

Supelco®

Analytical Products

Spectroquant® Prove Connect

to LIMS

MERCK

Data Transfer from Spectroquant® Prove / Prove plus with Prove Connect (LIMS)

Thank you for choosing Prove Connect.

Prove Connect to LIMS (in the following referred to as Prove Connect) is a desktop application to connect your Spectroquant® Prove / Prove plus instruments to laboratory software systems such as laboratory information management systems (LIMS), and electronic laboratory notebooks (ELNs). The software receives measurement data from Spectroquant® Prove / Prove plus instruments via network connection (LAN) for further processing with your LIMS/ELNs.

Prove Connect runs as a service and supports the XML and CSV file format. This allows an easy integration of Spectroquant® Prove / Prove plus instruments into an existing laboratory IT infrastructure.

Installation

System Requirements

Prove Connect supports the following instruments:

- Spectroquant® Prove 100 / Prove 100 plus
- Spectroquant® Prove 300 / Prove 300 plus

- Spectroquant® Prove 600 / Prove 600 plus

The software requires a computer with the following specification:

- Microsoft Windows 7 SP1, Windows 8, Windows 10
- 1 GB of free disk space
- 4 GB of RAM
- Network Connection (LAN)

Other configurations may work but are not supported.

Installing Prove Connect

Windows administrator rights are required for installing Prove Connect. Please download the installation file and start the installation of Prove Connect by double click.

Starting the Installation

After a double click, a start screen will appear. Please click on "Install" **1** (Figure 1) to start the installation.

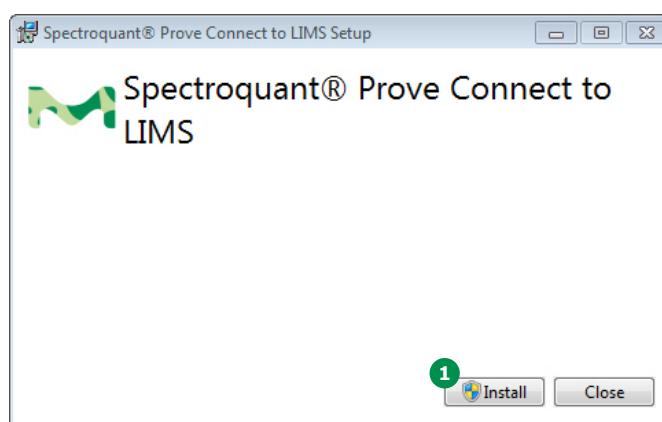


Figure 1 - Screenshot of installer's start screen

The setup wizard will guide you through the installation process. Click on "Next" **2** (Figure 2) to continue with the installation, "Back" **3** to return to the former step, e.g. to correct information, and on "Cancel" **4** to abort the installation. In the latter case, Prove Connect will not be installed on your computer.

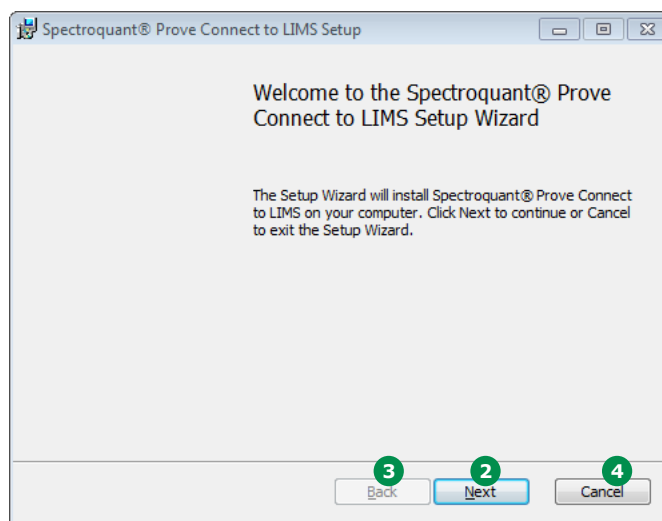


Figure 2 - Screenshot of setup wizard

Review the End-User License Agreement

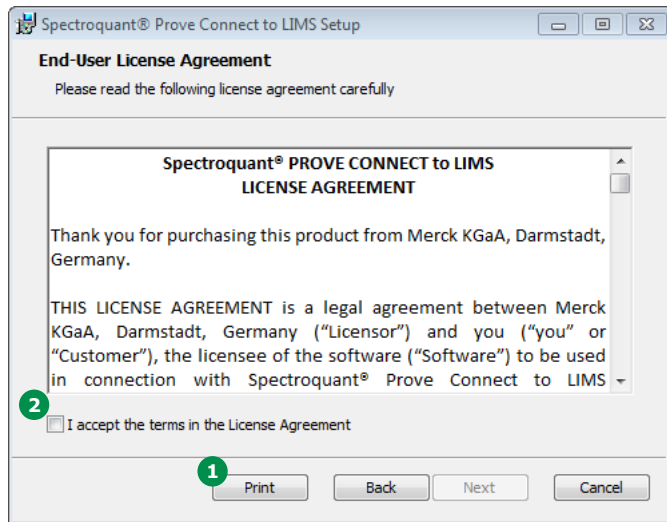


Figure 3 - Screenshot of the End-User License Agreement (EULA)

The installation process requires you to review and accept the end-user license agreement (EULA). Read the license agreement by scrolling down the text. You can also print the text by clicking the "Print" button **1** (Figure 3). Once you are finished, check **2**, if you agree.

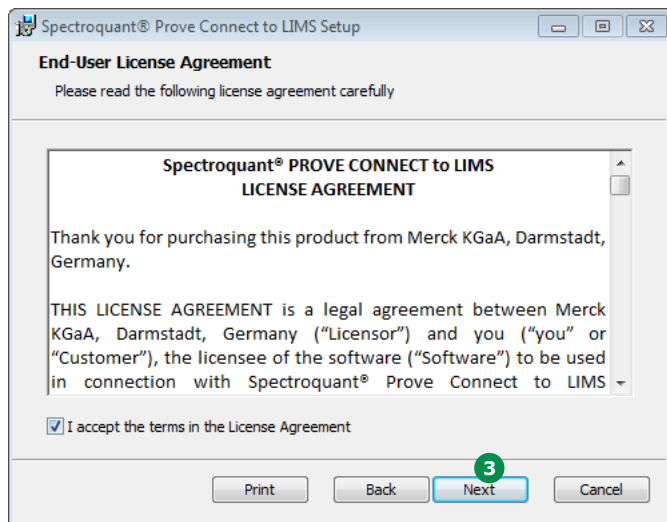


Figure 4 - Screenshot when accepting the EULA

Once the checkbox "I accept the terms in the License Agreement" is checked, the "Next" **3** (Figure 4) button is activated, and you can proceed with the software installation by clicking it.

Destination Folder

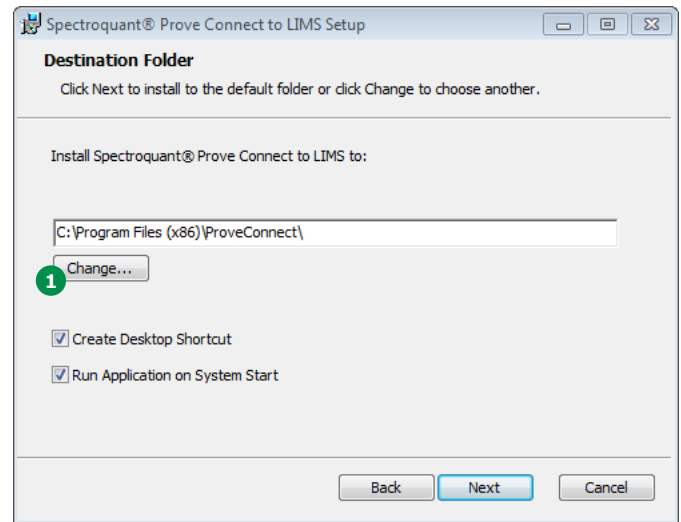


Figure 5 - Selection of destination folder for software installation

1. If you would like to install Prove Connect into another folder than the predefined directory given in Figure 5, please define the installation folder by clicking the "Change" button **1** (Figure 5). A dialog window opens (Figure 6) that allows you to select or create the new installation folder.

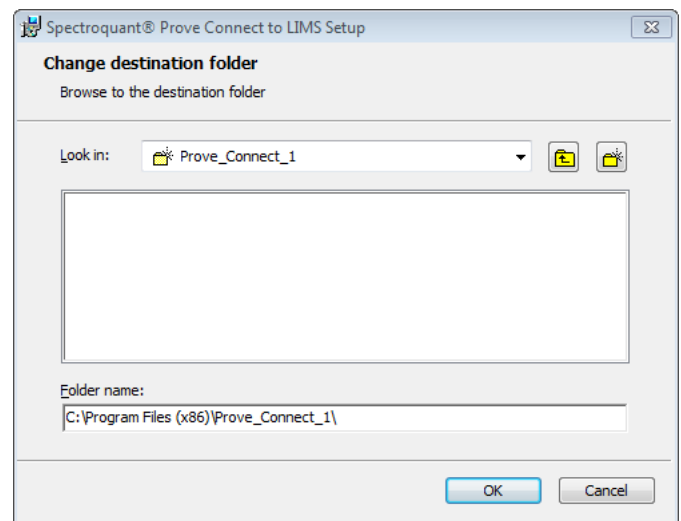


Figure 6 - For selection of an installation folder other than the predefined directory, this dialog window will open

If the folder does not exist, the new directory will be created. After clicking "OK" the dialog window is closed, and the selected path is displayed in the destination folder screen (Figure 7).

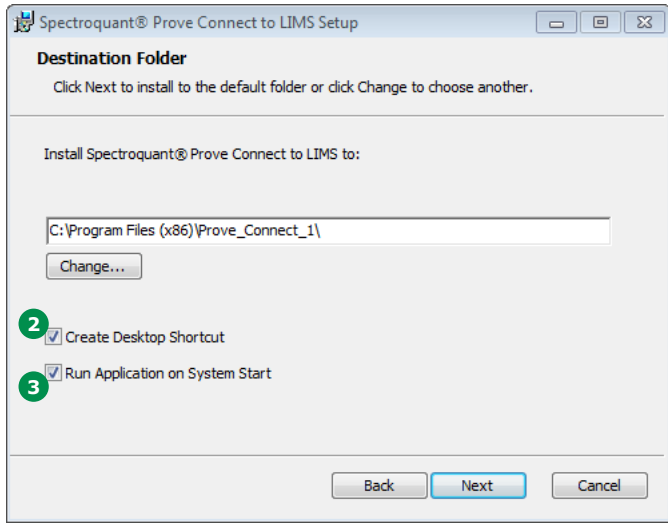


Figure 7 - Example for a non-predefined destination folder (Prove_Connect_1) for software installation

2. Please check **2** (Figure 7), if you would like to create shortcuts on your desktop.
3. Please check **3** (Figure 7), if the application should be started automatically started with the System Start
4. Click "Next" to continue.

Ready to Install

All settings are defined now. Click "Install" **1** (Figure 8) to continue with the installation.

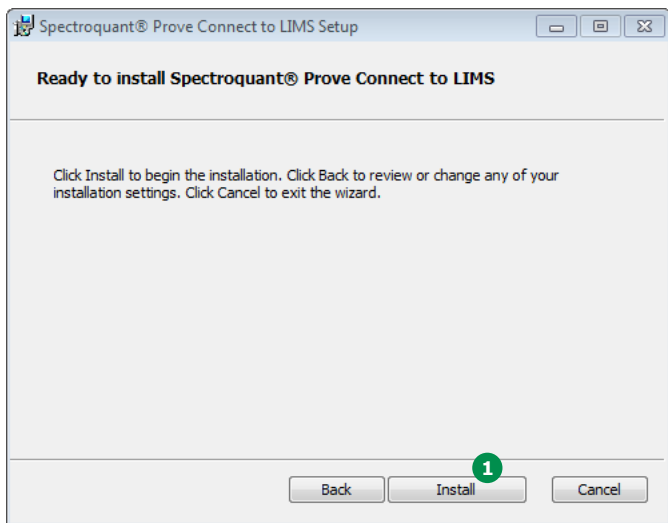


Figure 8 - Final window before installation starts

Installation Process

During the installation process the installer copies the required files to the PC. A progress bar indicates the status of the installation process.

Installation Completed

The setup wizard informs you, that the installation is completed (Figure 9). Click on "Finish" **1** (Figure 9) to exit the wizard.

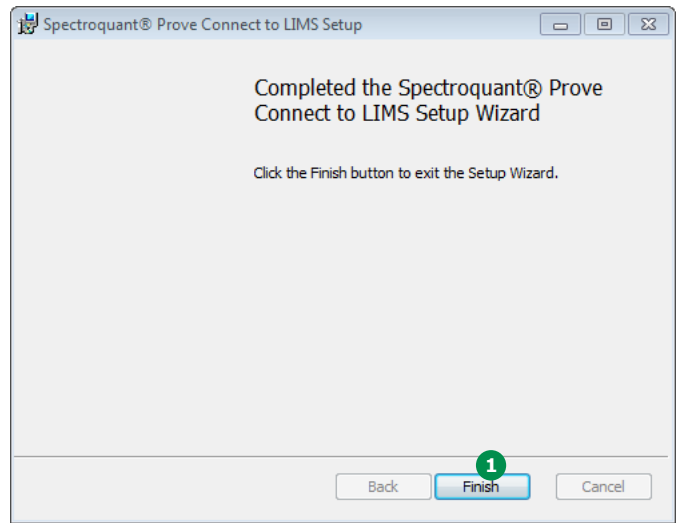


Figure 9 - Confirmation of successful installation by setup wizard

The following screen (Figure 10) informs you, that Spectroquant® Prove Connect to LIMS is now installed and ready to use.

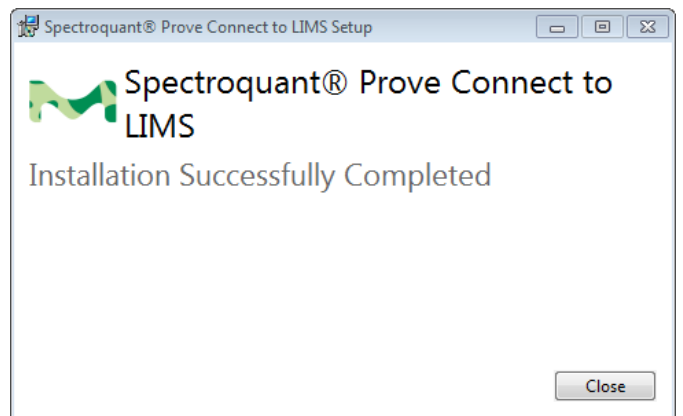


Figure 10 - Confirmation of successful installation by installer

Software Activation using the License Key

Please make sure, that you have the order confirmation email containing your license key at hand. You can retrieve the license key again from your personal Prove Connect download page. Enter the following link into the address list of your web browser and follow the instructions:

<http://www.merckmillipore.com/DE/de/analytix-and-sample-preparation/spectroquant-prove/spectroquant-prove-connect/pT6b.qB.o88AAAFcFEoTySCM,nav>

or

<https://www.sigmaaldrich.com/DE/en/products/analytical-chemistry/photometry-and-rapid-chemical-testing/photometry-instruments-kits-and-accessories/spectroquant-prove-connect-to-lims>

When you start the software for the first time, it requests you to enter the license key.

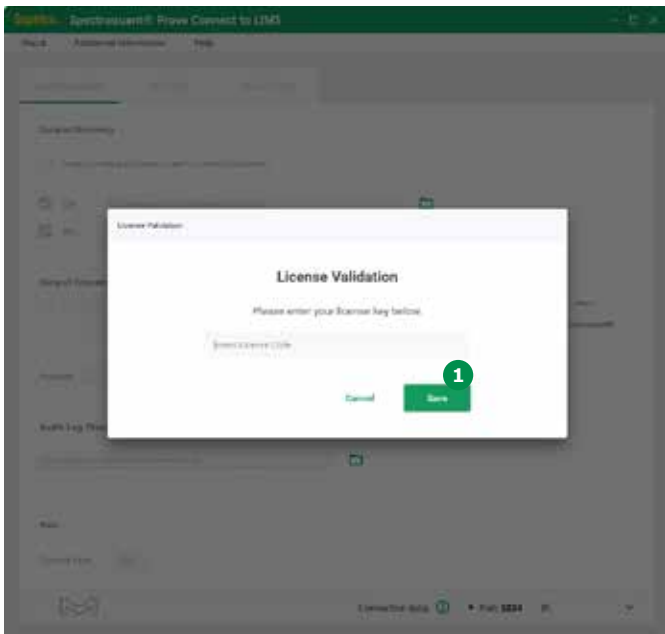


Figure 11 - Welcome screen of Prove Connect to LIMS software at first start asking you to enter the license code

Please enter the license key by copying it from the order confirmation email or download page and click on "Save" **1** (Figure 11) to store it. The software is now ready to connect with the Prove instrument(s).

Connecting Spectroquant® Prove / Prove plus to the Network

Use the Ethernet port **1** (Figure 12) on the back side of the instrument to connect the Spectroquant® Prove / Prove plus to a local network (LAN).

A network cable (RJ45) is required (not included).

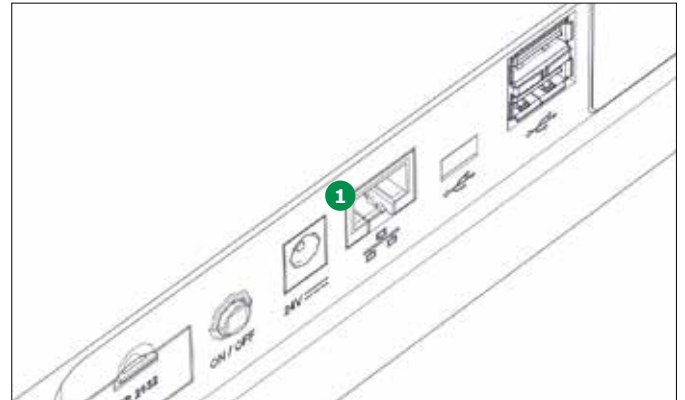


Figure 12 - Schematic drawing of back of the Spectroquant® Prove / Prove plus device with the LAN port

NOTE

After physically connecting the Spectroquant® Prove / Prove plus to the network (re)start the instrument.



Figure 13 - Screen of Spectroquant® Prove / Prove plus after clicking on "System"

1. To configure the network in the Spectroquant® Prove switch to "Network" **2** (Figure 13) on the Prove's System screen.

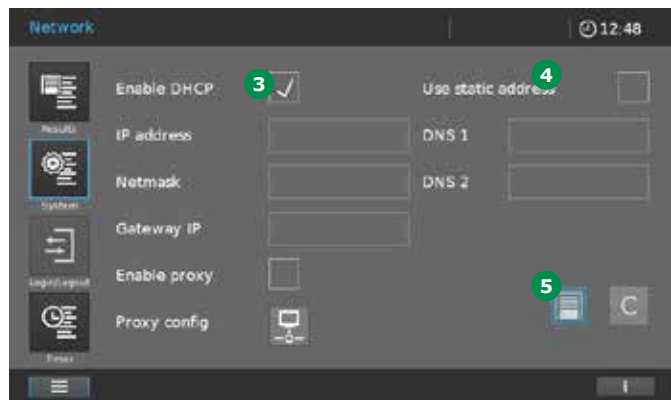


Figure 14 - After clicking on "Network" in the previous window (Figure 13), this window will appear

2. Select "Enable DHCP" 3 (Figure 14) if a DHCP-server is available in the network or select "Use static address" 4 and enter the network parameters (IP address, netmask, gateway, proxy) provided by your system administrator into the configuration menu.
3. To confirm click the Save button 5.

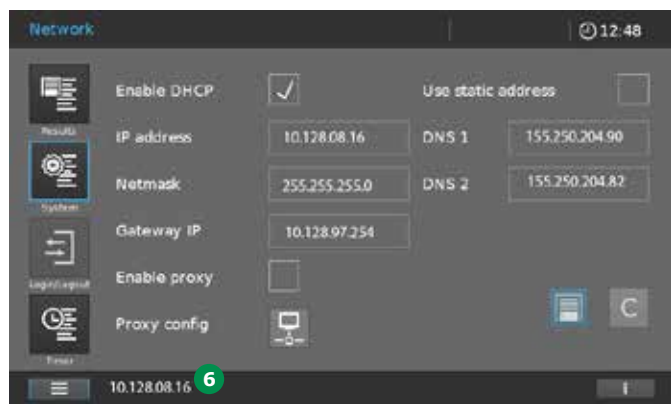


Figure 14 - After clicking on "Network" in the previous window (Figure 13), this window will appear

When the network connection of the Spectroquant® Prove / Prove plus is established an IP address 6 (Figure 15) appears in the status bar.

Establishing the Connection and Starting the Program

Starting Prove Connect

If "Run Application on System Start" was selected during installation (Figure 7), Prove Connect will be started, when the user logs in to Windows.

Prove Connect can also be started manually from the Windows start menu, a desktop short-cut or from the installation directory by double-clicking on the Prove Connect icon.

The PC needs to be connected to the same local network as the Spectroquant® Prove / Prove plus you would like to connect. To setup Prove Connect in the Spectroquant® Prove / Prove plus instrument you need your PC's IP address. This address needs to be entered in the Spectroquant® Prove / Prove plus settings as described below.

There are three options to connect your Spectroquant® Prove / Prove plus instrument to Prove Connect:

- Via DHCP as described below
- Via proxy as described on page 9
- Via static IP as described on page 12

Connecting Spectroquant® Prove / Prove plus Instrument to Prove Connect via DHCP

NOTE

Make sure a firmware version 1.4.5 or a more recent update is installed on the Prove to enable the connection to Prove Connect.

Connect the Spectroquant® Prove / Prove plus instrument to your local network.



Figure 16 - Screen of Spectroquant® Prove / Prove plus after clicking on "System"

1. Enable Prove Connect in the Prove System menu **1** (Figure 16).

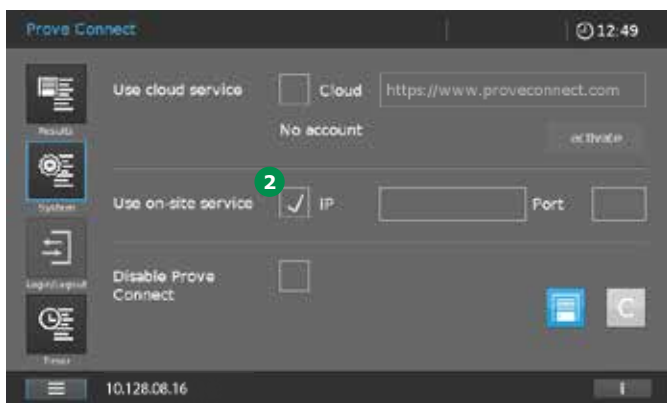


Figure 17 - After clicking on "Prove Connect" in the previous window (Figure 16), this window will appear.

2. Set the checkmark for Use on-site service **2** (Figure 17). Don't save or close this window yet.

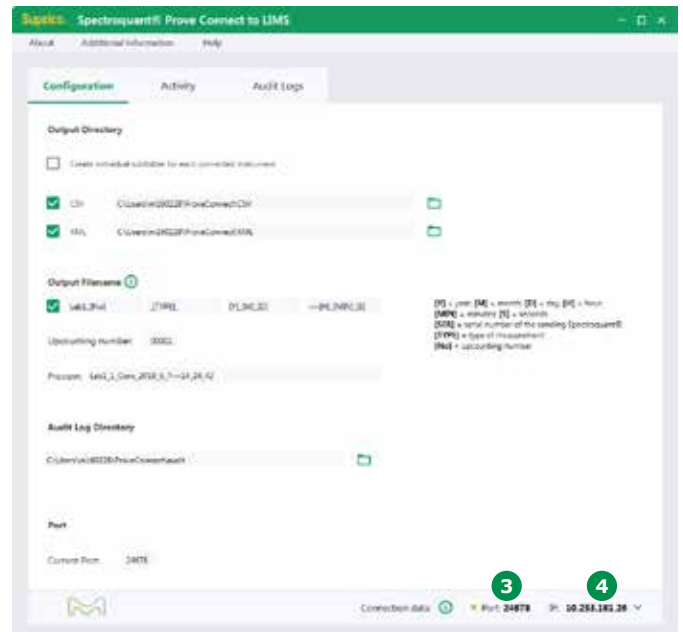


Figure 18 - Screenshot of Prove Connect for setup of network connection

3. Enter the Port **3** and IP address **4** shown in the Prove Connect to LIMS status bar (Figure 18) into the instrument (Figure 20).

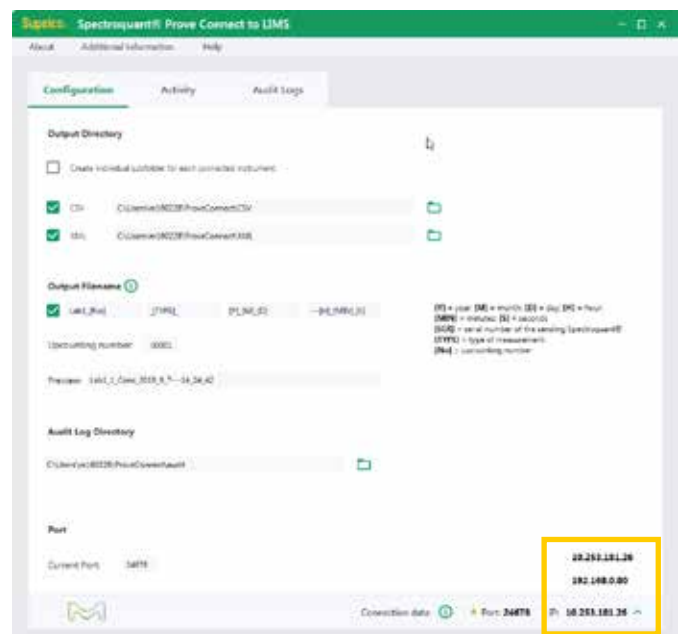


Figure 19 - Screenshot of Prove Connect for setup of network connection after clicking on the arrow next to **4** in Figure 18

To support the identification of the correct IP in more complex network environments, a list of all the PC's IP addresses is shown after clicking the arrow-button besides of the IP address (Figure 19).

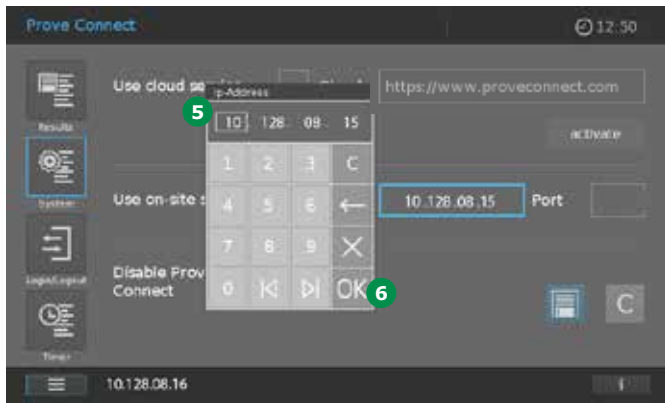


Figure 20 - Screen of Spectroquant® Prove / Prove plus (Figure 17) with entered IP address of the PC on which Prove Connect runs

4. On the Spectroquant® Prove / Prove plus, click in the field "IP address" (text box with the blue border) and the entry field appears **5** (Figure 20).
5. Enter the IP address **4** (Figure 18) into the instrument.
6. Confirm the entered IP address with "OK" **6** (Figure 20).

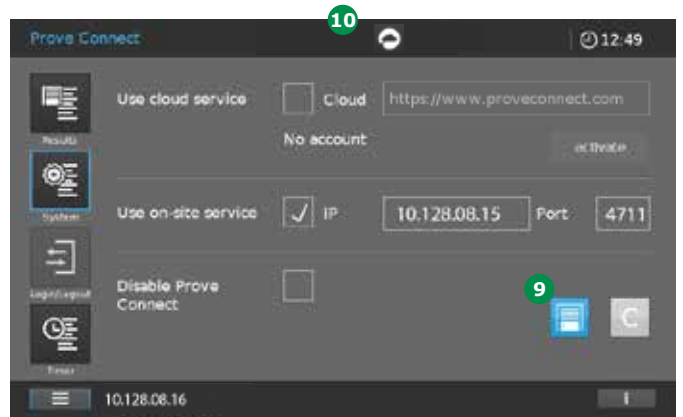


Figure 22 - Screen of Spectroquant® Prove / Prove plus with all network details

10. After setting all parameters (Checkmark, IP, and Port), press the save icon **9** (Figure 22).

The Spectroquant® Prove / Prove plus is now connected to your local network. When the connection is established the cloud icon **10** (Figure 22) appears in the instrument display.

NOTE

The company's firewall may block the Prove to establish a connection. Please contact your system administrator to configure an exception rule for the Prove instrument. Only system administrators or experienced users should configure the firewall, as a misconfiguration bears a risk for attacks from the external network.

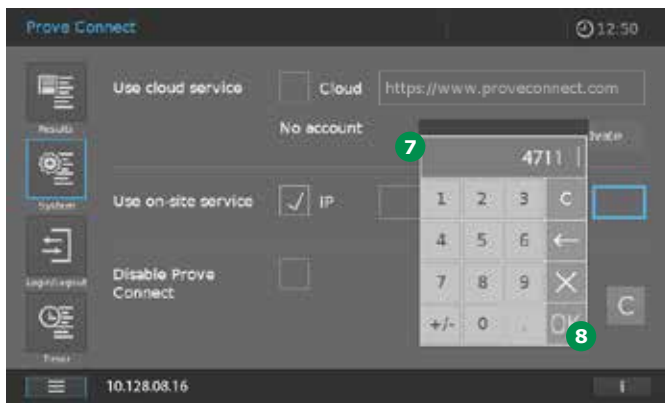


Figure 21 - Screen of Spectroquant® Prove / Prove plus (Figure 17) with entered Port of the PC on which Prove Connect runs

7. Open the field: Port (text box with the blue border). The entry field appears **7** (Figure 21).
8. Enter the Port **3** (Figure 18) shown in Prove Connect into the instrument.
9. Confirm the entered Port with "OK" **8** (Figure 21).

The Spectroquant® Prove / Prove plus is now ready to transfer data to Prove Connect. All measurements are now transferred to the Prove Connect application.

Connecting Spectroquant® Prove / Prove plus Instrument to Prove Connect via proxy

Connecting a network connection via a proxy please proceed as follows.



Figure 23 - Screen of Spectroquant® Prove / Prove plus after clicking on "System"

NOTE

These settings should be made by your system administrator.

Connect the Spectroquant® Prove / Prove plus instrument to the network.

1. Open the Network tab **1** (Figure 23) in the Prove System menu.

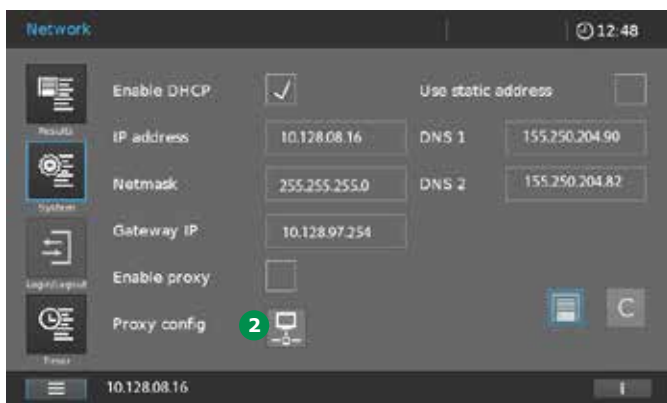


Figure 24 - After clicking on "Network" in the previous window (Figure 23), this window will appear

2. Open the Proxy config **2** in the Network menu (Figure 24).

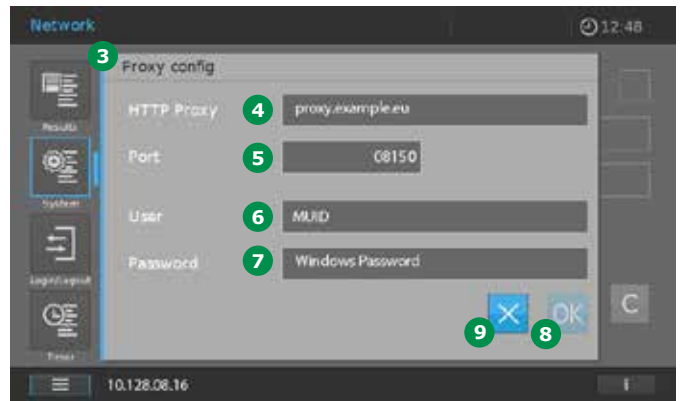


Figure 25 - Proxy configuration menu of the Prove

3. The Proxy config menu opens **3** (Figure 25). By pressing the entry field the keyboard appears to set the following parameters: HTTP Proxy **4**, Port **5**, User **6** and Password **7**. By pressing the "OK" button **8** the parameters are stored in the instrument and the menu closes. By tapping the "X" button **9** all parameters are discarded and the menu closes.

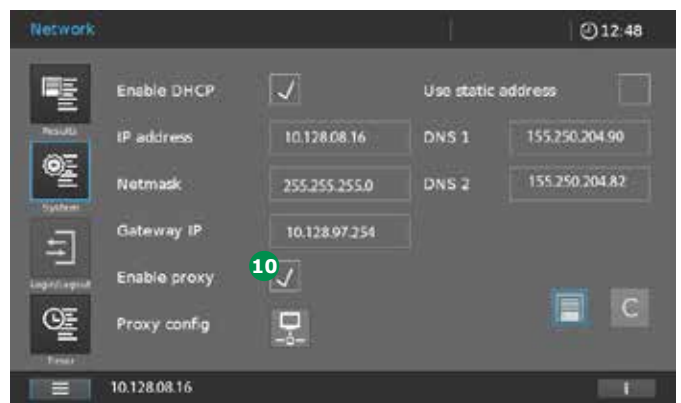


Figure 26 - After closing the previous window shown in Figure 25, the network window will appear again

4. Enable proxy **10** in the Network menu (Figure 26) and click on the "save" button. You will be redirected to the system screen as shown in Figure 27.



Figure 27 - Screen of Prove's system menu

5. Enable Prove Connect in the Prove System menu **11** (Figure 27).

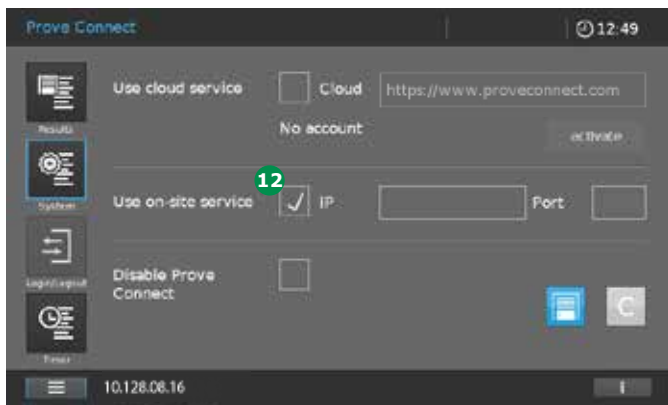


Figure 28 - Screen of "Prove Connect" menu

6. Set the checkmark for Use on-site service **12** (Figure 28).

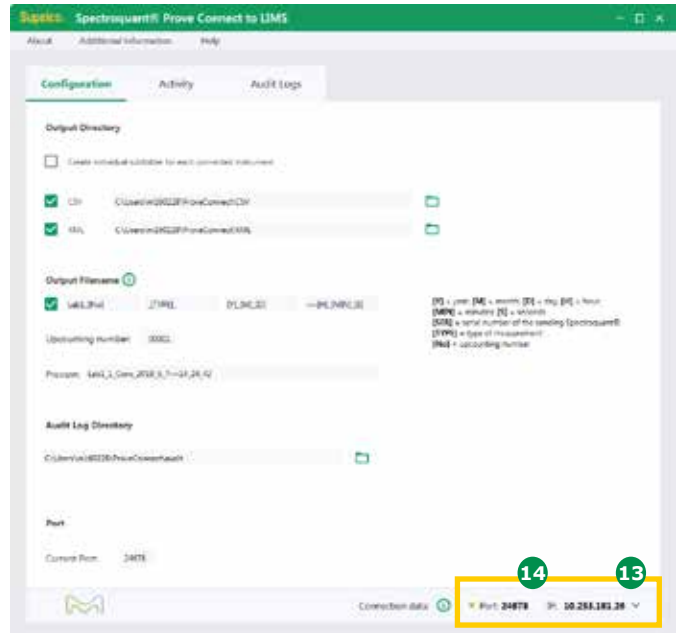


Figure 29 - Screenshot of Prove Connect for setup of network connection

7. Enter the IP address **13** and Port **14** (Figure 29) of the computer Prove Connect is running on into the Prove instrument.

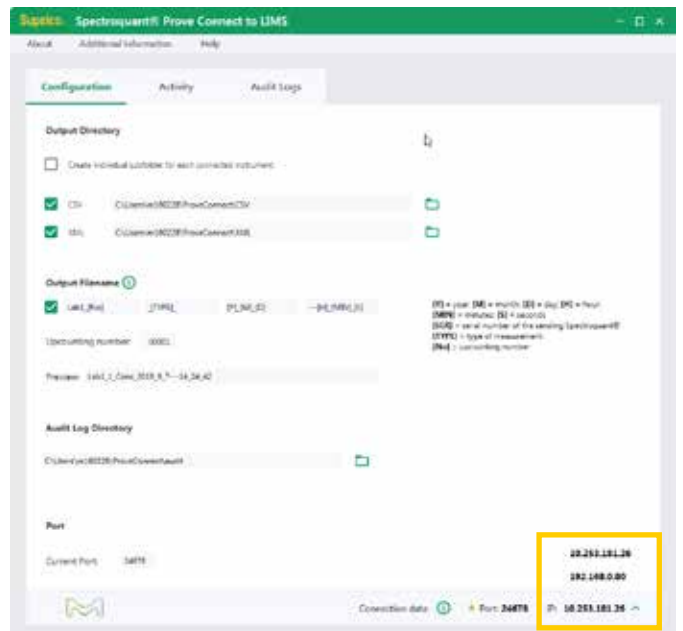


Figure 30 - Screenshot of Prove Connect for setup of network connection after clicking on the arrow next to the IP address

To support the identification of the correct IP in more complex network environments, a list of all the PC's IP addresses is shown after clicking the arrow button besides the IP address.

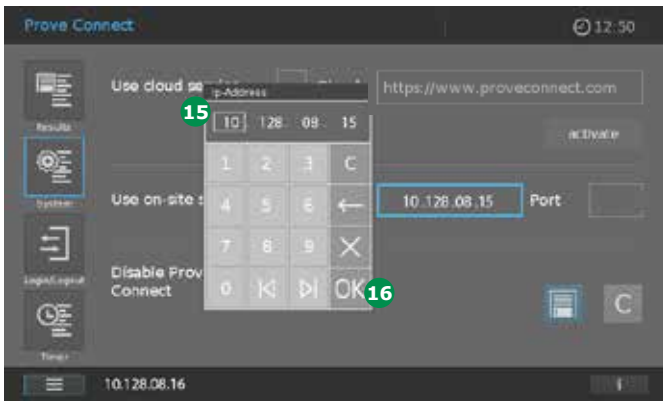


Figure 31 - Screen of Spectroquant® Prove / Prove plus (Figure 28) with entered IP address of the PC on which Prove Connect runs

8. On the Spectroquant® Prove / Prove plus, click in the field "IP address" (text box with the blue border) and the entry field appears **15** (Figure 31).
9. Enter the IP address **13** (Figure 29) into the instrument.
10. Confirm the entered IP address with "OK" **16** (Figure 31).

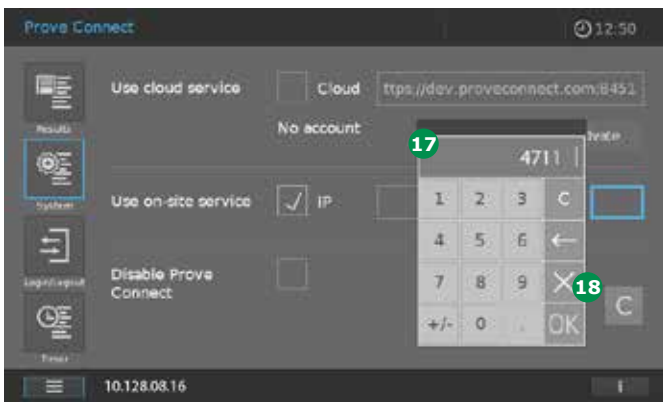


Figure 32 - Screen of Spectroquant® Prove / Prove plus (Figure 28) with entered Port of the PC on which Prove Connect runs

11. Click in the field: Port (text box with blue border). The entry field appears **17** (Figure 32).
12. Enter the Port **14** (Figure 29) into the instrument.
13. Confirm the entered Port with "OK" **18** (Figure 32).

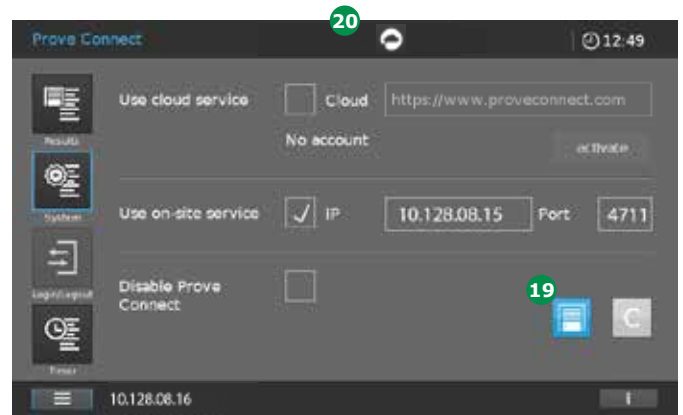


Figure 33 - Screen of Spectroquant® Prove / Prove plus with all network details

14. After setting all properties (Checkmark, IP and Port) press the save icon **19** (Figure 33).

The Spectroquant® Prove / Prove plus is now connected to your local Network. When the network is established the cloud icon **20** appears in the instrument display (Figure 33). The Spectroquant® Prove / Prove plus is now ready to transfer data to Prove Connect. All measurements are now transferred to the Prove Connect application.

Connecting Spectroquant® Prove / Prove plus Instrument to Prove Connect via static IP

To set the network connection via a static IP please proceed as follows.

NOTE

These settings should be made by your system administrator.

Connect the Spectroquant® Prove / Prove plus instrument to your local network.



Figure 34 - Screen of Spectroquant® Prove / Prove plus after clicking on "System"

1. Open the Network tab **1** (Figure 34) in the Prove System menu.

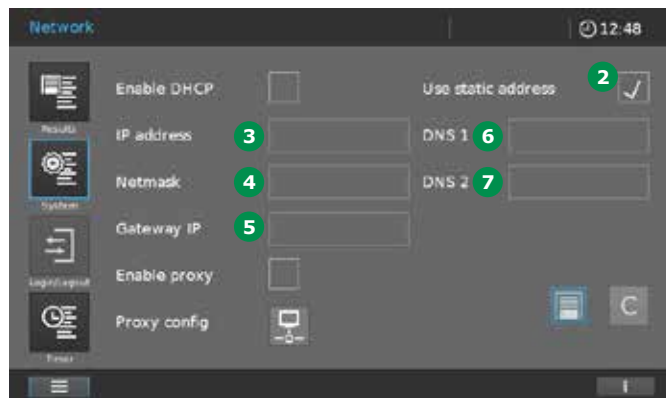


Figure 35 - After clicking on "Network" in the previous window (Figure 34), this window will appear

2. Enable "Use static address" **2** in the Network menu (Figure 35).
3. All parameters are discarded and your system administrator can set the static network parameters. By tapping into the respective entry field a keyboard appears. Accept the parameters by pressing "OK". IP address **3**, Netmask **4**, Gateway IP **5**, DNS 1 **6**, DNS 2 **7**. By pressing the "Safe" button the parameters are stored in the instrument and the menu closes. By tapping the "X" button all parameters are discarded and the menu closes.



Figure 36 - Screen of Spectroquant® Prove / Prove plus after closing the "Network" window (Figure 35)

4. Enable Prove Connect in the Prove System menu **8** (Figure 36).

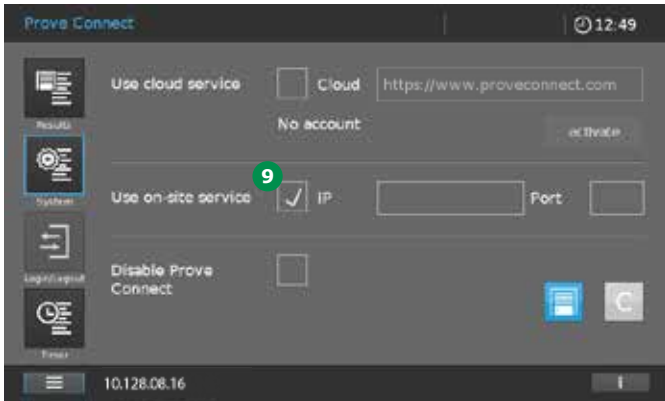


Figure 37 - Screenshot of Prove Connect menu after clicking on it in Figure 36

- Set the checkmark for "Use on-site service" 9 (Figure 37).

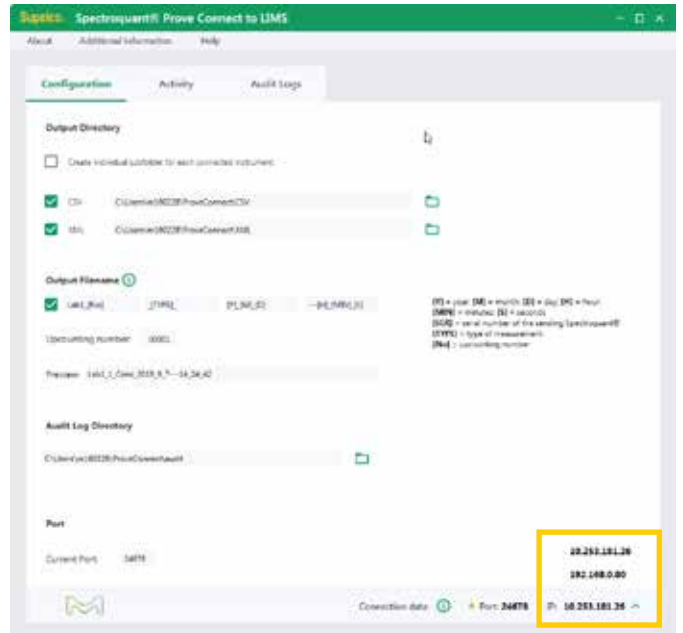


Figure 39 - Screenshot of Prove Connect for setup of network connection after clicking on the arrow next to the IP address

To support the identification of the correct IP in more complex network constellation, a list of all the PC's IP addresses is shown after clicking the arrow button besides the IP address (Figure 39).

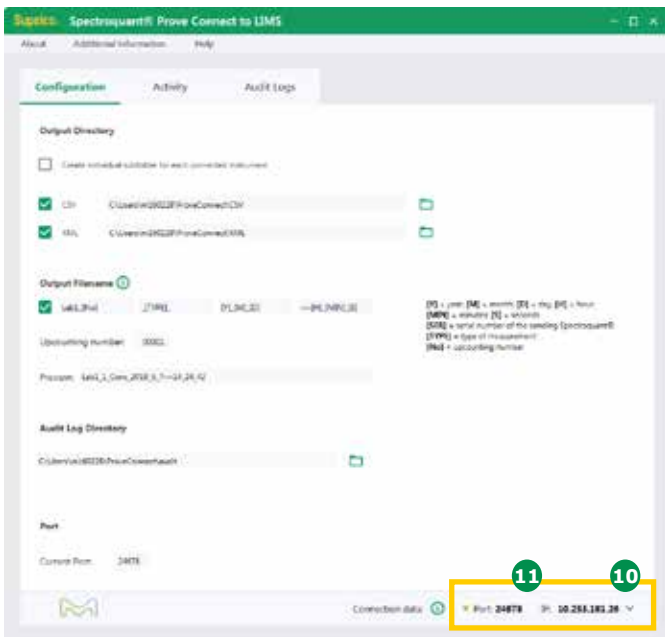


Figure 38 - Screenshot of Prove Connect for setup of network connection

- Enter the IP address 10 and Port 11 (Figure 37) shown in the Prove Connect to LIMS status bar into the instrument.



Figure 40 - Screen of Spectroquant® Prove / Prove plus (Figure 37) with entered IP address of the PC on which Prove Connect runs

- Click in the field: IP address (text box with blue border). The entry field appears 12 (Figure 40).
- Enter the IP address 10 (Figure 38) into the instrument.
- Confirm the entered IP address with "OK" 13 (Figure 40).

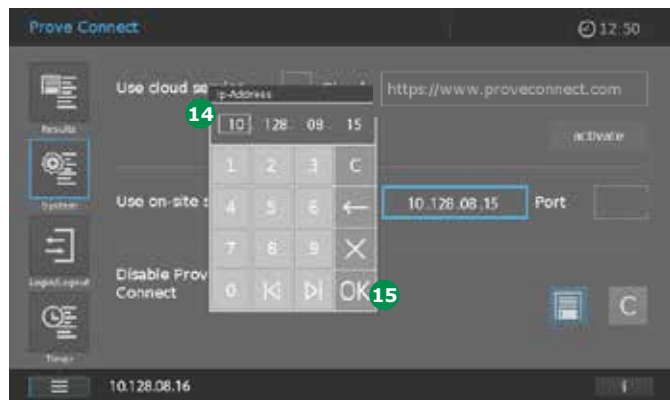


Figure 41 - Screen of Spectroquant® Prove / Prove plus (Figure 37) with entered IP address of the PC on which Prove Connect runs

10. Click in the field: Port (text box with the blue border). The entry field appears 14 (Figure 41).
11. Enter the Port 11 (Figure 38) into the instrument.
12. Confirm the entered Port with "OK" 15 (Figure 41).

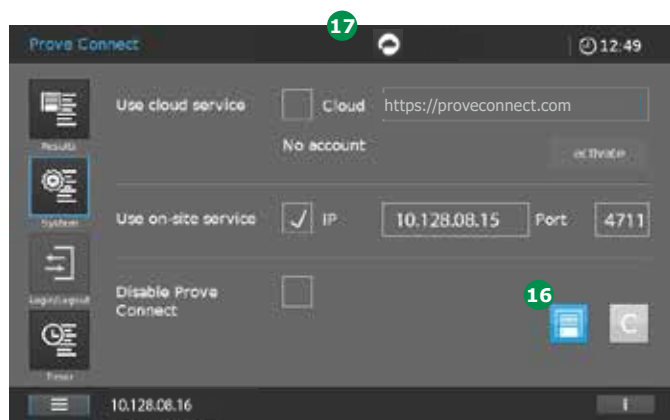


Figure 42 - Screen of Spectroquant® Prove / Prove plus with all network details

13. After setting all parameters (Checkmark, IP and Port) press the save icon 16 (Figure 42).

The Spectroquant® Prove / Prove plus is now connected to the network.
 When the connection is established the cloud icon 17 appears in the instrument display (Figure 42).
 The Spectroquant® Prove / Prove plus is now ready to transfer data to Prove Connect.
 All measurements are now transferred to the Prove Connect application.

Most likely Connection Errors

- Please make sure to activate the data transfer option ("Use on-site service") in the Prove Connect menu on the Spectroquant® Prove / Prove plus.
- A firewall could block the Spectroquant® Prove / Prove plus trying to establish the connection to the Prove Connect software. Please contact your system administrator to check the settings.
- An old firmware version is used, so that you could not find the Prove Connect menu on the Spectroquant® Prove / Prove plus, please install a Spectroquant® Prove / Prove plus firmware version 1.4.5 or a more recent update on the Spectroquant® Prove / Prove plus.

Running Prove Connect to LIMS

Background Mode

As Windows service Prove Connect is usually running in the background mode.

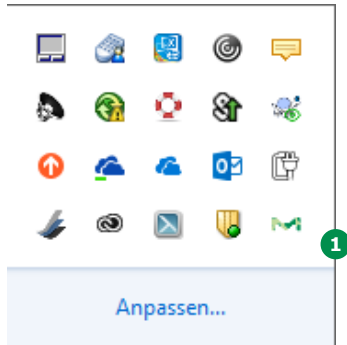


Figure 43 - Tray icons of Windows task bar

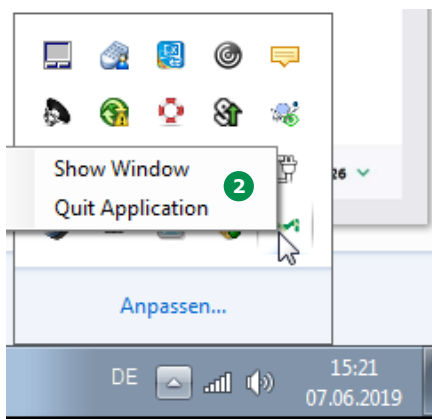


Figure 44 - Context menu after right-clicking on Prove Connect tray icon

Your computer shows a Prove Connect tray icon **1** (Figure 43) in the Windows task bar. Right-click on this icon opens a pop-up menu **2** (Figure 44) listing the following items:

“Show Window”: Prove Connect provides you a graphical user interface, the main window, that allows you to update the configuration settings, to retrieve information and to get an overview of the data transfer activities. The main window provides also access to an audit trail log.

“Quit Application” stops Prove Connect. Note that this will stop all connections between Spectroquant® Prove / Prove plus instruments and Prove Connect and, hence, the automatic transfer of measured data.

NOTE

The communication between the Prove instrument and the Prove Connect software is established via the network. Connecting the instrument or the computer that the Prove Connect software is installed on to the network could always bear a risk for attacks from the external network. Please make sure, to connect the devices only in the company network with a proper working firewall.

Prove Connect Main Window

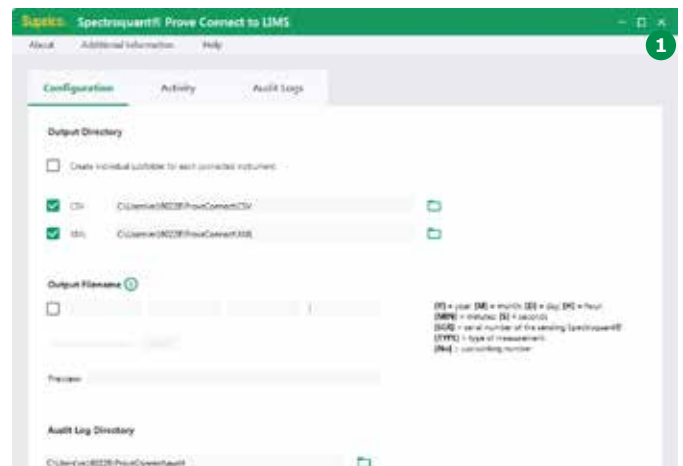


Figure 45 - Prove Connect's configuration tab

The Prove Connect Main window (Figure 45) allows you:

- To specify configuration settings for the data transfer
- To retrieve information about the software and help functions
- To get an overview of the data transfer activities as well as an audit trail

You can open the Prove Connect Main Window in the context menu of the Prove Connect system tray icon, when you click on “Show Window”. You can minimize, maximize and close the main window as usual by clicking the icons **1** (Figure 45) in the title bar.

Menu Bar



Figure 46 - Prove Connect’s menu bar

The Prove Connect Software’s menu bar (Figure 46) allows you to get more information about the software and related services.

About menu

The About menu leads you to a window showing the current software version, the license expiration date and the license key used for the activation of the software. Click on “OK” ① (Figure 47) to close the window.

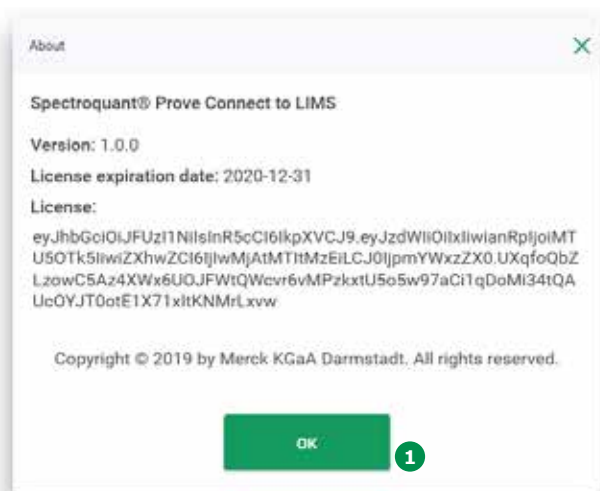


Figure 47 - Prove Connect’s About menu

Additional Information menu

You can retrieve the end-user license agreement in the EULA sub menu and information about the used third-party software in the “Used Software Licenses” sub menu of the Additional information menu.

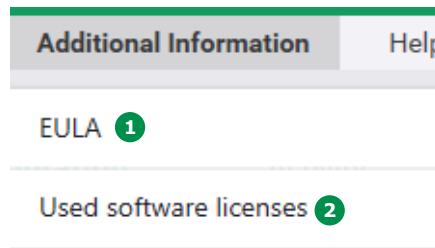


Figure 48 - Prove Connect’s Additional Information menu

If you click on the EULA sub menu ① (Figure 48), a PDF document is opened in your default Windows application, e.g. the Adobe Acrobat reader (Figure 49).



Figure 49 - Screenshot of EULA that was opened by clicking on the section in the previous window (Figure 48)

If you click on the “Used software licenses” sub menu ② (Figure 48), a text file is opened in your standard Windows application, e.g. Notepad (Figure 50). The file lists the used third-party licenses and their copyright information.



Figure 50 - Screenshot of “used software licenses” that was opened by clicking on the section in the previous window (Figure 48)

You can close the files in the respective applications.

Help menu

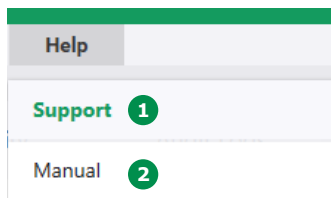


Figure 51 - Prove Connect’s Help menu

The help menu (Figure 51) allows you to open a PDF version of the user manual and shows you a support email address.

If you click on the “Support” sub menu 1 (Figure 51), a dialog window is opened that shows the support email address (Figure 52):



Figure 52 - Support pop-up that is opened by clicking on 1 in Figure 51

You can quit the window by clicking “OK”.

When you click on the “Manual” sub menu 2 (Figure 51), the PDF user manual is opened in your standard Windows application. You can close the file in your Windows application.



Figure 53 - Screenshot of manual that was opened by clicking on the 2 in the help menu (Figure 51)

Tab bar

The tab bar allows you to manage and supervise the data transfer activities of connected Prove instruments (Figure 54).



Figure 54 - Prove Connect’s tab bar

Configuration Tab

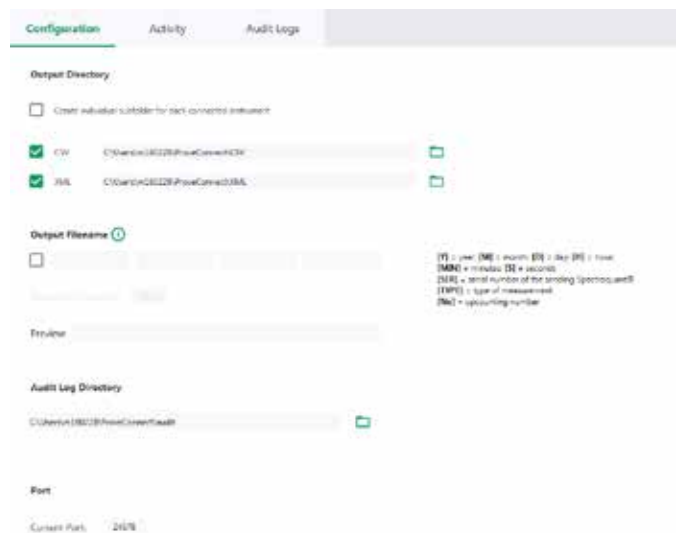


Figure 55 - Prove Connect’s configuration tab

Output Directory

Two output file formats can be selected: CSV and XML. To enable a data format, activate the corresponding checkbox ① (Figure 56) in the output directory section and select an output directory by clicking on ②.



Figure 56 - Section "Output Directory" in Prove Connect's configuration tab

The following directory selector allows you to specify the target directory of your Spectroquant® Prove / Prove plus data. The changes are instantly applied.

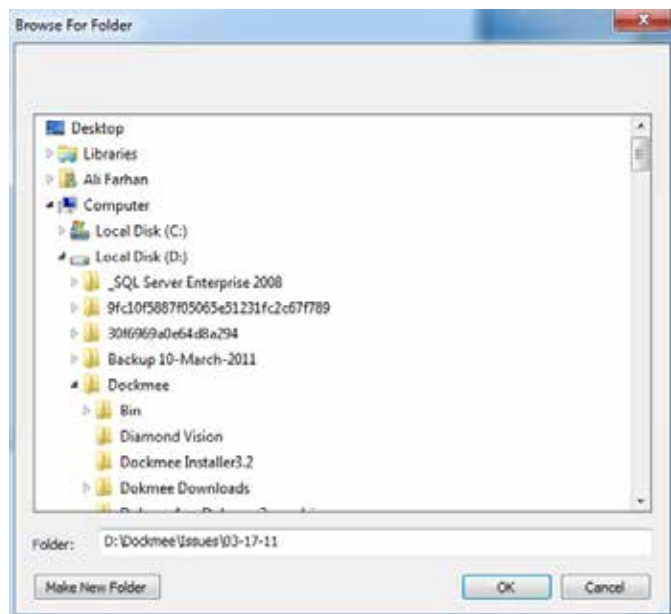


Figure 57 - Windows directory selector (BrowseForFolder)

It is possible, to create a separate subfolder for each Prove instrument that is connected to the software by checking ① in the output directory section.



Figure 58 - Section "Output Directory" in Prove Connect's configuration tab

Checking ① is effective for CSV and XML files. In both folders a subfolder is created, named by the serial number of the Prove instrument.

Output Filename

The output files are stored with a unique predefined filename. It has the following pattern: *instrument-[TYPE]_[ResultNo][MethodNo]*

Used abbreviations are defined in the following table:

Abbreviation	Explanation
[TYPE]	Current measurement mode
[ResultNo]	Result Number of the measurement stored on the Prove Instrument
[MethodNo]	Number of the used method in the method database

If you want to define your own pattern for the name of the CSV or XML output files, please activate the check box in the Output Filename section of the Configuration Tab ① (Figure 59).

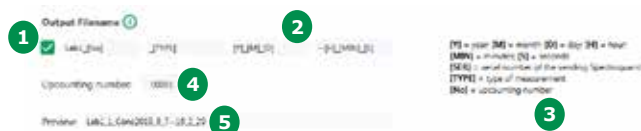


Figure 59 - Section "Output Filename" in Prove Connect's configuration tab

Four input fields are given **2**, which together form the filename. You can enter alphanumeric characters, special characters and the abbreviations in the square brackets listed on the right side of the output filename section **3**. The abbreviations **3** are automatically substituted by the current data during file storage. The following abbreviations are allowed:

Abbreviation	Data
[Y]	Is replaced by the current year of the file storage time
[M]	Is replaced by the current month of the file storage time
[D]	Is replaced by the current day of the file storage time
[H]	Is replaced by the current hour of the file storage time
[MIN]	Is replaced by the current minute of the file storage time
[S]	Is replaced by the current second of the file storage time
[SER]	Is replaced by the serial number of the instrument that transferred the measurement; in the preview a dummy value (0123456789) is shown
[TYPE]	Is replaced by the Prove measuring type of the data file that was currently transferred (Conc, Spectrum, Kinetics, Abs_Trans); In the preview a dummy value is shown (Conc)
[No]	Is replaced by an up-counting number; the number can be reset by defining an initial value in the text box 4

You can also define an up-counting number to be added anywhere in the filename. The number is then incremented by one with each stored measurement file up to 99999. An initial value can be entered in the text field "Up-Counting Number" **4**.

The preview **5** shows, how the filename would look like, in case, that a measurement would have been transferred right now. The abbreviations are already replaced by the current data.

When you don't configure the output filename, the output files are stored with a unique pre-defined filename. It has the following pattern: *instrument-[TYPE]_[ResultNo][MethodNo]*

Used abbreviations are defined in the following table:

Abbreviation	Explanation
[TYPE]	Current measurement mode
[ResultNo]	Result Number of the measurement stored on the Prove Instrument
[MethodNo]	Number of the used method in the method database

If you want to define your own pattern for the name of the CSV or XML output files, please activate the check box in the Output Filename section of the Configuration Tab **1** (Figure 59).

Audit Log Directory

The Audit Log Directory allows you to define the folder, in which the audit log files shall be stored. Click the folder icon **1** (Figure 60) to create or select a directory.



Figure 60 - Section "Audit Log Directory" in Prove Connect's configuration tab



Figure 61 - Section "Port" in Prove Connect's configuration tab
 In the Port section (Figure 61) you can define another port number, in case that the current port that was automatically chosen by the software is e.g. occupied by another Windows service.

When you click in the Port field **2** (Figure 61), a confirmation dialog is shown to warn that the change of the port number could inflict all current connections with Prove instruments.



NOTE

Only a system administrator should change the port configuration.

You can quit the window by clicking "OK". You can quit the window without changing the port configuration, by clicking "Cancel".

After you clicked on "Proceed" you can change the port number by entering a new value in the text box **1**. The changes are instantly applied. Remember that you must change the port in the Prove instrument settings as well.

Activity Tab

The Activity Tab (Figure 62) shows the last successfully established connections between the Prove instruments and the software. The overview is given in the form of a table that lists the serial number of the instrument **1**, its IP address **2** and the time of the last interaction with the software **3**. An additional comment is given **4**, in the case the instrument was disconnected after data transfer.

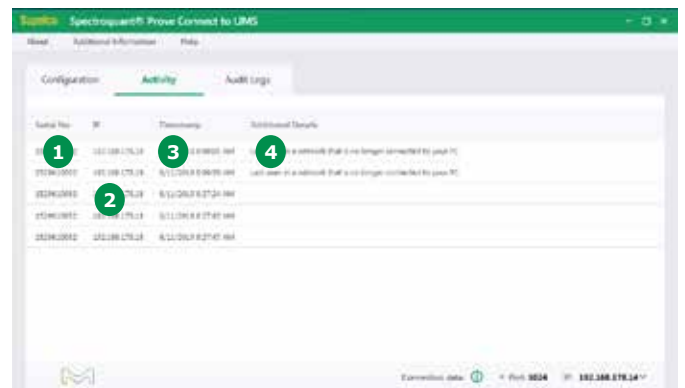


Figure 62 - Prove Connect's Activity tab

Audit Logs Tab

The Audit Logs Tab (Figure 63) shows a table with details of the data transfer activities that could be used for trace back e.g. in case of an audit.

The timestamp **1** column shows the date of the software action. The software can receive measurement data from the instrument (Receive-Action) and convert the data into the output file with subsequent file storage (Process Action). The second column **2** lists the names of the measurement raw data files, as they are originally stored on the Prove instrument. This information is important in case of an audit, as the filename and the information in the file cannot be changed by the user.

The third column **3** lists the serial number of the Prove instrument that transferred the data. The following two columns list the software actions **4**, please refer to the paragraph above, and their results **5**.

The last column **6** lists the name of the file, that was created by the software and stored in the user-specified folder on the PC or in the network. The new file is only produced during the software's Process Action, so that the column field is empty, when a Receive Action is reported.

Timestamp	Message	Serial No.	Action	Status	Additional Message
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Received	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Processed	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Received	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Processed	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Received	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Processed	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Received	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Processed	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Received	Success	
8/11/2018 8:00:00 AM	Instrument - CONN_471481_8348	11960000	Processed	Success	

Figure 63 - Prove Connect's Audit Logs tab

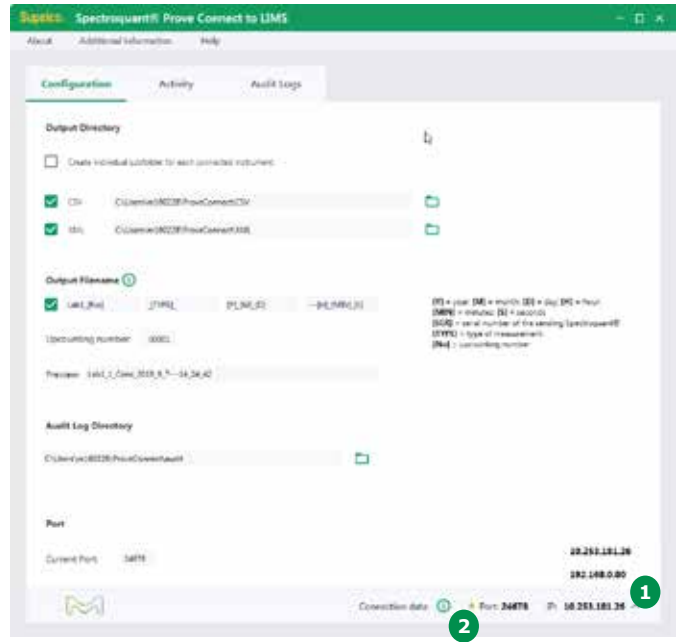


Figure 65 - Prove Connect's configuration tab

Status Bar

The status bar (Figure 64) at the bottom of the main window shows the IP address of the PC and the port number that should be entered in the Prove Instrument's Prove Connect menu for establishing the connection to the software, as described starting in section "Establishing the Connection and Starting the Program" on page 6.



Figure 64 - Prove Connect's status bar

In complex networks your PC could have more than one IP address and it could be not clear to which IP address the Prove should send its data depending on the network, the Prove itself is connected in. To assist you establishing a connection in those networks, the software shows a list of all IP addresses, when you click the arrow button **1** (Figure 65).

A status symbol **2** indicates whether the selected port is free for usage with Prove Connect (green) or occupied by another software (red).

Transferring Data from Spectroquant® Prove / Prove plus

Prove Connect acts as a background service waiting for data from Spectroquant® Prove / Prove plus instruments. If Prove Connect is enabled in the settings of the Spectroquant® Prove / Prove plus, all measurement data are transferred automatically.

If the Prove instrument is disconnected from the network, all measurement files that could not be transferred during the time that the network connection was interrupted, are transferred after the connection is reestablished, as long as the software is still running on the PC.

Prove Connect converts the data from the measurement into the selected output formats and saves them into the specified directories (see also Figure 58). This overall process happens seamlessly in the background. A potential target system (e.g. LIMS) needs be configured accordingly. The specific file format description can be found in the section Output Formats.

For monitoring the background process Prove Connect has an activity stream and an audit log. The description is found in the section Prove Connect Main Window starting on page 15. Log files are written to ensure full traceability. They are specified in more detail in section Log File.

Uninstalling Prove Connect

To uninstall Prove Connect, please use the “Add or Remove Programs” function in the Windows Control Panel. A dialog appears to confirm that you would like to modify the Prove Connect Software Setup (Figure 66).

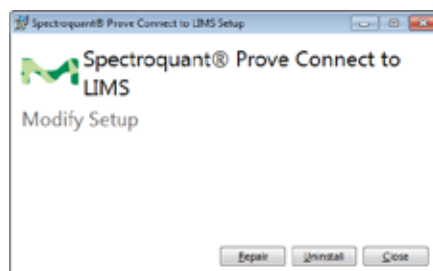


Figure 66 - Screenshot of setup wizard

Click the “Uninstall” button to start the uninstallation process. All program files and the application icon will be removed. After confirmation a progress bar appears indicating the progress of the uninstall process.

After Prove Connect has been successfully removed the following message appears (Figure 67). Press “Close” to close the window.



Figure 67 - Screenshot of setup wizard after successful uninstallation

NOTE

The log files and measurement files are not deleted after uninstalling Prove Connect.

Log File

The audit log files are generated daily. The log file contains the same information as the table in the Audit Logs tab (Figure 63). Each time a Prove Connect action takes place a new line is generated in the audit log file.

These log files can be found in the folder that is defined in the configuration tab of the Prove Connect main window.

Output Formats

Prove Connect provides two different output file formats:

1. CSV: Comma separated values: Text Text-based, human human-readable format.
2. XML: Original file format provided by Spectroquant® Prove / Prove plus

CSV

The CSV output format is structured in the following way. All fields are separated by a ";" character.

Device Information

The first section of the CSV file provides the following information about the instrument:

- Device type
- Device serial number
- Device software version of the method data base

The following table presents the device information section of a CSV output:

Devicename	Prove 600	
Serialnumber	1509600138	
VersionMDB	1.0.12	

Figure 68 - Screenshot of an example for a CSV-derived table with entries

Measurement-specific Information

The second part contains information provided about the sample and measuring results presented in one line composed of multiple columns details are not measurement-specific:

- timeStamp: time of the measurement in the following format YYMMDD_HMIN
- methodNr: the number of the used method in the method database
- methodName: the name of the method used
- ItemNo: the item number of the used test kit
- LotNo: the batch number of the used test kit
- expirationDate: the expiration date of the used test kit
- result: the measuring result
- unit: the dimension of the result
- citation unit: citation form
- dilution: dilution factor in case the sample was diluted
- sampleID: an alphanumeric string for the sample identification
- userId: the login name of the current user, when the user management was switched on
- resultNo: the number of the result on the Prove instrument
- resultClass: the measuring class, e.g. concentration, spectrum, kinetic, Abs_Trans
- pathlength: optical path length of the inserted cell
- analyteABS: the absorption value of the sample
- zaDate: date of the last zero adjustment measurement
- userRB: indication, whether the user performed a reagent blank measurement (true) or the factory reaction blank value is used (false)
- userRBValue: reagent blank value of the user's measurement
- userRBLotNo: lot number of the reagent used for the reagent blank measurement
- user RBDate: date of the user reagent blank measurement

- turbidityCorrection: indication, whether the turbidity correction function was activated (true) or de-activated (false)
- turbidityCorrectionValue. absorption value at the turbidity correction wavelength
- sampleBlank: indication, whether a sample blank was in effect (true) or not (false)
- sampleBlankValue: absorption value of the used sample blank
- userCal: indication, whether a user calibration was in effect (true) or not (false)
- userCalLotNo: lot number of the reagent used for the user calibration
- userCalDate: date of the user calibration measurement
- checkWLABsorption: absorption measured at an another wavelength ("plausibility" has to be activated to get a value).
- checkWLResult: result of the "plausibility check" (remark: plausibility check is only possible for some methods)

The following table gives an example of a concentration measurement

NOTE

Whereas the results are horizontally outputted in one line in the measuring file (separated by ";"), they are vertically listed in this section for a better readability .

timeStamp	190513_0805
methodNr	35
methodName	Nitrite
ItemNo	114547
LotNo	DEMO1506
expirationDate	991231_0000
result	0.542
unit	mg/l
citation	NO_2-N
dilution	0
sample ID	67
userId	anonymous
resultNo	199
resultClass	CONC
pathLength	16
analyteABS	1.971828
zaDate	190513_0805
userRB	false
userRBValue	0
userRBLotNo	
userRBDate	
turbidityCorrection	false
turbidityCorrectionValue	0
sampleBlank	false
sampleBlankValue	0
userCAL	false
userCALLotNo	
userCALDate	
checkWLABsorption	0
checkWLResult	

Kinetics

For a kinetics measurement, the following specific details are provided by Prove Connect:

- methodNr: the number of the used method in the method database
- pathlength: optical path length of the inserted cell
- resultClass: the measuring class, (in this case always kinetics)
- resultNo: the number of the result on the Prove instrument
- sampleID: an alphanumeric string for the sample identification
- timeStamp: time of the measurement in the following format YYMMDD_HMIN
- userId: the login name of the current user, when the user management was switched on
- mode: type of measurement (absorption or transmittance)
- duration: Duration of the measurement in seconds
- interval: Time interval between measurement points, in seconds
- delay: lead time to start the series of measurements
- wavelength: The fixed wavelength configured on the Prove instrument for the kinetics measurement
- result: A table composed of two columns: time and value, each entry in this table presenting a measurement value at a specific point of time

The following table presents a CSV output file of a kinetics measurement:

Devicename	Prove 600											
Serialnumber	1509600138											
VersionMDB	1.0.12											
methodNr	pathLength	resultClass	resultNr	sampleId	timeStamp	userId	mode	duration	interval	delay	WLO	
1201	0	KINETICS	54368	feli1	150807_1553	anonymous	ABSORPTION	60	5	60	500	
time	abs/trans@WLO											
0	0											
1	0											
2	0											
3	0											
4	0											
5	0											
6	0											
7	0											
8	0											

Figure 69 - Screenshot of a CSV-derived table for a kinetic measurement

Spectrum

For a spectrum measurement, the following specific details are provided:

- methodNr: the number of the used method in the method database
- pathlength: optical path length of the inserted cell
- resultClass: the measuring class, (in this case always spectrum)
- resultNo: the number of the result on the Prove instrument
- sampleID: an alphanumeric string for the sample identification
- timeStamp: time of the measurement in the following format YYMMDD_HMIN
- userId: the login name of the current user, when the user management was switched on
- mode: type of measurement (absorption or transmittance)
- wlStart: wavelength, at which the measurement was started
- wlEnd: wavelength, at which the spectrum measurement was ended
- wlDelta: wavelength increment chosen for the stepwise recording of the spectrum
- noiseOffset: offset value to reflect white noise
- result: a table with two columns: wavelength and value, each entry in this table presenting a measurement value for a specific wavelength (the wavelength values are equidistant)

The following table presents a CSV output file of a spectrum:

Devicename	Prove 600											
Serialnumbe	1527610039											
VersionMDB	1.0.12											
methodNr	pathLength	resultClass	resultNr	sampleId	timeStamp	userid	mode	wlStart	wlEnd	wlDelta	noiseOffset	
0	16	SPECTRUM	424	1234	150728_1323	BÄrrbel	ABSORPTION	250	550	d_5nm	0,05	
wavelength	value	min-max										
250	0,262											
255	0,211											
260	0,196	min										
265	0,261											
270	0,26											
275	0,547											
280	0,756	max										
285	0,615											
290	0,429											

Figure 70 - Screenshot of a CSV-derived table for a spectrum

Absorbance / Transmission Measurement

The CSV file of an absorbance or transmission measurement contains the following information:

- methodNr: the number of the used method in the method database
- pathlength: optical path length of the inserted cell
- resultClass: the measuring class, (in this case always Abs_Trans)
- resultNo: the number of the result on the Prove instrument
- sampleID: an alphanumeric string for the sample identification
- timeStamp: time of the measurement in the following format YYMMDD_HMIN
- userId: the login name of the current user, when the user management was switched on
- mode: type of measurement (absorption or transmittance)
- wavelength: wavelength, at which the measurement was recorded
- measValue: the absorbance or transmittance value measured at the wavelength

The following table presents a CSV output file of an absorbance or transmission measurement:

Devicename	Prove 600										
Serialnumbe	1529610052										
VersionMDB	1.0.12										
timeStamp	methodNr	methodNam	ItemNo	pathLength	resultClass	resultNr	sampleId	userId	mode	wavelength	measValue
20190611_07	0			16	ABS_TRANS	471621	5584	anonymous	ABSORPTION	500	0,235

XML

The original file format provided by Spectroquant® Prove / Prove plus is based on XML. This format is the basis to generate the other two formats. It is structured as follows:

Root Element

The first tag in the XML file is the root tag/element. It indicates the measurement type:

- 1-Concentration: <ConcMeasResult>
- 2-Kinetics: <KineticResult>
- 3-Spectrum: <SpectrumResult>
- 4-Abs/Trans: <AbsTransResult>

Result Header Element

The second tag is a generic tag that is not dependent on the measurement type. It is called "resultHeader" and provides information about the used device, user, method and other meta-data information such as the timestamp.

Result Header Attributes

The result header element contains the following attributes:

- resultClass: Indicating the measurement type (possible values: ABS-TRANS, CONC, KINETICS, SPECTRUM)
- userId: ID of the user who made the measurement
- sampleId: ID of the used sample

The following XML elements change between the different measurement types:

Measurement-specific Elements

Concentration

For a concentration measurement, the following specific elements are defined:

- ConcentrationResult: Defining the result of the measurement
- RenderedResult: Indicating the same information as displayed on the monitor of the Spectroquant® Prove / Prove plus device

The following example shows an XML file of a concentration measurement:

```
<?xml version="1.0"?>
- <ConcMeasResult>
  * <resultHeader versionMDB="1.0.12" class="Prove600" serialNo="1529610052" pathLength="16" timeStamp="2019-06-11T04:57:37.161Z" methodNr="55" resultNr="471617">
    <resultClass>CONC</resultClass>
    <userId>anonymous</userId>
    <sampleId>5580</sampleId>
  </resultHeader>
  * <testLotData expirationDate="2099-12-30T23:00:00.164Z">
    <lotNo>DEMO1506</lotNo>
  </testLotData>
  <methodConfiguration unit="0" citation="0" userZADate="2019-06-11T04:57:27.252Z" userCAL="false" userRBValue="0.0" userRB="false" sampleBlankValue="0.0"
    sampleBlank="false" turbidityCorrection="false" dilution="0"/>
  <concentrationResult concentration="3.1707869" checkWLAbsorption="0.0" tcAbsorption="0.0" analyteAbsorption="1.9576578"/>
  <renderedResult unit="mg/l" citation="PO_4-P" concentration="3.17"/>
</ConcMeasResult>
```

Kinetics

For a kinetics measurement, the following specific elements are defined:

- kineticsParam: Defining the instrument settings related to this type of measurement, such as the mode and the wavelength (settings are configured by the user before starting the measurement)
- measValues: Presenting the result value of each measurement point using the child elements "value" inside the child element "wavelength"

The following example shows an XML file of a kinetics measurement:

```
<?xml version="1.0"?>
- <KineticResult catalyticActivity="2.59095E-4">
  - <resultHeader versionMDB="1.0.12" class="Prove600" serialNo="1529610052" pathLength="16" timeStamp="2019-06-11T05:39:19.353Z" methodNr="0" resultNr="471624">
    <resultClass>KINETICS</resultClass>
    <userId>anonymous</userId>
    <sampleId>5586</sampleId>
  </resultHeader>
  - <kineticsParam interval="5" duration="30">
    <mode>ABSORPTION</mode>
    <wavelength>500</wavelength>
  </kineticsParam>
  - <measValues>
    - <wavelength>
      <value>0.23381245</value>
      <value>0.23372409</value>
      <value>0.23377019</value>
      <value>0.23393932</value>
      <value>0.23381448</value>
      <value>0.23369297</value>
      <value>0.23401995</value>
    </wavelength>
  </measValues>
</KineticResult>
```

Spectrum

For a spectrum measurement, the following specific elements are defined:

- spectrumParam: Indicating the instrument settings related to this type of measurement, such as mode and the wlDelta (wavelength increment), wlstart (initial wavelength), wlEnd (final wavelength)
- measValues: Presenting the result value of each measurement point using the child elements "float"

The following example shows an XML file of a spectrum measurement:

```
<?xml version="1.0"?>
- <SpectrumResult>
  - <resultHeader versionMDB="1.0.10" class="Prove600" serialNo="1643611698" pathLength="16" timeStamp="2017-06-09T11:24:58.326Z" methodNr="0" resultNr="1317">
    <resultClass>SPECTRUM</resultClass>
    <userId>anonymous</userId>
    <sampleId>0125</sampleId>
  </resultHeader>
  - <measValues>
    <float>0.052950654</float>
    <float>0.053409737</float>
    <float>0.053095005</float>
    <float>0.05379266</float>
    <float>0.054318134</float>
    <float>0.055269174</float>
    <float>0.05945932</float>
    <float>0.062856585</float>
    <float>0.064918905</float>
    <float>0.064369634</float>
    <float>0.06594166</float>
    <float>0.06584843</float>
    <float>0.066925645</float>
    <float>0.06582598</float>
    <float>0.0670058</float>
    <float>0.07033587</float>
    <float>0.07148241</float>
    <float>0.07367617</float>
    <float>0.074136026</float>
    <float>0.07688984</float>
    <float>0.07842573</float>
  </measValues>
  - <spectrumParam noiseOffset="0.05" wlEnd="900" wlStart="800">
    <mode>ABSORPTION</mode>
    <wlDelta>d_5nm</wlDelta>
  </spectrumParam>
</SpectrumResult>
```


Absorbance / Transmission Measurement

For an absorbance or transmittance measurement, the no specific elements are defined.

The XML file just contains the following keys:

- wavelength: wavelength, at which the measurement was recorded
- measValue: the measured value
- mode: type of measurement, absorbance or transmittance

The following example shows an XML file of an absorption/transmission measurement:

```
<?xml version="1.0"?>
- <AbsTransResult>
  * <resultHeader versionMDB="1.0.12" class="Prove600" serialNo="1529610052" pathLength="16" timeStamp="2019-06-11T05:35:39.717Z" methodNr="0" resultNr="471621">
    <resultClass>ABS_TRANS</resultClass>
    <userId>anonymous</userId>
    <sampleId>5564</sampleId>
  </resultHeader>
  <mode>ABSORPTION</mode>
  <wavelength>500</wavelength>
  <measValue>0.23520945</measValue>
</AbsTransResult>
```


Supelco[®]

Analytical Products

We provide information and advice to our customers on application technologies and regulatory matters to the best of our knowledge and ability, but without obligation or liability. Existing laws and regulations are to be observed in all cases by our customers. This also applies in respect to any rights of third parties. Our information and advice do not relieve our customers of their own responsibility for checking the suitability of our products for the envisaged purpose.

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the U.S. and Canada.

Merck Life Science KGaA, 64271 Darmstadt, Germany, Tel. +49(0)6151 72-2440

www.sigmaaldrich.com

© 2024 Merck KGaA, Darmstadt, Germany and/or its affiliates. All Rights Reserved. Merck, Supelco, and Spectroquant are trademarks of Merck KGaA, Darmstadt, Germany or its affiliates. All other trademarks are the property of their respective owners. Detailed information on trademarks is available via publicly accessible resources.

MERCK