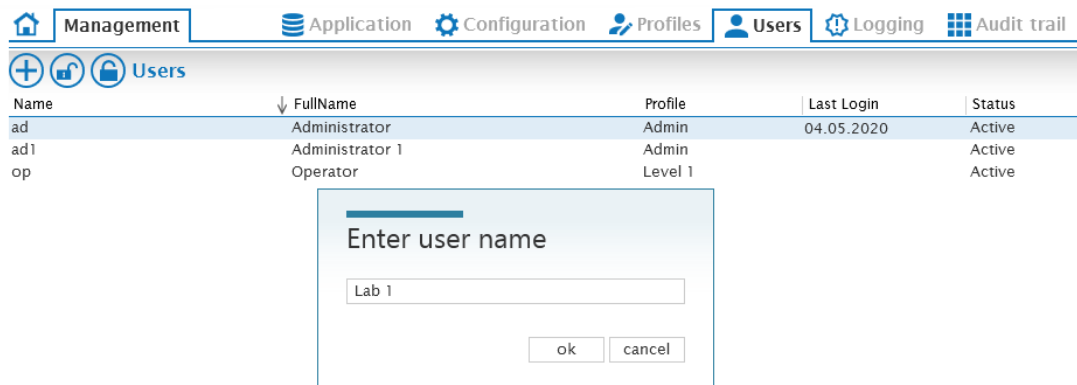
Three users are preset in the supplied databases. Two users have full administrator rights and one user has limited rights.

User name	Password	Full name	Level
ad	ad	Administrator	Admin
ad1	ad1	Administrator 1	Admin
op	op	Operator	Level 1

There must always be at least one user profile with full administrator rights!

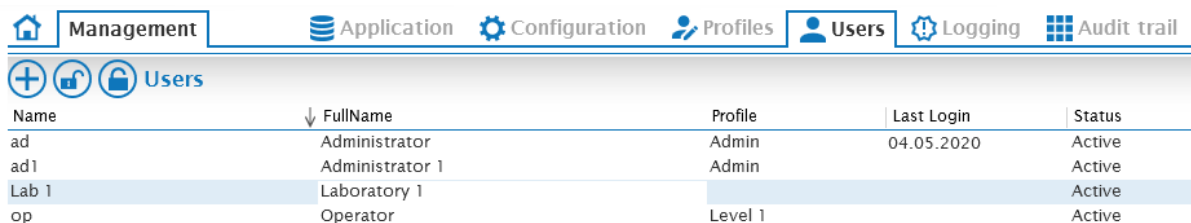
3.5.3 Creating new Users

Use  to create a new user. First the user name (login name resp. user ID) is entered.



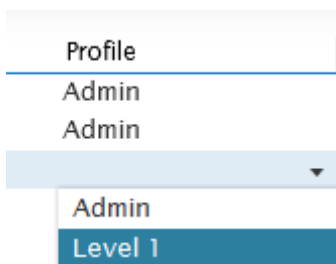
The screenshot shows the 'Users' management interface. The navigation bar includes 'Management', 'Application', 'Configuration', 'Profiles', 'Users', 'Logging', and 'Audit trail'. The 'Users' section is active, displaying a table with columns: Name, FullName, Profile, Last Login, and Status. The table lists three users: 'ad' (Administrator, Admin, 04.05.2020, Active), 'ad1' (Administrator 1, Admin, Active), and 'op' (Operator, Level 1, Active). A modal dialog box titled 'Enter user name' is open, with a text input field containing 'Lab 1' and 'ok' and 'cancel' buttons.

Then the full name is entered and a profile is assigned to the new user.



The screenshot shows the 'Users' management interface after a new user has been added. The table now includes a fourth user: 'Lab 1' (Laboratory 1, Admin, Active). The 'Profile' column for 'Lab 1' is highlighted, indicating it is selected. The navigation bar and other interface elements remain the same.

The user profile is selected via a drop-down menu in which the configured profiles are available for selection.




A new user must assign a password during the first login process. During the first login, the user name (User ID) is entered and confirmed with **ok** without entering a password.

A further window opens, in which the new password is assigned.

The password is active until expired or when an administrator has reset the account.

After entering a wrong password 6 times the account is automatically deactivated.

3.5.4 Reset account / Change password

To reset an account the  button is pressed. After the reset a new password needs to be assigned by the user.

Name	FullName	Profile	Last Login	Status
ad	Administrator	Admin	04.05.2020	Active
ad1	Administrator 1	Admin		Active
Lab 1	Laboratory 1	Level 1		Active
op	Operator	Level 1		Active

Reset

Sure to reset the Lab 1(Laboratory 1) account

The status of the user is changed to **Reset**

The next time the user logs in a new password needs to be assigned. Therefore the user id is entered and confirmed with **ok** without entering the password.

Login TitriSoft 3.4.0

Database

User name

Password

A further window opens, in which the new password is assigned.

Login TitriSoft 3.4.0

Old password


New password

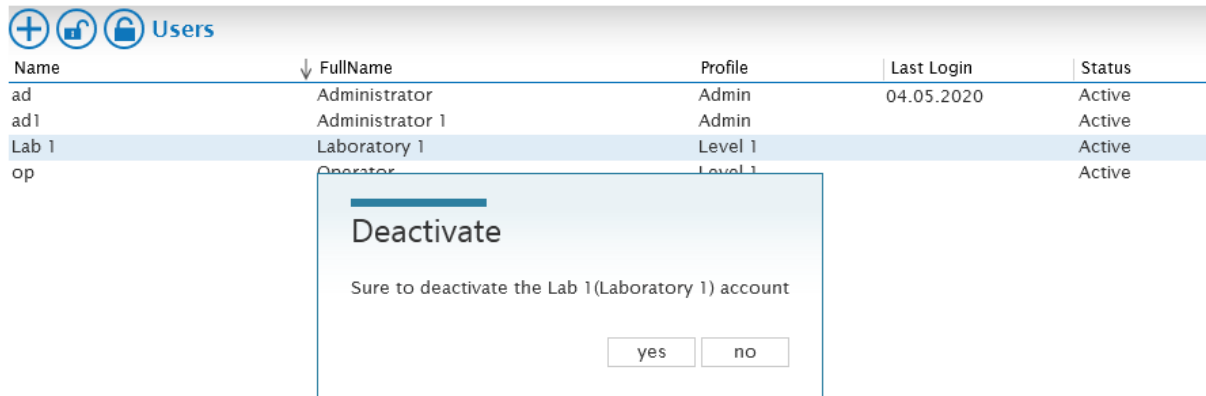
Confirm password

The new password must not be identical with the last two passwords used.

The password is active until expired or an administrator resets the account.

3.5.5 Deactivating an account

To deactivate an account the  button is pressed.

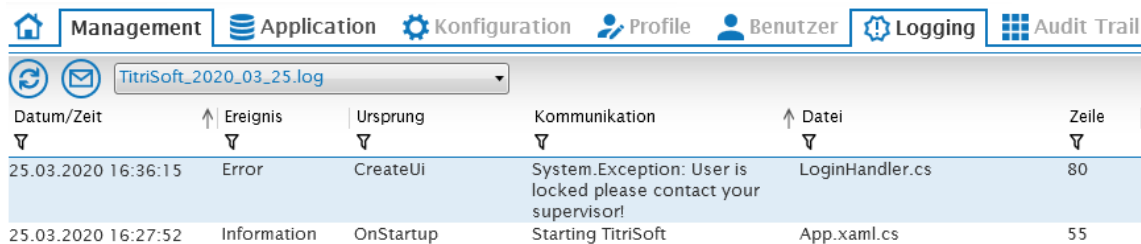


After deactivation the status of the user is changed to **Locked**. Deactivated users can no longer log in to TitriSoft.

To reactivate a deactivated user, the account must first be reset. Then the user can assign a new password.

3.6 Logging

Under **Logging** the communication of TitriSoft with the instruments is documented.




The log files are stored in the **Logging** subfolder. This is located in the same subfolder in which the **TitriSoft.exe** was installed.

Note: Log files are used for error analysis in case of problems with the RS communication!

3.7 Audit Trail

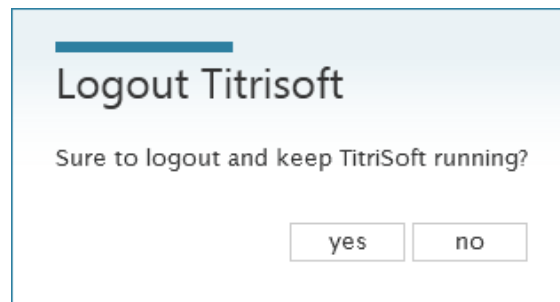
The Audit Trail is only available in the Pharma version of TitriSoft. Please refer to chapter **6. Pharma Version**.

3.8 Logout

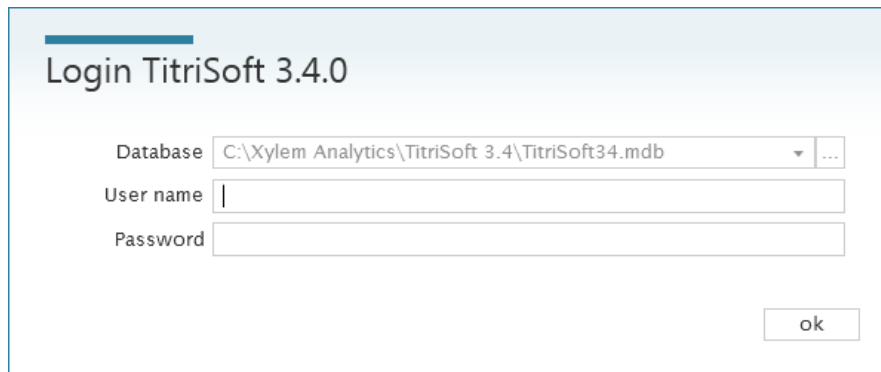
TitriSoft offers the possibility to log off or change a user. The Logout takes place via the button .



After confirmation of the logout the current user is logged out.



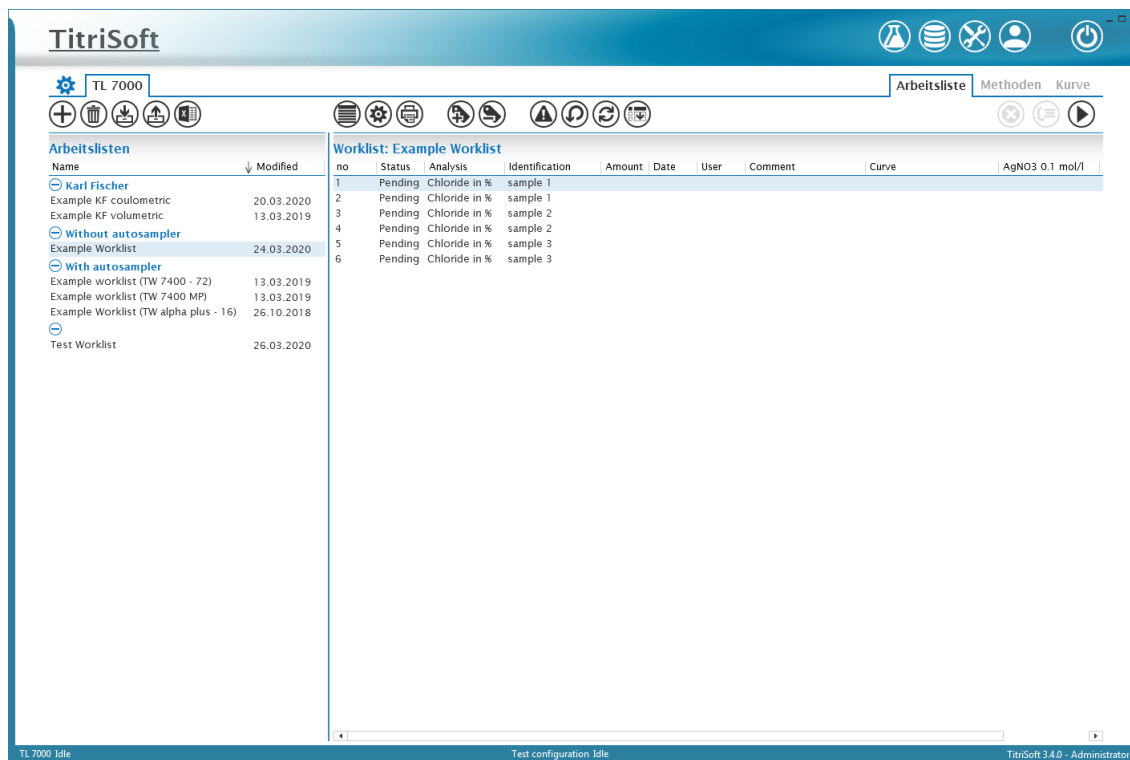
After logging out, the login window is displayed. TitriSoft continues working in the background.



The user from whom the sample was started is documented. When a new user logs in, the newly logged in user is documented. After a shift change it is thus traceable who was logged in to TitriSoft.

4 Titration Center









After each start of TitrSoft and login with user id and password the **Titration Center** opens automatically.









In the Titration Center the daily routine work is organized and performed. In the followed chapters the functionality of the Titration Center are explained.

4.1 Worklist Center

4.1.1 Functional overview

	Adding an deleting Worklists
	Im- and Exportieren of Worklists. See also chapter 4.1.2 Importing and exporting Worklists .
	Creates LIMS Excel-Templates.
	Organizes the coloms of the Worklist. See also chapter 4.1.3 Organizing Worklist columns .
	Opens the Worklist settings. See also Chapter 4.1.4 Worklist settings .
	Prints the current Worklist.
	Adding and removing of samples to the Worklist. After adding a sample the  of the column Analysis are used to select the analysis to be used. When adding samples afterwards this analysis is also automatically preselected for the coming samples.

	Setting a priority. This sample is given priority and measured as the next sample. The worklist is then processed normally.
	Resets a single sample or all samples to Pending state.
	Renumbers the samples in the worklist, e.g. after removing a sample.
	Cancels the active work list. The entire worklist is stopped immediately. The data of the current analysis is not saved.
	Skip the currently active titration block of a running method. This is mainly used to terminate titrations whose end criterion has not worked. All subsequent components such as calculations are carried out. The manual intervention is documented in the status of the sample.
	Starts a Worklist

4.1.2 Importing and exporting Worklists

Work lists can be exported and imported in a TitriSoft internal .tw file format. The worklist formats and settings are stored, allowing templates to be created.

4.1.3 Organizing Worklist columns

Title	In sample List	In Report	In Export
no	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Status	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Analysis	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Identification	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Amount	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Date	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
User	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Comment	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Position	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Curve	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
AgNO3 0.1 mol/l	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
EQ 1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Chloride [%]	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

The order of the columns in the worklists can be adjusted using the arrow keys. The checkboxes define which information should be displayed in the sample list, in the report (.pdf) and in the export (.xlsx or .csv).

4.1.4 Worklist settings

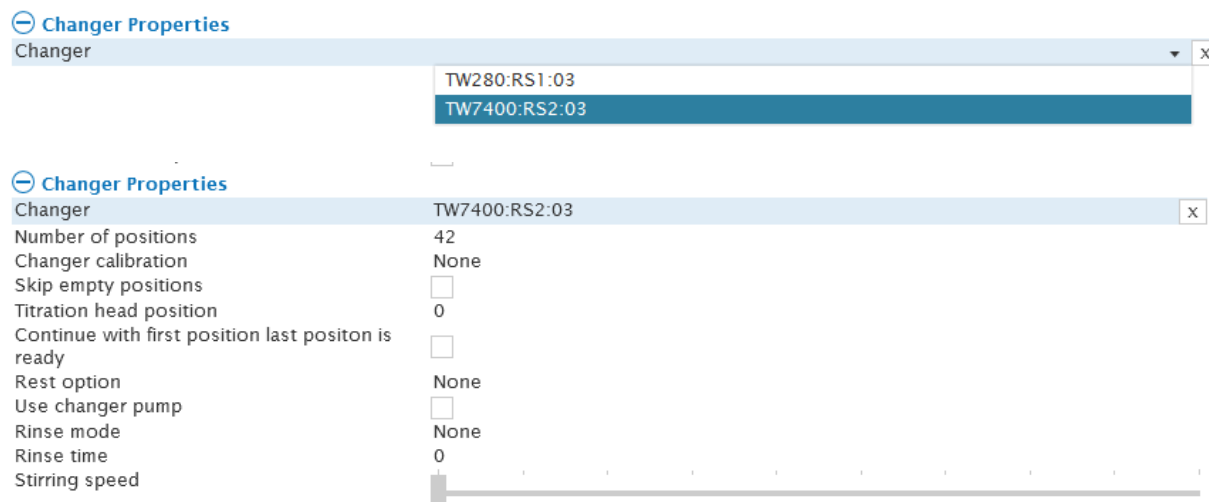


Name	Value
General	
Name	Example Worklist
Category	Without autosampler
Worklist type	Normal
Created by	Administrator
Created date	26.10.2018
Last modified	09.04.2020
Report Properties	
Report style	Curve list
Report title	
Is Landscape	<input type="checkbox"/>
Report on finish	<input type="checkbox"/>
Lims Import Properties	
Automatic import type	<input type="checkbox"/>
Export Properties	
Export on finish	None
Include date in export file name	<input type="checkbox"/>
Changer Properties	
Changer	

Name	Name of the Worklist
Category	Assigns a category to the worklist. Individual worklists can be grouped into freely definable categories for structuring purposes.
Worklist type	Normal or data collector. The Data Collector can be used if titration data should only be taken over from the titrator. The actual control of the titration is done by the titrator. Can only be used for volumetric or coulometric KF titrations.
Report style	Curve List, Sample List or Single Curve. Correspond to different printout formats .
Report title	Title that is printed as a header line on the report.
Is Landscape	When activated, the report is arranged in landscape format .
Report on finish	When activated, a report is automatically generated at the end of a work list. After activation, a storage path can be selected.
Automatic import type	Automatic import of a LIMS file to transfer sample information to the work list.
Export on finish	When activated, a .csv, .xlsx or .xslm file is automatically created when a worklist is completed. After activation a storage path can be selected.
Include date in export file name	When activated, a date and time are automatically added to the file name. Otherwise, an existing file will be overwritten.
Changer	When using a sample changer, it is selected here. For the settings see chapter 4.1.4.1. Using a sample changer.

4.1.4.1 Using a sample changer

Connected sample changers can be selected via a drop-down menu.



Number of positions	Corresponds to the number of positions of the plate or rack of the sample changer.
Changer calibration	When activated, a calibration of a pH electrode is carried out when a work list is started (2- or 3-point). The definition of the buffers to be used is made on the titrator.
Skip empty positions	Only for sample changers with beaker sensor. When activated, positions without beaker are skipped.
Titration head position	Defines the percentage by which the head is lowered during a titration.
Continue with first position last position is ready	When activated, the system continues with the first position after a complete run through the rack. Otherwise, the worklist finishes after one run.
Rest option	The sample changer moves to this position at the end of a work list.
Use changer pump	When activated, the pump is used for rinsing. The head position during rinsing can be defined. The positions in which the pump rinses are defined under the item Rinse mode. If None is selected here, the pump cleans in the sample position.
Rinse mode	Defines the positions in which the rinsing takes place. If no pump is active, the rinsing takes place in the beakers of the defined positions.
Rinse time	Defines the period for which the rinsing is to be carried out.
Stirring speed	Defines the stirring speed during the rinsing process. Not active when a pump is used.

4.2 Analysis Center













TitriSoft Worklist Analysis Curve

TL 7000

Analysis		Alkalinity (p+m)		Alkalinity (p+m)	
Name	Modified	Name	Value		
Methods					
Alkalinity (p+m)	04.05.2020	End point titration Titroline 7000:RS1:01:pHA 8,0; buret: Titroline 7000:RS1:01		Analysis Description	
Bases (non-aqueous)	26.10.2018	Formula: XatY(8,2)		Name	Alkalinity (p+m)
Beispiel Sample-Variable	24.03.2020	Formula: Result["ml at pH 8.2"]*Titer["HCl 0.1 mol/l"]*1000/Amount		Archived (not available in worklist)	<input type="checkbox"/>
Blank Bromine number	11.03.2019	End point titration Titroline 7000:RS1:01:pHA 4,1; buret: Titroline 7000:RS1:01		Version	1
Blank TAN ASTM 664	26.10.2018	Formula: XatY(4,3)		Category	Methods
Blank TBN ISO 3771	26.10.2018	Formula: Result["ml at pH 4.3"]*Titer["HCl 0.1 mol/l"]*1000/Amount		Created by	Administrator
Bromine number	11.03.2019			Created date	23.10.2018
Ca + Mg	26.10.2018			Last modified	04.05.2020
Chloride in %	26.10.2018			Analysis Properties	
Chloride in mg/l	26.10.2018			Stirrer	
COD Blank	26.10.2018			Balance	None
COD Sample	26.10.2018			Analysis Comment	
FOS/TAC	26.10.2018			Comment	
H2O2 (Ce(SO4)2)	26.10.2018				
Hydrochlorides	26.10.2018				
Mercaptane	13.03.2019				
Methode Nachrichten	26.03.2020				
pH Stat (Enzyme Kinetic)	23.03.2020				
pH Stat (Soil Samples)	26.10.2018				
pH strong acid	26.10.2018				
pH strong bases	26.10.2018				
SO2	11.03.2019				
Surfactants, anionic	13.03.2019				
Surfactants, cationic	13.03.2019				
TAN ASTM 664	26.10.2018				
TBN ISO 3771	26.10.2018				
Total acidity (pH 8.2)	26.10.2018				
Total Hardness	26.10.2018				
Karl Fischer Titrations					
KF Sample	13.03.2019				
KF Titer	26.10.2018				
Standardisation					
Titer AgNO3 0.1 mol/l	26.10.2018				
Titer COD	25.10.2018				
Titer EDTA 0.1 mol/l	26.10.2018				
Titer HCl 0.1 mol/l	26.10.2018				
Titer HClO4 0.1 mol/l	26.10.2018				
Titer KOH	11.03.2019				
Titer Na2S2O3 0.1 mol/l	26.10.2018				
Titer NaOH 0.1 mol/l	26.10.2018				

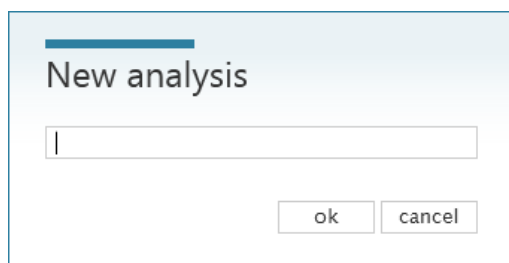
TL 7000 Idle TitriSoft 3.4.0 - Administrator

4.2.1 Functional overview

	Adds a new analysis. See also chapter 4.2.2 Adding a new analysis .
	Copies an existing method.
	Deleting a method.
	Importing an analysis
	Exporting an analysis
	Archive a method. This is no longer available in the worklist.
	Add titration commands to the method. See also chapter 4.2.3 Titration commands .
	Add logical queries to a method. See also chapter 4.2.4 Logical commands .
	Add automatic messages to a method. See also chapter 4.2.5 Interaction commands .
	Deletes an already inserted block from a method.
	Prints the currently displayed version of a method.
	Switches between the versions of a method. If a method was used for a titration at least once and then changed, the version number is automatically incremented and this version is used for the next titration. Old versions can be viewed and printed, but can no longer be used.

4.2.2 Adding a new analysis

After adding a new analysis, a name is assigned



The image shows a dialog box titled "New analysis". It has a light blue header bar with a white title "New analysis". Below the title is a text input field. At the bottom of the dialog, there are two buttons: "ok" and "cancel".

In the right window of the Analysis Center, the general information and settings of the method are displayed.

Alkalinity (p+m)

Name	Value
⊖ Analysis Description	
Name	Alkalinity (p+m)
Archived (not available in worklist)	<input type="checkbox"/>
Version	1
Category	Methods ...
Created by	Administrator
Created date	23.10.2018
Last modified	04.05.2020
⊖ Analysis Properties	
Stirrer	x
Balance	None
⊖ Analysis Comment	
Comment	

Name	Name of the analysis. Can be changed at any time (except pharma version for revised/approved analysis)
Category	Assigns a category to the analysis. Individual analyses can be grouped into freely definable categories for structuring purposes.
Stirrer	Defines the device that is to be used to control the stirrer. If a sample changer is used, its stirrer is used automatically regardless of the setting.
Balance	When using a balance to transfer sample weights, you can define here whether the transferred weight must be within defined limits (InRange) or is generally required (Required). Values that are outside the InRange limits are marked in red. With Required, the method can only be executed if a sample weight has been transferred or entered.
Comment	A manual comment can be added to an analysis method.

4.2.3 Titration commands

Various titration commands can be freely added for the execution of an analysis.


Titration loop
Calculation
Measurement
Dose Chemical
Delay time
Stirring speed
Clear curve
IO box
Direct command
ISE

4.2.3.1 Titration loops

Note: Titration loops only carry out the actual titration (measuring and dosing). Equivalence or end points are determined and documented using a calculation command.

4.2.3.1.1 Endpoint titrations

End point titration Titroline 7000:RS1:01:pHA 4,1; buret: Titroline 7000:RS1:01


Name	Value
Options	
Type	EndPoint
Parameter	Titroline 7000:RS1:01:pHA
Buret	Titroline 7000:RS1:01
Chemical	HCl 0.1 mol/l ...
Fill option	Finish
Stirring speed	
End criteria	
End value	4,1 ...
Use end volume	<input checked="" type="checkbox"/>
End volume	20 ...
End delay (sec)	10
Linear Step	0,02
Delta Value	1
Drift settings	
Measurement speed	Custom
Attenuation	None
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Slope Settings	
Slope type	Custom down
Maximal dose volume	1
Minimal dose volume	0,05
Slope by max. dose volume	10
Slope by min. dose volume	120
Display Settings	
Custum axis	<input type="checkbox"/>

Type	Defines the titration type, here Endpoint
Parameter	Defines the device with which the measurement is performed and the parameter to be measured (e.g. pH value)
Buret	Defines the instrument with which the titration reagent is to be dosed.
Chemical	Name of the reagent to be dosed. This must match the reagent name stored on the exchangeable head. Only in this way the stored concentration of the reagent is automatically taken over or, in the case of standardization/titer determination, stored on the exchangeable head.
Fill Option	Defines the time of automatic filling.
Stirring speed	Defines the stirring speed during the titration.
End value	Measuring value at which the titration stops automatically.

Use end volume	End volume at which the titration stops automatically, if activated. Recommended as safety criterion.
End delay (sec)	Time frame for which the end point must be held.
Linear Step	Step size for the linear titration part.
Delta Value	Delta criterion to the final value from which the dynamic titration changes to the linear titration.
Measurement speed	Defines the time after which a measured value is recorded and the next dosing step is carried out. Predefined or user-specific speeds can be used.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Slope type	Defines the slope type (rising/falling) and the step sizes in the dynamic part of the titration. Predefined or user-specific speeds can be used. If end values are used as end criteria, the slope type defines in which direction the end value lies (rising or falling curve).
Maximal dose volume	Maximum dosing step, which is applied on the slope at max. dosing volume.
Minimal dose volume	Minimum dosing step, which is applied on the slope at min. dosing volume.
Slope by max. dose volume	Slope of the titration curve at which the maximum dosing step is dosed.
Slope by min. dose volume	Slope of the titration curve at which the minimum dosing step is dosed.
Custom axis	User-specific axes can be defined for the titration graphics.

4.2.3.1.2 Linear Titration

Lineaire titration Titroline 7000:RS1:01:pHA 8,0; buret: Titroline 7000:RS1:01


Name	Value
Options	
Type	Lineair
Parameter	Titroline 7000:RS1:01:pHA
Buret	Titroline 7000:RS1:01
Chemical	HCl 0.1 mol/l ...
Fill option	Never
Stirring speed	
End criteria	
Use end value	<input type="checkbox"/>
Use end volume	<input checked="" type="checkbox"/>
End volume	20 ...
Number of EQ's	1
EQ Sensitivity	150
Linear Step	0,02
Drift settings	
Measurement speed	Custom
Attenuation	None
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Slope Settings	
Slope type	Down
Display Settings	
Custum axis	<input type="checkbox"/>

Type	Defines the titration type, here Linear
Parameter	Defines the device with which the measurement is performed and the parameter to be measured (e.g. pH value)
Buret	Defines the instrument with which the titration reagent is to be dosed.
Chemical	Name of the reagent to be dosed. This must match the reagent name stored on the exchangeable head. Only in this way the stored concentration of the reagent is automatically taken over or, in the case of standardization/titer determination, stored on the exchangeable head.
Fill Option	Defines the time of automatic filling.
Stirring speed	Defines the stirring speed during the titration.
Use end value	Measuring value at which the titration stops automatically if activated.
Use end volume	Final volume at which the titration stops automatically if activated. Recommended as safety criterion.
Number of EQ's	Number of EQ's to be used as stop criteria.

EQ Sensitivity	Slope of the titration curve from which a peak is to be evaluated as EQ.
Linear Step	Step size of the linear titration
Measurement speed	Defines the time after which a measured value is recorded and the next dosing step is carried out. Predefined or user-specific speeds can be used.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Slope type	Defines the slope type (rising/falling) and the step sizes in the dynamic part of the titration. Predefined or user-specific speeds can be used. If end values are used as end criteria, the slope type defines in which direction the end value lies (rising or falling curve).
Custom axis	User-specific axes can be defined for the titration graphics.

4.2.3.1.3 Dynamic Titration

Dynamic titration Titroline 7000:RS1:01:pHA 8,0; buret: Titroline 7000:RS1:01


Name	Value
Options	
Type	Dynamic
Parameter	Titroline 7000:RS1:01:pHA
Buret	Titroline 7000:RS1:01
Chemical	HCl 0.1 mol/l ...
Fill option	Never
Stirring speed	
End criteria	
Use end value	<input type="checkbox"/>
Use end volume	<input checked="" type="checkbox"/>
End volume	20 ...
Number of EQ's	1
EQ Sensitivity	150
Drift settings	
Measurement speed	Custom
Attenuation	None
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Slope Settings	
Slope type	Custom down
Maximal dose volume	1
Minimal dose volume	0,05
Slope by max. dose volume	10
Slope by min. dose volume	120
Display Settings	
Custom axis	<input type="checkbox"/>

Type	Defines the titration type, here Dynamic
Parameter	Defines the device with which the measurement is performed and the parameter to be measured (e.g. pH value)
Buret	Defines the instrument with which the titration reagent is to be dosed.
Chemical	Name of the reagent to be dosed. This must match the reagent name stored on the exchangeable head. Only in this way the stored concentration of the reagent is automatically taken over or, in the case of standardization/titer determination, stored on the exchangeable head.
Fill Option	Defines the time of automatic filling.
Stirring speed	Defines the stirring speed during the titration.
Use end value	Measuring value at which the titration stops automatically if activated.
Use end volume	Final volume at which the titration stops automatically if activated. Recommended as safety criterion.
Number of EQ's	Number of EQ's to be used as stop criteria.
EQ Sensitivity	Slope of the titration curve from which a peak is to be

	evaluated as EQ.
Measurement speed	Defines the time after which a measured value is recorded and the next dosing step is carried out. Predefined or user-specific speeds can be used.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Slope type	Defines the slope type (rising/falling) and the step sizes in the dynamic part of the titration. Predefined or user-specific speeds can be used. If end values are used as end criteria, the slope type defines in which direction the end value lies (rising or falling curve).
Maximal dose volume	Maximum dosing step, which is applied on the slope at max. dosing volume.
Minimal dose volume	Minimum dosing step, which is applied on the slope at min. dosing volume.
Slope by max. dose volume	Slope of the titration curve at which the maximum dosing step is dosed.
Slope by min. dose volume	Slope of the titration curve at which the minimum dosing step is dosed.
Custom axis	User-specific axes can be defined for the titration graphics.

4.2.3.1.4 pH-Stat Titration

pH Stat titration Titroline 7000:RS1:01:pHA 7; buret: Titroline 7000:RS1:01

Name	Value
Options	
Type	pHStat
Parameter	Titroline 7000:RS1:01:pHA
Buret	Titroline 7000:RS1:01
Chemical	NaOH 0.1 mol/l ...
Fill option	Never
Stirring speed	
End criteria	
Use end volume	<input type="checkbox"/>
Ph stat value	7
Linear Step	0,02
Delta Value	1
End time	600
Measurement interval (sec)	10
Drift settings	
Measurement speed	Custom
Attenuation	None
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Slope Settings	
Slope type	Custom up
Maximal dose volume	1
Minimal dose volume	0,02
Slope by max. dose volume	15
Slope by min. dose volume	230
Display Settings	
Custom axis	<input type="checkbox"/>

Type	Defines the titration type, here Linear
Parameter	Defines the device with which the measurement is performed and the parameter to be measured (e.g. pH value)
Buret	Defines the instrument with which the titration reagent is to be dosed.
Chemical	Name of the reagent to be dosed. This must match the reagent name stored on the exchangeable head. Only in this way the stored concentration of the reagent is automatically taken over or, in the case of standardization/titer determination, stored on the exchangeable head.
Fill Option	Defines the time of automatic filling.
Stirring speed	Defines the stirring speed during the titration.
Use end volume	Final volume at which the titration stops automatically if activated. Recommended as safety criterion.
pH-Stat value	pH value to be maintained during the stating phase.
Lineare Step	Step size for the linear titration part which is used to adjust the pH value.

Delta Value	Delta criterion from which the pretitration phase changes to the linear titration phase.
End time	Period over which the pH-stat titration is to be carried out.
Measurement intervall (s)	Distance between the data points of the pH-Stat curve.
Measurement speed	Defines the time after which a measured value is recorded and the next dosing step is carried out. Predefined or user-specific speeds can be used.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Slope type	Defines the slope type (rising/falling) and the step sizes in the dynamic part of the titration. Predefined or user-specific speeds can be used. If end values are used as end criteria, the slope type defines in which direction the end value lies (rising or falling curve).
Maximal dose volume	Maximum dosing step, which is applied on the slope at max. dosing volume.
Minimal dose volume	Minimum dosing step, which is applied on the slope at min. dosing volume.
Slope by max. dose volume	Slope of the titration curve at which the maximum dosing step is dosed.
Slope by min. dose volume	Slope of the titration curve at which the minimum dosing step is dosed.
Custom axis	User-specific axes can be defined for the titration graphics.

4.2.3.1.5 Photometric Titrations

To carry out a photometric titration, the photometric sensor OptiLine 6 is required. The measuring channel mVE is selected in the titration loop. Photometric titrations are usually carried out linearly, but can also be carried out dynamically depending on the titration course.

⊖ Optiline settings

Wave length	470nm
Intensity	40
Smoothing	None

Wavelength	Selection of the wavelength at which the titration is to be carried out. This depends on the indicator used and the resulting maximum potential difference before and after the color change.
Intensity	Percentage intensity of the LED used. The mV value at the beginning of the titration should be at about 1000.
Smoothing	Use of a smoothing of the measurement signal in case of noisy curves.

4.2.3.2 Calculations

A calculation generates results that are stored in the database. For titrations it is recommended to first calculate equivalence or end points and to carry out all further calculations with these calculated results.

Formula:

Name	Value
⊖ Calculation	
Type	Result
Result	...
Decimals	5
Smoothing	None
Maximums EQ's	-
Formula	...
Marker	None
⊖ X window	
Use X window	<input type="checkbox"/>
⊖ Y window	
Use Y window	<input type="checkbox"/>

Type	Defines the result respectively variable type. See also chapter 4.2.3.2.1 Result type .
Result	Name of the result. New names can be entered using <input type="text"/>
Decimals	Number of decimal places with which the result is to be specified.
Smoothing	Defines the number of data points used for the EQ calculation
Maximum EQ's	Maximum number of expected EQ's.
Formula	<input type="text"/> opens the formula editor to calculate the result. See also chapter 4.2.3.2.2. The Formula editor .
Marker	Sets a marker in the titration graphic (e.g. for EQ's) for the calculated result.

Use X window	Defines an evaluation window based on the x-axis.
Use Y window	Defines an evaluation window based on the y-axis.

4.2.3.2.1 Result type

Chemical
Global
Result
Sample

Chemical	If this type of variable is selected, the result is automatically transferred to the attachment used for titration and stored as titre. Note: The variable name must match the name stored on the exchangeable head!
Global	A global variable that can be used across methods. Example: Result of a blank titration.
Result	A local result variable.
Sample	A sample variable used for variable numerical sample properties such as density.

Example 1: Result - Variable

The Result variable is the most commonly used result variable. EQ's, measuring or final values are usually stored as a result - variable.

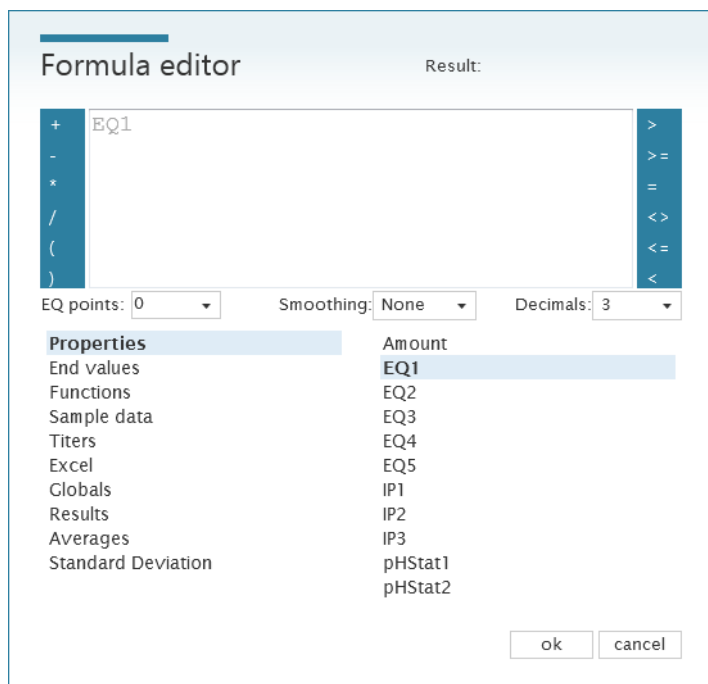
A result variable can be created in the Management Center, but also directly in the Analysis Center. Pushing opens an input window for entering the variable name, here EQ1.

Formula:

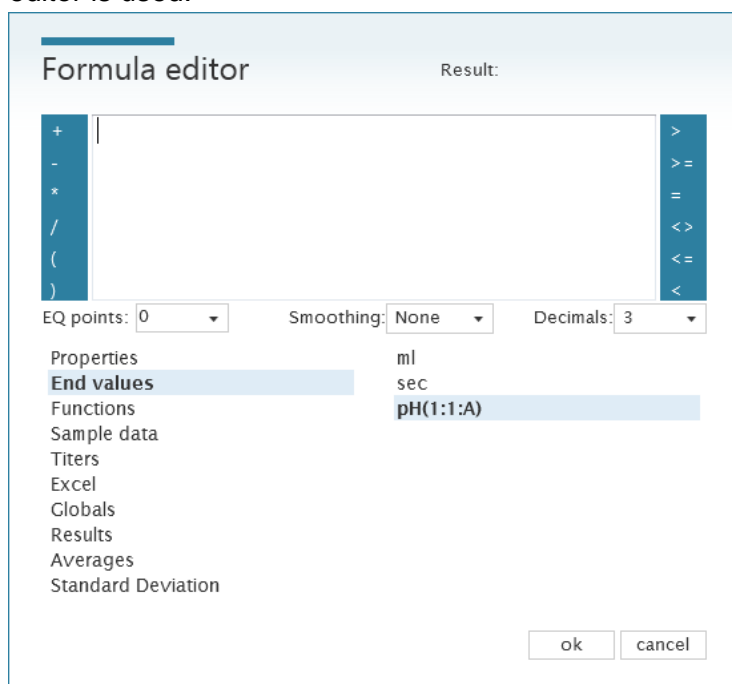
Name	Value
Calculation	
Type	Result
Decimals	3
Smoothing	None
Maximums EQ's	2
Formula	<input type="text" value="..."/>
Marker	None
X window	
Use X window	<input type="checkbox"/>
Y window	
Use Y window	<input type="checkbox"/>

Enter Result name

The calculation is done with the formula editor. In this example, the first of two expected equivalence points is calculated.



To document a measured value or a dosed volume, the **End values** menu in the formula editor is used.

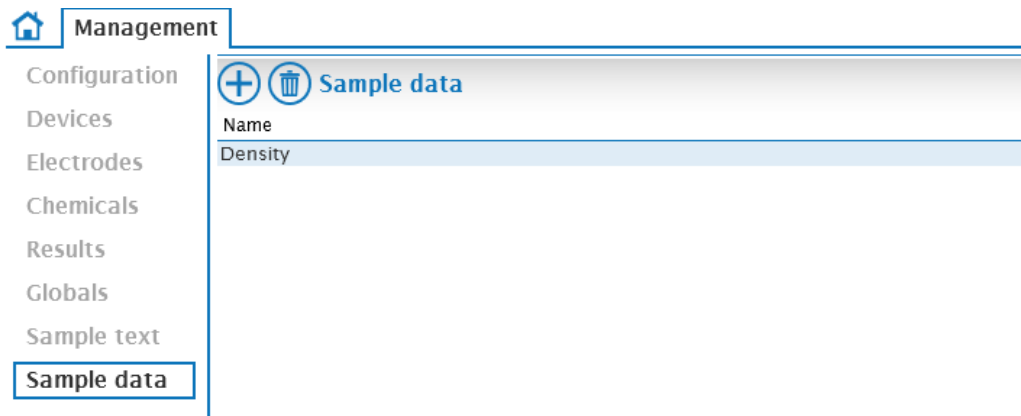


With this function the last measured value is calculated, e.g. a pH value but also a dosed volume using **ml**.

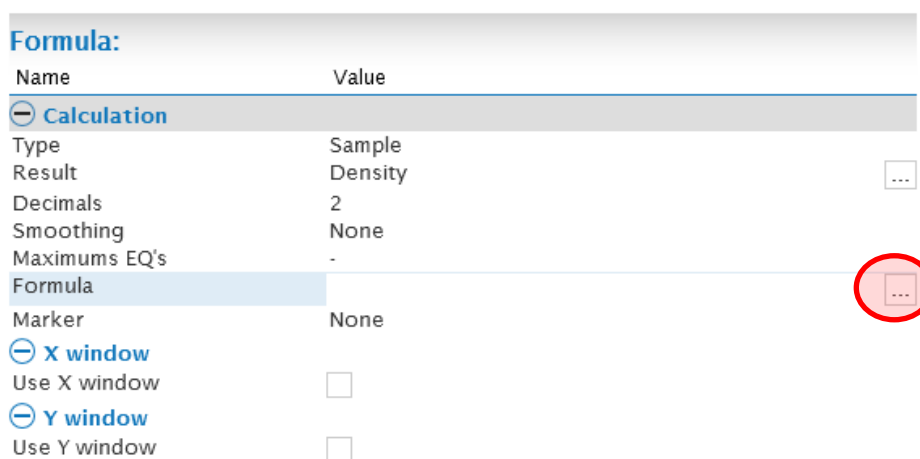
Results of the type Result are only available within one method for the respective sample. They are available for further calculations in the formula editor under **Results**.


Example 2: Sample-Variable

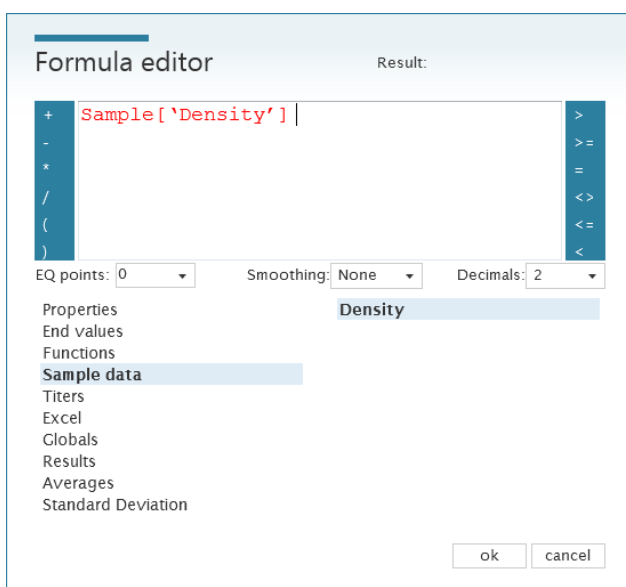
In the Settings Center a new variable is added via the + symbol.



In a calculation, the variable type **Sample** is selected and the corresponding variable is chosen.



Via  opens the formula editor. The corresponding variable is found under **Sample data** and is selected by double-clicking and confirmed with ok



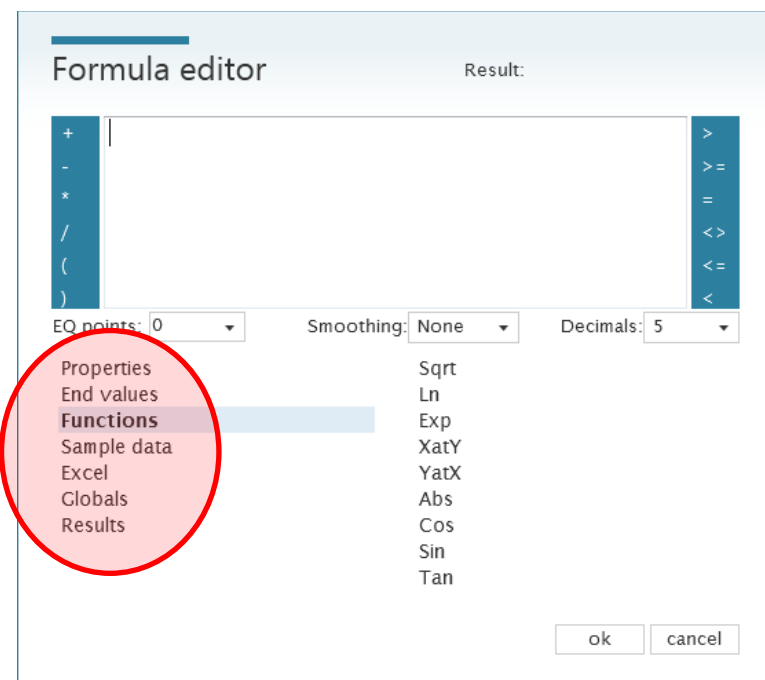
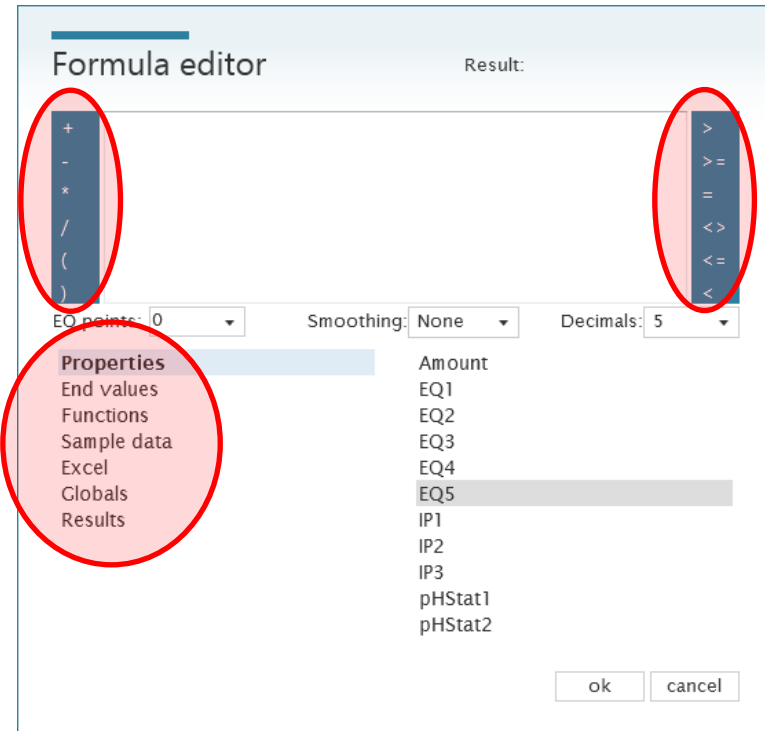
When the method is selected in the work list, the sample variable appears as a numeric input field. Alternatively, a variable created in the Settings Center can be used directly in a calculation, for example of a result variable. In this case the input field also appears automatically in the worklist.

Worklist: Example Worklist

no	Status	Analysis	Identification	Amount	Date	User	Comment	Curve	Density
1	Pending	Example Sample variable							

4.2.3.2.2 The Formula editor

General calculation symbols are located at the right and left edge of the editor. Variables and further calculation functions can be found in the submenus below.



Properties	Amount	Weighing of the sample.
	EQ1 – EQ5	Calculates up to 5 EQ's in the titration curve.
	IP1 – IP3	Calculates up to three intersection points.
	pHStat1 – pHStat2	In preparation.
End values	e.g. ml, pH, s	Corresponds to the last measured value at the end of a titration or a measurement.
Functions	Sqrt	Calculates the square root of a number.
	Ln	Calculates the natural logarithm of a number.
	Exp	Calculation of an exponential function.
	XatY;YatX	Calculates an x-value for a given y-value respectively a y-value for a given x-value.
	Abs	Calculates the absolute value of a number.
	Cos;Sin;Tan	Calculation of trigonometric functions.
Sample data	e.g. Density	Provides variable sample data for further calculation.
Excel		For external calculation using macro-based Excel sheets.
Globals		Use of results that are stored as global variables.
Results	z.B. ml at EQ1	Use of already calculated local results for further calculation.

4.2.3.3 Measuring command

A measuring command only carries out the actual measurement. The measured value must be documented by a calculation module.

Measure: Titroline 7000:RS1:01:pHA

Name	Value
Options	
Parameter	Titroline 7000:RS1:01:pHA
Stirring speed	
Delay (sec)	0
Delay message	
Drift settings	
Measurement speed	Custom
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Attenuation	None

Parameter	Defines the device with which the measurement is performed and the parameter to be measured (e.g. pH value)
Stirring speed	Defines the stirring speed during the measurement.
Delay (sec)	Defines a waiting period that starts after the measurement.
Delay message	A freely definable message that is displayed in the status line during the waiting period.
Measurement speed	Defines the time after which a measured value is recorded. Predefined or user-specific speeds can be used.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.

4.2.3.4 Dosage command

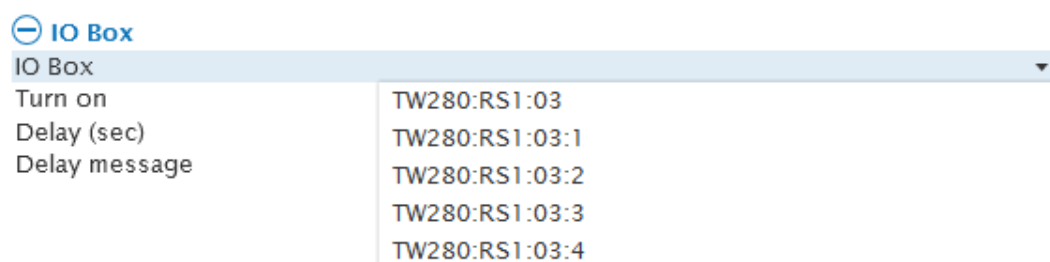
DoseVolume: 10 HCl 0.1 mol/l from Titroline 7000:RS1:01	
Name	Value
⊖ Dose	
Buret	Titroline 7000:RS1:01
Chemical	HCl 0.1 mol/l ...
Volume	10 ...
Delay (sec)	0
Do measurement	<input type="checkbox"/>
Fill option	Never

Buret	Defines the device with which the reagent is to be dosed
Chemical	Name des zu dosierenden Reagenzes. Dieser muss mit dem auf dem Wechsellaufsatz gespeicherten Reagenznamen übereinstimmen. Nur so wird die gespeicherte Konzentration des Reagenzes automatisch übernommen.
Volume	Specifies the volume to be dosed. Press ... to open the formula editor.
Delay (sec)	Defines a waiting period that starts after the dosage.
Messung durchführen	When activated, a measured value is automatically recorded after dosing.
Fill Option	Defines the time of automatic filling.

4.2.3.5 Delay time, Stirring speed and Clear curve

Delay time	Insert a waiting time. A message can be displayed during the waiting period.
Stirring speed	Inserting a stirring speed. A waiting time and message displayed during the waiting time can also be set.
Clear Curve	Resets a titration graphic e.g. after a predosage (dosing command) has been carried out, whose volume is not to be taken into account for the titration.

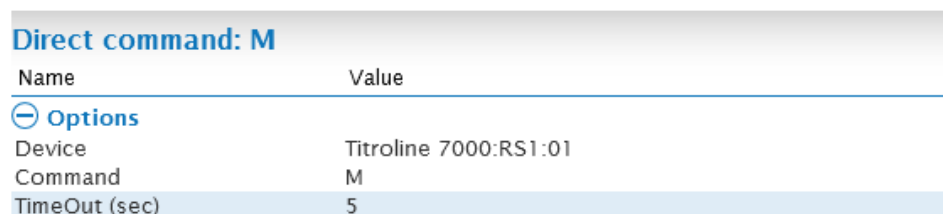
4.2.3.6 IO-Box



If a pump MP25 is directly connected to the sample changer, it can be switched on here for a defined period of time. This is done by selecting the port without address, here **TW280:RS1:03**.

An optional IO-Box for the use of additional accessories can also be connected to a sample changer. The port of the IO-Box is controlled by selecting the corresponding port 1 - 4 of the IO-Box to which the accessory is connected.

4.2.3.7 Direct command



Device	Device to which an RS command is to be sent.
Command	RS command, which is sent to the device as a direct command.
TimeOut (sec)	Waiting time which is kept after sending the direct command.

A list of the most important RS commands can be found in the corresponding device manuals.

4.2.3.8 ISE

ISE Calibration with

Name	Value
Options	
ISE type	Calibration
Parameter	Addition
Stirring speed	Calibration
Delay (sec)	
Delay message	
ISE options	
Electrode	
Measured value	...
Concentration	...
Drift settings	
Measurement speed	Turbo

4.2.3.8.1 ISE – Calibration

ISE Calibration with Titroline 7000:RS1:01:mVA

Name	Value
Options	
ISE type	Calibration
Parameter	Titroline 7000:RS1:01:mVA
Stirring speed	
Delay (sec)	0
Delay message	
ISE options	
Electrode	
Measured value	...
Concentration	...
Drift settings	
Measurement speed	Custom
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Attenuation	None

ISE type	Type of ISE measurement, here Calibration.
Parameter	Defines the device used for measurement and the parameter to be measured (e.g. mV).
Stirring speed	Defines the stirring speed during the measurement.
Delay (sec)	Defines a waiting period that starts after the measurement.
Delay message	A freely definable message that is displayed in the status line during the waiting period.
Electrode	Selection of the electrode for which the calibration data are recorded. This must be created in advance (see also chapter 3. Settings Center).
Measured value	Result variable to which the measured value is stored.

Concentration	Sample variable on which the concentration associated with the measured value is stored. The concentration is entered in the input field of the Worklist.
Measurement speed	Defines the time after which a measured value is recorded. Predefined or user-specific speeds can be used.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.

4.2.3.8.2 ISE - Measurement







ISE Measurement with Titroline 7000:RS1:01:mVA

Name	Value
Options	
ISE type	Measurement
Parameter	Titroline 7000:RS1:01:mVA
Stirring speed	
Delay (sec)	0
Delay message	
ISE options	
Electrode	
Measured value	...
Result	...
Decimals	-
Drift settings	
Measurement speed	Custom
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Attenuation	None

ISE Typ	Type of ISE measurement, here Calibration.
Parameter	Defines the device used for measurement and the parameter to be measured (e.g. mV).
Stirring speed	Defines the stirring speed during the measurement.
Delay (sec)	Defines a waiting period that starts after the measurement.
Delay message	A freely definable message that is displayed in the status line during the waiting period.

Electrode	Selection of the electrode for which the calibration data are recorded. This must be created in advance (see also chapter 3. Settings Center).
gemessener Wert	Result variable to which the measured value is stored.
Ergebnis	Result variable to which the concentration is stored, calculated from the measured value and the calibration line.
Decimals	Number of decimal places with which the result is to be specified.
Measurement speed	Defines the time after which a measured value is recorded. Predefined or user-specific speeds can be used.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.

4.2.3.8.3 ISE - Addition

ISE Addition with Titroline 7000:RS1:01:mVA	
Name	Value
Options	
ISE type	Addition
Parameter	Titroline 7000:RS1:01:mVA
Stirring speed	
Delay (sec)	0
Delay message	
ISE options	
Electrode	
Concentration	
Start Volume	
Result	
Decimals	-
Buret	
Number of additions	0
Volume	
Drift settings	
Measurement speed	Custom
Measurement period (s)	2
Delta mV/minute	20
Minimum time (s)	2
Maximum time (s)	15
Attenuation	None

ISE type	Type of ISE measurement, here Calibration.
Parameter	Defines the device used for measurement and the parameter to be measured (e.g. mV).
Stirring speed	Defines the stirring speed during the measurement.
Delay (sec)	Defines a waiting period that starts after the measurement.
Delay message	A freely definable message that is displayed in the status line during the waiting period.
Electrode	Selection of the electrode for which the calibration data are recorded. This must be created in advance (see also chapter 3. Settings Center).
Concentration	Sample variable, via which the concentration of the standard to be added is specified.
Start Volume	Sample variable used to specify the starting volume (sample volume including TISAB).
Result	Result variable to which the concentration is stored, calculated from the measured value and the calibration line.
Decimals	Number of decimal places with which the result is to be specified.
Buret	Burette that doses the addition standard.
Number of additions	Specification of the number of standard additions to be performed.
Volume	Indication of the volume to be dosed per addition step.
Measurement speed	Defines the time after which a measured value is recorded. Predefined or user-specific speeds can be used.
Measurement period (s)	Period used to record a measured value.
Delta mv/Minute	Stability criterion for the next dosing step of the titration.
Minimum time (s)	Minimum time to wait for the next dosing step.
Maximum time (s)	Maximum time to wait for the next dosing step.
Attenuation	Use of a smoothing of the measurement signal. Usually used for non-aqueous titration.

4.2.4 Logical Commands

The following loops / queries are executed as long as the criterion formulated in the condition is fulfilled. The criterion is defined in the formula editor of the respective query.

Repeat
While loop
If statement
Sleep Analysis


Repeat	The number of repetitions to be performed is defined in the loop condition.
While loop	The commands in the loop are executed as long as the criterion is fulfilled.
If statement	The commands in the loop are executed if the criterion is fulfilled.
Sleep Analysis	In preparation.

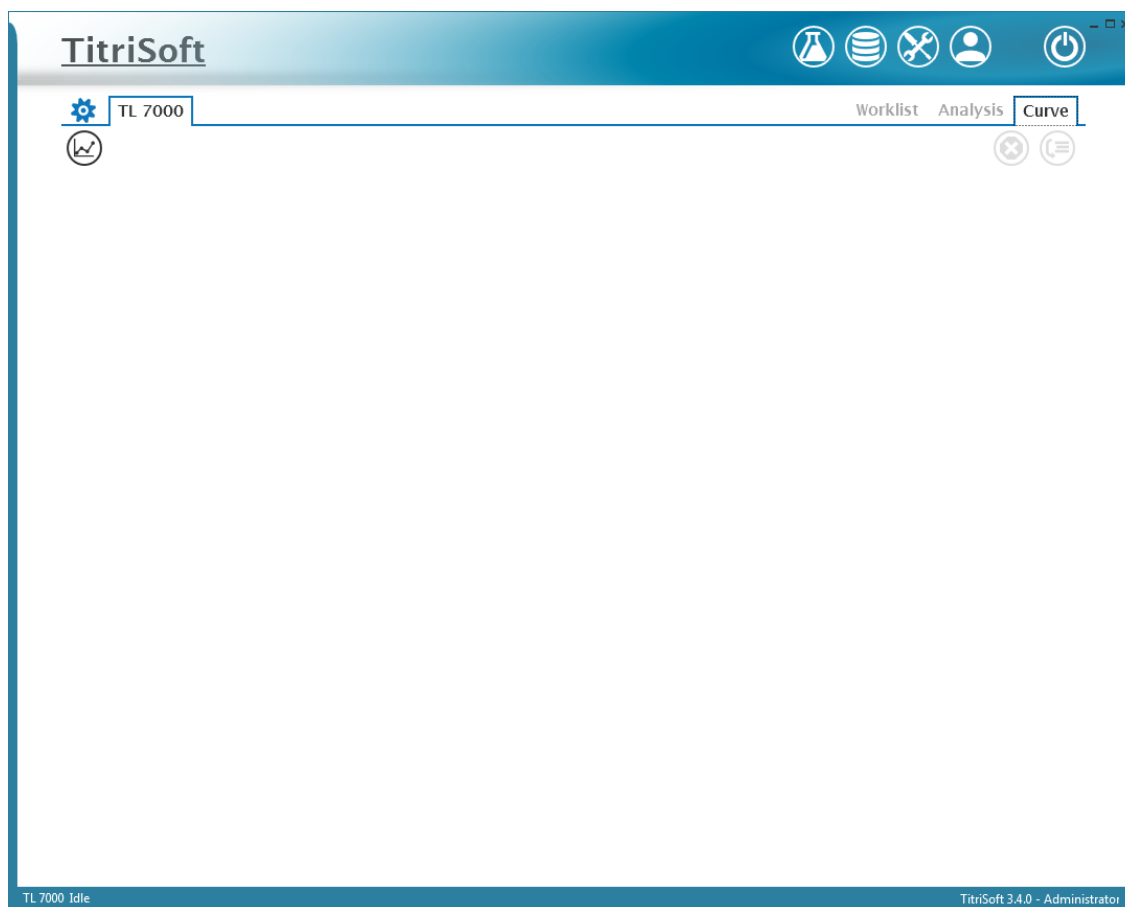
4.2.5 Interaction commands


Message box
Input box
Amount box
Sample text

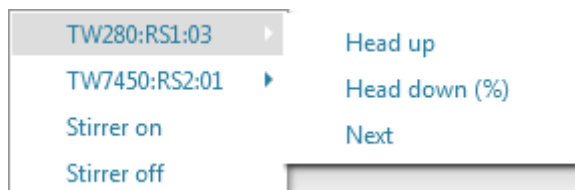
Message box	A title and a message can be entered. After confirming the message, the method continues with the next block.
Input box	A command prompt appears. The input is stored on a freely definable variable type.
Amount box	A prompt for an initial weight (Amount) appears. If the balance is connected, the window can optionally close as soon as data has been received.
Sample text	When using the method, an additional sample text variable is displayed in the work list as an input field.

4.3 Curve and Quick access to the Sample Changer

In the **Curve** area, the online curve of the titration is displayed in large size during a titration. The titration points can optionally be displayed via the  symbol.



Direct commands can be sent to a sample changer via the  symbol. This symbol can be reached from any window in the Titration Center.



Head up	Moves the head of the selected sample changer to the highest position.
Head down (%)	Lowers the head of the sample changer by the specified percentage.
Next	Moves the sample changer to the next position.
Stirrer on	Switches on the stirrers of all connected devices.
Stirrer off	Switches off the stirrers of all connected devices.

4.4 Example sequence of a method

In the following, the procedure of a method is explained in more detail using an example. TitrISOft is supplied with an Examples database that contains further method examples.

Procedure of the example method:

Analysis Example sequence of a method	
Example sequence of a method	
Measure: Titroline 7800:RS1:01:pHB	
Formula: End['pH(1:1:B)']	
DoseVolume: 30 Water from Titroline 7000:RS1:02	
Clear curve data	
Dynamic titration Titroline 7800:RS1:01:mVA ;; buret: Titroline 7800:RS1:01	
Formula: EQ1	
Formula: Result['EQ 1']*Titer['AgNO3 0.1 mol/l']*0.1*35.453/Amount	

1. Measurement

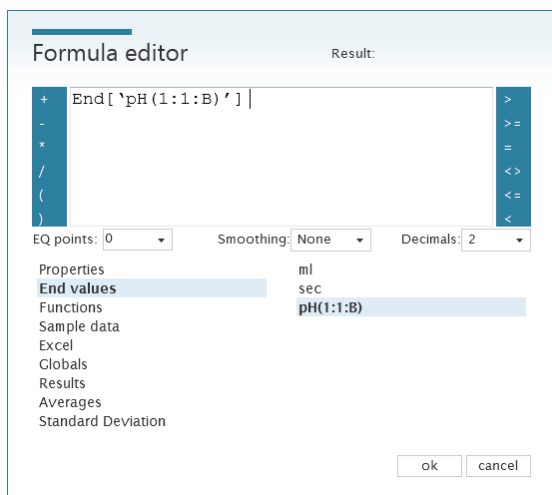
At the beginning of the method the start pH value of the sample is measured. This module only carries out the measurement of the pH value, the documentation is carried out in step 2. A TL 7800 is used, measuring channel B.

Measure: Titroline 7800:RS1:01:pHB	
Name	Value
Options	
Parameter	Titroline 7800:RS1:01:pHB
Stirring speed	<input type="range"/>
Delay (sec)	0
Delay message	
Drift settings	
Measurement speed	Normal

2. Calculation of the Start pH value

A calculation module is inserted to document the pH value. The pH value is selected in the formula editor of this command under the section End values.

Formula: End['pH(1:1:B)']	
Name	Value
Calculation	
Type	Result
Result	Start pH <input type="button" value="..."/>
Decimals	2
Smoothing	None
Maximums EQ's	-
Formula	End['pH(1:1:B)'] <input type="button" value="..."/>
Marker	None
X window	
Use X window	<input type="checkbox"/>
Y window	
Use Y window	<input type="checkbox"/>



The numbers in brackets stand for: RS1, device address 1, measuring channel B.

3. Dilution of the sample

A dosing command is used to dilute the sample with 30 ml water. A TL 7000 with address 2 is used as dosing burette.

Dosiere Volumen: 30 Wasser von Titroline 7000:RS1:02	
Name	Value
⊖ Dosieren	
Bürette	Titroline 7000:RS1:02
Reagenz	Wasser ...
Volumen	30 ...
Wartezeit (s)	0
Messung durchführen	<input type="checkbox"/>
Füll-Optionen	Finish

4. Reset of the Titration curve

A **Clear Curve** is used to reset the curve before titration. Otherwise the 30 ml predosage volume of water would be included in the titration curve.

Note: If a pre-titration is carried out, no Clear Curve module would be used.

5. Dynamic Titration

A dynamic titration with AgNO₃ on mV is performed. Measuring channel A is used to determine the chloride content of the sample.

Dynamic titration Titroline 7800:RS1:01:mVA ;; buret: Titroline 7800:RS1:01	
Name	Value
Options	
Type	Dynamic
Parameter	Titroline 7800:RS1:01:mVA
Buret	Titroline 7800:RS1:01
Chemical	AgNO ₃ 0.1 mol/l ...
Fill option	Finish
Stirring speed	
End criteria	
Use end value	<input type="checkbox"/>
Use end volume	<input checked="" type="checkbox"/>
End volume	20 ...
Number of EQ's	1
EQ Sensitivity	100
Drift settings	
Measurement speed	Custom
Attenuation	None
Measurement period (s)	3
Delta mV/minute	10
Minimum time (s)	3
Maximum time (s)	15
Slope Settings	
Slope type	Medium down
Display Settings	
Custom axis	<input type="checkbox"/>

6. Calculation of the equivalence point

After a titration the equivalence point must be calculated. This is done using a calculation command.

Formula: EQ1	
Name	Value
Calculation	
Type	Result
Result	EQ 1 ...
Decimals	3
Smoothing	None
Maximums EQ's	1
Formula	EQ1 ...
Marker	Blue box
Formula calculates	X-value
X window	
Use X window	<input type="checkbox"/>
Y window	
Use Y window	<input type="checkbox"/>

In the formula editor, EQ1 is selected from the **Properties**.

Formula editor

Result:

EQ1

EQ points: 0 Smoothing: None Decimals: 3

Properties	Amount
End values	EQ1
Functions	EQ2
Sample data	EQ3
Titers	EQ4
Excel	EQ5
Globals	IP1
Results	IP2
Averages	IP3
Standard Deviation	pHStat1
	pHStat2

ok cancel

7. Calculation of the result

The chloride concentration is also calculated using a calculation command.

Formula: Result['EQ 1']*Titer['AgNO3 0.1 mol/l']*0.1*35.453/Amount

Name	Value
Calculation	
Type	Result
Result	Chloride [%]
Decimals	2
Smoothing	None
Maximums EQ's	-
Formula	Result['EQ 1']*Titer['AgNO3 0.1 mol/l']*0.1*35.453/ Amount
Marker	None
X window	
Use X window	<input type="checkbox"/>
Y window	
Use Y window	<input type="checkbox"/>

In the formula editor, the required characteristics are selected in the individual sections. The calculated result for the EQ can be found under the heading **Results**, the concentration of the AgNO3 solution under **Titers** and the sample weight under **Properties**. The factor 0.1 is used to convert the result into %, the second factor 35.453 corresponds to the molar mass of chloride.

Formula editor

Result:

Result['EQ 1']*Titer['AgNO3 0.1 mol/l']*0.1*35.453/Amount

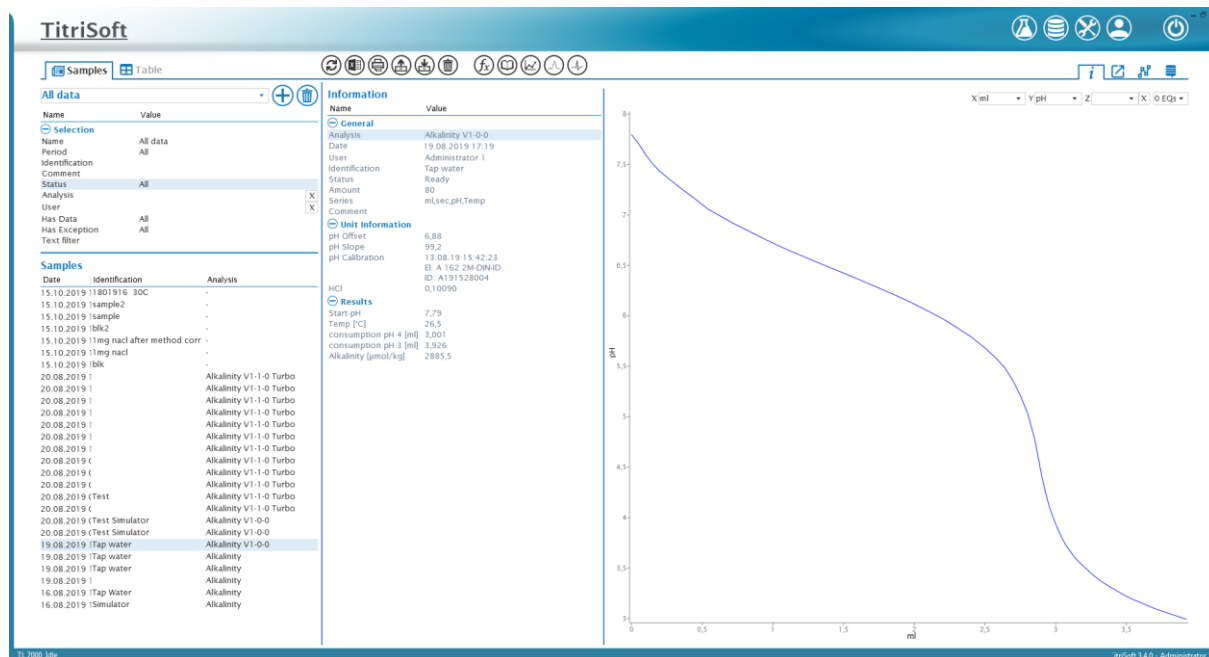
EQ points: 0 Smoothing: None Decimals: 2

Properties	Amount
End values	EQ1
Functions	EQ2
Sample data	EQ3
Titers	EQ4
Excel	EQ5
Globals	IP1
Results	IP2
Averages	IP3
Standard Deviation	pHStat1
	pHStat2

ok cancel


5 Database Center

The database center is opened via the  button.







All measured results can be viewed in the database center. Results-related metadata are documented here. The displayed data can be filtered by selection criteria, which are described in the following chapter.

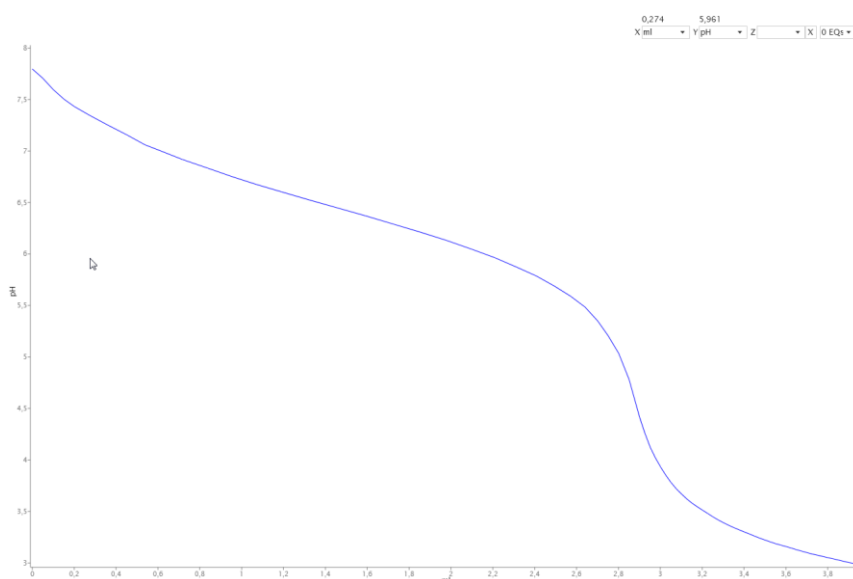
5.1 Selection area

	Adding or deleting selections
Name	Name of the Selektion
Period	Displays data for the defined period.
Identification	Displays all samples with the entered sample identification.
Comment	Displays all samples with the entered comment.
Status	Filters according to a sample status (e.g. Ready or Aborted).
Analysis	Displays the results that have been measured with the selected method.
User	Filters according to a user who performed the measurement.
Has Data	Displays only results that contain data, contain none or all.
Has Exception	Displays only results that have exceptions, have none, or all results.
Text filter	Filters according to further text criteria, e.g. sample text variables.

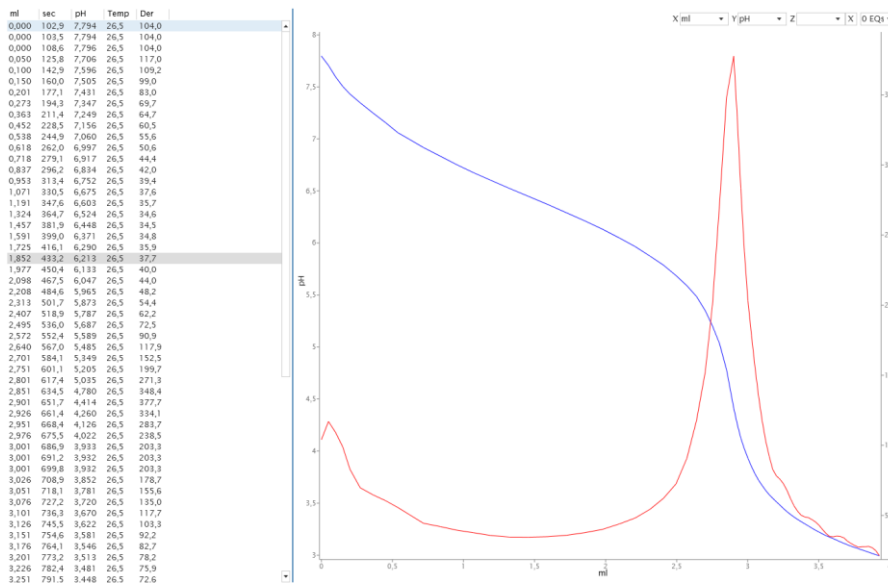
5.2.2 View overview

	Display of sample information including all linked metadata such as user, method used and instruments used.
	Display of the titration curve. See also chapter 5.2.2.1 Titration curve und titration data .
	Display of the titration data. See also chapter 5.2.2.1. Titration curve und titration data .
	Display of the method data used including statistical values such as version number, creator and date of creation.

5.2.2.1 Titration curve und titration data



The titration curve is visible in each of the points listed in chapter **5.2.2 View Overview**. In the upper right-hand area the representation of the curve can be adapted to suit the user. The unit of the x and y axis as well as an optional secondary axis z can be selected. Furthermore, up to 5 EQ's can be displayed. The display of the EQ's calculated in the method is not affected by this. Via the buttons the first or second derivative can be added. The absolute values of the derivatives are displayed below the titration data.



5.3 Table view



Checkboxes can be used to switch sample information on or off in the table view.







Columns

Name	Used
Alkalinity [µmol/kg]	<input checked="" type="checkbox"/>
Amount	<input checked="" type="checkbox"/>
consumption pH 3 [ml]	<input checked="" type="checkbox"/>
consumption pH 4 [ml]	<input checked="" type="checkbox"/>
HCl	<input type="checkbox"/>
NaOH	<input type="checkbox"/>
pH Calibration	<input type="checkbox"/>
pH Offset	<input type="checkbox"/>
pH Slope	<input type="checkbox"/>
Start-pH	<input type="checkbox"/>
Temp [°C]	<input type="checkbox"/>

The table view shows the sample results in tabular form. It can be sorted by date in descending or ascending order.

Date	Identification	Analysis	Name	Alkalinity [µmol/kg]	Amount	consumption pH 3 [ml]	consumption pH 4 [ml]
16.08.2019 10:08	Simulator	Alkalinity	Administrator 1	964,624099	50	1,482	1,107
16.08.2019 13:19	Tap Water	Alkalinity	Administrator 1		50	4,563	3,438
19.08.2019 16:00		Alkalinity	Administrator 1			4,716	3,566
19.08.2019 16:25	Tap water	Alkalinity	Administrator 1		100	4,457	3,357
19.08.2019 17:01	Tap water	Alkalinity	Administrator 1		80	3,953	3,003
19.08.2019 17:19	Tap water	Alkalinity V1-0-0	Administrator 1	2885,5	80	3,926	3,001
20.08.2019 08:34	Test Simulator	Alkalinity V1-0-0	Administrator 1		53		
20.08.2019 08:35	Test Simulator	Alkalinity V1-0-0	Administrator 1	2025,5	53	2,461	2,211
20.08.2019 08:43		Alkalinity V1-1-0 Turbo	Administrator 1			0,936	0,511
20.08.2019 08:48	Test	Alkalinity V1-1-0 Turbo	Administrator 1		57	1,282	1,057
20.08.2019 08:55		Alkalinity V1-1-0 Turbo	Administrator 1			0,675	0,550
20.08.2019 08:57		Alkalinity V1-1-0 Turbo	Administrator 1	75,53		0,859	0,634
20.08.2019 09:19		Alkalinity V1-1-0 Turbo	Administrator 1			1,618	1,418
20.08.2019 15:00		Alkalinity V1-1-0 Turbo	Administrator 1		52	0,850	0,775
20.08.2019 15:04		Alkalinity V1-1-0 Turbo	Administrator 1	1054,09	53	0,777	0,577
20.08.2019 15:06		Alkalinity V1-1-0 Turbo	Administrator 1	2097,98	51	1,440	1,115
20.08.2019 15:09		Alkalinity V1-1-0 Turbo	Administrator 1		25	1,992	1,742
20.08.2019 15:12		Alkalinity V1-1-0 Turbo	Administrator 1		65	0,923	0,698
20.08.2019 15:19		Alkalinity V1-1-0 Turbo	Administrator 1		20	0,793	0,743
20.08.2019 15:26		Alkalinity V1-1-0 Turbo	Administrator 1	8546,96	23	2,197	1,997

5.3.1 Functional overview

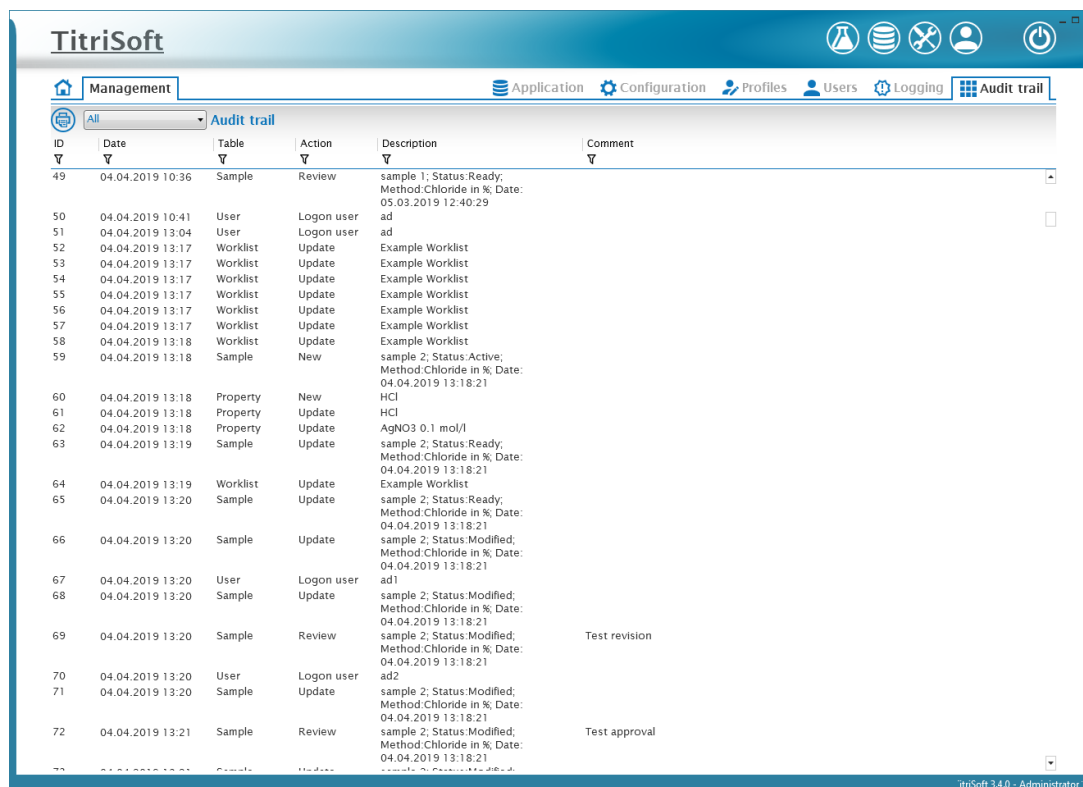
	Refreshing the view while the work list is running.
	Export of the sample list to Excel.
	Export of the sample list as .csv file.
	Print the sample list. Various display options are available (List Report and Single Curve).
	Import and export of sample results.
	Delete sample results.

6 Pharma version

A separately available pharmaceutical version of TitrSoft fulfills further requirements of pharmaceutical guidelines such as CFR 21 Part 11 of the FDA or Eudralex Volume 4, Annex 11 of the European Union. The standard TitrSoft version already meets many requirements for the regulated area. The following chapters list the differences between the pharmaceutical version and the standard version.

6.1 Audit Trail

The Audit Trail is available in the Settings Center.



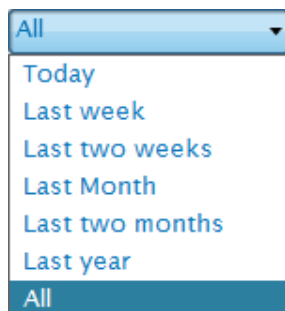
The screenshot shows the TitrSoft Audit Trail window. The window title is 'TitrSoft' and it has a navigation bar with 'Management' selected. The 'Audit trail' tab is active, displaying a table with the following columns: ID, Date, Table, Action, Description, and Comment. The table contains 23 rows of data, including entries for sample reviews, user logons, and worklist updates. Some entries have comments like 'Test revision' and 'Test approval'.

ID	Date	Table	Action	Description	Comment
49	04.04.2019 10:36	Sample	Review	sample 1; Status:Ready; Method:Chloride in %; Date: 05.03.2019 12:40:29	
50	04.04.2019 10:41	User	Logon user	ad	
51	04.04.2019 13:04	User	Logon user	ad	
52	04.04.2019 13:17	Worklist	Update	Example Worklist	
53	04.04.2019 13:17	Worklist	Update	Example Worklist	
54	04.04.2019 13:17	Worklist	Update	Example Worklist	
55	04.04.2019 13:17	Worklist	Update	Example Worklist	
56	04.04.2019 13:17	Worklist	Update	Example Worklist	
57	04.04.2019 13:17	Worklist	Update	Example Worklist	
58	04.04.2019 13:17	Worklist	Update	Example Worklist	
59	04.04.2019 13:18	Sample	New	sample 2; Status:Active; Method:Chloride in %; Date: 04.04.2019 13:18:21	
60	04.04.2019 13:18	Property	New	HCl	
61	04.04.2019 13:18	Property	Update	HCl	
62	04.04.2019 13:18	Property	Update	AgNO3 0.1 mol/l	
63	04.04.2019 13:19	Sample	Update	sample 2; Status:Ready; Method:Chloride in %; Date: 04.04.2019 13:18:21	
64	04.04.2019 13:19	Worklist	Update	Example Worklist	
65	04.04.2019 13:20	Sample	Update	sample 2; Status:Ready; Method:Chloride in %; Date: 04.04.2019 13:18:21	
66	04.04.2019 13:20	Sample	Update	sample 2; Status:Modified; Method:Chloride in %; Date: 04.04.2019 13:18:21	
67	04.04.2019 13:20	User	Logon user	ad1	
68	04.04.2019 13:20	Sample	Update	sample 2; Status:Modified; Method:Chloride in %; Date: 04.04.2019 13:18:21	
69	04.04.2019 13:20	Sample	Review	sample 2; Status:Modified; Method:Chloride in %; Date: 04.04.2019 13:18:21	Test revision
70	04.04.2019 13:20	User	Logon user	ad2	
71	04.04.2019 13:20	Sample	Update	sample 2; Status:Modified; Method:Chloride in %; Date: 04.04.2019 13:18:21	
72	04.04.2019 13:21	Sample	Review	sample 2; Status:Modified; Method:Chloride in %; Date: 04.04.2019 13:18:21	Test approval

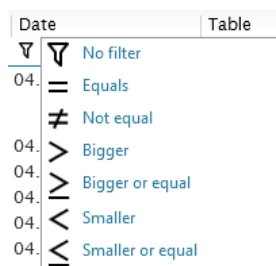
In addition to the automatic entries, a comment window opens for certain changes such as method adjustments. The comment is documented for the automatic entries. Additionally, a manual audit trail comment entry can be made at any time.



The entries displayed in the **Audit Trail** can be reduced using a time filter.



Additionally, each column can be filtered according to the following criteria.



The audit trail can be printed out at any time using the printer symbol.



6.2 Review and Approval of Analyses and Test results

Methods and analysis results can be reviewed with the following symbol.



Review Bases (non-aqueous)

User name

Password

After a review, a method/an analysis result can be approved.



A review cannot be performed by the same person who prepared a method or recorded an analytical result. The third level of final approval must be performed by a third person. Each check must be confirmed by entering the user ID and password. A comment window for the automatic audit trail entry opens.

A reviewed method or a reviewed result cannot be further modified or deleted. Archiving is still possible.

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