



7

Titration

TITRISOFT 3.5 TITRATION SOFTWARE

SI Analytics

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7. TitriSoft – simple and with strong benefits

TitriSoft 3.5

The titration software TitriSoft 3.5 is the optimal solution for your titration tasks. The software works under Windows version 10 or higher and supports your daily workflow in sample preparation, titration, and evaluation of the results. The software has been developed to be clear, logical and user-friendly.

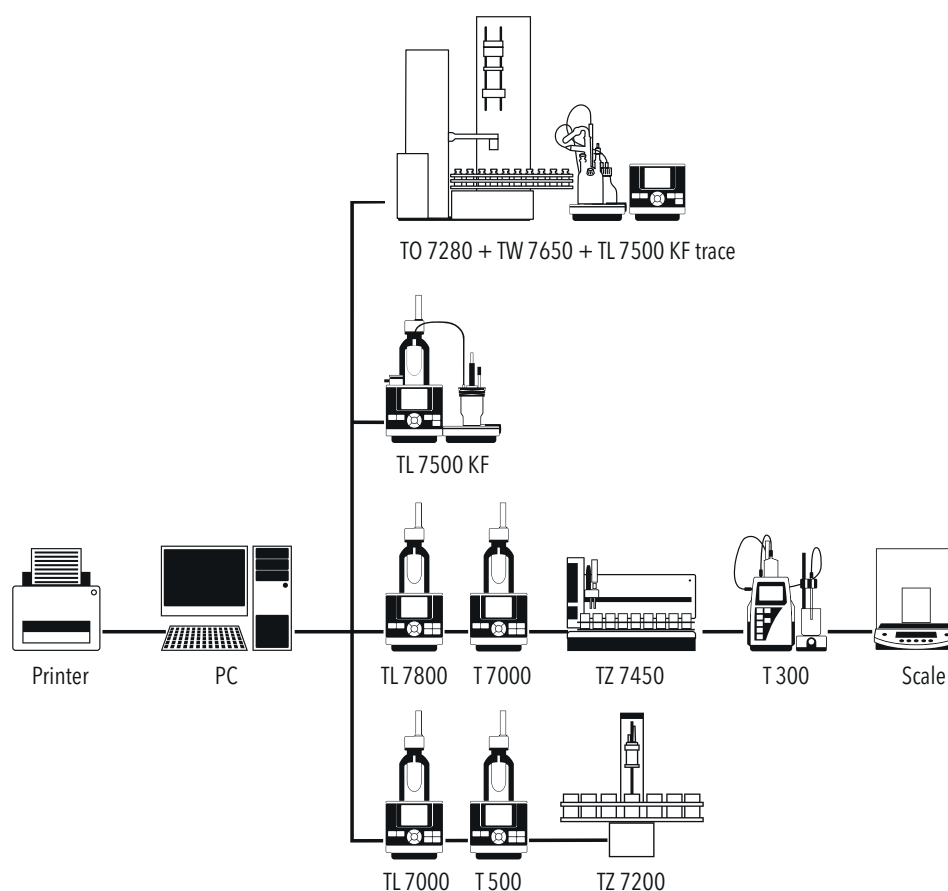
TitriSoft 3.5 allows to control the following devices with your PC:

- Titrators: TitroLine® 7000, 7750, 7800, 7500 KF, 7500 KF trace and alpha plus
- Sample changers: TW 7200 and TW 7450, TW alpha plus, TW 7400
- Piston burettes: TITRONIC® 300, universal, 500 and 110 plus
- Headspace Oven TO 7280 and sampler TW 7650
- Balances

You can connect the titration hardware to any free USB or serial interface of your PC. Each of these interfaces allows different device combinations (configurations). All devices connected to the PC can be used in all configurations. For the automation of titrations, e.g., the TitroLine® 7800 with our sample changer TW 7200 is controlled by the software. For more complex titration tasks with sample preparation you can first dose with piston burettes. Then carry out the titration with a TitroLine® 7000, 7750 or 7800.

Of course, you can also use the software exclusively for dosing tasks with piston burettes.

The image below shows possible device configurations.

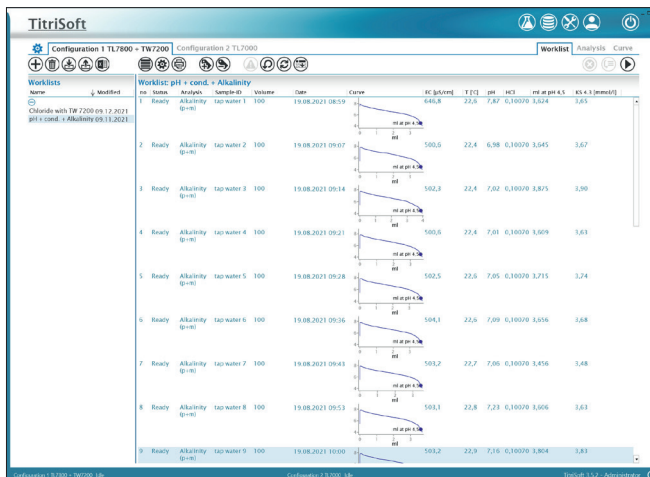


“Titrations Center”, the main menu

The different software tasks are assigned to five different centers:

- Settings
- Database
- Analysis
- Worklists
- Curve

Each of these centers can be chosen at the menu bar.

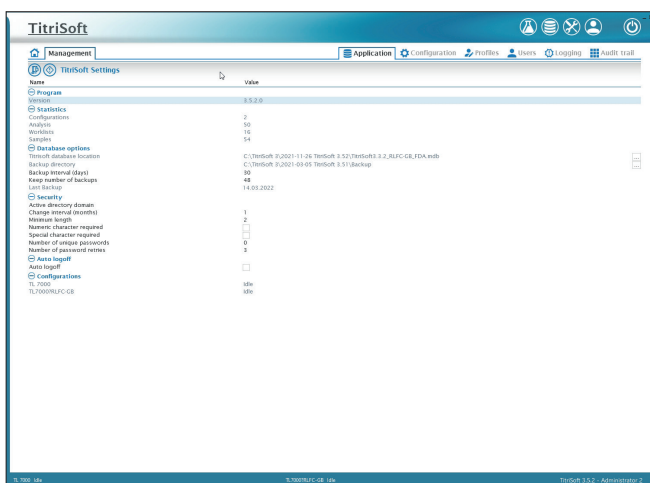


Titration Center

“Settings”, the system configuration

In the system configuration, the basic settings are made in “Application”. For example, the database is selected here, the backup directory is set, the password length is set, etc.

The devices, reagents, electrodes, and variables are managed in “Configuration”.



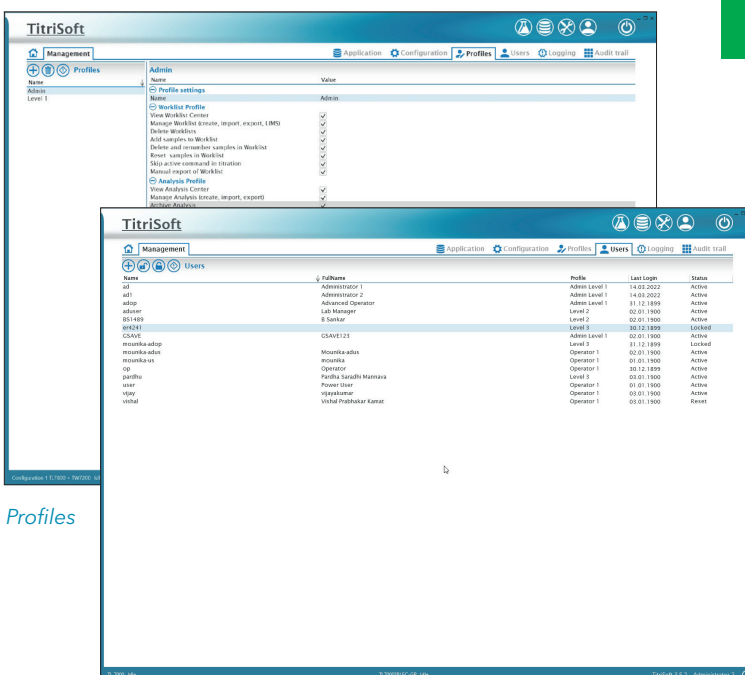
Settings

User profiles

Individual user profiles can be created in “Profiles”. The number of profiles is unlimited and each profile can allow different permission. See page 63, “Controlled access”.

User

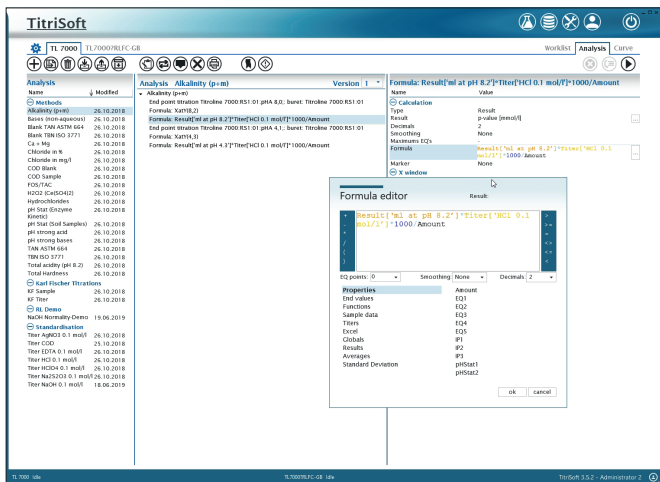
Under “User”, each user is assigned a profile. The number of users is unlimited.



Profiles

Users

Software

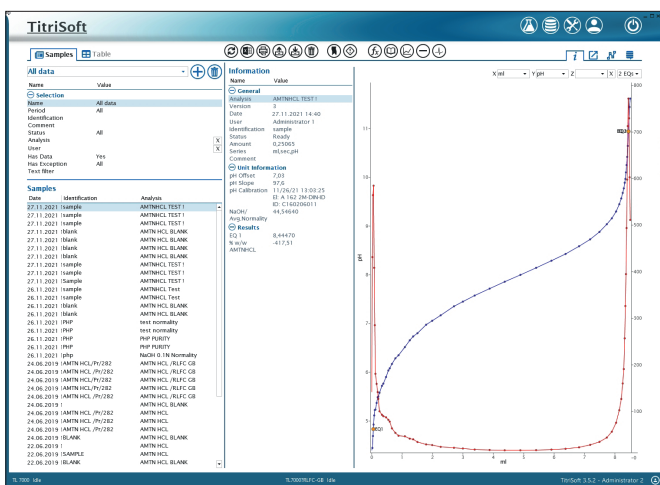


Analysis

“Analysis”, your methods center

This is where you set up and save your titration methods. Even complex methods can be installed with a few mouse clicks. Adjustment of the titration parameters is facilitated by the use of symbolic slide controls. Functions such as waiting time, IF loops, repetition, dosings and measurements in addition to the titration parameters and calculation formulas provide virtually unlimited options for method procedures.

These results lists can also be exported in Excel format, printed or saved as a PDF file.



Database

“Database”, your data storage

Titration curves, results, measured values and used methods of all titrations are stored in the database. These data can be selected by sample name, date, user, and method and loaded in a few seconds.

You can display the information of the performed titrations as a graphic, result or measured value listing. Each stored titration can be subsequently optimized according to your needs. For example, you can add, save, and print subsequent calculations with the curve. A subsequent data export in ASCII or Excel format is possible at any time. In the TitriSoft 3.5 new filter functions have been added. Individual filters can be set by date, user, method, and the selected records are then listed as table form. These results lists can also be exported in Excel format, printed or saved as a PDF file.

“Worklists”, your clearly structured workplace

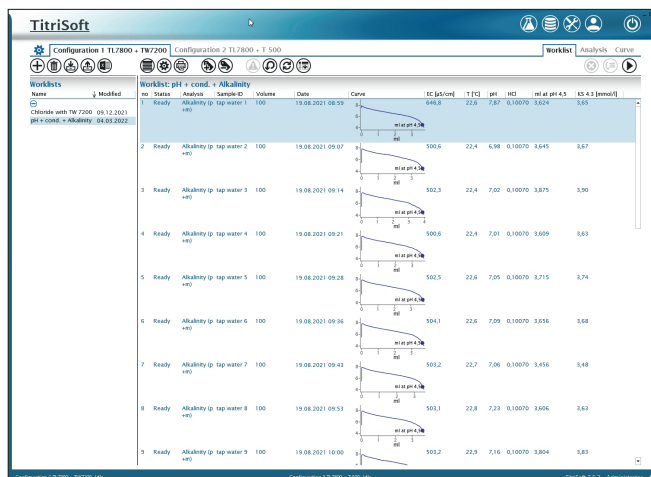
“Worklists” is the place where you carry out your daily jobs, i.e. select methods, enter sample names and origin weighed-in quantities, start the work list and display (and print out if desired) the results at the end of a titration. The worklist shows the individual samples with the associated methods and their characteristics such as sample name, number, status, date, time, results, and events and other freely configurable sample data, e.g., density.

During the process you can follow the titration under “Curve” or directly via the worklist. You can, however, simply allow the samples to be processed in the background and use the PC for other tasks or start an additional titration with another configuration in parallel.

When working with the TW 7200, TW 7450 and TW 7650 sample changer, you can adjust various settings such as skip empty items, rinse and waiting options.

From version 3.5, the headspace oven TO 7280/ sampler, as well as the control of the TL 7500 KF trace are also directly supported.

Documentation, which is in accordance with GLP and ISO 9000 directives, can be produced in a number of different forms; tables, lists, curves or individual printouts with curves. In addition, results can be saved in ASCII or CSV format, external documentation programs may be accessed and results transferred directly, e.g., into a LIMS.



Worklists

TitriSoft 3.5-System requirements

For optimal and fast working with the TitriSoft 3.5 software your system should be equipped as shown below:

- Interface: a free USB- or RS232-interface per configuration
- Computer: Pentium (Dual-Core) 2
- GHz or higher (I3 or higher recommended)
- Operating system: Windows 10 (32/64 bit) or higher
- RAM: minimum 4 GB (8 GB or more recommended)
- Hard disk: minimum free storage volume 200 MB
- Graphics card: minimum resolution 1280 x 1024, 1920 x 1200 recommended

TitriSoft 3.5 P requirements are identical

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TitriSoft 3.5 P – simply reliable ...

In this case, the “P” stands for “pharmaceutical”.

The TitriSoft 3.5 P fully meets all requirements of the FDA 21 CFR Part 11 regulation regarding „Electronic Records“, „Electronic Signature“ and „Audit Trail“.

The FDA (Food and Drug Administration of the USA) 21 CFR Part 11 regulations describe how to deal with electronically stored data (“Electronic Records”) and how to prepare electronic signatures (“Electronic Signature”).

These regulations are binding for all companies offering medical, pharmaceutical, or food products and services in the USA.

The regulations are relating to:

- the handling of electronically stored data: Electronic Records.
- the creation of electronic signatures: Electronic Signatures
- the traceability of all steps and settings carried out on the instrument (“Audit Trail”)

Comparison between TitriSoft 3.5 and 3.5 P

Functions	TitriSoft 3.5	TitriSoft 3.5 P
Electronic records	■	■
Electronic Signatures	—	■
Audit Trail	—	■
Controlled Access	■	■
Copies of Records	■	■
Straightforward procedure	■	■
All types of titrations	■	■
Comfortable worklists	■	■
Online titration curves	■	■
Clear documentation	■	■
Perfect titration control by PC	■	■
Parallel titration (with multiple configurations, also with a TL 7800 and a piston burette; see page 65)	■	■

Controlled Access

The controlled access guarantees that only authorized individuals have access to the software functions, according to your company's security policy and the FDA requirements.

By creating individual profiles, each user can be assigned appropriate access to the software.

The screenshot shows the TitriSoft Management interface. On the left, a sidebar lists user profiles: Admin, Level 1, Level 2 (highlighted with an orange circle), and Operator. The main area displays the configuration for the 'Level 2' profile. It is organized into sections: Profile settings, Worklist Profile, Analysis Profile, and Management Profile. Each section contains a list of permissions with checkboxes indicating whether they are enabled for the profile.

Name	Value
Level 2	
Profile settings	
Name	Level 2
Worklist Profile	
View Worklist Center	<input checked="" type="checkbox"/>
Manage Worklist (create, import, export, LMS)	<input checked="" type="checkbox"/>
Delete Worklists	<input type="checkbox"/>
Add samples to Worklist	<input checked="" type="checkbox"/>
Delete and renumber samples in Worklist	<input 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 type="checkbox"/>
Review Analysis	<input type="checkbox"/>
Approve Analysis	<input 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 type="checkbox"/>

User Profiles

Ordering Information TitriSoft 3.5 /3.5 P

Type No.	Order No.	Description
TZ 3571	285217950	Titration software TitriSoft 3.5 for all TitroLine® 7XXX titrators and piston burettes TITRONIC® 300/500, and for all sample changers
TZ 3572	285217960	Titration software TitriSoft 3.5 P. Same as TitriSoft 3.5, but 21 CFR, part 11 compliant
TZ 3573	285217970	Update older TitriSoft versions to version 3.5
TZ 3574	285217980	Update older TitriSoft P versions to version 3.5 P
TZ 3575	285217990	Upgrade TitriSoft 3.5 to TitriSoft 3.5 P

ID	Date	Table	Action	Description
1	14.03.2022 15:35	User	TitriSoft Open	
2	14.03.2022 15:35	User	Logon user	ad
3	14.03.2022 15:35	Worklist	New	Example KF coulometric
4	14.03.2022 15:35	User	TitriSoft Close	
5	14.03.2022 15:36	User	TitriSoft Open	
6	14.03.2022 15:36	User	Logon user	ad
7	14.03.2022 15:37	Configuration	New	Titration 1
8	14.03.2022 15:38	Analysis	New	HCl
9	14.03.2022 15:38	AnalysisMethod	New	HCl (1)
10	14.03.2022 15:38	AnalysisMethod	Update	HCl (1)
11	14.03.2022 15:38	AnalysisMethod	Update	HCl (1)
12	14.03.2022 15:38	AnalysisMethod	Update	HCl (1)
13	14.03.2022 15:38	Property	New	pH Offset
14	14.03.2022 15:38	Property	New	pH Slope
15	14.03.2022 15:38	Property	New	pH Calibration

Audit Trail

Audit Trail

The 21 CFR Part 11 prescribes that, creating methods, modifying passwords or saving results, has to generate an entry in the Audit Trail.

TitriSoft 3.5 P automatically generates an entry in the Audit Trail table, as soon as an access to the database has taken place. The local time and the GMT are automatically stored together with this entry in the Audit Trail. Each entry also asks for a comment.

The Audit Trail or parts of it can be printed out, or a human-readable digital copy of it, e.g. a PDF file can be generated.

Date	Identification	Analysis
27.11.2021	1sample	AMTNHCL TEST !
27.11.2021	1sample	AMTNHCL TEST !
27.11.2021	1sample	AMTNHCL TEST !
27.11.2021	1blank	AMTN HCL BLANK
27.11.2021	1blank	AMTN HCL BLANK
27.11.2021	1blank	AMTN HCL BLANK
27.11.2021	1blank	AMTN HCL BLANK
27.11.2021	1sample	AMTNHCL TEST !
27.11.2021	1sample	AMTNHCL TEST !
27.11.2021	1Sample	AMTNHCL TEST !
26.11.2021	1sample	AMTNHCL Test
26.11.2021	1sample	AMTNHCL Test
26.11.2021	1blank	AMTN HCL BLANK
26.11.2021	1blank	AMTN HCL BLANK
26.11.2021	1PHP	test normality
26.11.2021	1PHP	test normality

Electronic records

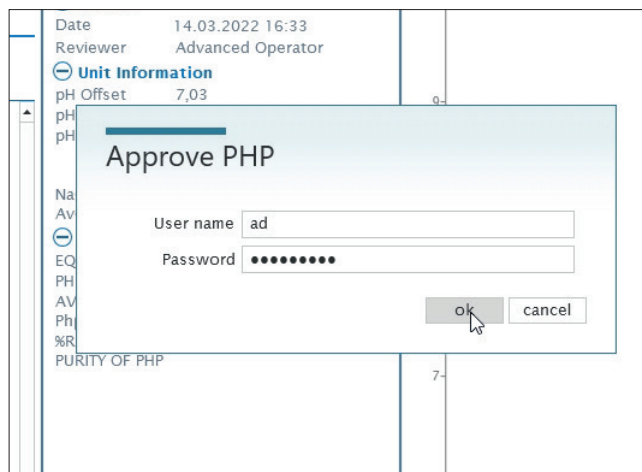
Electronic Records

The 21 CFR Part 11 prescribes how to safeguard and store the generated results over time.

Besides regularly making backup copies of the complete database, it is possible to generate readable digital copies of the results, methods, worklists, the Audit Trail, the user administration and the configuration(s). For that purpose, a PDF writer is integrated in the software. The purchase of expensive third-party software for generating PDF files is not necessary. Of course, the database is password protected against unauthorized access.

Electronic Signature

Digital analysis results have to be as reliable as classical, manually checked results with a handwritten signature. A digital signature, which is as safe as a handwritten one, can be placed to approve all electronic records. The approver has to enter the name and an additional password. The electronic signature is stored together with the signer's function, the reason of signing and the date and time.



Electronic Signature

Parallel titration with TitroLine® 7800 and TitriSoft 3.5/3.5 P

In combination with the new TitriSoft 3.5/3.5 P it is possible to carry out a so-called „parallel“ titration, e.g., with a TitroLine® 7800 and a TITRONIC®300/500 piston burette. This means that you only need one titrator and one piston burette to carry out two titrations simultaneously, in parallel.

Typical example: With a TitroLine® 7800 and a sample changer, acid-base titrations are carried out in one configuration. The pH electrode is connected to measuring input A. At the same time, a titration of

chloride is carried out with a second configuration. The silver electrode is connected to measuring input B. The titration is carried out with a TITRONIC® 500 piston burette.

