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iCAP 7000 Plus Series ICP-OES

Software Manual

Qtegra ISDS Software 2.10 SR3

BRE0015330 Revision C January 2019

ThermoFisher SCIENTIFIC

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For Research Use Only. Not for use in diagnostic procedures.

History

The following table lists the changes within this document.

Rev.	Section/Link	Title
A	Detector Setup Wizard	Description of Detector Setup Wizard.
A	Saving as HTML File, page 6-6	Description of Report export format HTML.
A	Table 3-5	Description of new User Groups.
A	Displaying Reports	Description of Mass Calibration Report.
A	page 3-9	Added a Tip when opening an empty History window.
A	Table 14-11	Updated Automatic LabBook backup settings table.
A	To open a signed or locked LabBook	Description of 'locked' state of a signed LabBook.
A	Individual columns in the Sample List	Description of how to add additional Sample List columns.
A	Access Rights	Description of Access Rights applet.
A	File Access Rights	Description of File Access Rights applet.
A	To add a Windows user to a Qtegra user group	Description of how to add a Windows user to a Qtegra group.
A	Table 4-6	Update table to explain events of Qtegra System Log.
A	Table 8-1	Update table of Reports supplied with Qtegra.
A	Figure 6-5	Description of Report button in LabBook History window.
C	Categories	Making SD and %RSD values available for exports and queries.
C	To create a prepFAST method	Extended description of prepFAST methods.

Rev.	Section/Link	Title
C	page 10-41	Extended description of Quality Control results shown in the Comment tile of the Concentrations view.
C	page 13-10	Clarification for Update Calibration.

Contents

1

Using This Manual

This chapter provides information about this manual.

Contents

About this Manual

This *Software Manual* introduces the Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software suite and describes the configuration and operation of the iCAP™ 7000 Plus Series ICP-OES instrument with Qtegra ISDS Software. For information about the operating procedures for the iCAP 7000 Plus Series ICP-OES system, we recommend that you read the *Operating Manual*.

With Qtegra ISDS Software, the Configurator tool is provided to set up Configurations and settings specific to your individual systems and users. In the Qtegra tool you have access to the creation of Templates and LabBooks, can query results, manage your files, look for help. Here you define the Template's settings and create your LabBook for measurement.

Who Uses this Guide

This *iCAP 7000 Plus Series ICP-OES Software Manual* is intended for all personnel the need to perform measurements with the iCAP OES mass spectrometer.

Scope of this Guide

The *iCAP 7000 Plus Series ICP-OES Software Manual* includes the following chapters:

- Chapter 3: "Configurator" describes the Configurator tool, which contains all tools necessary to configure and adjust the Qtegra ISDS Software framework for your laboratory.

- Chapter 4: "Qtegra" describes the principal tool for preparing and running measurements. The Qtegra tool is the main Qtegra ISDS Software module and is used to design, start and stop the measurements.
- Chapter 5: "Templates" describes the analytical workflow for sample measurement that is defined in a Template.
- Chapter 6: "LabBooks" describes that LabBooks are based on the settings specified in the Templates in Qtegra. These setting can still be adjusted in the LabBook before the measurements is run.
- Chapter 8: "Qtegra Reports" describes the necessary steps to create and execute Reports using the Qtegra Report Editor.
- Chapter 9: "Method Parameters" describes the Method Parameters, which are dependent on the evaluation method assigned to the LabBook.
- Further chapters describe the evaluation methods and their typical use case.
- Additional chapters describe the basic mathematical methods used by Qtegra ISDS Software. This includes information about statistical calculations, linear and polynomial regression as well as Gaussian error estimation for regression analysis.

Related Documentation

In addition to this *Software Manual*, Thermo Fisher Scientific provides the following documents for the iCAP 7000 Plus Series ICP-OES instrument:

- *Operating Manual*
- *Consumables and Parts Catalog*
- *Installation Guide*
- *iCAP 7000 ICP-OES Spectrometer Qtegra ISDS Software Installation Procedure* (section 2 of 3)
- *Data Processing Algorithms Manual*

The *Operating Manual* represents the Original Operating Instructions. Thermo Fisher Scientific provides this *Software Manual* as additional reference documents for the iCAP 7000 Plus Series ICP-OES instruments.

A printed version of the *Operating Manual* is shipped with the instrument.

Typographical Conventions

This section describes typographical conventions that have been established for Thermo Fisher Scientific manuals.

Signal Words

Make sure you follow the precautionary statements presented in this manual. The special notices appear different from the main flow of text:

Tip Points out possible material damage and other important information in connection with the instrument.

Data Input

Throughout this manual, the following conventions indicate data input and output via the computer:

- Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
- Input that you enter by keyboard is identified by quotation marks: single quotes for single characters, double quotes for strings.
- For brevity, expressions such as "choose **File > Directories**" are used rather than "pull down the File menu and choose Directories."
- Any command enclosed in angle brackets < > represents a single keystroke. For example, "press **<F1>**" means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, "press **<Shift>** + **<F1>**" means press and hold the <Shift> key and then press the <F1> key.
- Any button that you click on the screen is represented in bold face letters. For example, "click **Close**".
- Procedures often end with "click **OK**", which is omitted in many cases. "Click **Save** to save your changes" is also no more shown as the final step.

Topic Headings

The following headings are used to show the organization of topics within a chapter:

Chapter 1 Chapter Name

Second Level Topics

Third Level Topics

Fourth Level Topics

Contacting Us

There are several ways to contact Thermo Fisher Scientific. You can use your smartphone to scan a QR Code, which opens your email application or browser.

Contact	Link / Remarks	QR Code
Brochures and Ordering Information	www.thermofisher.com/icp-oes	
Service Contact	www.unitylabservices.com	
Technical Documentation SharePoint	❖ **To get user manuals for your product** 1. With the serial number (S/N) of your instrument, request access on our customer SharePoint as a customer at www.thermoscientific.com/Technicaldocumentation 2. For the first login, you have to create an account. Follow the instructions given on screen. Accept the invitation within six days and log in with your created Microsoft™ password. 3. Download current revisions of user manuals and other customer-oriented documents for your product. Translations into other languages may be available there as well.	
Customer Feedback	❖ **To suggest changes to this manual** You are encouraged to report errors or omissions in the text or index. Send an email message to the Technical Editor at documentation.bremen@thermofisher.com.	

2

Introduction to Qtegra ISDS Software

This *Software Manual* describes the Thermo Scientific Qtegra Intelligent Scientific Data Solution (ISDS) configurable software package for elemental analyses for configuration and operation of the Thermo Scientific iCAP 7000 Plus Series ICP-OES. Qtegra ISDS Software is a true end-to-end solution for workflow-driven analysis. You can use this suite of applications for a variety of Thermo Fisher Scientific products.

The main Qtegra ISDS frameworks introduced in this chapter are:

Contents

Firmware Update

When a firmware update is available, the **Firmware Update** dialog opens automatically if the controlling computer has access to the Internet, see Figure 2-1.

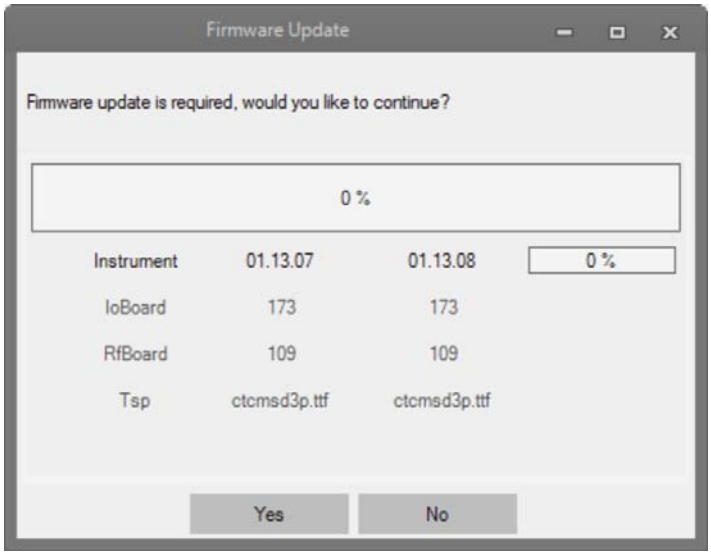


Figure 2-1. Firmware Update dialog

❖ **To install the firmware update**

1. Click Yes.
2. Follow the instructions.

Setting User Levels

Qtegra ISDS Software is used by different people with different functions. At the beginning, Qtegra ISDS Software is installed and configured. These steps usually are done by an Administrator. In the daily laboratory use, a Qtegra User prepares the measurement, for example, the User selects or creates a LabBook to be scheduled.

When you open additional Qtegra ISDS Software tools, for example, Instrument Control, you need QtegraAdministrator rights. Without these rights a message box is shown that explains that required privileges to run the program are missed. How to set the Qtegra ISDS Software user levels is described in this chapter.

The Qtegra ISDS Software user levels are defined over the Windows User rights. To grant all Qtegra ISDS Software users access to the desired user interface, Windows™ offers two options to be performed by an Administrator.

❖ **To display the Users and Groups folders**

1. Open **Start > Windows Administrative Tools > Computer Management**.
2. In the Computer Management window, expand **System Tools** and **Local Users and Groups**. The **Users** and **Groups** folders are shown. See Figure 2-2.

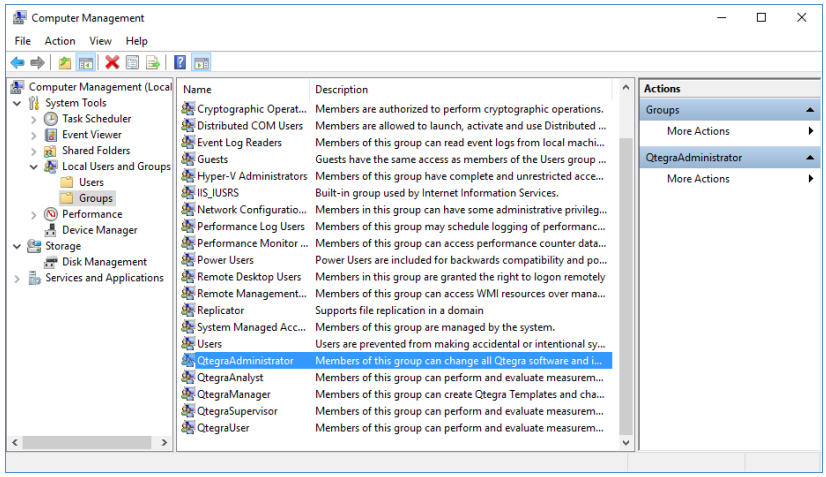


Figure 2-2. Computer Management window

Or, an Administrator opens the Microsoft Management Console (MMC).

❖ **To open the Microsoft Management Console (MMC)**

1. Click the **Start** button.

2. Type `mmc` into the search box and press **<Enter>**. After confirming the User Account Control message, the Console window opens, see Figure 2-3.

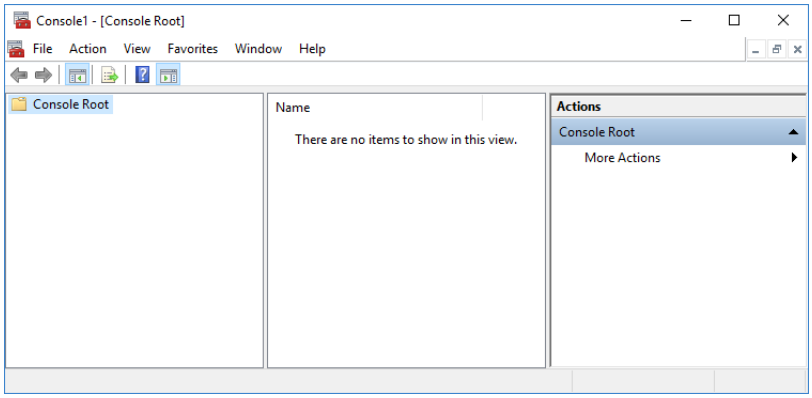


Figure 2-3. Console window

3. In the left pane, click **Local Users and Groups**.

4. If you do not see Local Users and Groups, it is probably because that snap-in has not been added to Microsoft Management Console. Follow these steps to install it:

   a. In the Console window, click **File > Add/Remove Snap-in**.

   b. Select **Local Users and Groups**, and then click **Add**. See Figure 2-4.

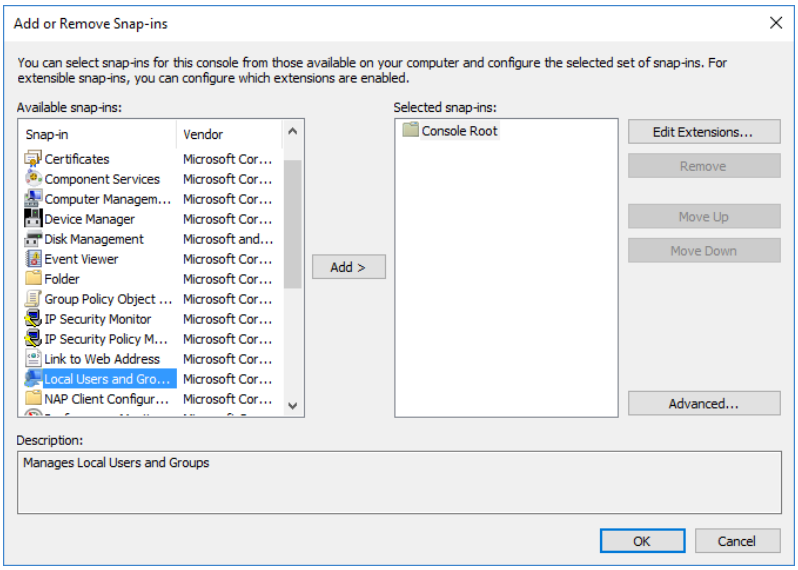


Figure 2-4. Adding Local Users and Groups

   c. In the **Choose Target Machine** dialog, select **Local computer**, and then click **Finish**.

d. Click **OK** to close the **Add or Remove Snap-ins** dialog. The entry **Local Users and Groups (Local)** is shown, see Figure 2-5.

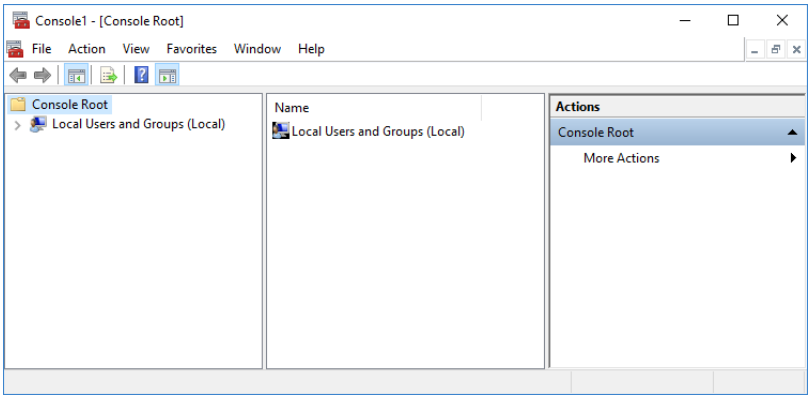


Figure 2-5. Console with Local Users and Groups

5. Double-click **Local Users and Groups** to expand the entry.

6. Double-click the **Groups** folder.

Tip If the Qtegra groups are not available on your Windows system, the installation process obviously failed. Nevertheless, you can add the Qtegra groups to Windows.

❖ **To create Qtegra user groups if these groups are not available**

1. Click **Action > New Group**, see Figure 2-6.

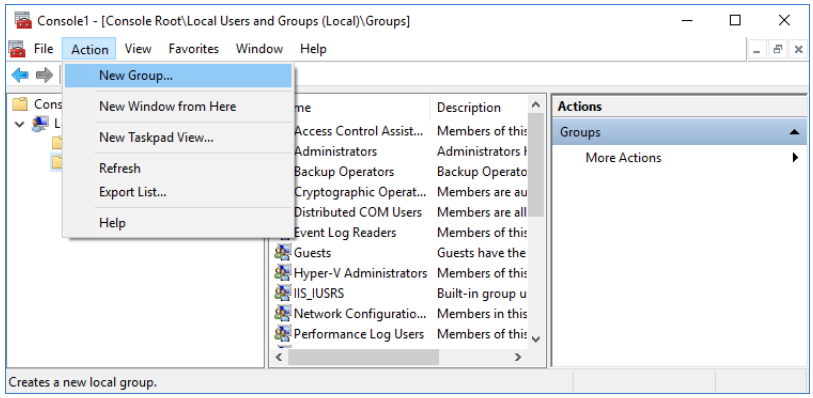


Figure 2-6. Creating new group

2. In the **New Group** dialog, enter *QtegraAdministrator* as Group name. Members of this group can change all Qtegra ISDS Software and instrument settings.

3. Repeat step 1 up to step 2 for *QtegraSystemAdministrator*, *QtegraDataAdministrator*, *QtegraManager*, *QtegraSupervisor*, *QtegraAnalyst*, and *QtegraUser,* where members of this group have roles as described in Table 3-5.

4. Double-click the desired Qtegra group and click **Add** to add all desired Windows users to this Qtegra group. Standard Windows dialogs guide you through the selection of users.

   a. In the first step, enter the desired users (see Figure 2-7).

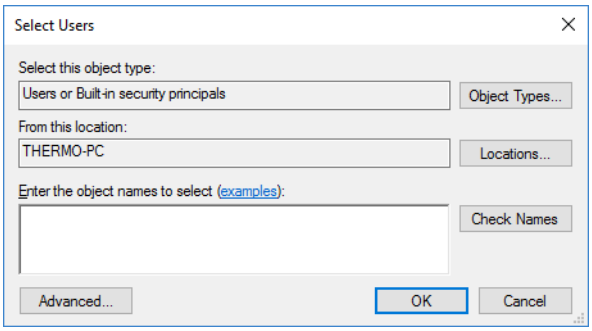


Figure 2-7. Selecting Windows users

-or-

   b. Click **Advanced** to open the extended search dialog (see Figure 2-8).

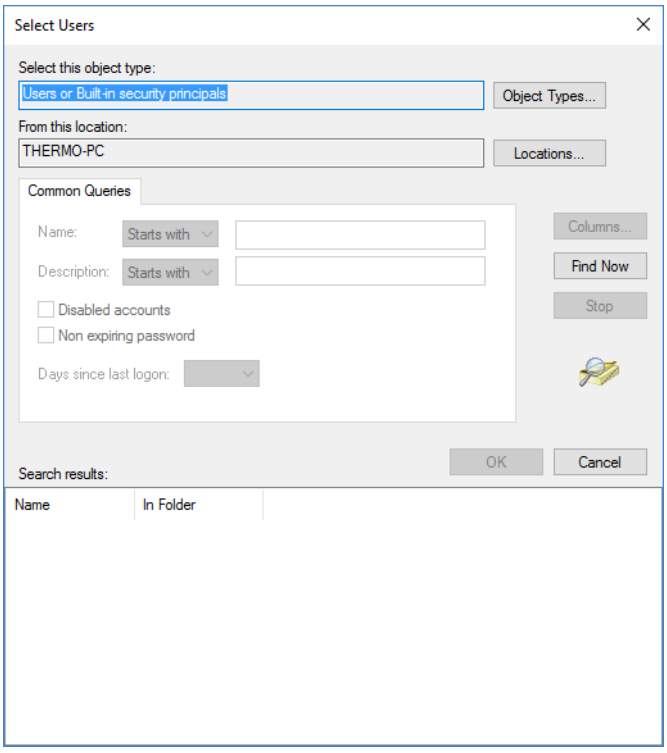


Figure 2-8. Advanced search for Windows users

   c. As final step of your user selection, click **OK** to close all dialogs.

After login, every Windows user on the Qtegra ISDS PC automatically is granted access with his or her Qtegra role that is defined by membership in one of the Qtegra user groups.

Tip If a single Qtegra ISDS user is added to more than one Qtegra user group, the user has the rights of the highest group in the hierarchy.

The following examples shows how to add a user to a Qtegra user group. The user ("Thermo") is configured on the system and has Windows rights.

❖ **To add a Windows user to a Qtegra user group**

1. Right-click the Windows Start menu and select **Computer Management** from the shortcut menu.

2. In the left pane, expand **Local Users and Groups** and select **Users**.

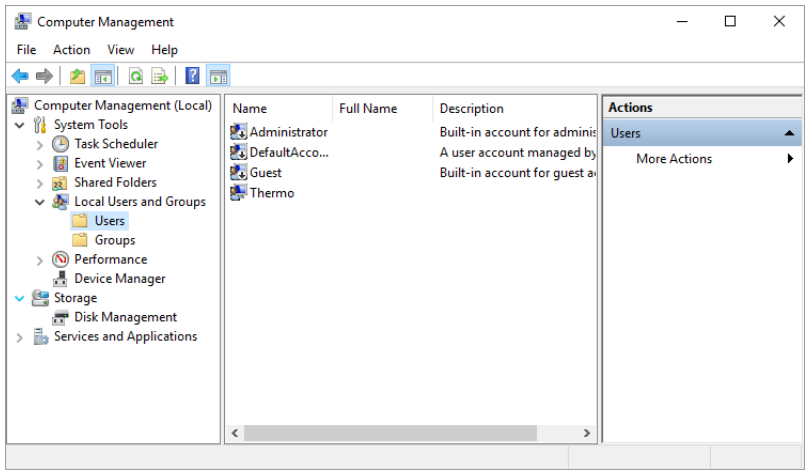


Figure 2-9. Expanding current Local Users and Groups

3. In the middle area, select the user ("Thermo") you wish to add to a Qtegra user group.
   The right pane shows the user and the **More Actions** item.

4. Click **More Actions** and select **Properties** from the shortcut menu.
   The **Thermo Properties** dialog opens.

5. Select the **Member Of** tab.

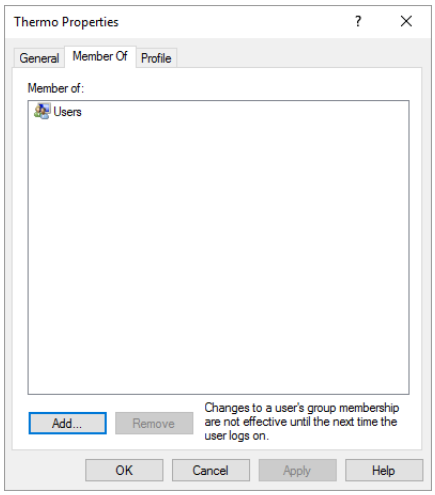


Figure 2-10. Member Of tab of the selected user

6. Click **Add** to open the **Select Groups** dialog.

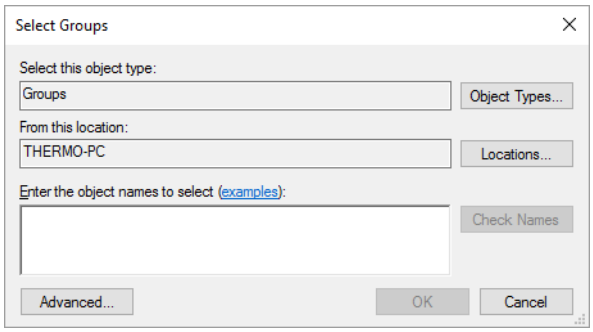


Figure 2-11. Select Groups dialog

7. In the lower field, enter the object name, that means, enter the Qtegra user group, for example "`qtegraanalyst`". Make sure to type the correct (part of the) Qtegra user group.

8. Click **Check Names** to verify the object name.
In our example, the name will change to "THERMO-PC\QtegraAnalyst", where the prefix comes from your PC name.

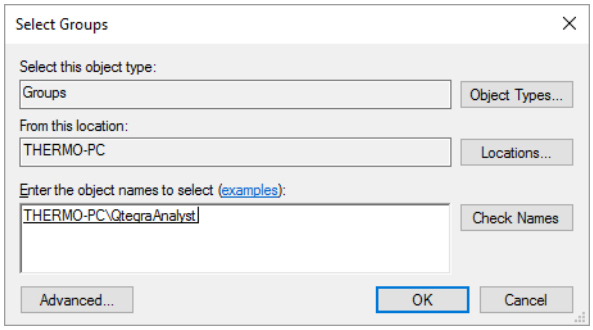


Figure 2-12. Updated object name

9. Click **OK** to see the additional membership in the **Properties** dialog.

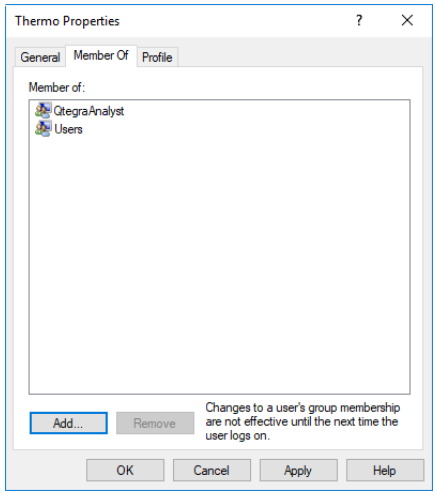


Figure 2-13. Member Of tab with new membership

10. Close the Properties dialog. Close the Computer Management window.

After next login, the user “Thermo” can start Qtegra and operates as a QtegraAnalyst.

Quick Start

The Thermo Fisher Scientific field service engineer installs the iCAP 7000 Plus Series ICP-OES at your site. He also sets up the Qtegra ISDS Software for first use.

Five Clicks to get a Result

1. Open your LabBook.
   A LabBook contains all the details that are relevant to your experiment, for example, all the instrument's parameters, sample information, and data collection and reporting parameters.

2. Click the Get Ready button.
   The Get Ready button communicates with the instrument to start the peristaltic pump, ignite the plasma, allow it to warm up, and do a performance check. In the time it takes you to prepare your calibration standards and load them into the autosampler, the instrument has done everything it needed to be prepared for the day's analysis.

3. Load your sample information.
   Qtegra ISDS Software is flexible, so you can type your sample names in one by one, or you can import your entire sample from an external spreadsheet.

4. Analyze your samples.
   Once your samples are added to the LabBook, you are ready to start your analysis. A single click loads the LabBook into the scheduler and runs it.

5. Export your data.
   Whether you want your data electronically or in a hard copy, data reporting can be done with a single button click. Export your data into one of the pre-loaded Report templates or create your own Report template.

Configurator Overview

The Configurator tool is used by your network Administrator and your laboratory manager. Different applets are provided to edit general settings of the hardware and software and to configure and adjust the Thermo Scientific Qtegra ISDS framework for your laboratory. For details on the Configurator tool, see "Configurator" on page 3-1.

The user interface of the Configurator tool is shown in Figure 2-14:

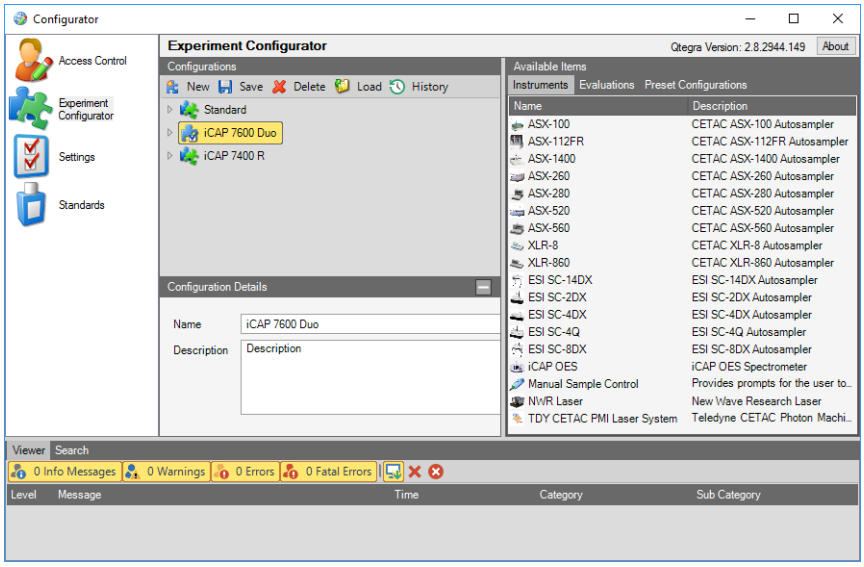


Figure 2-14. User interface of Configurator

Table 2-1 gives a short description of each applet.

Table 2-1. Applets of the Configurator

Applet		Description
	Access Control	Allows the Administrator to define the access permissions for the different programs and applications in the user interface.
	Access Rights	Introduced with Qtegra ISDS Software version 2.10, allows to control the access permissions by granting or denying access to the Qtegra applications in general and the Configurator applets in particular.
	Experiment Configurator	Allows the Administrator to define instrument settings, communication ports, and combine instrument sets and evaluation strategies for a specific Experiment Configuration. Templates and LabBooks created in Qtegra are based upon these Configurations.
	Reports	Allows the Administrator to create new and to edit existing Report templates.

Table 2-1. Applets of the Configurator, continued

Applet		Description
	Settings	Gives access to the settings database (registry) and controls default settings such as the default directory path for Qtegra. The settings stored here should not normally need any modifications.
	Signature Workflow	Signatures allow to document that a workflow stage (*Acquired, Verified* and *Approved*) has been performed by a known person. Each stage can be revoked. In the Configurator, the stages are defined and the access rights for signing and revoking are set individually for all user groups.
	Standards	Central database editor for stock solutions and standards.

Qtegra Overview

The Qtegra tool is the main Qtegra ISDS module and is used to design, start and stop the measurements. The **Home Page** tab offers access to all pages of the Qtegra tool. By default, the Home Page opens on the **Dashboard** page.

Tip If you can read **Unreleased and untested version!** on the Dashboard page, your version of Qtegra is not released for scientific purposes, but only as an internal test version, which may be unstable. Please contact your Thermo Fisher Scientific field service engineer to get a released version.

The analytical workflow is based on the design of a measurement in a Template. Sample analysis and data acquisition is then performed in LabBooks created from the Template with appropriate information on the samples. For details on the Qtegra tool, see "Qtegra" on page 4-1.

The user interface of the Qtegra tool is shown in Figure 2-15:

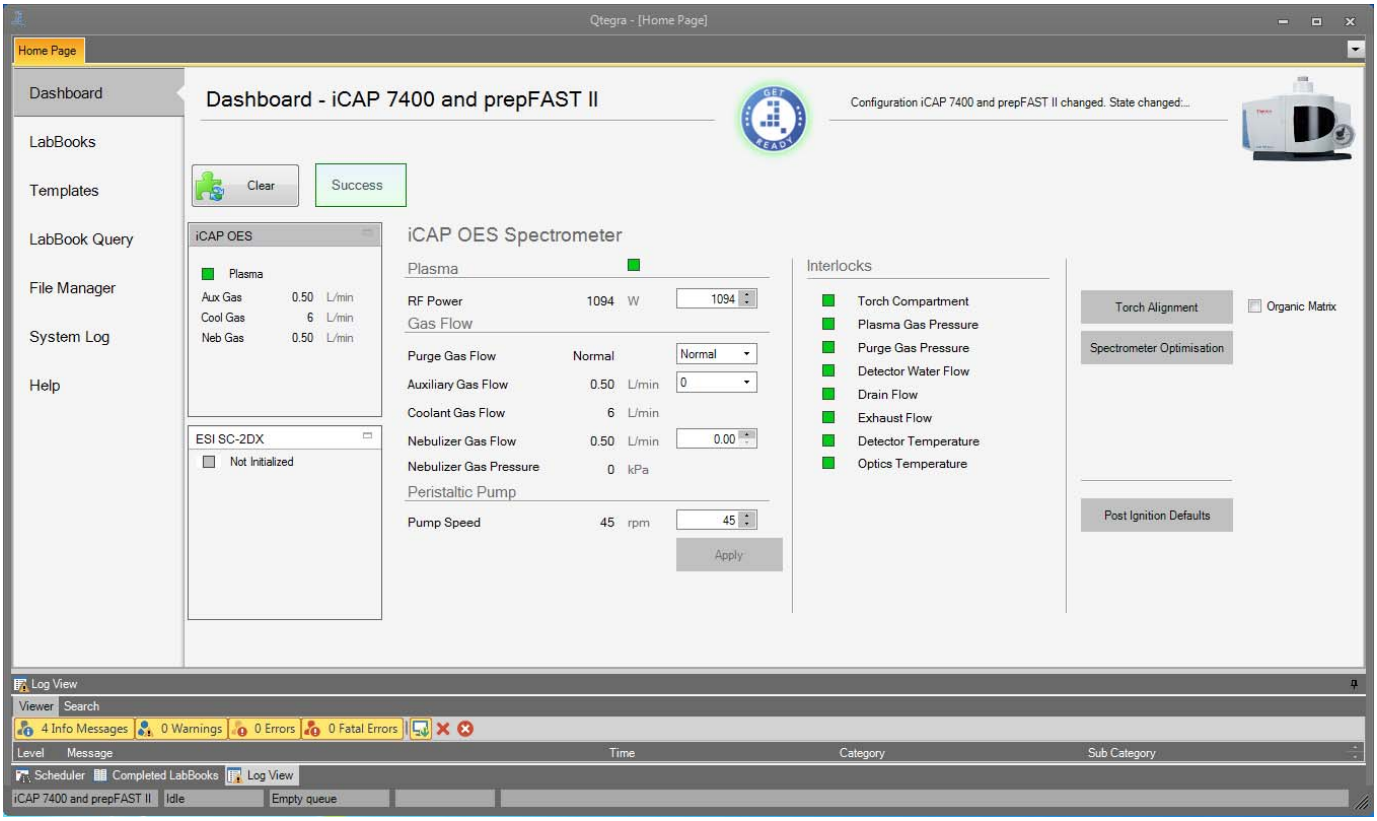


Figure 2-15. User interface of Qtegra

Central Data Storage

Native instrument data are usually stored on the local computer and final results are stored in LIMS by utilizing synchronization tools. In some cases, it could be of advantage if the native data files are stored in a central location rather than on the local PC.

Qtegra ISDS Software offers the capability to use network location for manual synchronization or as a central data repository. Technically it utilizes symbolic links, offered by the Windows 7 and successor operating systems, which are underlying the permissions of the active directory.

Prerequisites

If you plan to enable chained links Windows needs to be prepared for the handling of this. This can be easily achieved by calling the Windows command on the command line. Press **<Win> + <R>** and type
`fsutil behavior set SymlinkEvaluation R2R:1`

Please note that you must call this command with evaluated privileges. To achieve this, call the **Command Prompt** with right-click by using **Run as administrator**.

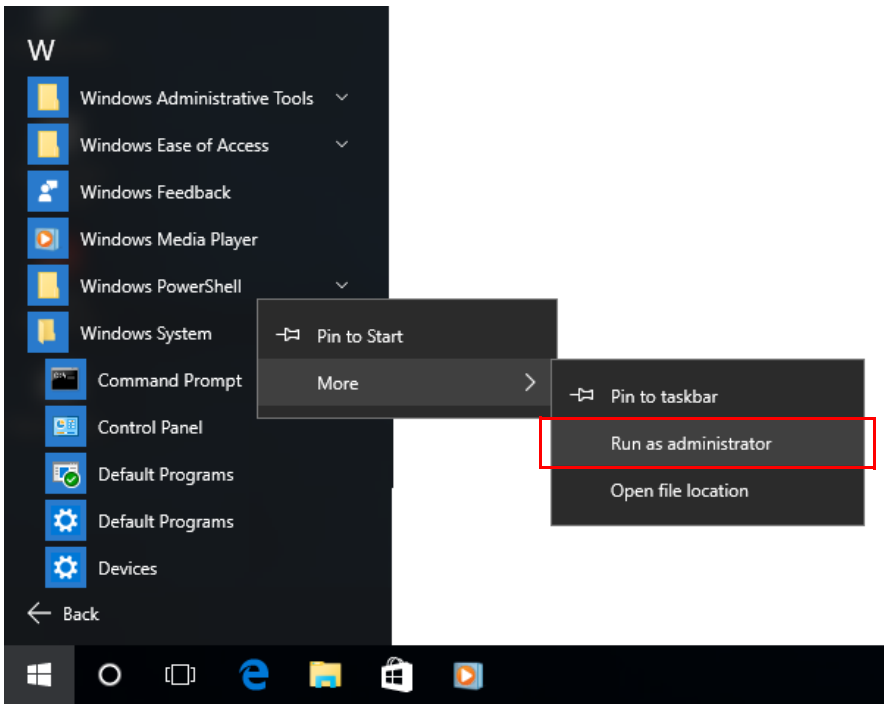


Figure 2-16. Shortcut menu of cmd.exe

By default, the File Service of Qtegra ISDS Software does not have access to the server location, therefore it must be decorated with credentials, which are sufficient to log on to the server.

❖ **To set the access permission for the File Service**

1. Open the **Computer Management** window and navigate to **Services and Applications > Services.**

2. Double-click **File Service** to open the Properties window, see Figure 2-17.

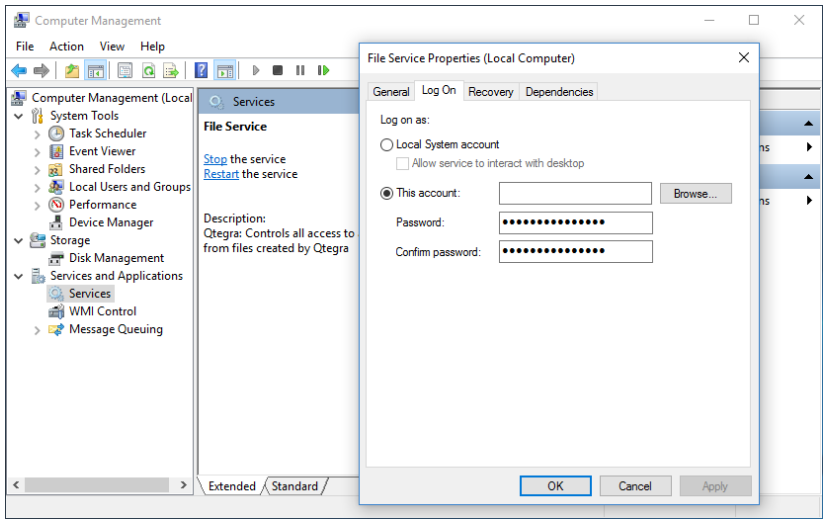


Figure 2-17. File Service Properties window

3. On the **Log On** tab, type the credentials (for example, user name and password) required to access the remote server.

4. Confirm with **OK** and - as prompted - restart the service.

5. Confirm the following message box with **Yes**, since restarting File Manager forces the restart of a couple of dependent services.

Using Network Locations

Qtegra ISDS Software offers some build-in functionality to handle network links located in the **File Manager**. You may also use this link for local folders.

❖ **To create a link to an external location**

1. From the **Qtegra - [Home Page]** navigation pane, click **File Manager**.
   The **File Manager** page opens with the tree structure and list view.

2. Under **Workspace** or from the list view, right-click the desired folder, and from the shortcut menu, select **Create Link to Folder**.

The standard Select Folder dialog opens to select the folder you want to link, see Figure 2-18.

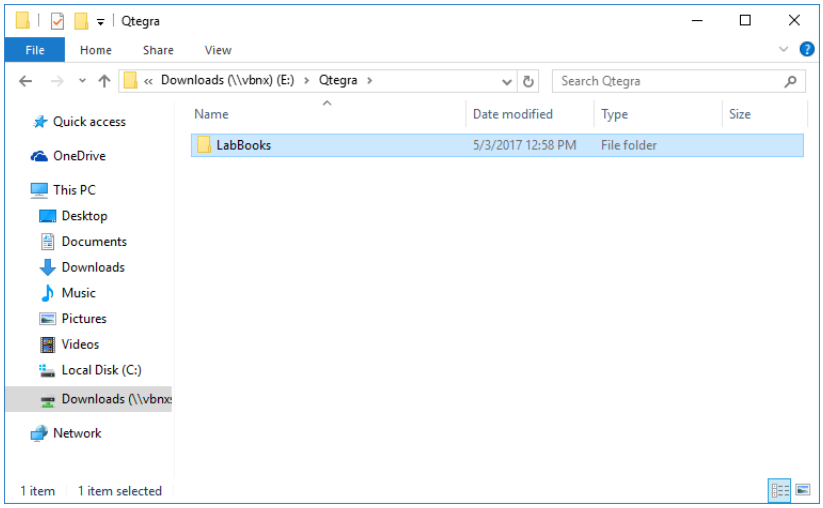


Figure 2-18. Select Folder dialog

Tip You can select a local folder as well as a network location. Make sure to have sufficient credentials for the network file service when accessing a network folder. For details on credentials, see "Prerequisites" on page 2-14.

3. To confirm your selection, click **Select Folder**.
An editor opens and gives the option to type a name for the newly created folder link, see Figure 2-19.

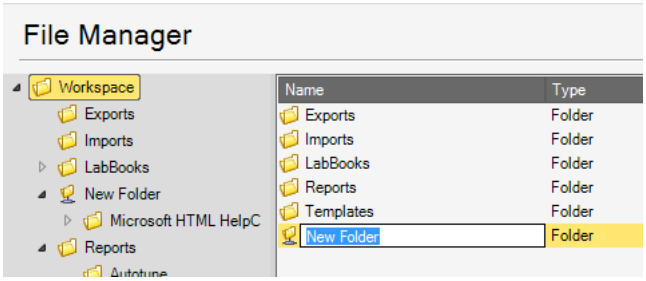
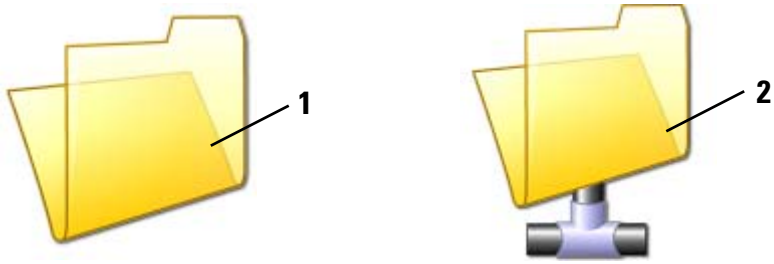


Figure 2-19. Renaming folder link

4. Type the desired name.



Labeled Components: 1=folder, 2=folder link

Figure 2-20. Icons for folders and folder links

To distinguish folders from links, Qtegra ISDS Software displays links with a different icon. While normal folders are displayed within a standard folder symbol (**1** in Figure 2-20), linking folders are represented with a connector on the bottom (**2** in Figure 2-20).

Tip We do not recommend to store the results of your measurement directly from the acquisition onto network locations if the network is not 100% reliable. This could cause a data loss for the measured sample.

Whenever you are browsing for a file (LabBook, Template, or others), the folder link (indicated by special icon) is displayed beside the other folders.

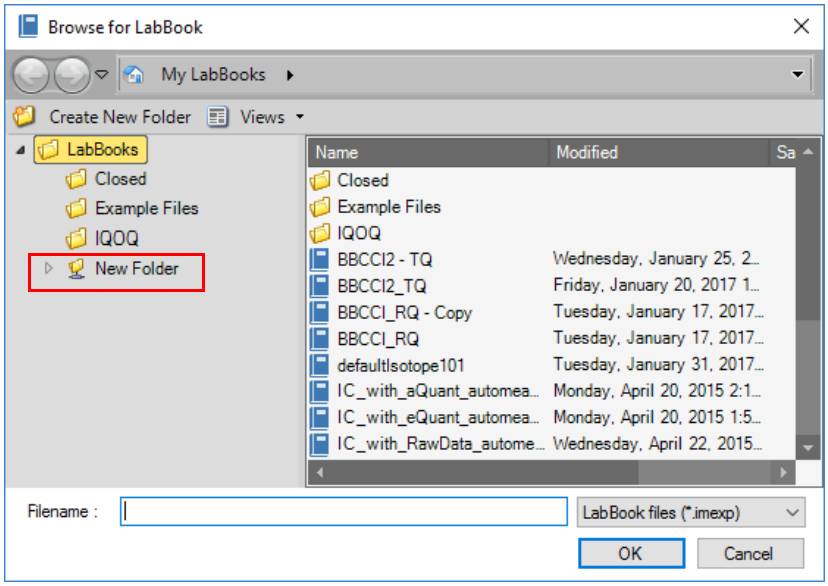


Figure 2-21. Folder link in Browse for file dialog

Tip The Browse for file dialogs also offer the above described function to create a folder link, see Figure 2-22.

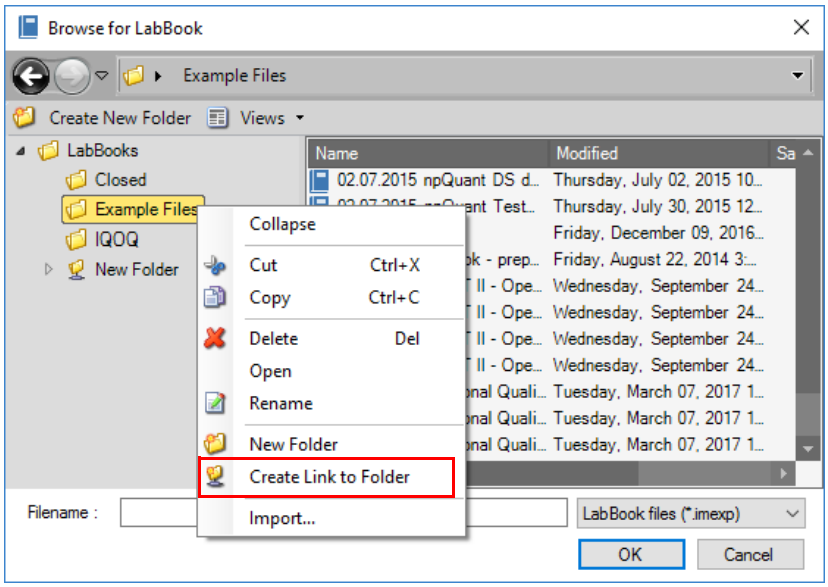


Figure 2-22. Create Link to Folder command in Browse for file dialog

A link can also be removed from the Qtegra File Manager.

❖ **To delete a link to an external location**

1. From the shortcut menu of the selected item, click **Delete**.
   Note that only the link is deleted and not the folder nor the content of the folder.

While the delete command deals with the link the copy command will copy the content of the folder to another location but not to the link.

❖ **To copy a link to another location**

1. From the shortcut menu of the selected folder link, click **Copy**.
2. Select the folder you want the content of the folder link to be copied, and then from the shortcut menu, click **Paste**.
   The content will be copied soon. This may take a few seconds as all subfolders are also copied.

Qtegra LabBook Signing

For good laboratory practice and standard compliance Thermo Scientific Qtegra ISDS Software offers the ability to sign LabBooks. Qtegra ISDS Software uses the user's certificate storage offered by Microsoft Windows.

In order to use the signing features for LabBooks inside Qtegra ISDS Software it is necessary to have a valid certificate, which includes a private key. Normally valid certificates will be provided by the laboratory IT administrators or by a trust center. Two typical service providers are:

- http://www.trustcenter.de/ (Germany)
- http://www.verisign.com/ (US)

Almost all trust center companies offer a free certificate for private use, which may serve for testing. Another option to receive a valid certificate is to use the below described built-in feature of Windows.

Creating a Self-Signed Signature

Tip In order to be able to create a self-sign signature you must have administrator rights. Ask your Administrator.

The file encryption feature of Windows uses a certificate and its private key for encrypting your hard drive. Therefore, it is possible to use the available wizard to generate a self-signed certificate.

❖ **To generate a self-signed certificate**

1. Open **Control Panel > User Accounts**.
2. Select **Manage your file encryption certificate**, see Figure 2-23.

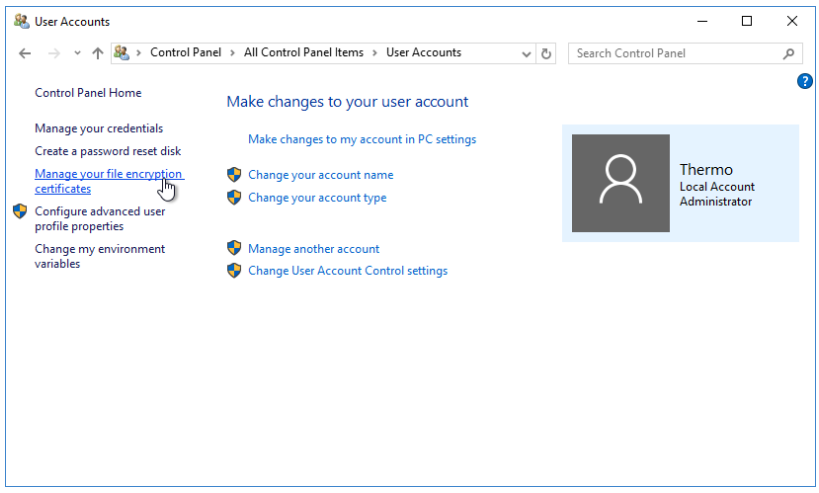


Figure 2-23. Make changes to your account

The **Encrypting File System** wizard opens, see Figure 2-24.

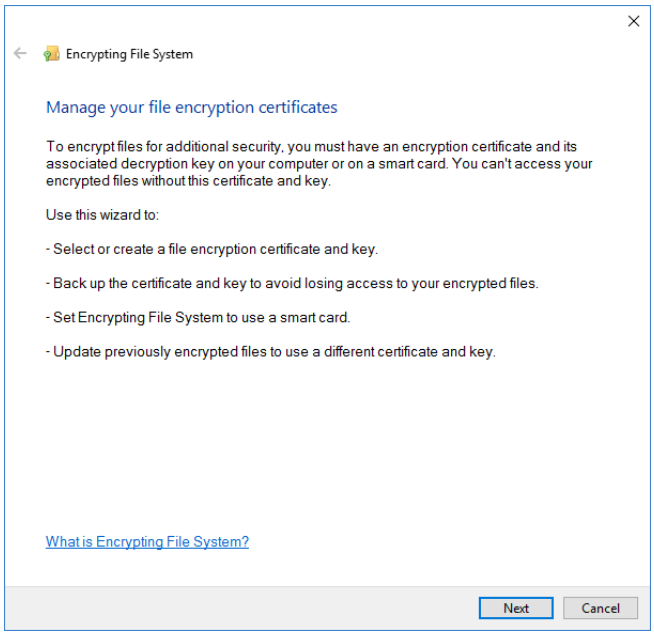


Figure 2-24. Encrypting File System wizard start

3. Click **Next**.
4. Select **Create a new certificate** and click **Next**, see Figure 2-25.

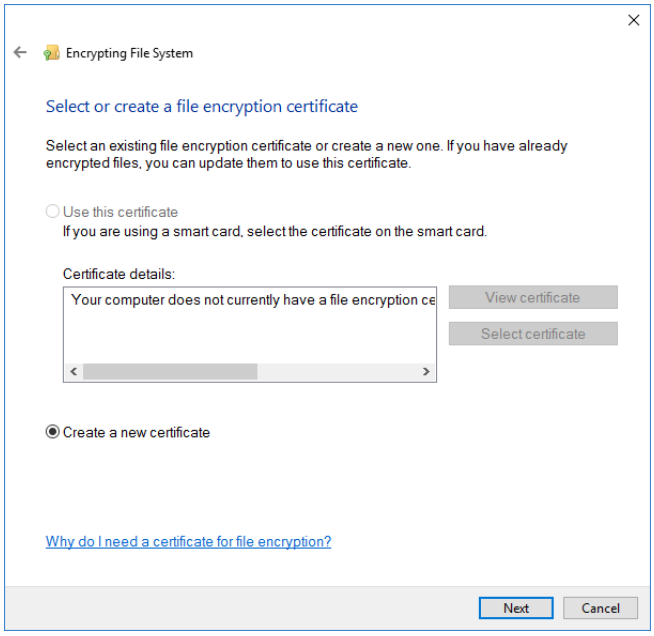


Figure 2-25. Selecting to create a new certificate

5. Select the first radio button **Make a self-signed certificate and store it on my computer** and click **Next**, see Figure 2-26.

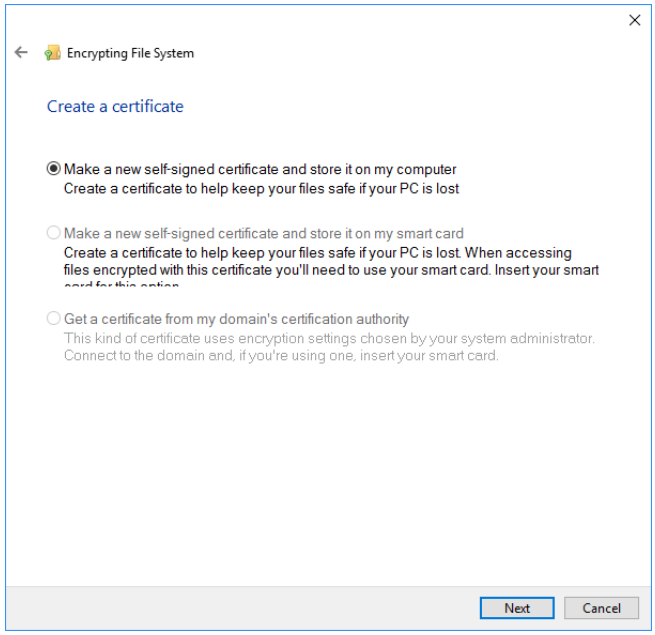


Figure 2-26. Selecting a self-signed certificate

After a short time period the new certificate will be available to the system.

6. Select **Back up later** if you only intend to use this certificate for testing, see Figure 2-27.

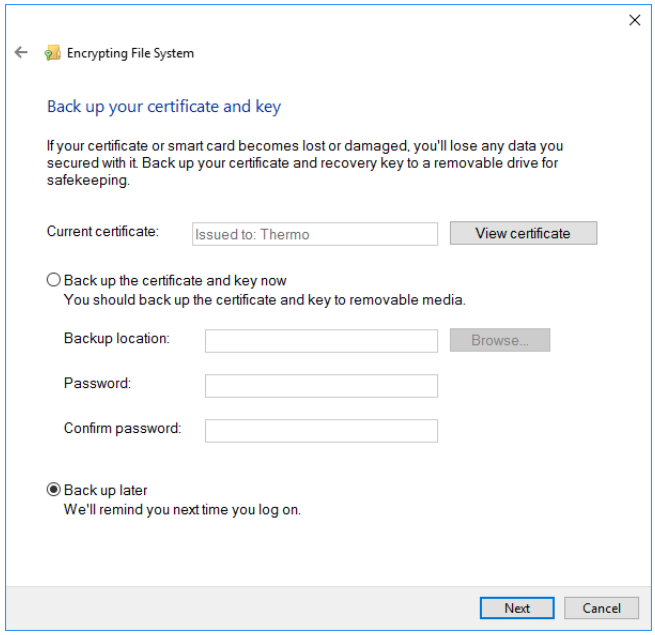


Figure 2-27. Selecting back-up for self-signed certificate

Tip If you wish to back up the key now, select the first option, select the back-up location and enter a password.

7. Do not change your current encryption settings, see Figure 2-28, and click **Next**.

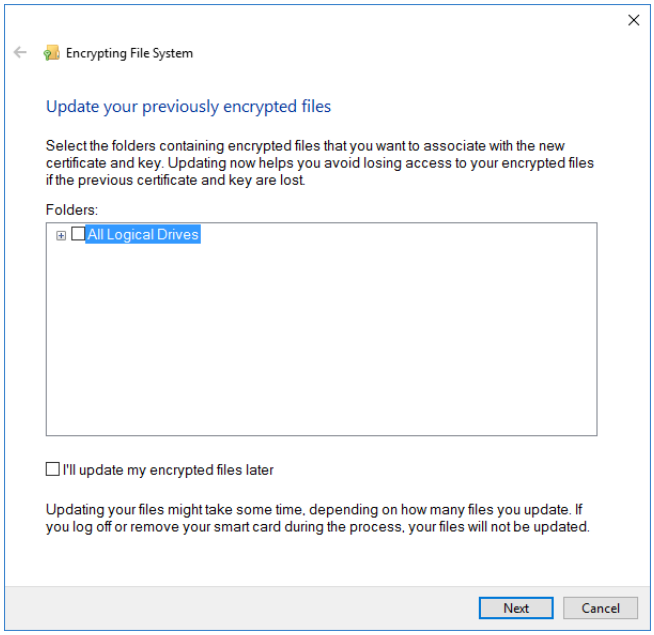


Figure 2-28. Selecting encryption settings

8. Finish the **Encrypting File System** wizard, see Figure 2-29.

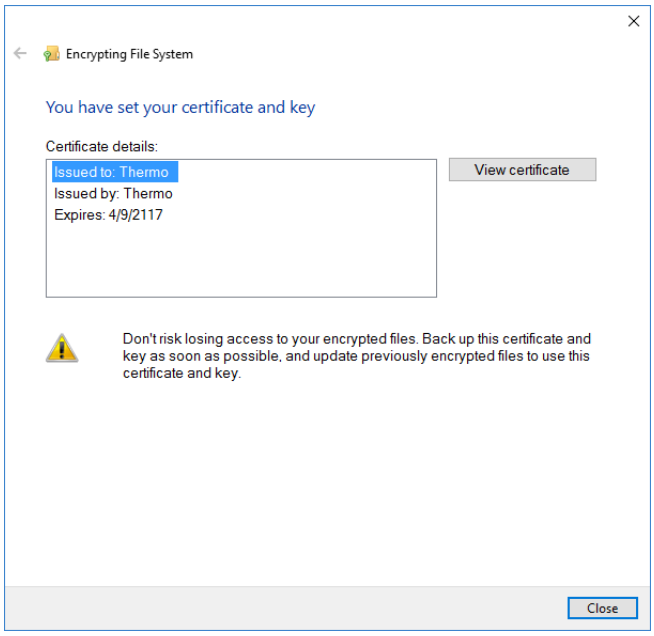


Figure 2-29. Finishing Encrypting File System wizard

9. Click **Close**.

You can now sign a LabBook. Qtegra ISDS Software offers the signing feature for every measured LabBook.

The Certificate Manager

The Certificate Manager can be called by pressing **<Win> + <R>** and typing `certmgr.msc` in the Run dialog. It can be used to explore and maintain currently installed certificates, see Figure 2-30.

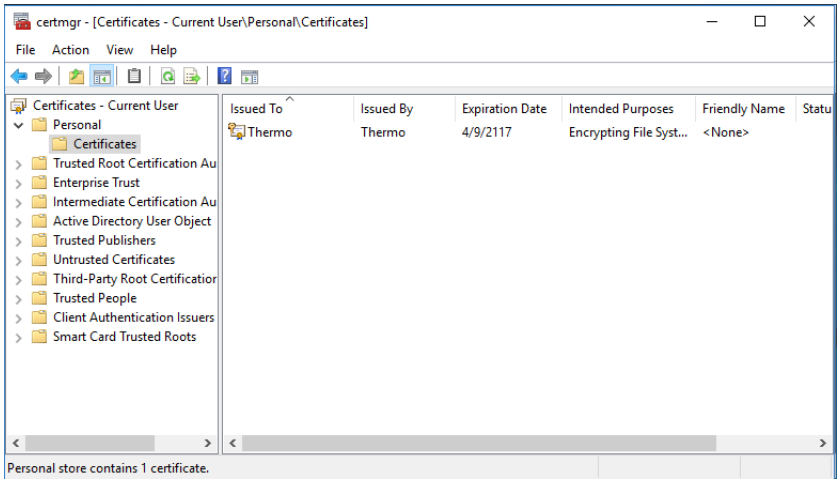


Figure 2-30. Certificate Manager

Using a Centralized Certification Authority (CA)

In this scenario, a Windows server of the domain is running as a certification authority (CA) where a domain user can request trusted certificates from the server. These certificates can be used by Qtegra ISDS Software to sign a LabBook. In order to simplify the example, there is only one Windows Server 2012 r2 running the Active Directory Service. The current Domain is called “CERTTEST” and the server is also acting as the certification authority, which can be achieved by running Active Directory Certificate Services.

Request Certificate from Server

This step is only necessary for setting-up a new domain user. Already existing users should have their certificate with the private key on there main computer - the computer which is used for signing emails. With the domain setup and the certification authority in place, the following steps are necessary to request a certificate for a user.

❖ To request a certificate

1. Log on to the machine or to one of the machines, which should be available for signing.

2. Press **<Win> + <R>** and then type `certmgr.msc` in the Run dialog to start the Windows Certificate Manager, see Figure 2-31.

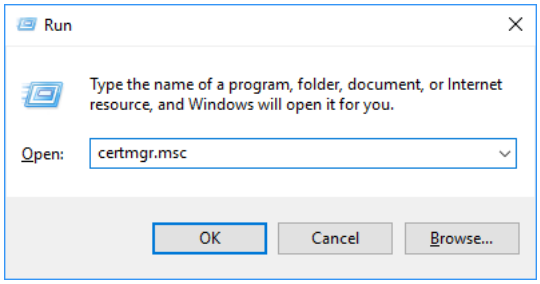


Figure 2-31. Starting the Windows Certificate Manager

The Certificate Manager displays the certificate storage of the current user, see Figure 2-32.

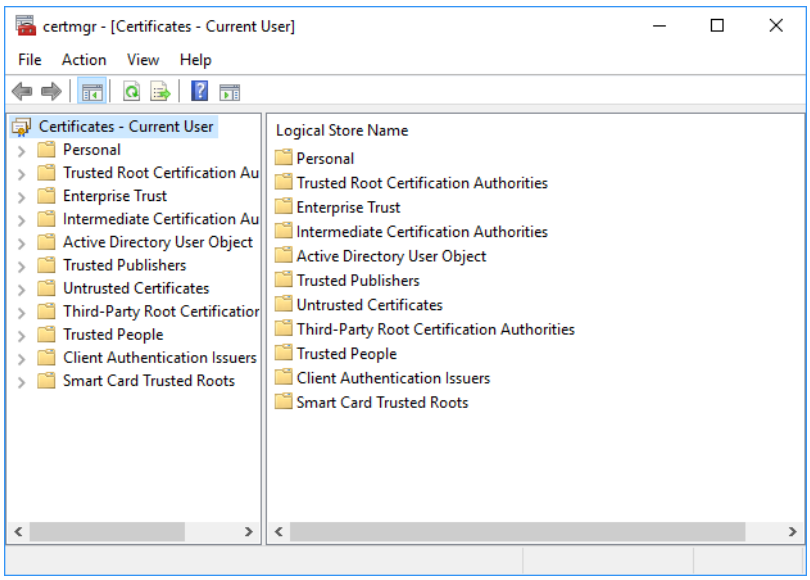


Figure 2-32. Certificate Storage of current user

3. Right-click the **Personal** folder and select **Request New Certificate** from the shortcut menu, see Figure 2-33.

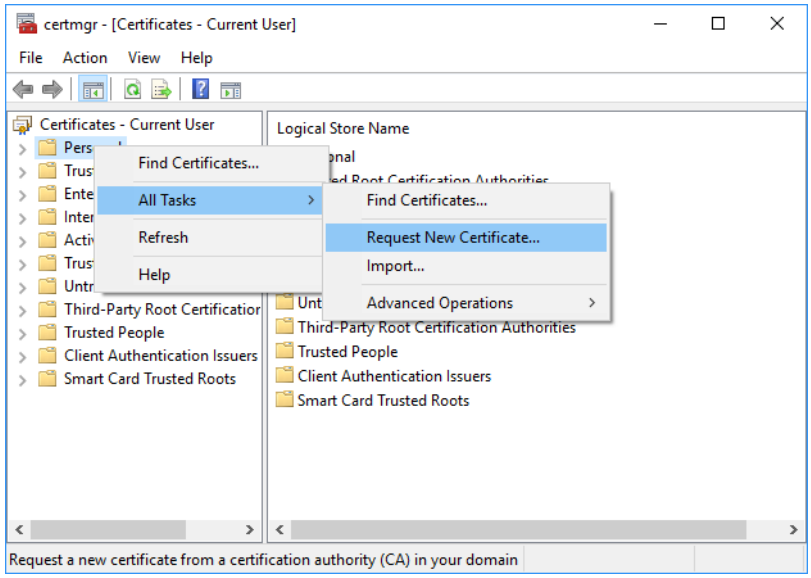


Figure 2-33. Request New Certificate

4. Follow the steps presented by a **Certificate Enrollment** wizard, see Figure 2-34.

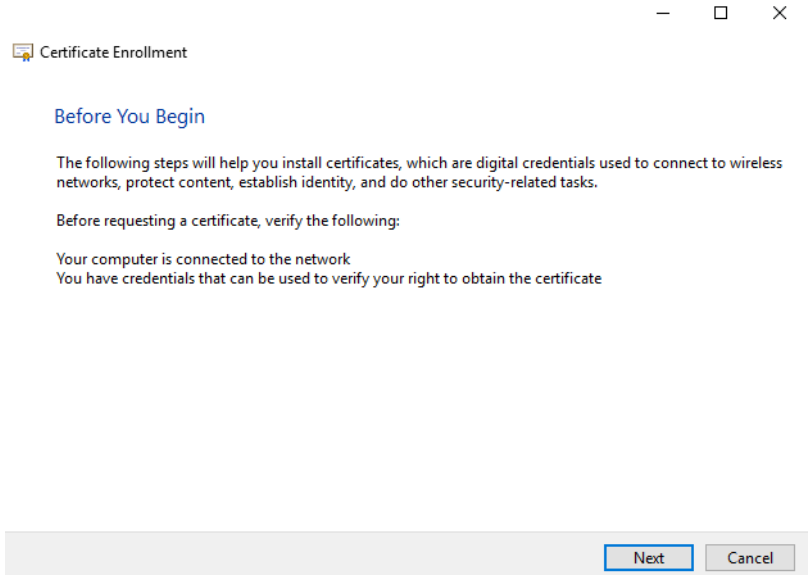


Figure 2-34. Certificate Enrollment Wizard start

5. Select the certificate enrollment policy, see Figure 2-35.

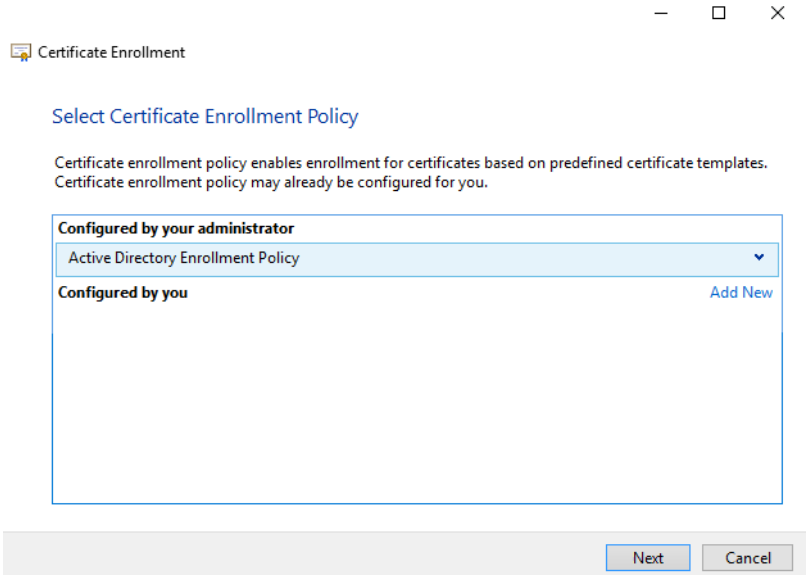


Figure 2-35. Selecting Certificate Enrollment Policy

6. Click **Next**.

7. In the **Request Certificates** dialog, choose **User** certificate, which allows Secure Email, see Figure 2-36.

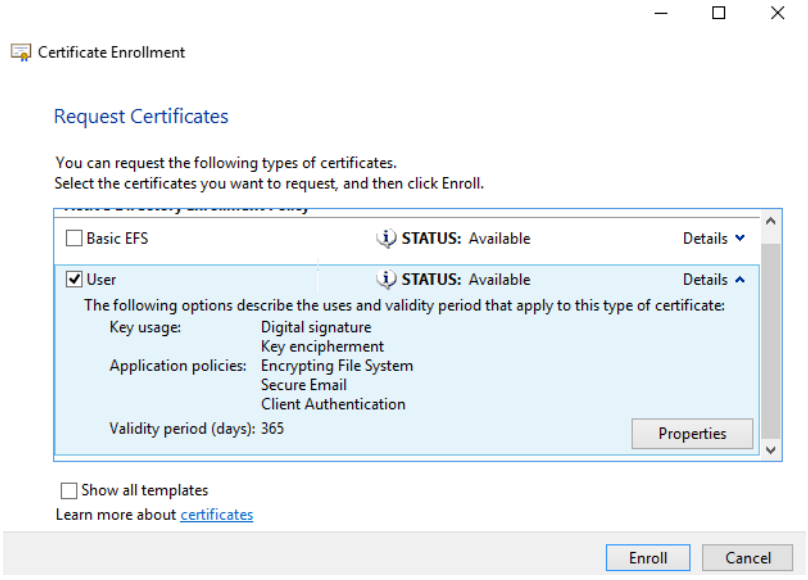


Figure 2-36. Requesting New Certificate

8. Click **Enroll** to display the Certification Installation Results page, see Figure 2-37.

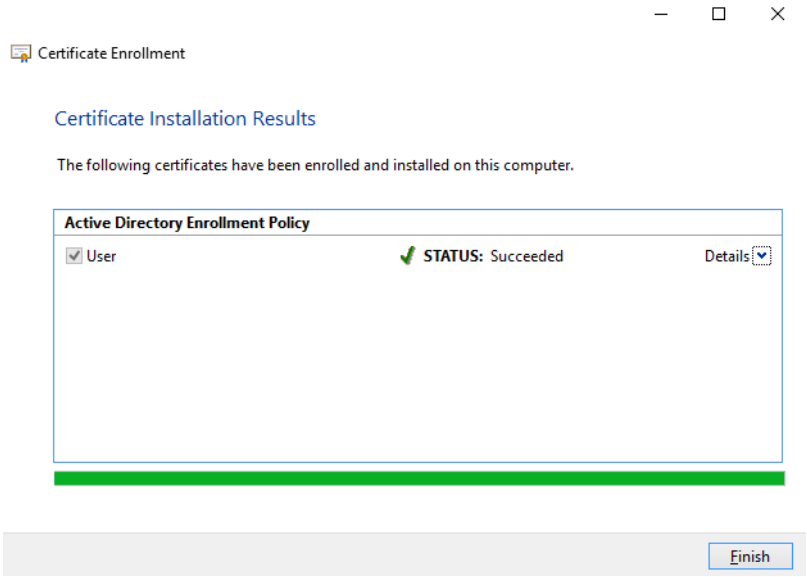


Figure 2-37. Finishing Certificate Enrollment

9. Click **Finish**.

   The private key is now stored locally in your personal certificate storage, see Figure 2-38.

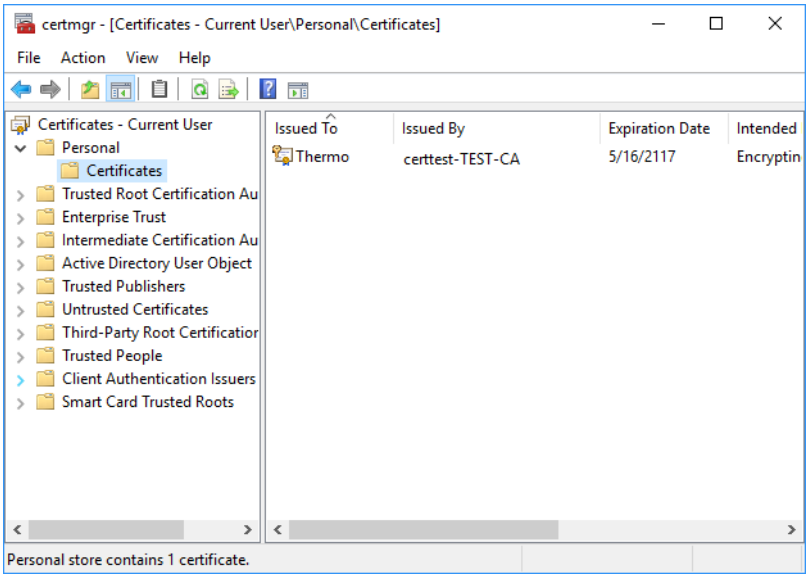


Figure 2-38. Certificate storage for current user

Tip It is one of the fundamentals of asymmetric cryptography that the private key is never known by a server.

Export Certificate with Private Key

The following simple steps are required to export a user certificate.

❖ **To export a user certificate**

1. Log on to the machine and user, which contains the certificate with the private key in the users certificate storage.
2. Start the Windows Certificate Manager as described in "Request Certificate from Server" on page 2-23.
3. Select the certificate to-be-exported in the **Personal** folder.
4. Choose **Export** from the shortcut menu, see Figure 2-39.

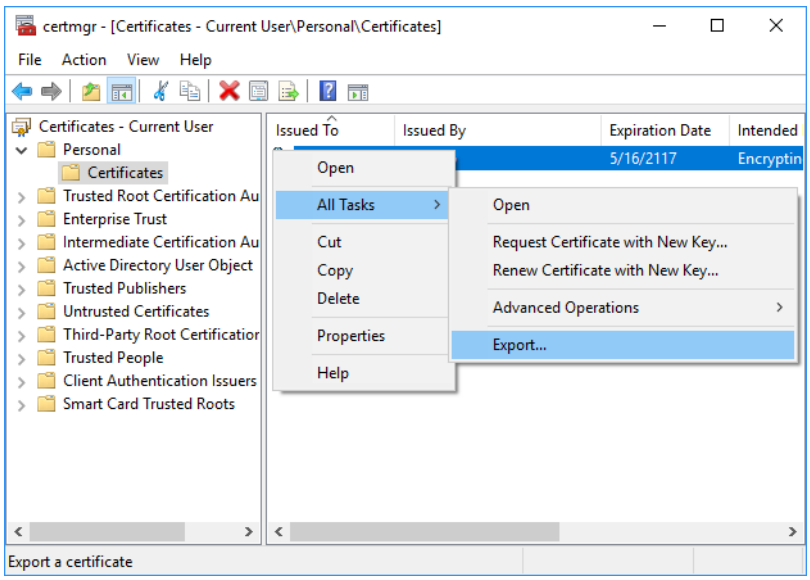


Figure 2-39. Exporting certificate

5. Follow the **Certificate Export Wizard**, see Figure 2-40.

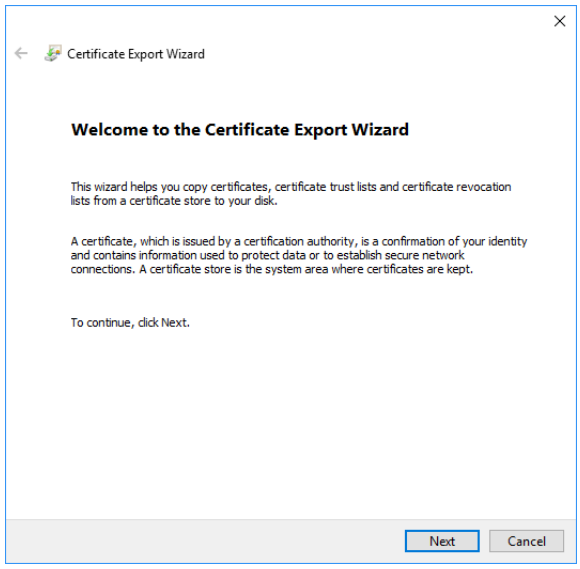


Figure 2-40. Certificate Export Wizard

6. Choose to export the private key, see Figure 2-41.

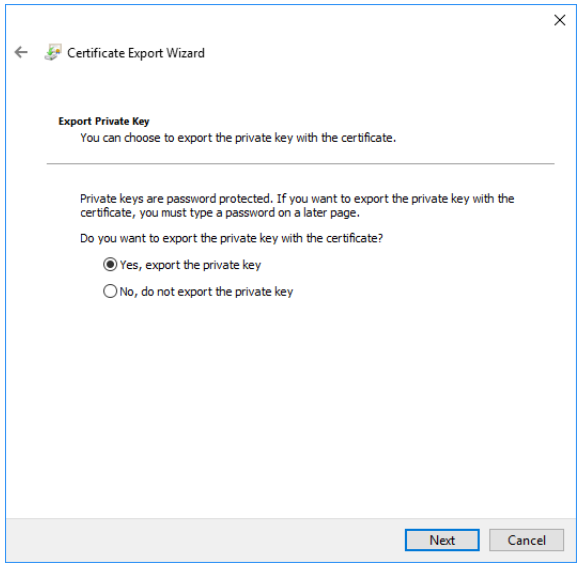


Figure 2-41. Selecting export of private key

7. Select the file format, see Figure 2-42.

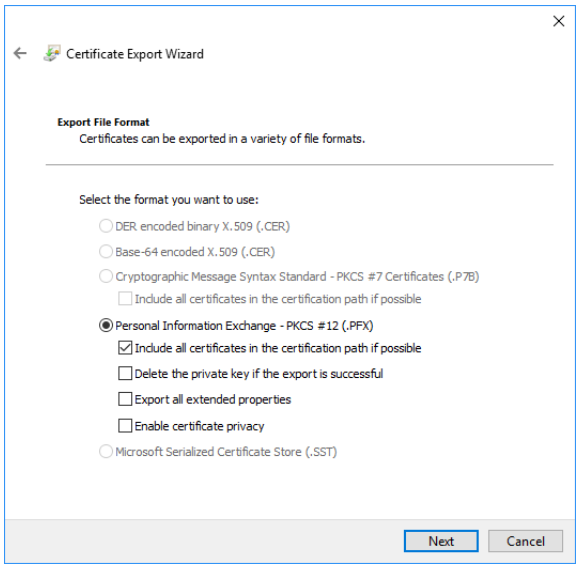


Figure 2-42. Selecting file format for private key

8. Make sure to set an export password to protect your private key, see Figure 2-43.

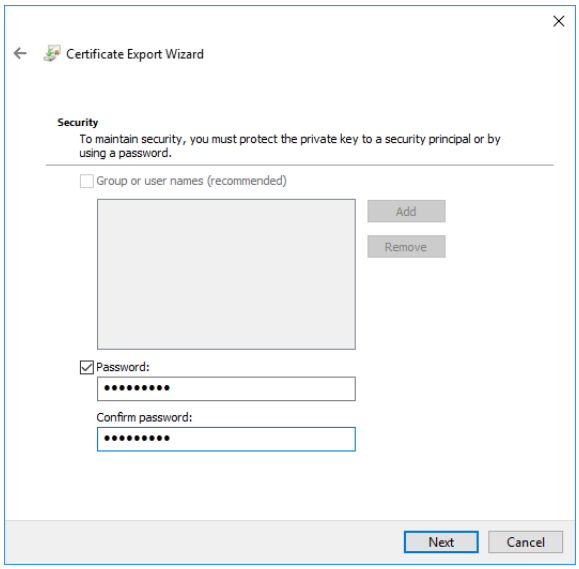


Figure 2-43. Entering password for private key

9. Select a file name and a location for the export, see Figure 2-44.

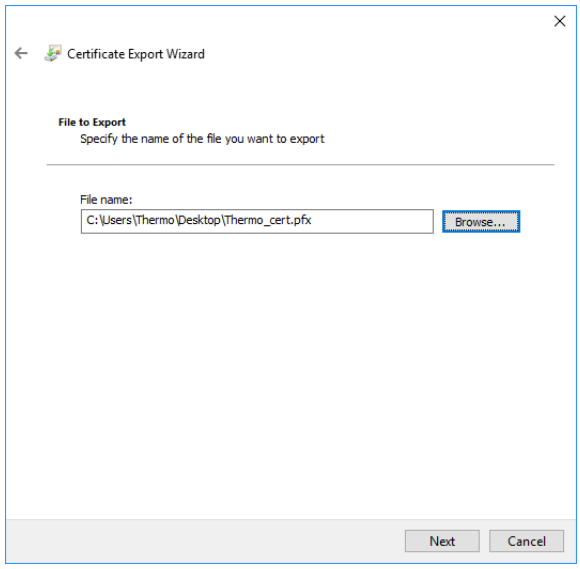


Figure 2-44. Entering file name and location for private key

10. Click **Finish** to complete the **Certificate Export Wizard**, see Figure 2-45.

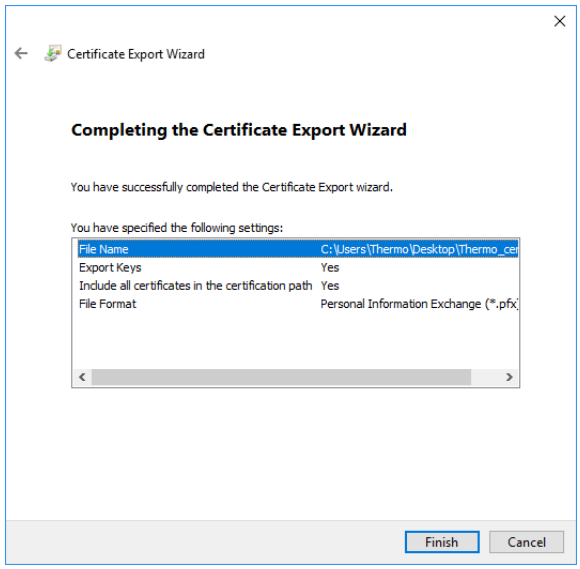


Figure 2-45. Completing the Certificate Export Wizard

After a successful export, a PFX file will be available in the selected export folder.

Import Certificate with Private Key on a Different Machine

The following simple steps are required to import a user certificate.

❖ To import a private key

1. Log on to the machine where you want to access your private key (for example, for signing of LabBooks with Qtegra ISDS Software) with your domain user login.
2. Locate the PFX file, which was created during the exportation of your certificate (see "Export Certificate with Private Key" on page 2-28).
3. Double-click the PFX file to start the Certificate Import Wizard and follow the steps.
4. Choose Current User, see Figure 2-46.

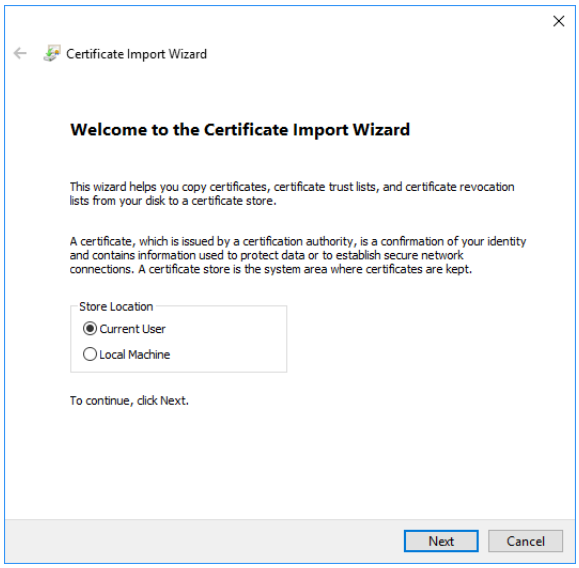


Figure 2-46. Certificate Import Wizard

5. In the wizard, select the PFX file, see Figure 2-47.

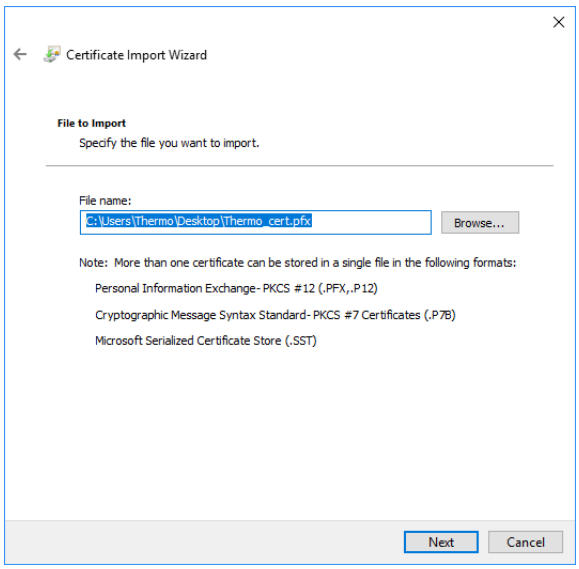


Figure 2-47. Selecting PFX file

6. Enter the password that you have specified during export, see Figure 2-48.

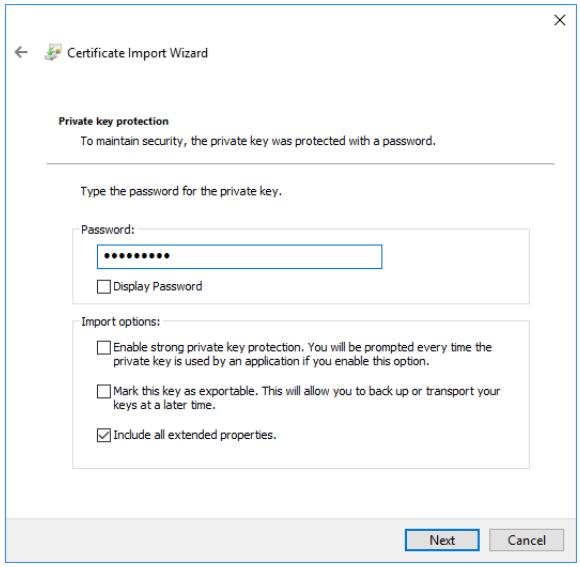


Figure 2-48. Entering password

7. Select the option to automatically select the certificate store, see Figure 2-49.

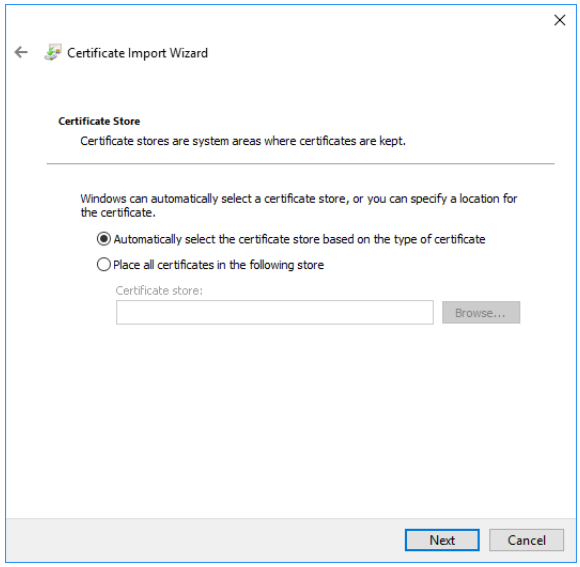


Figure 2-49. Selecting certificate store

8. Click **Finish** to complete the wizard, see Figure 2-50.

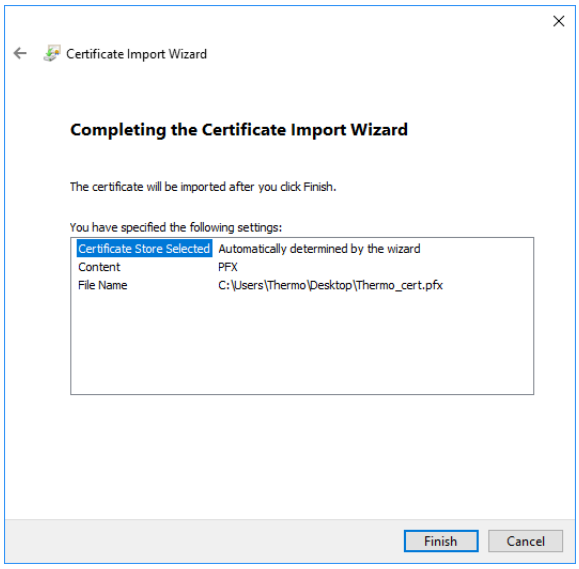


Figure 2-50. Completing the Certificate Import Wizard

Signing in Qtegra ISDS Software

There are two possibilities to sign a Qtegra LabBook with the credentials of a certain user:

- If the Qtegra ISDS Software is installed under the account of the specific user, the user can sign the LabBook from within his/her account.
- Qtegra ISDS Software allows the current user to change credentials for signing.

❖ **To sign a Qtegra ISDS Software LabBook with user login**

1. Log on with your domain user login if the Qtegra ISDS Software is installed under your account.
2. Select **Signing** in a completed LabBook.

3. Click **Sign**, see Figure 2-51.

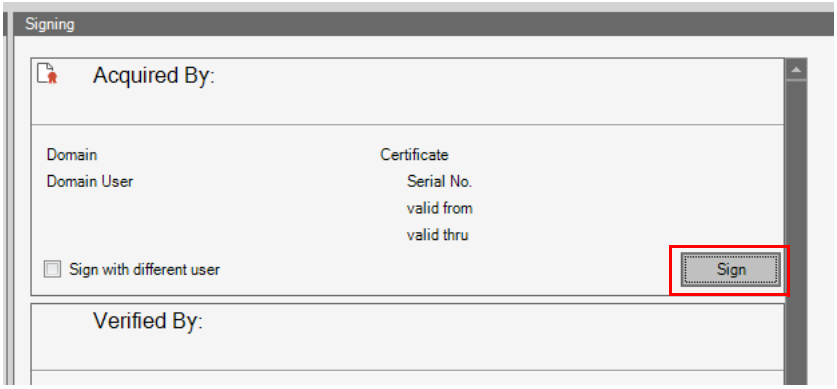


Figure 2-51. Signing LabBook

4. In the **Select certificate for signature** dialog, choose an available certificate.

❖ To sign as different user

1. Select the **Sign with different user** check box, see Figure 2-52.

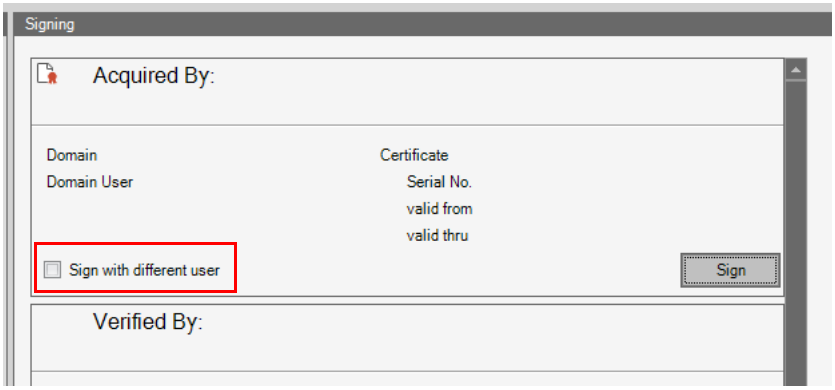


Figure 2-52. Signing LabBook with different user

2. Click **Sign** and type the necessary credentials (user name and password for the different user), see Figure 2-53.

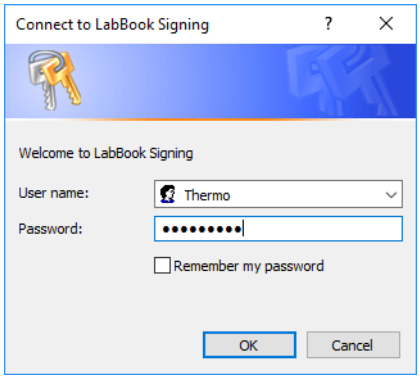


Figure 2-53. Entering password

Tip In order to access a user profile, it is currently necessary to be signed-in on the current machine to be able to use the "Sign with different user" feature. This issue will be fixed in future versions.

Final Note

Concerning security issues and in order to avoid spreading ones private key over multiple machines, signing of LabBooks can also be performed offline - disconnected from the instrument. Using the Qtegra ISDS **File Manager** feature **Create Link To Folder** (see Figure 2-54) allows to connect to a shared folder making LabBooks available to multiple users. The LabBook to-be-signed can be opened in that location and signed locally with the current credentials.

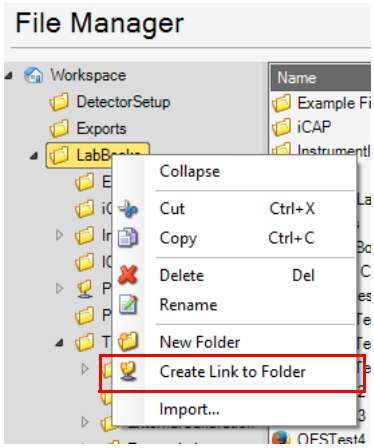


Figure 2-54. Folder shortcut menu item Create Link to Folder

Compliance with your SOP

Each organization has rules, policies, procedures, and standards which are written in the Standard Operating Procedures (SOP). Such an SOP can follow Part 11 in Title 21 of the *Code of Federal Regulations, Electronic Records, Electronic Signatures* (21 CFR Part 11) which includes the U.S. federal guidelines for storage and protection of electronically stored data and the application of electronic signatures. These guidelines have been developed to ensure that electronic records are reliable, authentic and comprehensible.

An important implication in 21 CFR Part 11 is that organizations must implement rules to confirm that proper methods, procedures, and controls are in place. As a result prevention of data falsification, data reconstruction and system security must be addressed.

Qtegra ISDS Software provides a wide range of features, which enable laboratories to operate within SOP compliance. These features include audit trails, support for electronic signatures and tools for the integrated data management.

Table 2-2. Qtegra supported sections of 21 CFR Part 11

Section	Title
11.10	Controls for closed systems
11.30	Controls for open systems
11.50	Signature manifestations
11.70	Connection signature / document
11.100	General requirements for electronic signatures
11.200	Electronic signatures components and controls
11.300	Controls for identification codes / passwords

Your SOP should require both technical and procedural compliance. To achieve technical compliance, the organization must use software that contains the required security features and functions. To achieve procedural compliance, your organization must establish SOP and policies that define how to use processes and systems in a compliant matter.

Configuring the system to be compliant with SOP

❖ **To set Qtegra to be compliant with your SOP**

1. Open the **Configurator**.
   The list of applets, the display region for applet settings and the viewer region are shown.

2. From the **Configurator** list of applets, select **Settings**.

3. In the display region for applet settings, expand **Settings** and then expand **Compliance Settings**. See Table 2-3 for details on compliance parameters.

Table 2-3. Compliance Settings parameters

Tree item	Default	Recommended	Comment
Enable global compliance	True	True	Beside other settings, a true global compliance value removes any limitation on the number of files with the .log extension. Without limitation, a Qtegra user in a regulated environment can maintain a complete set of log files that provide full information, for example, during an audit.
Enable compliant system log	False	True	If system event logging is set to *True*, every log on and off from users to and from the system is logged.
LabBook > **Prevent exporting and reporting of modified LabBooks**	False	True	If set to *True*, the **Export** button (and **<Ctrl> + <E>** function of the LabBook toolbar is disabled after the LabBook evaluation results have been modified. The **Save Report** function is also disabled but shows the results of the modified LabBook.
LabBook > **Prevent multiple signing by a single user**	False	True	If set to *True*, a user can only sign a single stage of a LabBook. After a stage has been signed, the next Sign button remains disabled for the current user.
LabBook Backup > **Automatic backup after analysis**	False		See Table 14-11 for details on automatic backup settings.
LabBook Backup > **Backup folder**	Workspace		
LabBook Backup > **Backup suffix**	<empty>		
Two stage identity checks > **Require for Commenting**	False	True	Activate an additional ID check (that means, the user must re-enter his password) before a LabBook or Template is saved.
Two stage identity checks > **Require for Exporting**	False	True	Activate an additional ID check (that means, the user must re-enter his password) before a LabBook is exported.

Table 2-3. Compliance Settings parameters, continued

Tree item	Default	Recommended	Comment
Two stage identity checks > **Require for Reporting**	False	True	Activate an additional ID check (that means, the user must re-enter his password) before a Report is generated.
Two stage identity checks > **Require for Signing**	False	True	Activate an additional ID check (that means, the user must re-enter his password) before a LabBook is signed or a signature is revoked.

4. Close the Configurator tool and switch to Qtegra.

Qtegra ISDS Software implements some of these controls directly and relies on the security functions in your computer operating system for other parts, namely:

- The audit trail
  Every alteration of a Template or LabBook is recorded in the history of each. These can be viewed, compared, exported or printed.
- Electronic signatures
  With Qtegra ISDS Software it is possible to electronically sign each LabBook with so-called digital SSL certificates that are issued by Trusted CA Certificate Authorities.
- The Qtegra ISDS Software layer controls the file operations.
- The Administrator restricts user access and controls software feature access through the Access Control (part of the Qtegra ISDS Configurator tool).

  Tip During installation, the Qtegra ISDS Software setup creates the Windows groups QtegraUser, QtegraSupervisor, QtegraAnalyst, QtegraManager, and QtegraAdministrator. QtegraSystemAdministrator and QtegraDataAdministrator must be added manually (see page 2-5). No other Qtegra ISDS Windows groups are allowed – all Qtegra ISDS users will have to be assigned to one of the supplied Windows groups. Qtegra ISDS Software allows to change the Windows group names. Domain groups can not be added to Qtegra ISDS Windows groups.
- Your computer security functions manage user authorization.
- The Windows permission management maintains electronic record security.

Resetting the system to ignore compliance with SOP

By default, Qtegra ISDS Software is configured to prevent changes to the Sample List during measurement of a LabBook. This is done in order to provide maximum data traceability during analysis in a SOP

compliant environment. In this default state, if changes are necessary, you must stop the LabBook before you can change the Sample List. Any changes to the Sample List can then be commented and captured in Audit Trail.

❖ **To allow changes to the sample list during measurement**

1. In the **Configurator** tool, **Settings** applet, **Settings** section, **Compliance Settings** group, set the **Enable global compliance** value to *False* to allow these changes nevertheless.

2. You may also set the **Enable compliant system log** value to *False* to stop system event logging, which would ignore compliance with SOP, too.

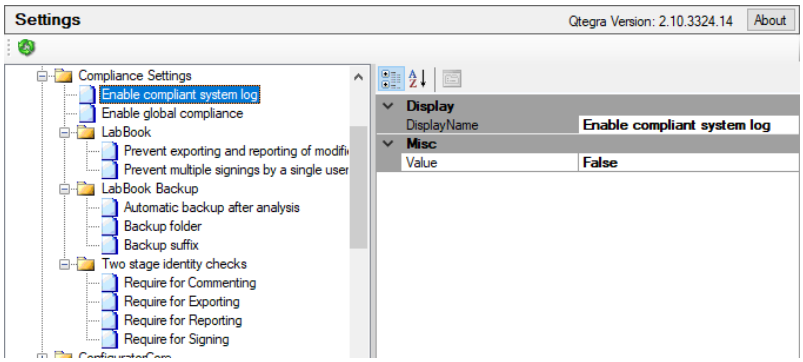


Figure 2-55. SystemEventLog setting

Tip When the Enable global compliance value is set to *False*, changes to the Sample List in a running LabBook are not captured in the Audit Trail. Moving, deleting, or renaming a Template or LabBook then is no more logged.

Advanced Audit Policy

In order to log account activities, for example, “User account management logs” (see Figure 2-58) the Administrator must adjust the Windows OS to enable the logging for Windows and Qtegra ISDS Software.

This section describes how to enable the Advanced Audit Policy for Qtegra ISDS Software System Event logging.

Tip This instruction shows how to change the Windows settings with regard to the Local Group Policy. These changes are only necessary when Qtegra ISDS Software is used in laboratories regulated under 21 CFR Part 11 compliance.

❖ To enable the Advanced Audit Policy

1. In the Configurator tool, Settings applet, expand Settings > Compliance Settings, and select the **Enable compliant system log** item. Make sure that Misc > Value is set to *True*.

2. In Windows, press **<Win> + <R>** and type `gpedit.msc` in the Run dialog to open the Local Group Policy Editor.

3. In the **Local Group Policy Editor**, expand the folder tree under Computer Configuration, see Figure 2-56.

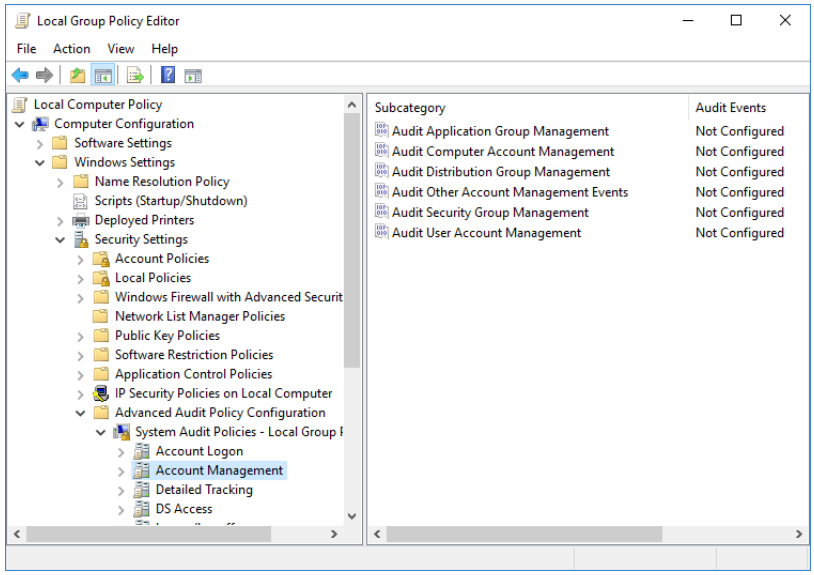


Figure 2-56. Expanded folder tree for System Audit Policies

Expand Local Computer Configuration > Windows Settings > Security Settings > Advanced Audit Policy Configuration > System Audit Policies - Local Group Policy Object.

4. Select the following items and change their Audit Events setting from *Not Configured* to *Success and Failure*. To do so, right-click the

subcategory items and select **Properties** from the shortcut menu. The Properties setting dialog opens, see Figure 2-57.

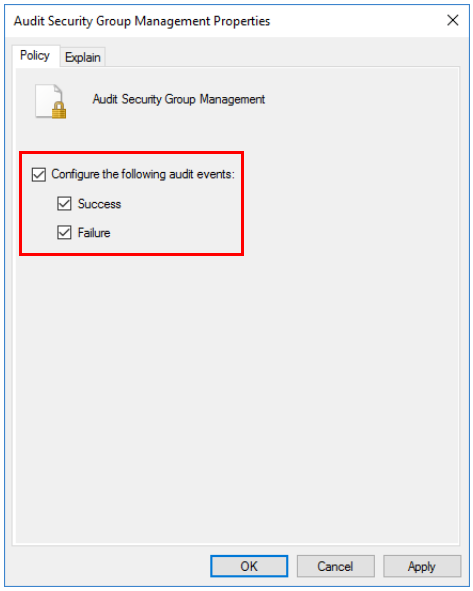


Figure 2-57. Properties setting dialog with activated check boxes

5. Set these properties for Account Management, see Figure 2-58.

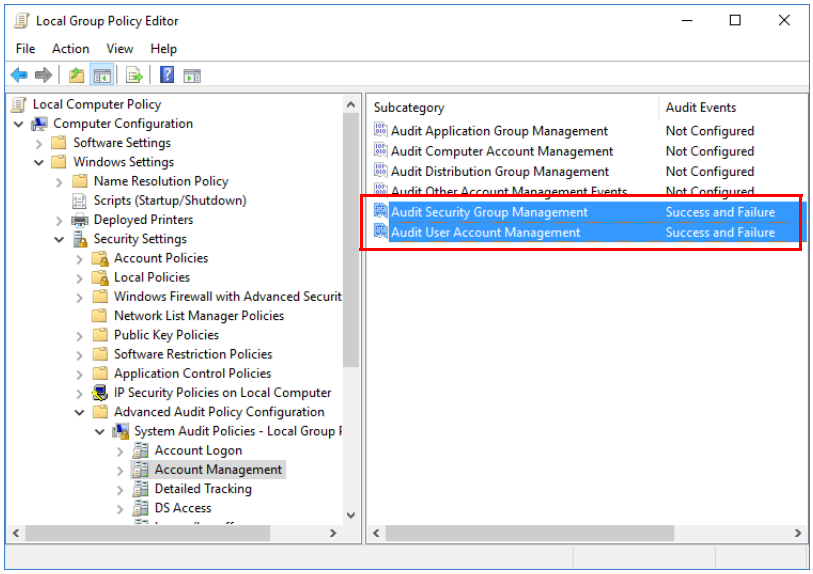


Figure 2-58. Account Management setting

6. Set these properties for Logon/Logoff, see Figure 2-59.

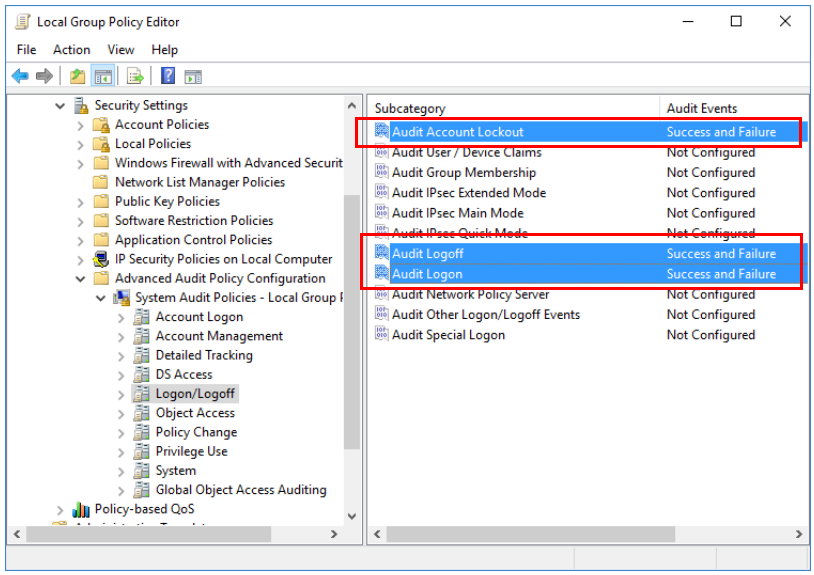


Figure 2-59. Logon/Logoff setting

7. Set these properties for Policy Change, see Figure 2-60.

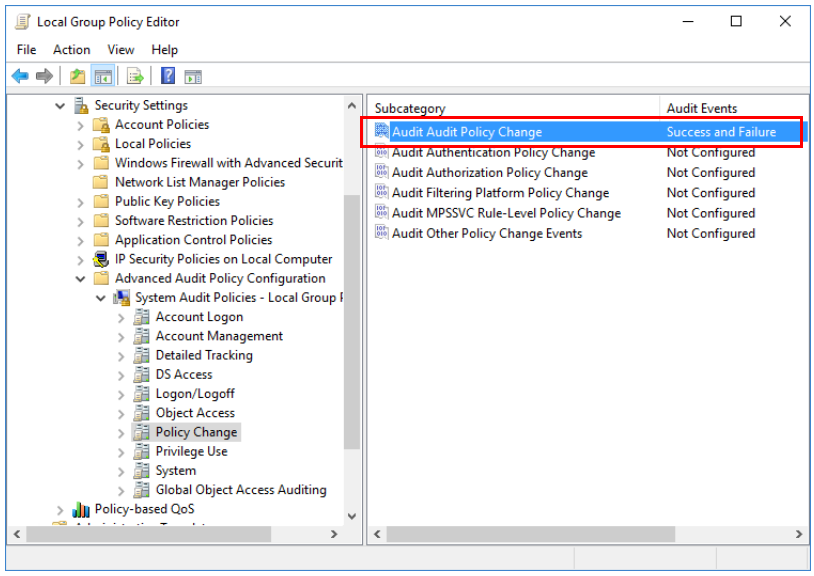


Figure 2-60. Policy Change setting

8. Set these properties for System, see Figure 2-61.

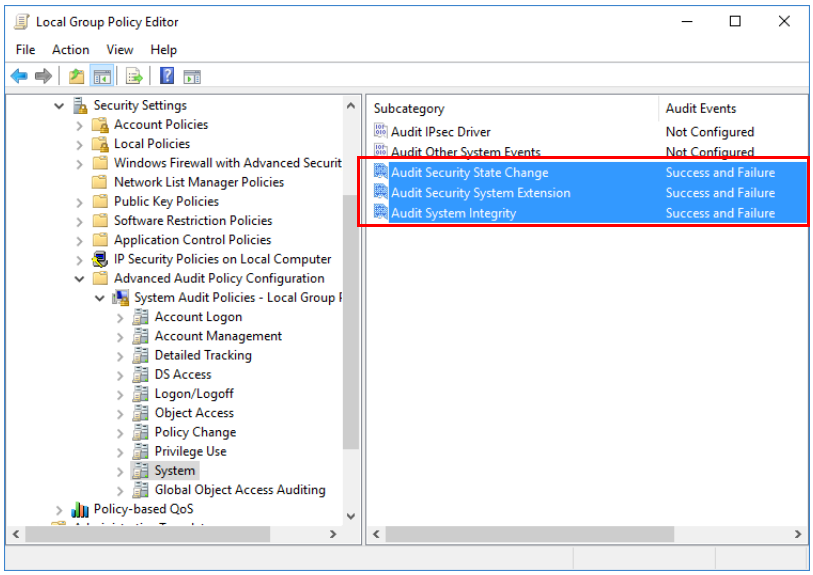


Figure 2-61. System setting

9. To activate the changes in the Windows log, navigate to Computer Configuration > Windows Settings > Security Settings > Local Policies > Security Options and change the value from *Not Defined* to *Enabled*. To do so, right-click the subcategory items and select **Properties** from the shortcut menu.
The Properties setting dialog opens, see Figure 2-62.

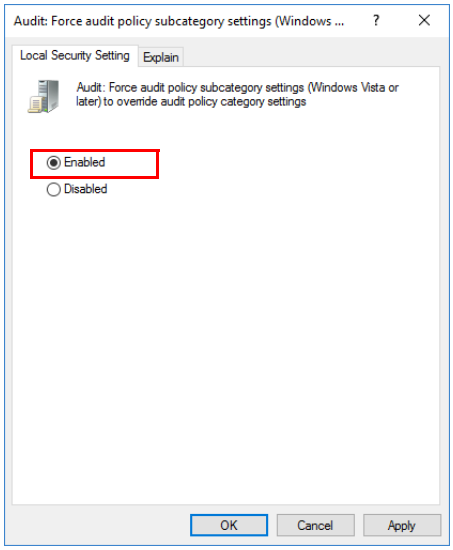


Figure 2-62. Properties setting dialog with Enabled option

10. Set this property for Security Options, see Figure 2-63.

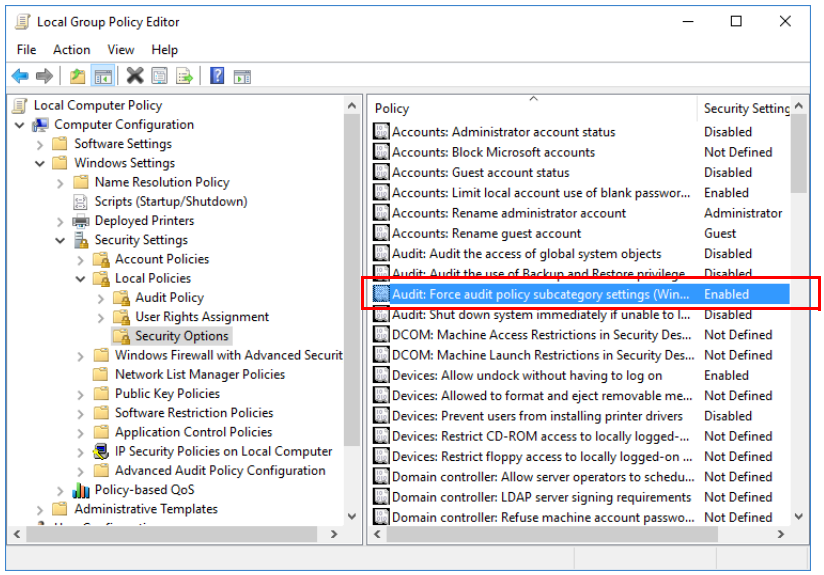


Figure 2-63. Security Options setting

11. Close the Local Group Policy Editor.

12. Restart your computer.

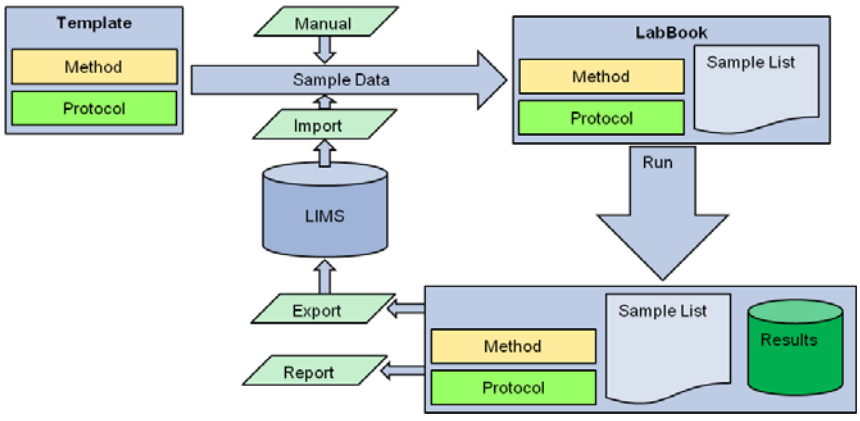


Figure 2-64. LIMS integration

Installation Qualification Operational Qualification (IQ/OQ)

Since version 2.4 of Qtegra ISDS Software, the setup procedure ends with an Installation Qualification (IQ) including an Operational Qualification (OQ). Both qualifications ensure that your instrument works as specified.

The IQ/OQ is run once after every Qtegra ISDS Software installation or upgrade, whereas IQ is run on every start of Qtegra ISDS Software. Results are protocoled in the Log View and displayed as information when IQ is run without failures and as error when there occurred a problem.

Tip Any changes to the IQOQ LabBooks cause an IQ failure when Qtegra ISDS Software is started. To avoid this failure never change the originally delivered and installed files. If changes in an example LabBook are necessary, safe a copy of this LabBook.

The full IQ/OQ package is only available as part of the *iCAP OES Qualification Kit*. With this kit there is no limit on the frequency with which the IQ/OQ process can be performed. It can be run as often as the system SOP requires.

After the installation, the IQ/OQ procedure starts automatically and displays the following window, see Figure 2-65.

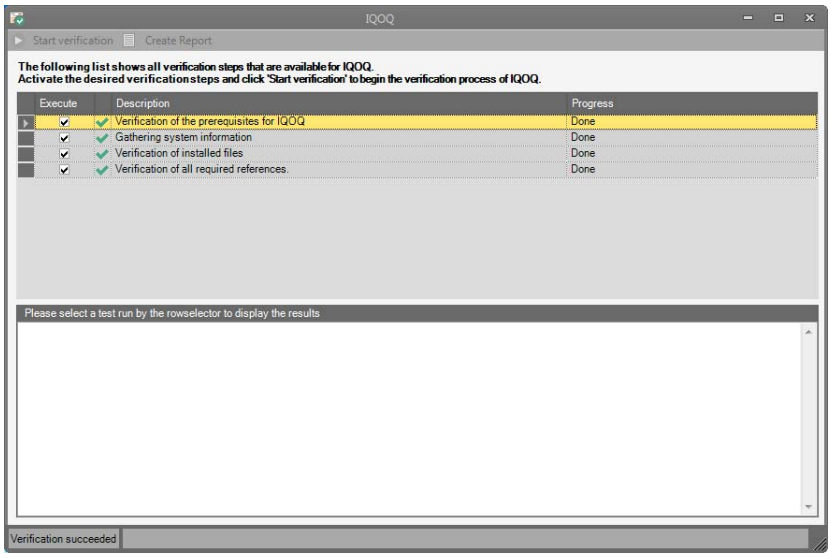


Figure 2-65. IQ/OQ status window

The IQ steps ensure that all the files and assemblies necessary to run any part of the IQ/OQ procedure are found in the correct versions and locations. They also ensure that all files necessary for running the Qtegra ISDS Software are installed in the correct location and have the correct size and name. The OQ step ensures the accurate evaluation of the LabBooks.

A more comprehensive summary of the result for each test is shown in the lower part of the IQOQ window, when you click the desired line selector to the most left of the table.

The IQ/OQ Report is saved to **C:\Users\<User>\Documents\Thermo\Qtegra\IQOQ** and opens automatically in your PDF viewer. It can be saved to another location or printed out as a hard-copy for storage, see Figure 2-66.

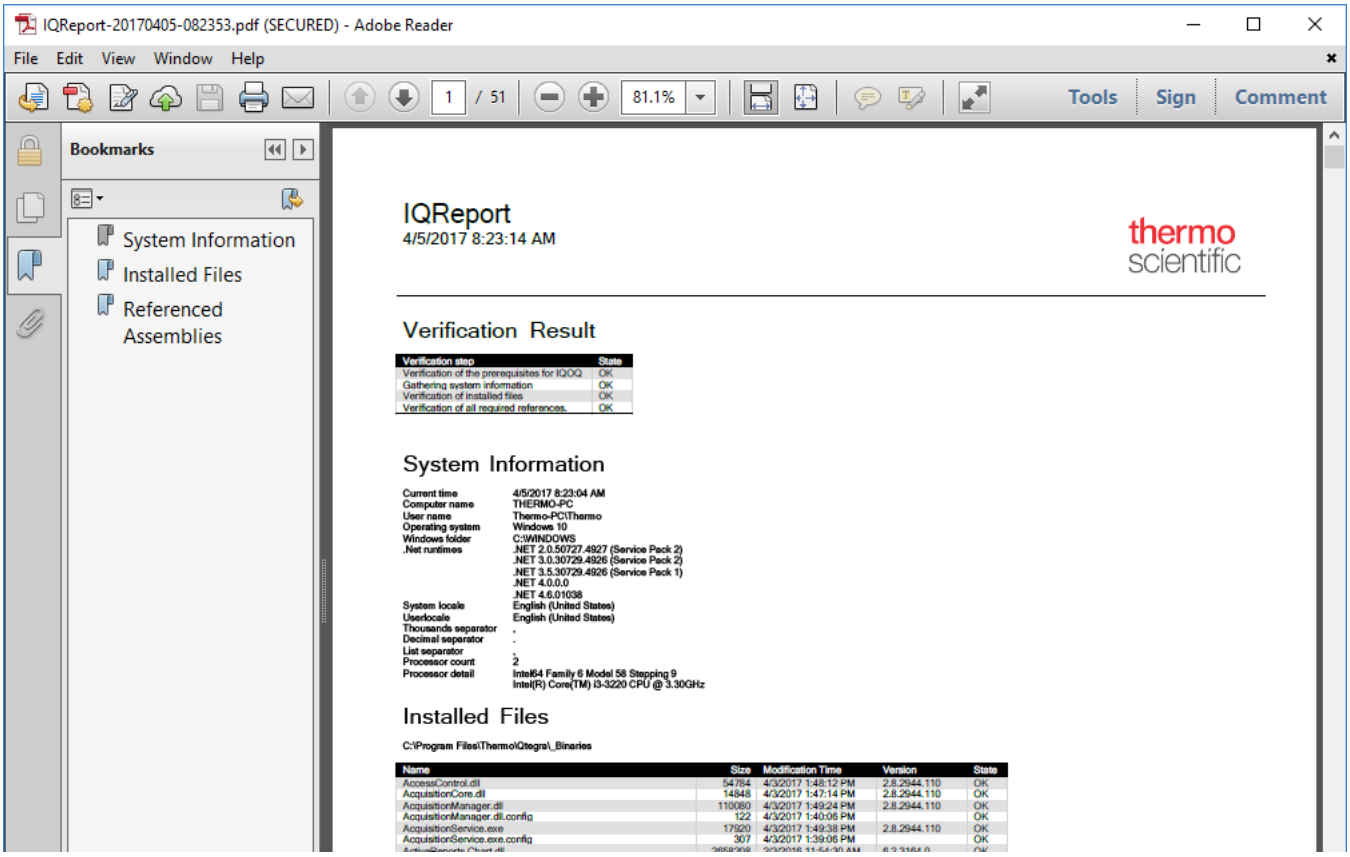


Figure 2-66. Part of an IQ/OQ Report

Configurator

The Configurator tool contains all tools necessary to configure and adjust the Qtegra ISDS Software framework for your laboratory.

Contents

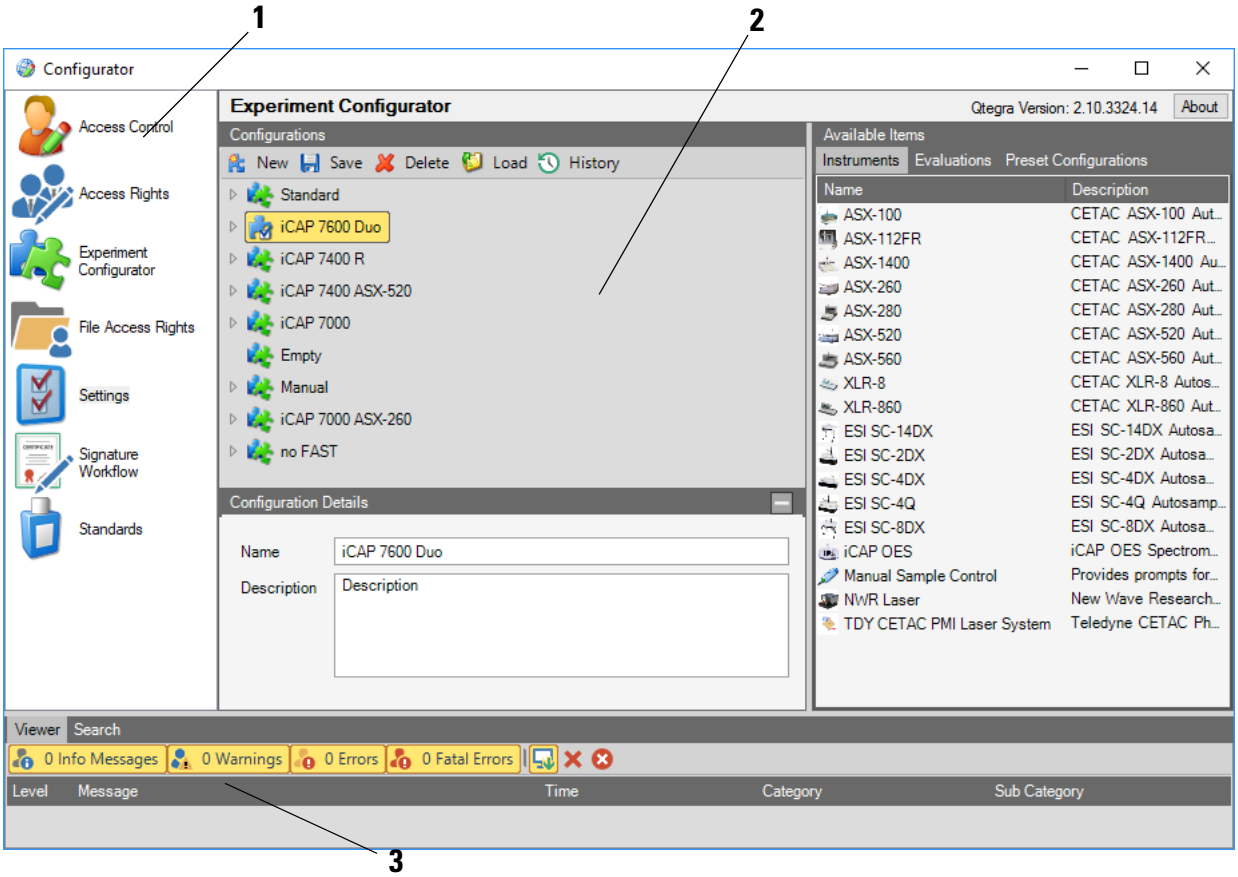
❖ To open the Configurator tool

1. Click **Start > Thermo Qtegra > Configurator** to open the Configurator.
   -or-
   Create a desktop shortcut to **Configurator** and double-click this icon.

   The list of applets, the display region for applet settings and the viewer region are shown.

User Interface of the Configurator Tool

The Configurator tool has three regions, as shown in Figure 3-1:



Labeled Components: 1=list of applets, 2=display region for applet settings, 3=viewer region

Figure 3-1. User interface of the Configurator tool

The list of applets (see also "Configurator Overview" on page 2-11) shows the icons for all applets available in the Configurator tool. The applet settings are displayed when you click the icon.

Tip By default, Enable global compliance is set to *True*. The Configurator will therefore only show a reduced list of applets. To see all applets as shown here, switch off the global compliance parameter. For details, see "Configuring the system to be compliant with SOP" on page 2-37.

Viewer Region

The **Viewer** region (see Figure 3-2) of the Configurator tool displays a list of log files, such as errors and warnings.

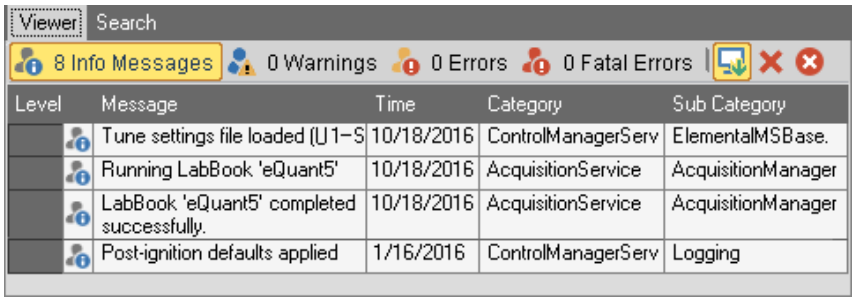


Figure 3-2. Viewer region of the Configurator tool

Tip The Viewer region is also shown in Qtegra and in the Instrument Control tool (see "Log View Region" on page 4-38).

For details on the Viewer region tools, see "Log View" on page 4-88.

Access Control

The **Access Control** applet of the Configurator tool allows the Administrator to control the Virtual instruments, Virtual evaluations, and User Actions.

❖ **To open the Access Control**

1. From the **Configurator** list of applets, select **Access Control**.

With the Access Control applet, the responsible person defines who has access to parts of programs and what type of access permission is granted or denied to a user group. Figure 3-3 shows a typical structure.

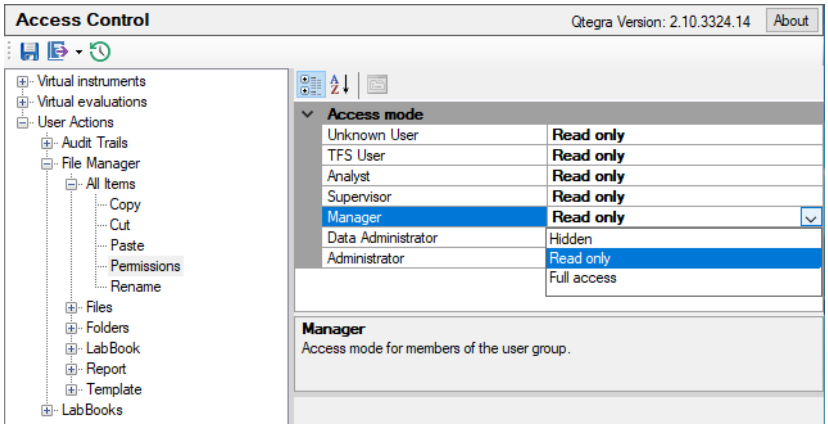


Figure 3-3. Layout of the Access Control applet

Granting Access Rights

In the Access Control applet, you can define for each user group, which buttons and controls are visible and activated.

❖ **To grant or deny access to the user interface**

1. Expand **Virtual instruments**, **Virtual evaluations**, or **User Actions** and the tree items below.
   The **Access mode** settings are shown on the right.
2. Click the user group for which you wish to change the access rights, for example, **Normal user**.
3. Click  to expand the list of access rights, see Figure 3-3.
4. Select the new access right for the user group, for example, *Read only*.
   The new access rights are defined for the expanded component.

Access rights can be granted on three major components Audit Trails, File Manager, and LabBooks.

Table 3-1. Access rights for Audit Trails

Audit Trail	Description
History > Export	Allows the user to export the history entries. Default is *Full access* for Normal user.
History > View	Allows the user to view the history entries. Default is *Full access* for Normal user.
System Log > Export	Allows the user to export the system log entries. Default is *Full access* for Normal user.
System Log > Show All	Allows the user to show the entire list of log entries in the System Log page, which is controlled by the Show All check box. See "System Log Page" on page 4-69. Default is *Full access* for Normal user.
System Log > View	Allows the user to view the system log entries. Default is *Full access* for Normal user.

Table 3-2. Access rights for the File Manager page

File Manager	Description
All Items	Allows the user to copy, cut, paste, and rename the items. Default is *Full access* for Normal user.
Files	Allows the user to delete, export, and import files to Qtegra ISDS Software. Default is *Full access* for Normal user.
Folders	Allows the user to create links, delete, and create new folders on the File Manager view. Default is *Full access* for Normal user.
LabBook	Allows the user to copy, create, cut, delete, edit, and paste LabBooks on the File Manager view. Default is *Full access* for Normal user.
Report	Allows the user to copy, create, cut, delete, edit, and paste Reports on the File Manager view. Default is *Full access* for Normal user.
Template	Allows the user to copy, create, cut, delete, edit, and paste Templates on the File Manager view. Default is *Full access* for Normal user.

Table 3-3. Access rights for LabBooks

LabBooks	Description
Electronic Signatures	Allows the user to sign (and lock) different stages of a LabBook and to revoke the signature. Default is *Full access* only for Administrator and Data Administrator.
Evaluation Results	Allows the user to include and exclude data entries to and from the eQuant Evaluation Concentration Ratios view, the Concentrations view, and the Survey Concentrations view. Allows the user to include and exclude data entries to and from the Raw Data Raw Intensities view, the Raw Intensity Ratios view, and the Survey Intensities view. Default is *Full access* for Normal user.
Method Development	Allows the user to copy, create, cut, and paste Element Finder and Plasma Optimization methods. Allows the user to create LabBooks from Method Development and to perform Actions. Default is *Full access* for Normal user.
Method Parameters	Allows the user to edit and modify the Method Evaluations, Instruments, Interference Correction, and Standards data. Default is *Full access* for Normal user.
Sample List	Allows the user to add, copy, delete, edit, and move samples in the Sample List. Default is *Full access* for Normal user except Quality Control with *Full access* for the Data Administrator only.
Settings	Gives the user access to Flags and Limits. Default is *Full access* for Normal user.

Types of access rights that can be granted or denied are listed in Table 3-4.

Table 3-4. Access rights for Qtegra

Name	Description
Full access	The user can both see the certain program, application, or menu item and edit the settings.
Read only	The user can only see the certain program, application, or menu item; changes are not allowed.
Hidden	Same as *Read only*: The user can only see the certain program, application, or menu item; changes are not allowed.

Tip **Full access** rights by default are granted to the *System Administrator, Administrator, Data Administrator, Manager, Supervisor, Analyst*, and normal *User* groups. Users who have not been assigned (by the Windows administrator) to a Qtegra ISDS Software group belong to the *Unknown user* group. For this group, every access mode is set to **Read only**.

Setting History and System Log Export and View Rights

To be compliant with quality requirements, an Administrator may set or reject the access rights for the history and system log function of Qtegra ISDS Software.

Tip The following steps refer to the history function. Replace "History" by "System Log" to adapt the description accordingly.

❖ **To set the access rights on the history or system log function**

1. Expand **User Actions > Audit Trails > History**.
2. Select the **Export** or **View** item.
   The **Access mode** settings are shown on the right.
3. Click the user group for which you wish to change the access rights, for example, **Normal user**.
4. Select the new access right (*Hidden, Read only*, or *Full access*) and enter a comment.
   The new access rights are defined for this item and affect the history of LabBooks, Templates and Tune Settings.

Generating an Access Control Report

For each user action, you can export the access control permissions to get an overview of your settings.

❖ To generate an access control Report

The print out shows the access control permissions focused on the **User Actions** component.

1. Expand **Export** to show the menu and select the file format for the Report.

   a. Select **Save as HTML** to compile an HTML Report that is shown in your browser.
   The Browse For Folder dialog is opened to select the folder where you want to save the HtmlReport folder with the *index.html* file and all images used.

   b. Select **Save as PDF** to compile a PDF Report that is shown in your PDF viewer.
   The Save As dialog is opened to select the folder and to type the file name of the PDF file.

   c. Select **Save as RTF** to generate a Report that is displayed in Microsoft Word or your alternative RTF viewer.
   The Save As dialog is opened to select the folder and to type the file name of the RTF file.

   d. Select **Save as XML** to generate a Report that is displayed in your browser.
   The Browse For Folder dialog is opened to select the folder where you want to save the XML output.

The Report shows a matrix of *Full access* for full access rights and *Hidden* or *Read only* for denied access rights, see Figure 3-4.

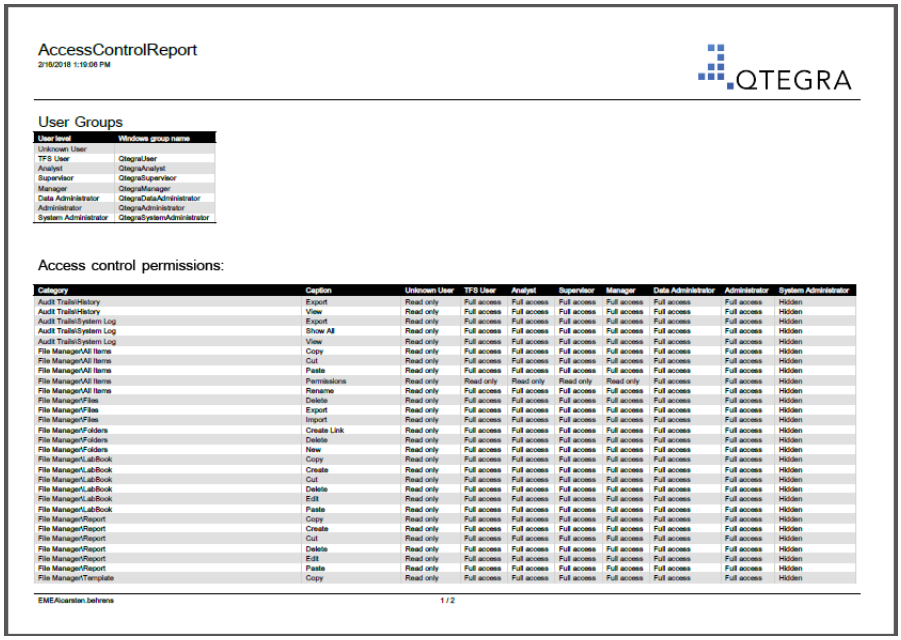


Figure 3-4. Detail view of an access control Report

Viewing History Entries

Tip Viewing and exporting the history is only available if the Enable global compliance value is set to *True*.

❖ **To view, compare and export the history of entries**

1. In the **Access Control** applet, click **History** to open the History window.

   Tip The History window is only opened when entries are available. You will neither see the History window nor get any notification that your click has been executed if no history entries are available.

2. To compare the history entries, press **<Ctrl>** or **<Shift>** and select the range of history entries you wish to compare.

   Tip Qtegra ISDS Software allows the selection of any number of entries for comparison purposes but only 2 history entries can be exported for comparison.

3. Click **Compare** to compare the selected entries.
   The Comparison dialog opens and shows all selected entries column by column.

4. Resize or minimize the Comparison dialog to make all entries visible. The column header shows the date of selected entry with the oldest version left and the newest version right.

5. Click the triangle in front of the items to collapse and expand the items to focus on the interesting parts.

6. Select **Show differences only** if you wish to view only the differences, which is the default setting.
   When removing the tick, Qtegra ISDS Software needs a few seconds to update the list and to show all history entries. Differences then are shown in bold letters.

7. Click **Close** to close the Comparison dialog.

8. Expand the Export button to select the file format for the history export.

   a. Select **Save as HTML** to compile a HTML history that is displayed in your browser.
      The Save As dialog is opened to select the folder where you want to save the HTML output.

   b. Select **Save as PDF** to compile a PDF history that is displayed in your PDF viewer.
      The Save As dialog is opened to select the folder and to type the file name of the PDF file.

c. Select **Save as RTF** to generate a history that is displayed in Microsoft Word or your alternative RTF viewer.
The Save As dialog is opened to select the folder and to type the file name of the RTF file.

d. Select **Save as XML** to generate a history that is displayed in the browser.
The Browse For Folder dialog is opened to select the folder where you want to save the XML output.

9. Click **Close** to close the History window.

Access Rights

The **Access Rights** applet of the Configurator tool introduced with Qtegra ISDS Software version 2.10 allows to control the access permissions by granting or denying access to the Qtegra applications in general and the Configurator applets in particular.

This applet shows one matrix of all Qtegra user groups and the Qtegra applications, that means, the Configurator, InstrumentInstall, Qtegra, and ServiceStatus tools. The second matrix shows all Qtegra user groups and the Configurator applets, see Figure 3-5 with the default settings.

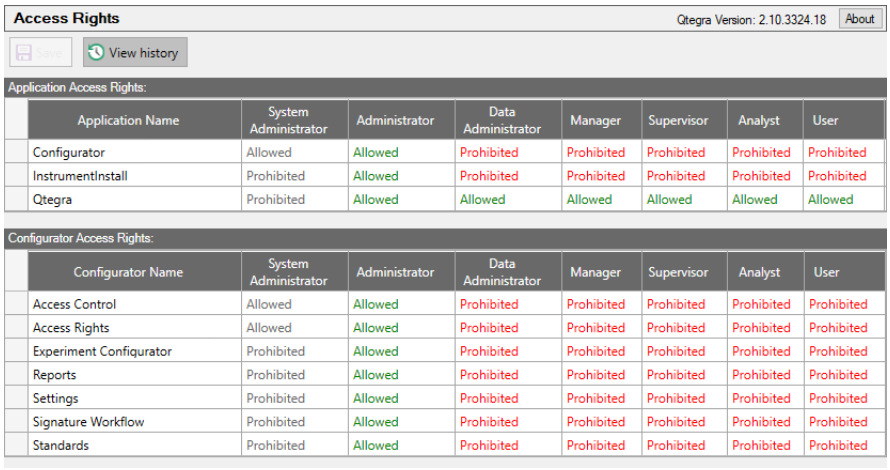


Figure 3-5. Layout of the Access Rights applet

If a cell of the matrix shows green ‘Allowed’, members of the corresponding Qtegra user group can run the application or open the Configurator applet. The default settings give the Administrator access to all applications and applets. The settings for the System Administrator can not be changed and are therefore displayed in gray.

When opening an application with insufficient user rights, a message is shown, see Figure 3-6.

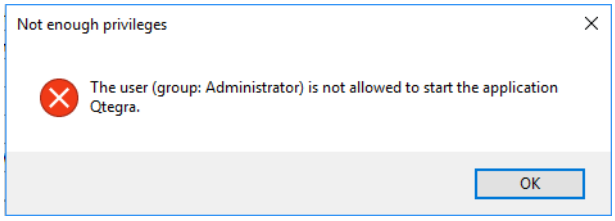
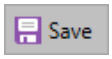


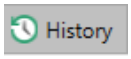
Figure 3-6. Message for insufficient privileges

The application itself is not opened.

Tip By default, the minimum user level for **Applications** (except Qtegra) and **Configurators** is defined as Administrator. Other user groups cannot open these programs.



After selecting *Prohibited* or *Allowed* from the listbox, click outside the matrix to enable the **Save** button. Click **Save** to make your changes available after a comment was entered in the confirmation dialog.



Click **History** to view, compare and export the history of a Configuration. See "Viewing History Entries" on page 3-9 for details.

User Roles

During setup of Qtegra ISDS Software, Thermo Fisher Scientific provides the user groups shown in Table 3-5. The Windows user installing Qtegra ISDS Software is added to the Administrator group.

Table 3-5. User roles provided by Qtegra

Name[a]	Description
System Administrator*	The System Administrator has only access to the Configurator tool to set up the user group functionality.
Administrator	The Administrator is responsible for the instrument setup, configuration settings and technical services. By default, the Administrator has full access to all programs and applications available except Post Analysis Manipulation.
Data Administrator*	The Data Administrator is responsible for the acquired data. By default, the Data Administrator has full access to programs and applications available and to Post Analysis Manipulation.
Manager	The Manager is responsible for method setup/creation and instrument maintenance. By default, the Manager has limited access to programs and applications. The access rights are granted by the Administrator by changing the minimum required user level for the selected application.
Supervisor	The Supervisor is an optional user role with some extended access rights that are defined in your environment. By default, the Supervisor has limited access to programs and applications. The access rights are granted by the Administrator by changing the minimum required user level for the selected application.

Table 3-5. User roles provided by Qtegra, continued

Name[a]	Description
Analyst	The Analyst is an optional user role with some extended access rights that are defined in your environment. By default, the Analyst has limited access to programs and applications. The access rights are granted by the Administrator by changing the minimum required user level for the selected application.
User	The User is responsible for sample measurement. By default, the User has limited access to programs and applications. The access rights are granted by the Administrator by changing the minimum required user level for the selected application.

[a] The Qtegra user group marked with an asterisk is not created during installation. See page 2-5 for creation of Qtegra user groups.

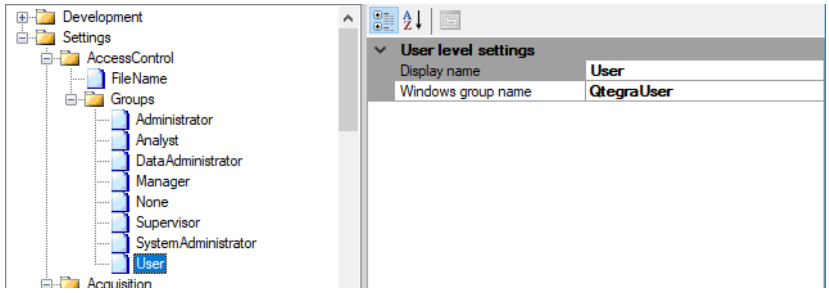
Changing the Group name or User name

If policies or internal rules require, you can change the Windows group name or the User name provided by Qtegra ISDS Software.

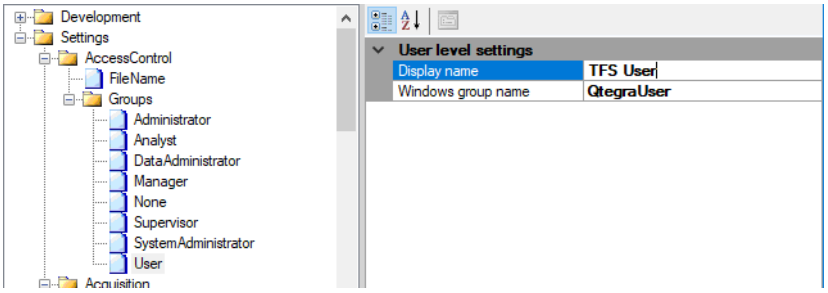
IMPORTANT There is a risk of losing access. If you are a member of the Administrator group, which actually should be changed, make sure to temporarily become a member of another group with the right to use the Configurator. After successful verification of your Group name change, remove yourself from the other group.

❖ **To change a Windows Group name or Display name for the user**

1. In the **Settings** applet, expand **Settings > Groups**.
2. Select the group item you want to rename, for example, *User*. The right pane displays the current values.

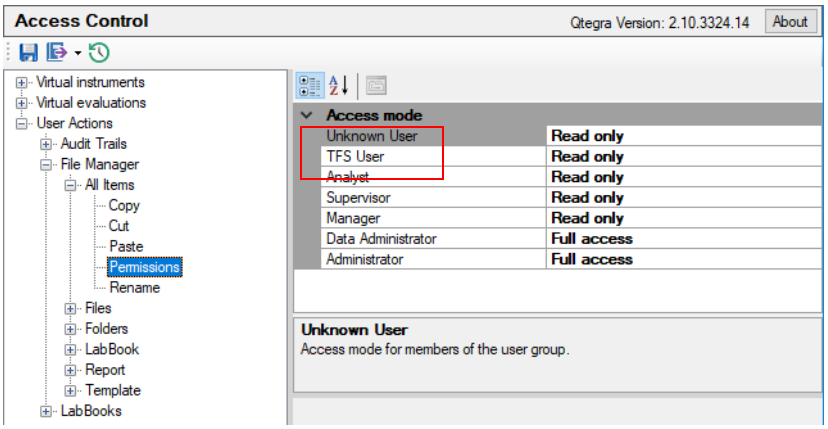


3. Click into the field you want to change and type the desired name for the *Display name* or for the *Windows group name*. There is no restriction regarding the characters.



IMPORTANT While changing the **Windows group name**, make sure to change this name also in the **Windows Computer Management** under System Tool > Local User and Groups > Groups. Otherwise, users of the renamed group can no more run the Qtegra ISDS Software.

4. Stop typing with **<Enter>** and add your comment into the Confirmation dialog that is shown immediately.
The new value is shown in the list boxes, where you set the access control.



Tip When changing the **Windows user group** name, make sure to type the correct name of the Windows group. See"Setting User Levels" on page 2-3 for details.

Experiment Configurator

The **Experiment Configurator** applet of the Configurator tool combines instrument sets. Each combination is saved as specific Configuration for later use in the Qtegra ISDS Software when creating a LabBook or Template.

Tip Access to this module is defined in the "Access Control" on page 3-4. Generally, only the Administrator has full access to this module.

In the Experiment Configurator applet, all virtual instruments, virtual evaluation types and preset configurations are listed on tabbed pages, see Figure 3-7.

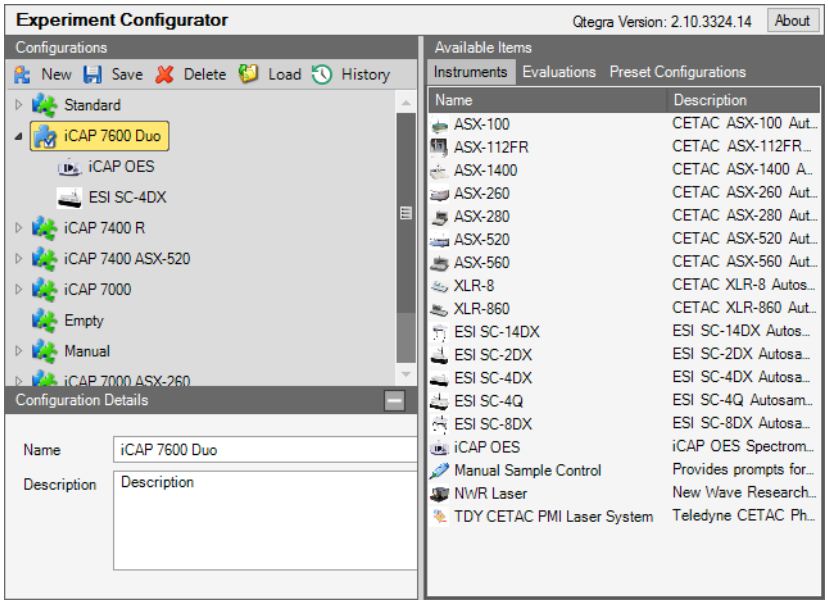


Figure 3-7. Layout of the Experiment Configurator applet

The commands available in Experiment Configurator are summarized in Table 3-6.

Table 3-6. Experiment Configurator commands

Commands	Description
	To create a new Configuration. Adds **New Experiment Configuration** to be renamed.
	To save the current Configuration.
	To delete the current Configuration.

Table 3-6. Experiment Configurator commands, continued

Commands	Description
	To load all current Configurations.
	To view, compare and export the history of a Configuration. See "Viewing History Entries" on page 3-9 for details.

❖ **To open the Experiment Configurator**

1. From the **Configurator** list of applets, select **Experiment Configurator**.

Creating a new Configuration

A Configuration provides Qtegra ISDS Software with the hardware parameters of your instruments. As Administrator, make sure that a Configuration based on your instrument is available.

❖ **To create a new Configuration**

1. From **Configurator > Experiment Configurator**, click **New** to add a new Configuration, see Figure 3-8.

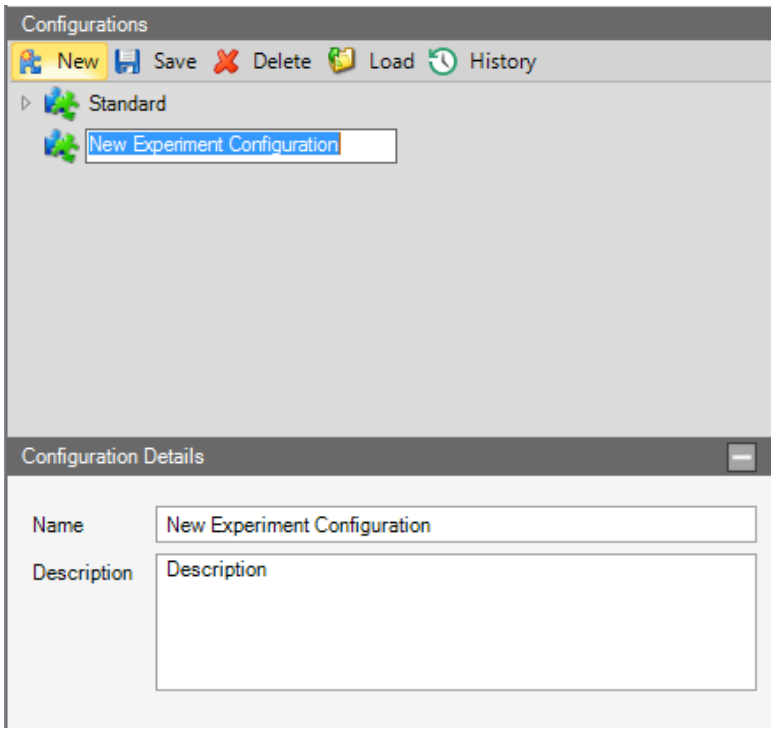


Figure 3-8. Add new Configuration

2. Type a name and click anywhere outside the field.
-or-

Press **<Enter>** to confirm.
The name is accepted as there are no restrictions with regard to the character range. The Configuration is displayed in the **Configuration Details** view.

3. Type a **Description** in **Configuration Details**.

4. From the right-hand pane of available **Instruments**, select your instrument, see Figure 3-7.

   All supported instruments and peripherals are listed in the **Instruments** tab.

5. Drag *iCAP OES* from the **Instruments** tab to your new Configuration and drop when + is shown, see Figure 3-9.

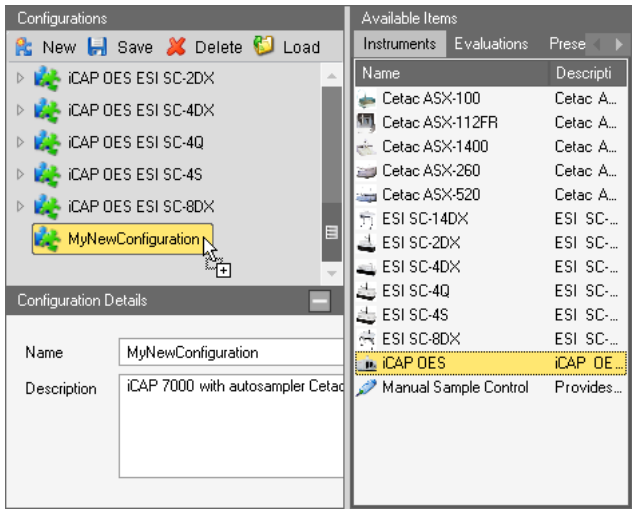


Figure 3-9. Add iCAP OES to your Configuration

The Configuration item is expanded and shows one instrument.

6. Drag the peripheral you wish to add from the **Instruments** tab to your new Configuration, see Figure 3-10.

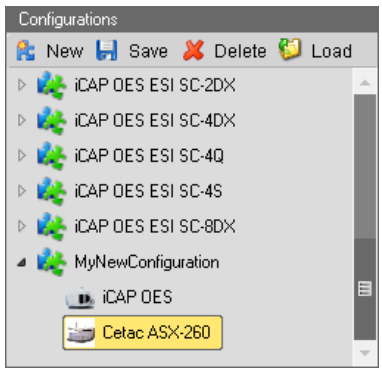


Figure 3-10. Instrument and autosampler added to your Configuration

❖ **To rename a Configuration**

1. From **Configurator > Experiment Configurator**, select the Configuration you wish to rename.
   The **Configuration Details** window shows the name and description.
2. In the **Name** field, change the name according to your needs.
3. Optionally, add or change the **Description**.

Editing the Settings of Instruments

In the Experiment Configurator applet, your Administrator edits the settings for the instrument in the Configurations field.

❖ **To edit the instrument or peripheral settings**

1. From **Configurator > Experiment Configurator**, open the list of Configurations and right-click the instrument or peripheral you wish to edit the settings for, see Figure 3-11.

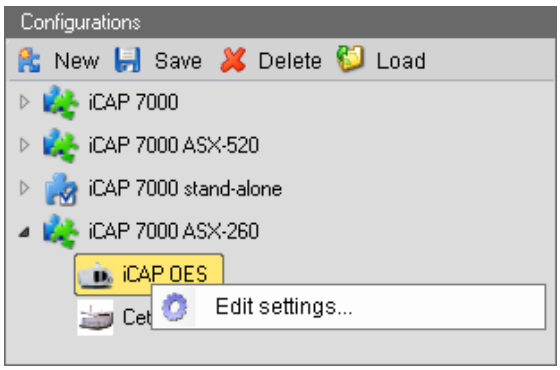


Figure 3-11. Right-click the instrument item to edit the settings

2. Click **Edit settings** to open the **Settings** dialog, see Figure 3-12.

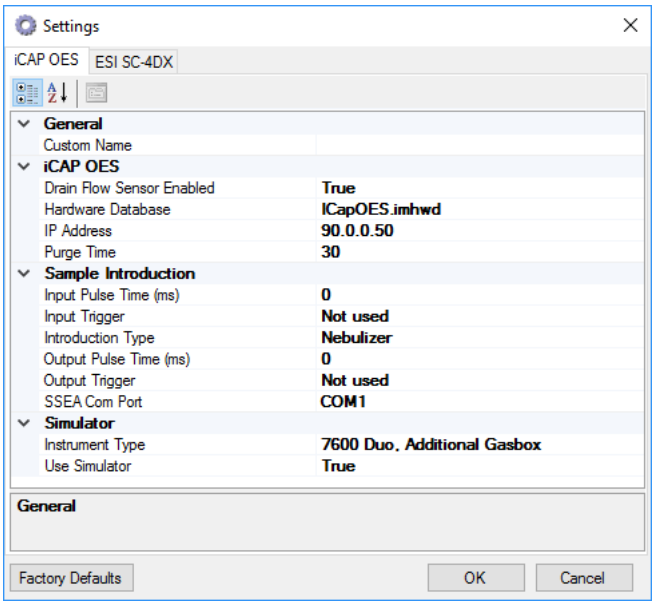


Figure 3-12. Settings dialog for iCAP OES in Configurator

3. The setting parameters are grouped, for example, **Sample Introduction** or **General**. When changing the values, take the description in the lower tile into account.

4. Click a cell to change the value.

If a drop-down menu is available for this cell, the drop-down arrow is shown, see Figure 3-13.
If the cell represents a Boolean variable, just double-click to switch between **True** and **False**.

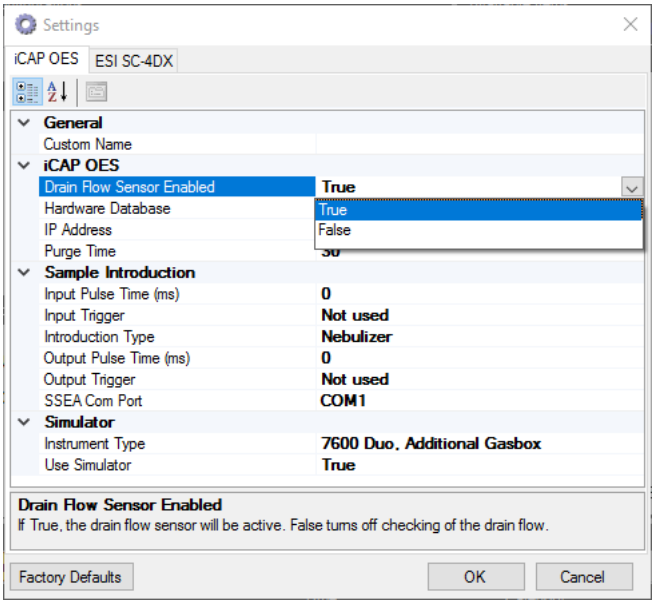


Figure 3-13. Drop-down menu of Settings in the Experiment Configurator

5. Select an item from the list.

6. Some peripherals provide several setting pages. Select the tabs, for example, *FAST Setup* and *Autosampler* to set up all parameters.

Enabling the Drain Flow Sensor

The Drain Flow Sensor is a unique safety and time saving device which uses a bubble counter to check that at least one bubble passes from the instrument spray chamber drain every two minutes. This ensures that if the sample introduction becomes blocked/sample tubing has detached that valuable time and gas is not wasted by continuing the run. This is also an excellent safety feature, as it will ensure a safe controlled shutdown from an automated sequence, activate nudge mode on the pump to save the tubing and leave everything ready for the user to assess and re-start the system, with no need to re-fill all the sample tubes.

This option allows you to enable/disable the drain flow sensor when using accessories that do not have a drain actively pumping liquid waste via the instrument peristaltic pump, for example, ultrasonic nebulizer or hydride accessory.

❖ **To enable the drain flow sensor of iCAP 7000 Plus Series ICP-OES**

1. From the **Configurator** list of applets, select **Experiment Configurator**.

2. In the list of **Configurations**, right-click the instrument you wish to enable the drain flow sensor for iCAP 7000 Plus Series ICP-OES.

3. Click **Edit Settings** (see Figure 3-11) to open the **Settings** dialog, see Figure 3-14.

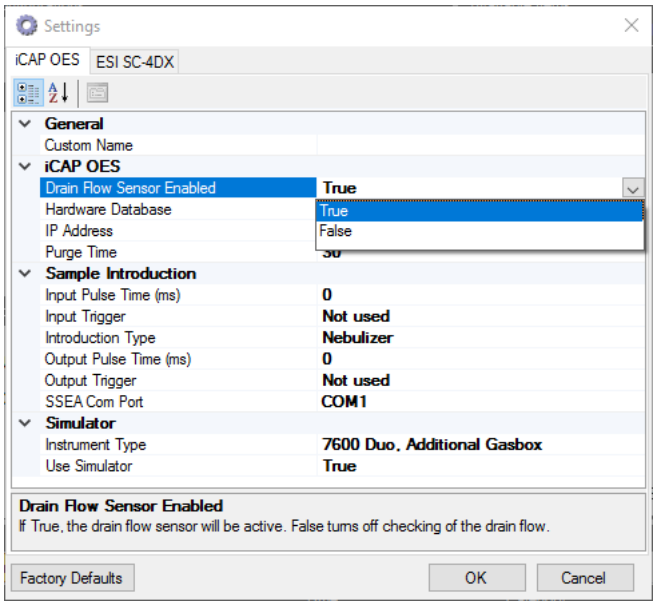


Figure 3-14. Drain flow sensor settings for iCAP OES in Configurator

4. In the **iCAP OES** tab, click the **Drain Flow Sensor Enabled** cell.
5. Click ⌄ to open the drop-down list and select **True**.

❖ **To reset settings to factory default**

1. From **Configurator > Experiment Configurator**, open the list of Configurations and right-click the instrument or peripheral you wish to reset the settings for, see Figure 3-11.
2. Click **Edit settings**.
3. In the **Settings** dialog, click Factory Defaults to reset all values to the defaults as set from the factory.

Managing Configurations

In the Experiment Configurator applet, Configurations can be loaded from the database, saved and activated as a preset, and deleted.

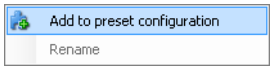
❖ **To load all Configurations from the database**

1. From **Configurator > Experiment Configurator**, click **Load** to load all Configurations from the database.
   The Configurations list is updated.

For typical applications with the iCAP 7000 Plus Series ICP-OES instrument, pre-configured system combinations are made available in the **Preset Configurations** tab by the Thermo Fisher Scientific field service engineer upon delivery of the system.

❖ **To create a Preset Configuration**

1. From **Configurator > Experiment Configurator**, open the list of Configurations and right-click the Configuration you wish to add to the list of Preset Configurations.



2. Select **Add to preset configuration** from the shortcut menu to add the Configuration to the list of Preset Configurations.

❖ **To activate a Preset Configuration**

1. Select the **Preset Configurations** tab.
2. Select the preset Configuration you wish to work with.

3. Drag the preset Configuration to **Configurations**, see Figure 3-15.

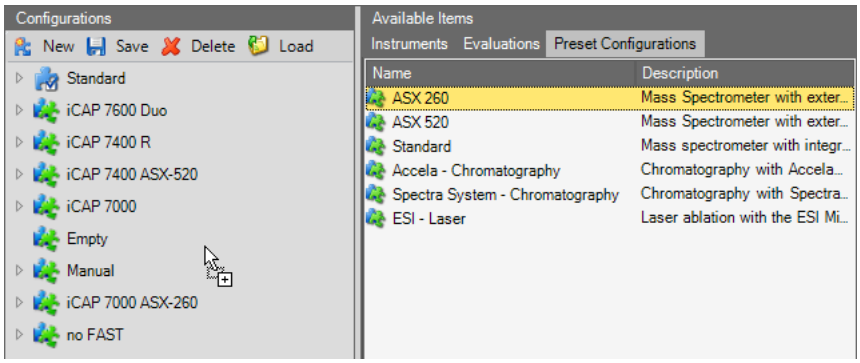


Figure 3-15. Selecting a preset Configuration

The preset Configuration is now added to the Configurations list.

❖ To delete a Configuration

1. From **Configurator > Experiment Configurator**, select the Configuration you wish to delete.

2. Click **Delete** to delete the selected Configuration.
A confirmation dialog opens.

3. Click **Yes** to delete the Configuration.

File Access Rights

The **File Access Rights** applet of the Configurator tool introduced with Qtegra ISDS Software version 2.10 allows to manage the file access by permissions. Especially the Qtegra System Administrator uses this applet as he has no access to the Qtegra File Manager.

With the File Access Rights applet, the responsible person defines the file access rights by selecting a principal and setting the permissions respectively on the file or folder level currently selected. Figure 3-16 shows a typical structure.

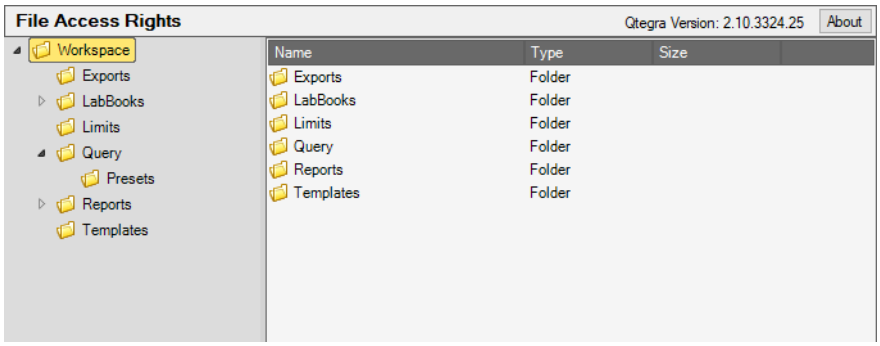


Figure 3-16. Layout of the File Access Rights applet

Refer to "Setting File Permissions" on page 4-60 for a detailed description on how to manage file permissions. Adapt the folder structure from the Qtegra File Manager page accordingly.

Reports

The **Reports** applet of the Configurator tool allows you to create new Report templates or to edit existing templates.

Tip By default, Enable global compliance is set to *True*. The Configurator will therefore only show a reduced list of applets. To see all applets as shown here, switch off the global compliance parameter.

The Reports applet (see Figure 3-17) determines the layout of the Reports.

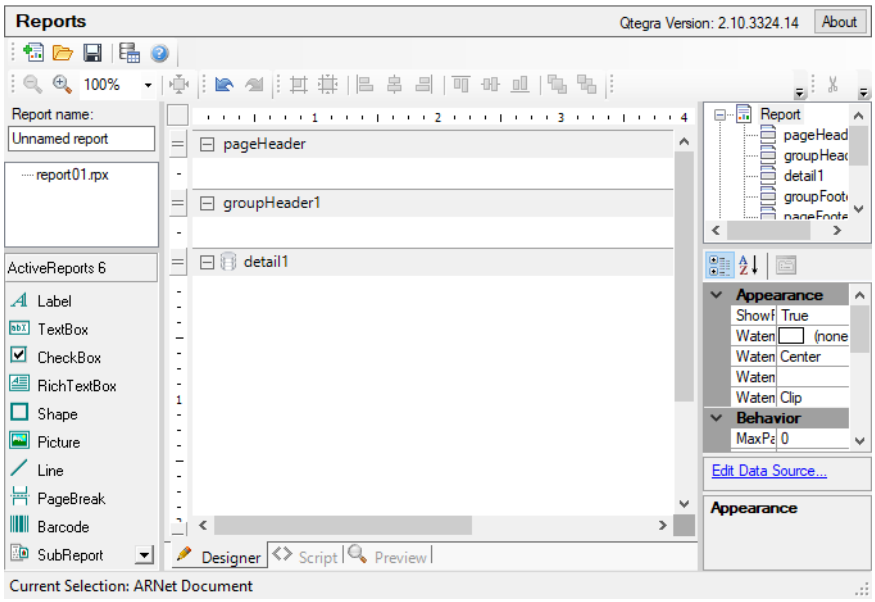


Figure 3-17. Layout of the Reports applet

The commands available in the Reports applet are summarized in Table 3-7.

Table 3-7. Reports commands

Commands	Description
	To create a new Report template.
	To open/load a Report in the file format *.imrep.
	To save the current Report template.
	To load a template from the XML database.

❖ **To open the Reports applet**

1. From the **Configurator** list of applets, select **Reports**.

❖ **To create a new Report template**

1. From **Configurator > Reports**, click **Create** to create a new Report template.
2. Type a **Report name**.
3. Configure the layout.

4. Click **Save** to save the Report template.
   The file is saved in the file format *.imrep.

❖ **To edit an existing Report template**

1. From **Configurator > Reports**, click **Load** and browse for the Report file.
2. Select the Report file you wish to edit.
3. Click **OK** to open the file.
4. Edit the file.

5. Click **Save** to save the Report template.

Settings

The **Settings** applet of the Configurator tool controls default settings, for example, the default directory path for Qtegra or the default settings for dwell time.

The Settings applet (see Figure 3-18) gives access to the settings database (registry).

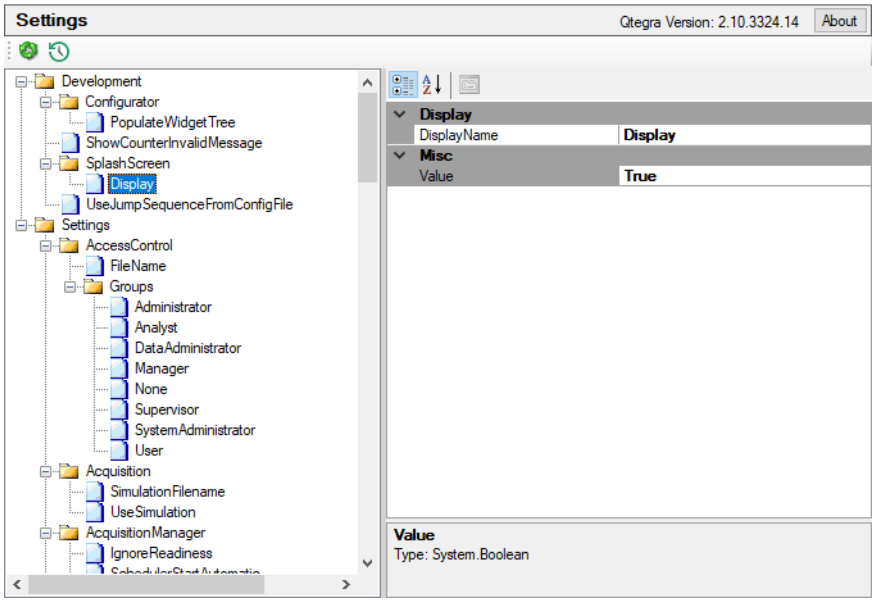


Figure 3-18. Layout of the Settings applet

❖ **To open the Settings applet**

1. From the **Configurator** list of applets, select **Settings**.
2. Scroll through the list of settings and select the item you want to change. Details of the selected item are displayed in the right-hand pane.
3. Click into the field where you want to change the value. In some cases, a listbox offers the values to be selected. In other cases, type the desired value. Be sure to type only valid values.

❖ **To enable debug messages**

1. From the **Settings** applet, expand **Settings > Logging** and click **ShowAll**.
2. Set the **Value** for **Misc** to **True**.

❖ **To enable extended debug logging in the Sample List**

1. From **Configurator > Settings**, expand **Logging** and click **SampleListSynchronisationLoggingEnabled**.

2. Set the **Value** for **Misc** to **True**.

Tip Activate this logging feature only if you experience unexpected issues in the Sample List. Better leave it *False* because otherwise a significant amount of log messages is added to the log files, which need to be stored.

Compliance Settings

For details, see "Compliance with your SOP" on page 2-37.

Viewing History Entries

For details, see "Viewing History Entries" on page 3-9.

Signature Workflow

Signatures allow to document that a workflow stage has been performed by a known person. By default, Qtegra ISDS Software provides the three stages *Acquired, Verified* and *Approved*. Each stage can be revoked. In the Signature Workflow applet of the Configurator, the stages are defined. In the Access Control applet of the Configurator, the access rights for signing and revoking are set individually for all user groups.

❖ **To define Signature Workflow stages**

1. Open Configurator > Signature Workflow.
   The currently available stages are shown.

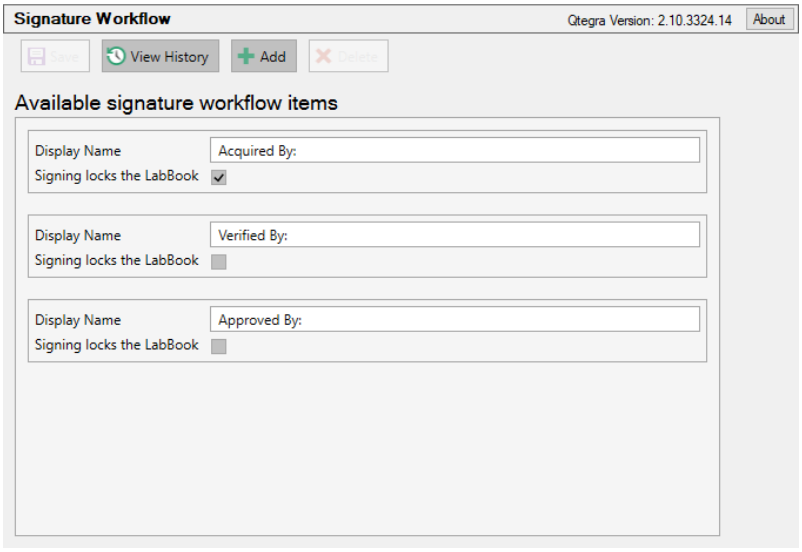


Figure 3-19. Default definition of the Signature Workflow

2. To rename the item, select an existing item and edit the **Display Name** if desired.
   The selected item gets yellow highlighted.

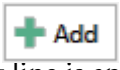
   Tip When changing the Display Name, always make sure that the items represent hierarchical levels. A typical signing workflow (*Acquired, Verified, Approved*) is shown by default. Do not re-order the workflow by renaming the items.

   Tip After changing the Display Name, the access rights remain as originally defined.

3. Tick **Signing locks the LabBook** to protect the LabBook against any changes after signing.
   In some cases it makes sense to lock a LabBook beginning with a higher level. After a LabBook is locked by signature, it always remains locked when getting the next signature.

As Qtegra ISDS Software provides three workflow items by default, you can add additional items or remove existing items.

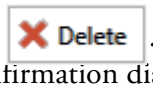
❖ To add workflow items

1. Open Configurator > Signature Workflow.
   The currently available stages are shown.
2. Click 

.
   A new line is appended to the list.
3. Change the **Display Name** according to your needs and tick **Signing locks the LabBook** if desired.
4. Drag the selected item to the desired position to represent the correct stage, that means, select the item and move the mouse pointer while the mouse button is pressed.

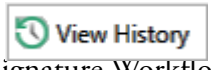
   Tip To make the new settings available, the Configurator tool must be restarted before the next step is performed.
5. Set the access rights for Sign and Revoke under Access Control > User Actions > LabBooks > Electronic Signatures. See "Granting Access Rights" on page 3-4.

❖ To delete workflow items

1. Open Configurator > Signature Workflow.
   The currently available stages are shown.
2. Select the stage you want to delete.
   The selected stage gets yellow highlighted.
3. Click 

.
   A confirmation dialog opens.
4. Click **Yes**.
   The workflow item is removed from the Signature Workflow view.

❖ To view the workflow history

1. Open Configurator > Signature Workflow.
   The currently available stages are shown.
2. Click 

.
   The Signature Workflow History window opens a list of available history entries.
3. Select the entries (press **<Ctrl>** to select multiple entries).
4. Click **Export** if you want to export the history as HTML, PDF, RTF, or XML.
   -or-
   Click **Compare** to show the differences between the Signature Workflow items.

To view, compare and export the history of the Configuration, see "Viewing History Entries" on page 3-9.

Standards

The **Standards** applet of the Configurator tool gives access to the standards database. New standard files, Internal Standard files and isotope dilution standard files are created here.

The Standards applet (see Figure 3-20) shows a list of standards on the left. On the right pane, the associated elements and their concentration in the standard solution are displayed as well as the periodic table.

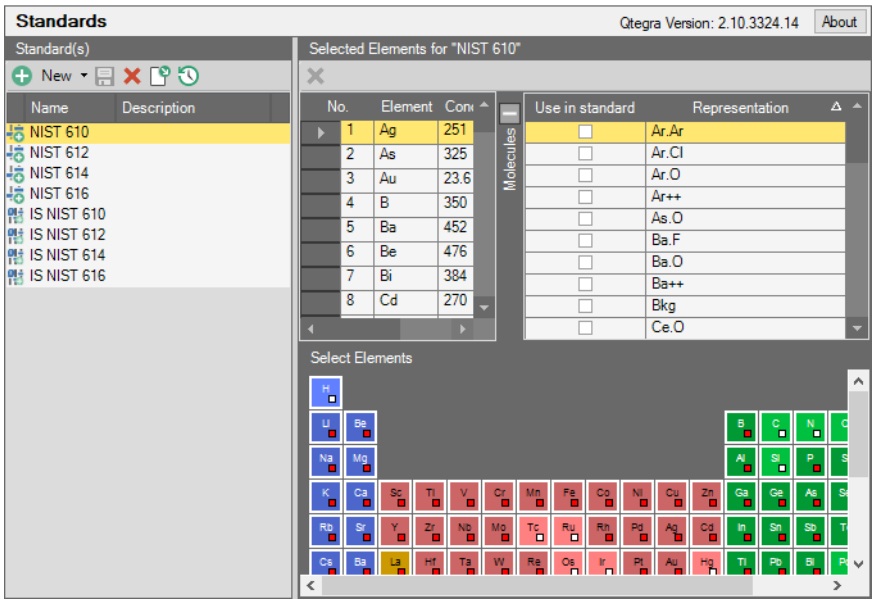


Figure 3-20. Layout of the Standards applet

The Standards commands are summarized in Table 3-8.

Table 3-8. Standards commands

Commands	Description
	To create a new standard or Internal Standard.
	To delete the selected standard(s).
	To load all standards from the preset standard database.
	To save the standards files to the database.
	To open the History for Standards dialog, where you can view, compare and export history entries. See "Viewing History Entries" on page 3-9 for details.

Tip Some standards offered to be created with the  menu are designed for other instruments rather than the iCAP 7000 Plus Series ICP-OES instrument.

❖ **To open the Standards applet**

1. From the **Configurator** list of applets, select **Standards**.

❖ **To load all standards from the standard database**

1. From **Configurator > Standards**, click **Load** to load all standards from the database.

❖ **To save standards to the standard database**

1. From **Configurator > Standards**, change or add standards according to your needs.

2. Click **Save** to save the standards to the database.

❖ **To delete standards from the standard database**

1. From **Configurator > Standards**, open the Standard(s) list and select the row you wish to delete.

2. Click **Delete**.
   A confirmation dialog opens.
3. Click **Yes**.
   The standard is deleted from the database.

❖ To select molecules as standard

1. From **Configurator > Standards**, open the Standard(s) list and on the top right, click the **collapse** button to expand the Molecules list. The Molecules list opens, see Figure 3-20.
2. To add molecules to your standard, tick **Use in standard** of the Molecules list.
   The molecule is immediately copied to your standard list.
3. Define the concentration and unit of the analytes as required.

Qtegra

Qtegra is the principal tool for preparing and running measurements. The Qtegra tool is the main Qtegra ISDS Software module and is used to design, start and stop the measurements.

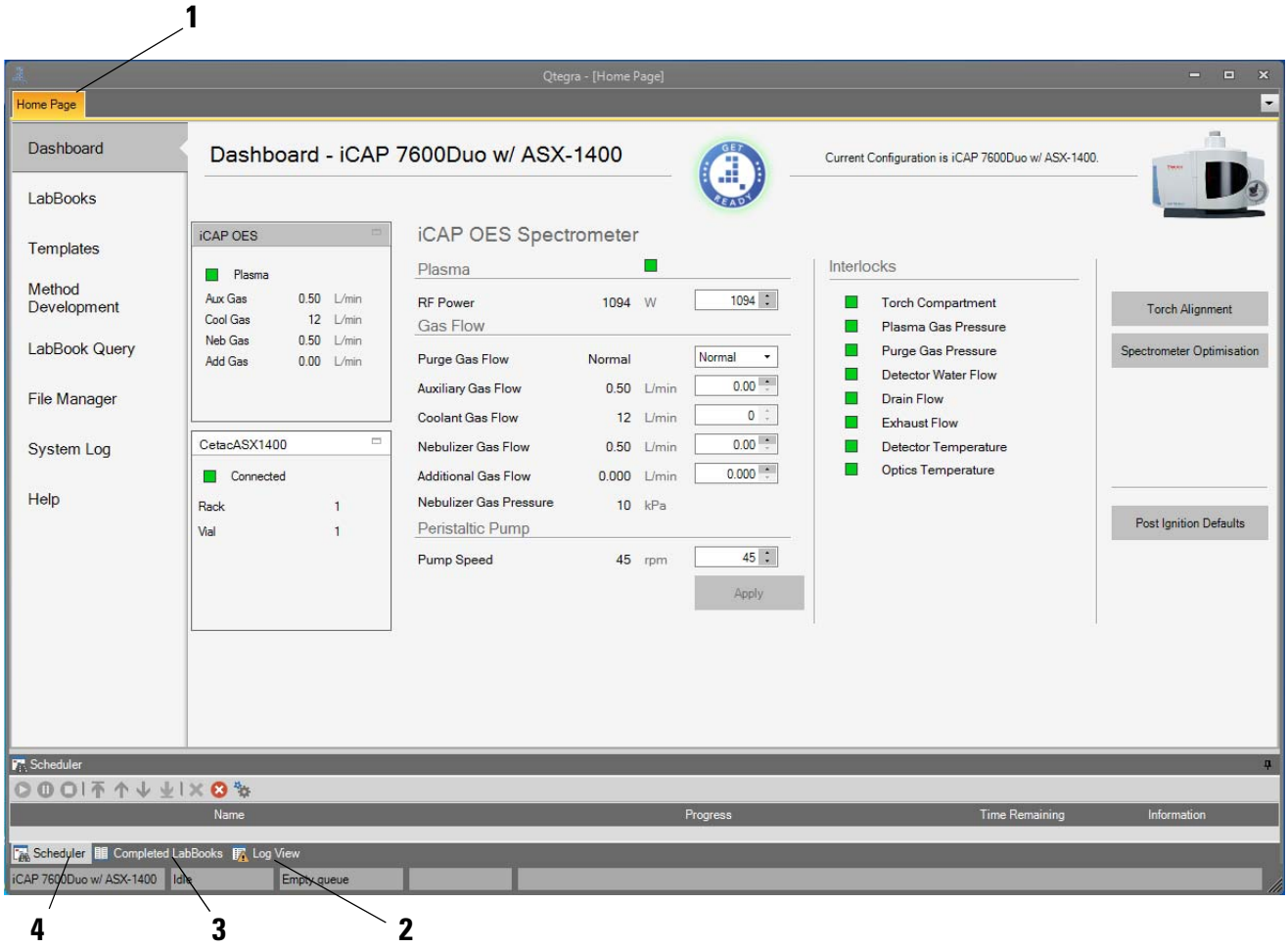
Contents

❖ To open the Qtegra tool

1. Double-click the icon on your desktop to open **Qtegra**.

User Interface of the Qtegra Tool

The user interface of the Qtegra tool is shown in Figure 4-1.



Labeled Components: 1=Home Page tab, 2=LogView tab, 3=Completed LabBooks tab, 4=Scheduler tab

Figure 4-1. Home Page of Qtegra

The **Home Page** (**1** in Figure 4-1) by default shows the Dashboard page. It gives access to all pages of the Qtegra tool for the creation and management of Template and LabBook files, for measurement, result analysis, and to the Help Page.

The **Log View** tab (**2** in Figure 4-1) shows system messages, warnings and errors of the iCAP 7000 Plus Series ICP-OES instrument.

The **Completed LabBooks** tab (**3** in Figure 4-1) lists the LabBooks previously run.

The **Scheduler** tab (**4** in Figure 4-1) lists all LabBooks assigned to be run.

❖ **To move the Scheduler, Log View or Completed LabBooks**

1. On the **Qtegra - [Home Page]**, right-click the **Scheduler, Log View** or **Completed LabBooks** title bar or tab.
   The shortcut menu opens, see Figure 4-2.

Figure 4-2. Shortcut menu of title bar

2. Select **Floating** to show the selected tab in a separate window. Move the window or resize as required.
3. Make sure **Auto Hide** is deselected.

   Tip You can click **Auto Hide** in the top right corner of a tab area to hide the selected tab when the cursor leaves this area and click to cancel.

4. Click and drag the title bar of **Scheduler, Log View** or **Completed LabBooks**.
5. Move the cursor over the position indicators, see Figure 4-3.

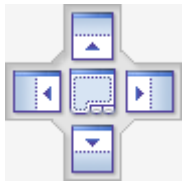


Figure 4-3. Position indicator to move tab

The selected tab is shown in the background, and the new position of the tab is indicated as colored, see Figure 4-4.

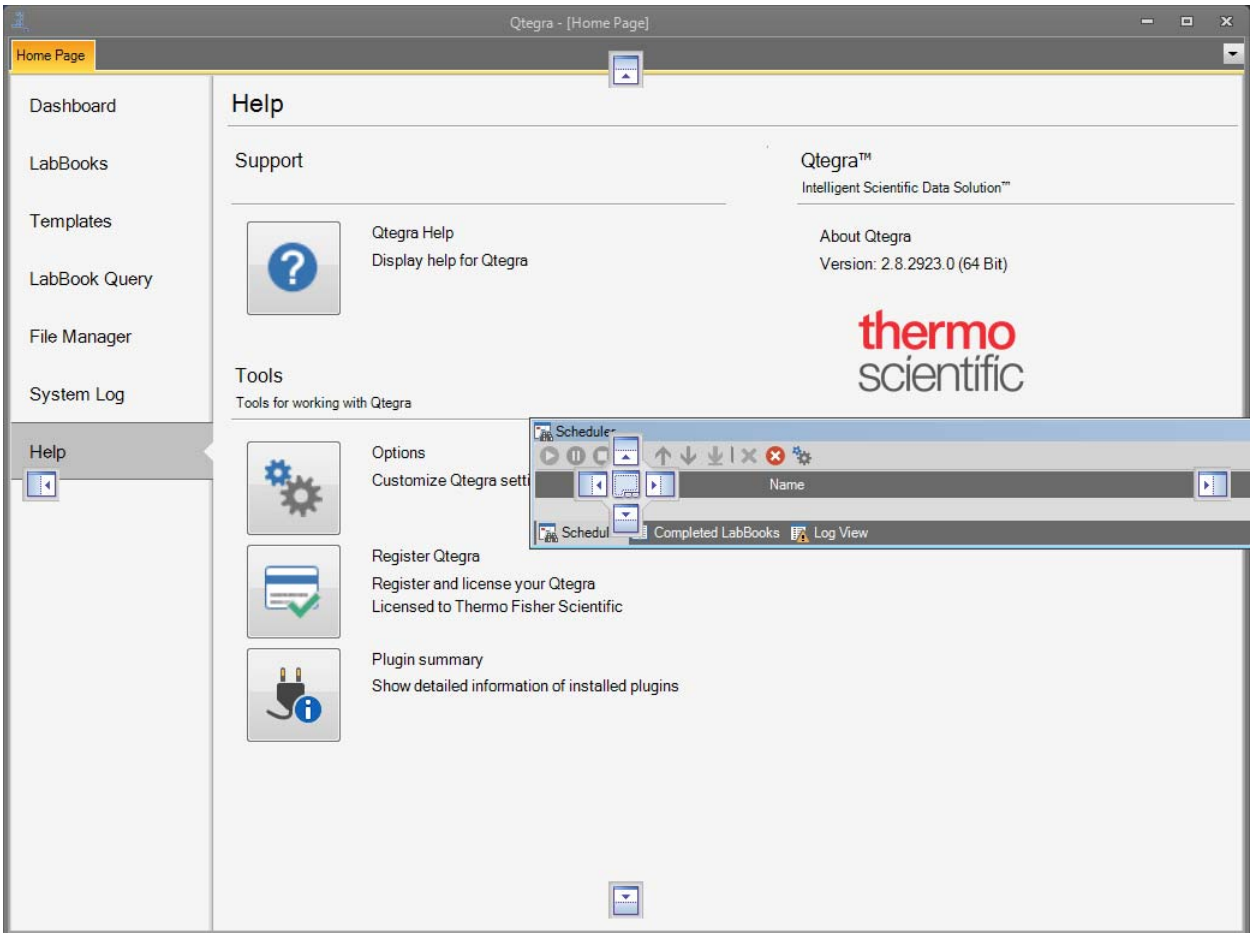


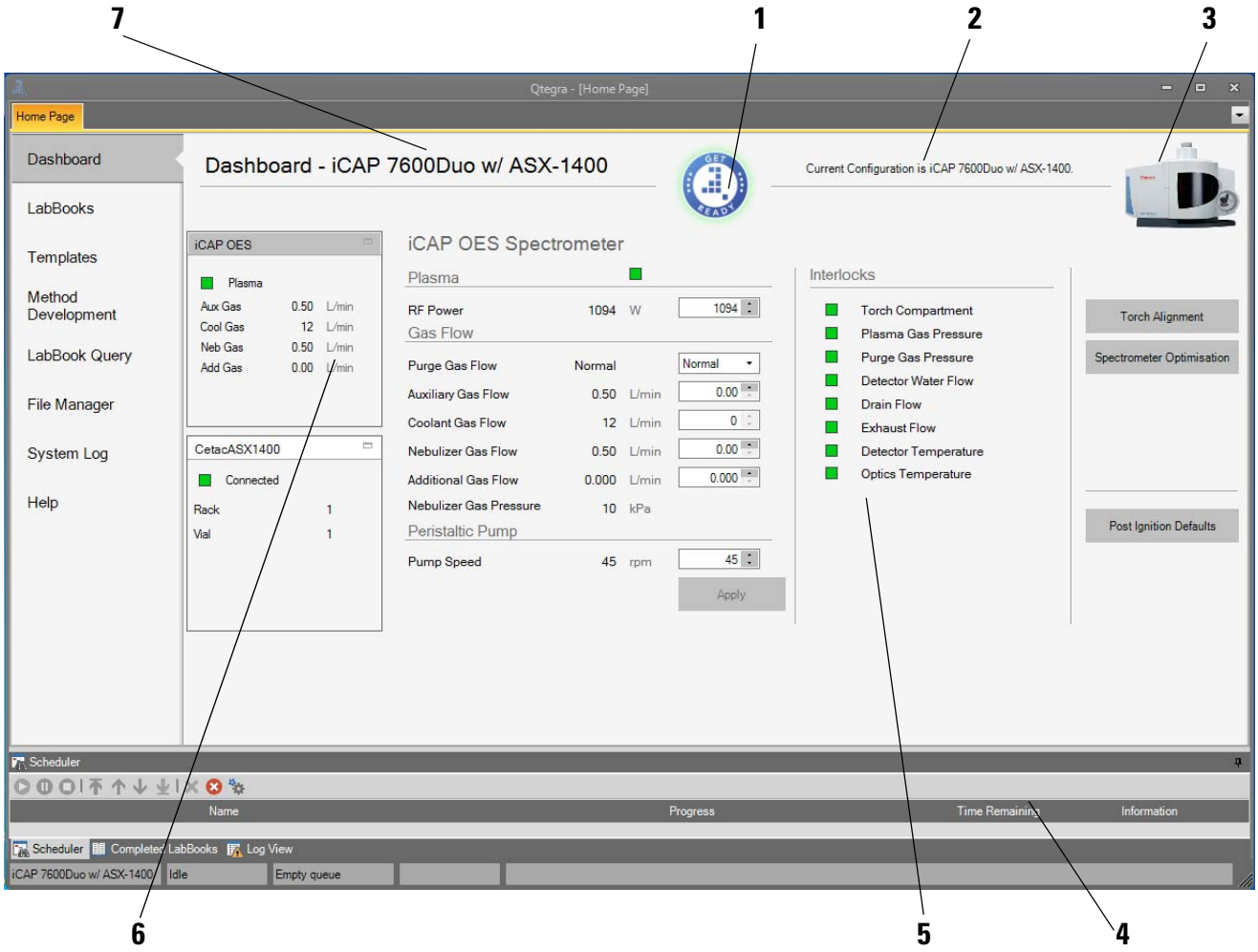
Figure 4-4. Moving the Scheduler tab

6. Drop the selected tab where you wish to place it.

Dashboard Page

The Home Page opens with the **Dashboard** page by default when you start the Qtegra tool.

The **Dashboard** page of Qtegra offers several functions to prepare the iCAP 7000 Plus Series ICP-OES system for measurement, close down the system or change the Configuration, and shows on one page the instrument controls and main settings of the iCAP 7000 Plus Series ICP-OES instrument, see Figure 4-5.



Labeled Components: 1=Get Ready button, 2=current Configuration status, 3=iCAP 7000 Plus Series ICP-OES thumbnail to change Configuration, 4=function buttons and check box for organic matrix (not shown), 5=important parameters of the iCAP 7000 Plus Series ICP-OES system, 6=instrument selector (peripheral selector), 7=current Configuration

Figure 4-5. Dashboard Page of Qtegra

The **Get Ready** button (**1** in Figure 4-5) gives access to the **Get Ready** procedure ("Getting Ready" on page 4-6). It also switches on and off the plasma to start and stop your iCAP 7000 Plus Series ICP-OES instrument.

Next to the **Get Ready** button, the action currently taken and the status of the current Configuration are displayed (**2** in Figure 4-5).

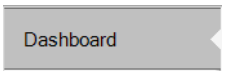
The iCAP 7000 Plus Series ICP-OES thumbnail (**3** in Figure 4-5) opens the **Select Configuration** dialog ("Changing the Configuration" on page 4-18). Here you can change the Configuration according to your system setup.

With the buttons at the right side (**4** in Figure 4-5) below the iCAP 7000 Plus Series ICP-OES thumbnail, the torch can be aligned, and spectrometer optimization and post ignition defaults can be set. When carrying out a torch alignment with organic samples, the check box on the right side should be selected.

The main part (**5** in Figure 4-5) of the Dashboard page presents an overview of all main settings of the iCAP 7000 Plus Series ICP-OES instrument. The parameters for the iCAP OES Spectrometer can be changed here and are set with the **Apply** button.

On top of the Dashboard page, the currently loaded Configuration (**7** in Figure 4-5) is displayed. Below, the progress of the Get Ready procedure is shown if activated.

❖ **To open the Dashboard page of Qtegra**



1. On the **Qtegra - [Home Page]** navigation pane, click **Dashboard**. The Dashboard page of Qtegra opens.

Getting Ready

The **Get Ready** procedure on the Dashboard page of Qtegra helps to start the instrument. It switches on the plasma and waits for the instrument to warm up. The Spectrometer Optimization is performed, followed by the performance checks if so defined.

The **Spectrometer Optimization** may be performed at any time, and is a routine, which ensures that the wavelengths are correctly located on the detector. This routine will automatically run when the plasma is ignited. During this routine, the pump will stop and the nebulizer gas will be turned off - this is because the routine uses plasma wavelength positions, so no sample is required.

Tip It is recommended that the Spectrometer Optimization is carried out prior to analysis.

The **Nebulizer Optimization** optimizes the nebulizer pressure settings for the performance tests.

Tip Standard concentric glass nebulizers are optimized for a flow of approximately 0.4 to 0.7 L/min. Ensure that gas flows in excess of 0.7 L/min are not used as this may result in sub-optimal performance. Other nebulizers may run at higher flows.

The performance checks are defined by the **Sensitivity**, **Relative Standard Deviation**, and **Detection Limit** tests.

Tip The performance checks should be run using the standard aqueous solutions kit.

Tip The performance checks should not be run using the Sprint Valve (7600 model only).

Once the Performance Report is passed, the instrument is ready for operation.

If the Performance Report fails, check for causes and run the tests again.

❖ **To prepare the iCAP 7000 Plus Series ICP-OES system for measurement**

1. On the Dashboard page, click the red **Get Ready** button. The **Get Ready** dialog opens, see Figure 4-6.

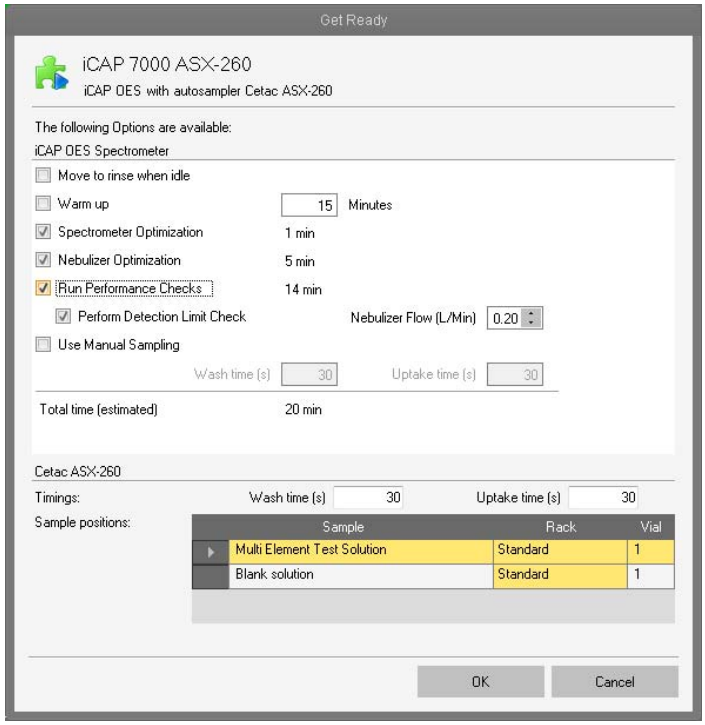


Figure 4-6. Get Ready dialog for iCAP 7000 Plus Series ICP-OES

2. **Move to rinse when idle** can be selected when using an autosampler if the probe has not been used for a while.
3. If you select **Warm up**, type the time in **Minutes**.
4. To optimize spectrometer parameters, select **Spectrometer Optimization**.
5. To optimize the nebulizer, select **Nebulizer Optimization**.

6. Select **Run Performance Checks**.

   Tip The performance check can also be run directly from the green **Get Ready** button, that is, without closing down the system first, see "Repeating Get Ready" on page 4-14.

7. If you select **Perform Detection Limit Check**, enter **Nebulizer Flow (L/Min)**.

8. If you run the tests using an autosampler, enter **Wash time (s)** and **Uptake time (s).** Set the **Rack** and **Vial** position for **Multi Element Test Solution** and **Blank solution** to define the **Sample positions**.

9. With **Manual Sampling**, type the **Wash time (s)** and the **Uptake time (s)**.
   The default for both of *30* s is usually sufficient.

   As good laboratory practice needs validated tests this item always is checked when you open this dialog.

10. If an autosampler is configured, for **Sample positions** in the lower extension of Figure 4-6, select the desired vials from the table to specify the sample positions for **Multi Element Test Solution** and **Blank solution**.

    From the **Position Kind** drop-down list, select *Vial* to move the probe to the rack and vial specified in the next columns. Select *Home* to move the probe to its home position. Select *Rinse* to move the probe into the rinse position where the probe is washed and moved up to rinse as often as set in the hardware.

    From the **Rack** drop-down list, select the desired rack number, where the vial is placed.

    Type the **Vial** number for each sample.

11. Click **OK**.
    The plasma is switched on. During warm-up the Dashboard shows the remaining warm-up time, see Figure 4-7.

Figure 4-7. Dashboard during warm-up

The **Get Ready** button shortly shows yellow until the state changes to ready while the plasma is switched on. When the warm-up starts the button is already green. After warm-up, the Spectrometer Optimization starts.
You can click **Skip** to skip the warm-up.

12. If you wish to stop the procedure, click **Stop**.

The **Spectrometer Optimization** is performed and if passed, the **Sensitivity** test starts, see Figure 4-8.

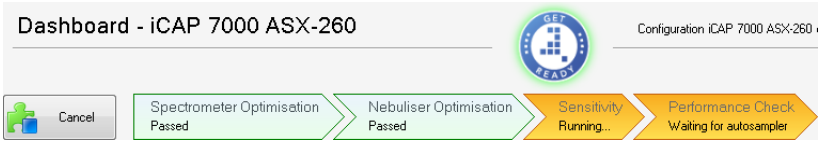


Figure 4-8. Dashboard starting the performance checks

With manual sampling, after the stabilization process, a dialog opens, see Figure 4-9.

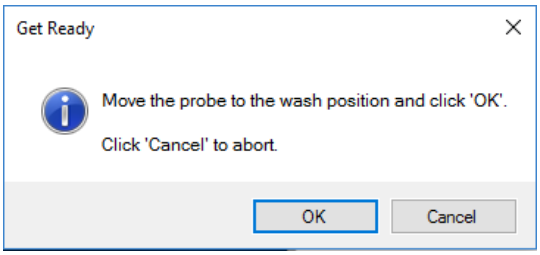


Figure 4-9. Waiting For Response dialog for wash position

13. Move the sample probe to the wash position and click **OK**.

    The washing starts. After washing, a dialog opens, see Figure 4-10.

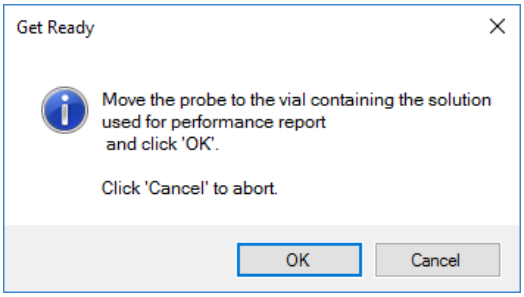


Figure 4-10. Waiting For Response dialog for standard solution

14. With manual sampling, aspirate your solutions according to the test and click **OK**.
    When using an autosampler, this is automatically performed.

    The sample uptake starts, followed by the performance test.

    The Performance Check is followed by the **Relative Standard Deviation** test and the **Detection Limit**.

    The procedure finishes and the display changes accordingly.

    As the entire Get Ready procedure (all options are activated in the Get Ready dialog) performs many steps, for example, the Warm up procedure, the Spectrometer Optimization, the Nebulizer

Optimization, and Performance Checks, then not all steps can be shown in the Dashboard. Instead, a horizontal slider is added below the Get Ready procedure icons to scroll through all steps.

The display shows **Failed** for tests that have not been passed successfully, see Figure 4-11.

Figure 4-11. Dashboard showing Get Ready failed

15. Click **View results** to open the Performance Report in a separate tab, see also "File Manager Page" on page 5-1 on location of Reports.

16. Click **Clear** to close Get Ready.

Additional Instrument Settings

On the Dashboard page of Qtegra, **Torch Alignment** and **Post Ignition Defaults** can be defined, and a button for **Spectrometer Optimization** is provided, see Figure 4-12.

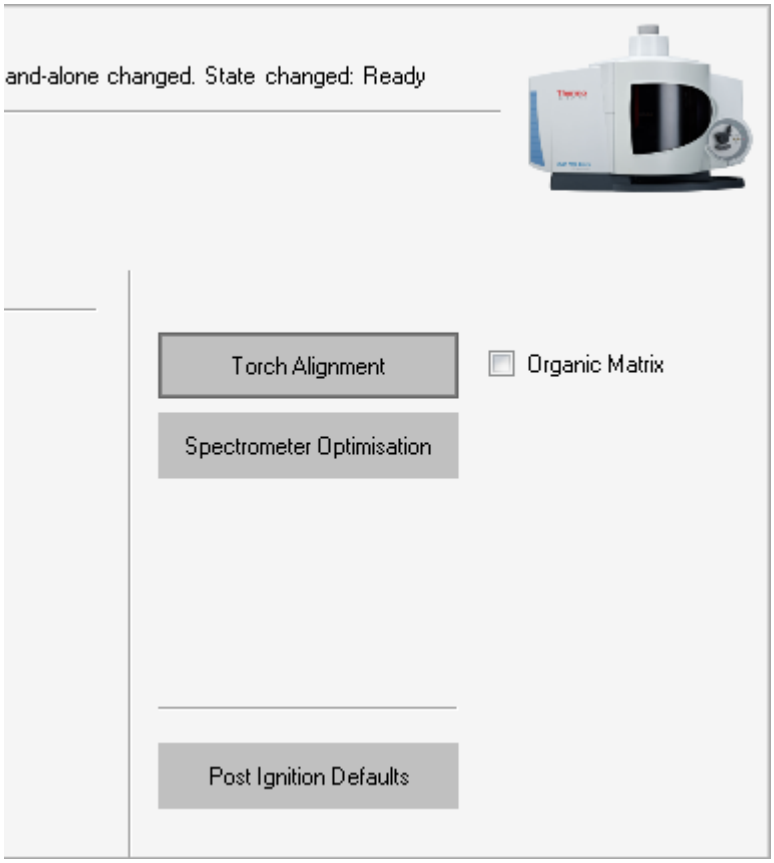


Figure 4-12. Additional function buttons on the Dashboard page

For maximum sensitivity and optimum results the alignment of the plasma image is critical. Whenever a torch has been removed or replaced in the instrument, or if the torch body or center tube has been replaced, a torch alignment procedure should be carried out.

The 2 ppm Zinc solution for **Torch Alignment** should be made up with either an aqueous or an organic matrix as required. The organic matrix is ideally kerosene.

Post Ignition Defaults can be set in order to immediately change start-up settings, all at the same time.

Spectrometer Optimization is a routine, which ensures that the wavelengths are correctly located on the detector. See also "Getting Ready" on page 4-6.

❖ **To align the torch of your iCAP 7000 Plus Series ICP-OES system**

1. On the Dashboard page, click **Torch Alignment**.
   The Waiting for user response dialog opens, see Figure 4-13.

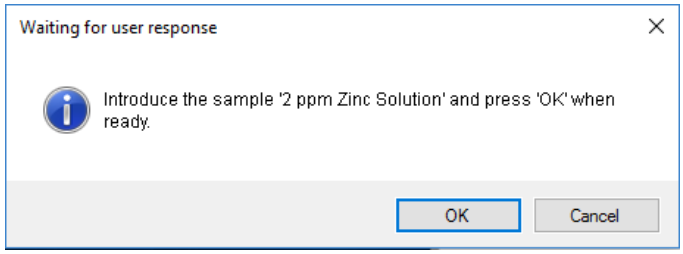


Figure 4-13. Waiting for response dialog Torch Alignment

2. Start aspirating the 2 ppm Zinc solution for some seconds.
3. Click **OK**.
4. Aspirate until the test is finished.
   The progress of the test can be followed in the message bar at the bottom of Qtegra, see Figure 4-14.

Figure 4-14. Torch Alignment progress message example

Four Alignment steps are performed. After *Radial, slit=UV* follows *Radial, slit=Vis*, *Axial, slit=UV*, and *Axial, slit=Vis*.
The message *Torch Alignment: Passed* is shown when the test succeeded.

❖ **To set post ignition defaults of your iCAP 7000 Plus Series ICP-OES system**

1. On the Dashboard page of Qtegra, click **Post Ignition Defaults**. The Post Ignition Defaults dialog opens, see Figure 4-15.

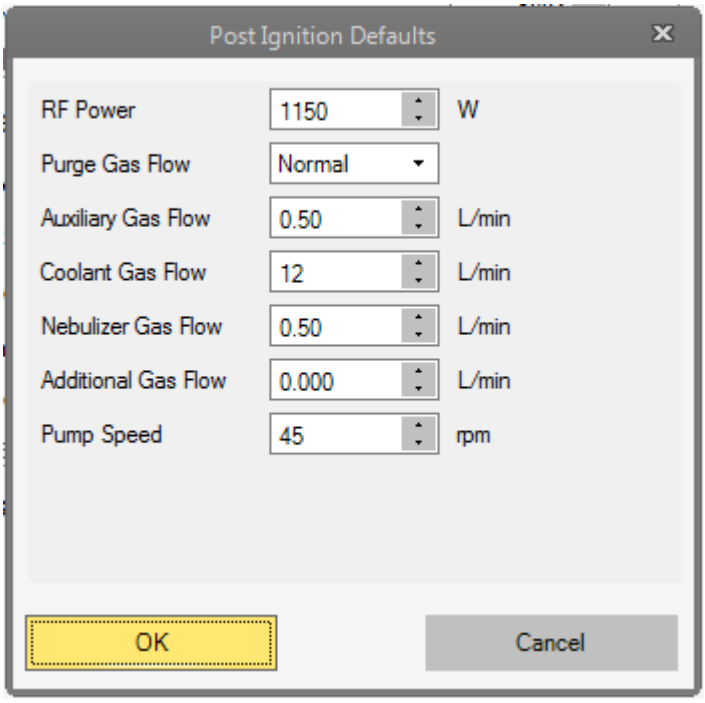


Figure 4-15. Post Ignition Defaults dialog

2. Select **RF Power** to change the value.
The default and range depend on the iCAP 7000 Plus Series ICP-OES model. For details, see "Measure Modes" on page 9-12.

3. Click the **Purge Gas Flow** edit box to select *Normal* or *High*.
The default and range depend on the iCAP 7000 Plus Series ICP-OES model.

4. Select **Auxiliary Gas Flow** to change the value.
The default and range depend on the iCAP 7000 Plus Series ICP-OES model. For details, see "Measure Modes" on page 9-12.

5. Select **Coolant Gas Flow** to change the value.
The coolant gas flow is only adjustable for iCAP 7600 instruments. For details, see "Measure Modes" on page 9-12.

6. Select **Nebulizer Gas Flow** to change the value.
The nebulizer gas is only adjustable for iCAP 7400 and iCAP 7600 instruments. For details, see "Measure Modes" on page 9-12.

7. Select **Additional Gas Flow** to change the value.
The additional gas flow is only adjustable for iCAP 7600 instruments that are fitted with a gas Mass Flow Controller. For details, see "Measure Modes" on page 9-12.

8. Select **Pump Speed** to change the value.
The default and range depend on the iCAP 7000 Plus Series ICP-OES model. For details, see Analysis Mode parameters in "Acquisition Parameters" on page 9-14.

9. Click **OK**.
These values are now applied as defaults whenever the instrument is switched on.

❖ **To optimize the spectrometer**

1. On the Dashboard page, click **Spectrometer Optimization**.
The spectrometer optimization starts. A message in the Log View shows when the process is finished.

Shutting Down the System

In your laboratory environment, the instrument remains in a ready state. Qtegra ISDS indicates this state with a green surrounded **Get Ready** button on the Dashboard page.

The iCAP 7000 Plus Series ICP-OES system can be shut down with the **Shut Down** option on the Dashboard page of Qtegra.

❖ **To close the iCAP 7000 Plus Series ICP-OES system down**

1. On the Dashboard page, click the green **Get Ready** button to display three options, see Figure 4-16.

Figure 4-16. Additional options on Get Ready button

Tip If the plasma is on, while you are opening this dialog, it is not automatically switched off.

2. Click **Shut Down**.
A message opens (see Figure 4-17) to ensure that the sample probe is removed from the analyte solution.

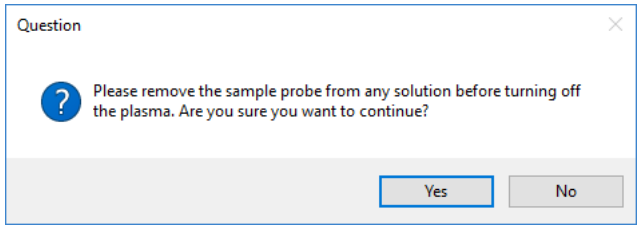


Figure 4-17. Remove probe message when shutting down the instrument

3. Remove the probe from the solution.
4. Click **Yes** to proceed with shutting down the system.
    a. If you click **Yes** (see Figure 4-17), the iCAP 7000 Plus Series ICP-OES system shuts down and the plasma switches off.
    b. Independent from any setting in the Configurator > Experiment Configurator > Peristaltic Pump Shutdown Behavior, the peristaltic pump is switched off.
    c. The instrument changes to *Not Ready*. The Get Ready icon changes to red.
    d. You may now work inside the instrument.

    -or-

    Click **No** (see Figure 4-17) if you wish to cancel the shut down process.
    a. If you click **No**, an Error message opens to inform about canceling the shut down, see Figure 4-18.

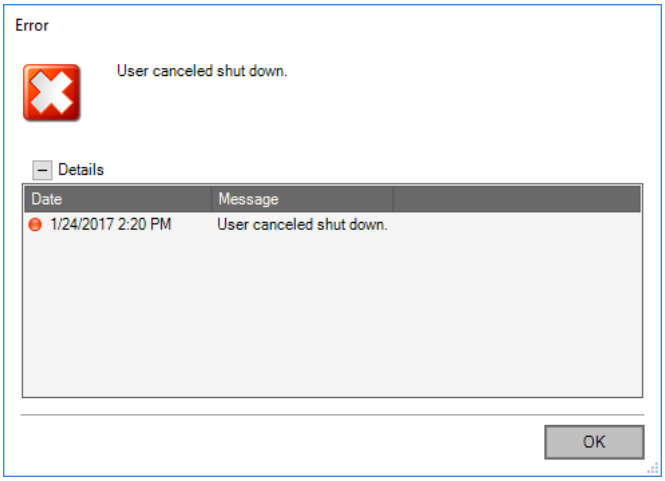


Figure 4-18. Canceling Shut Down error message

    b. Click **OK** to leave the instrument unchanged and in *Ready* state.
    c. The Get Ready button remains green.

Repeating Get Ready

The Get Ready procedure can be run for the iCAP 7000 Plus Series ICP-OES system directly with the Repeat Get Ready option from Get Ready button on the Dashboard page of Qtegra.

❖ **To repeat Get Ready directly from the Get Ready button**

1. On the Dashboard page, click the green **Get Ready** button to display three options, see Figure 4-16.

2. To set desired start parameters, click **Repeat Get Ready**. The Get Ready dialog opens with the settings last selected, see Figure 4-6.

   a. Set all parameters according to your needs. For details, see "Getting Ready" on page 4-6.

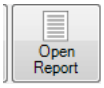
   b. Click **OK** to set the instrument into the Get Ready state.

Opening a Report

A performance Report for the iCAP 7000 Plus Series ICP-OES system can be accessed directly with the Show Report function on the Dashboard page of Qtegra.

❖ **To open a Performance Report directly from the Get Ready button**

1. On the Dashboard page, click the green **Get Ready** button to display three options, see Figure 4-16.



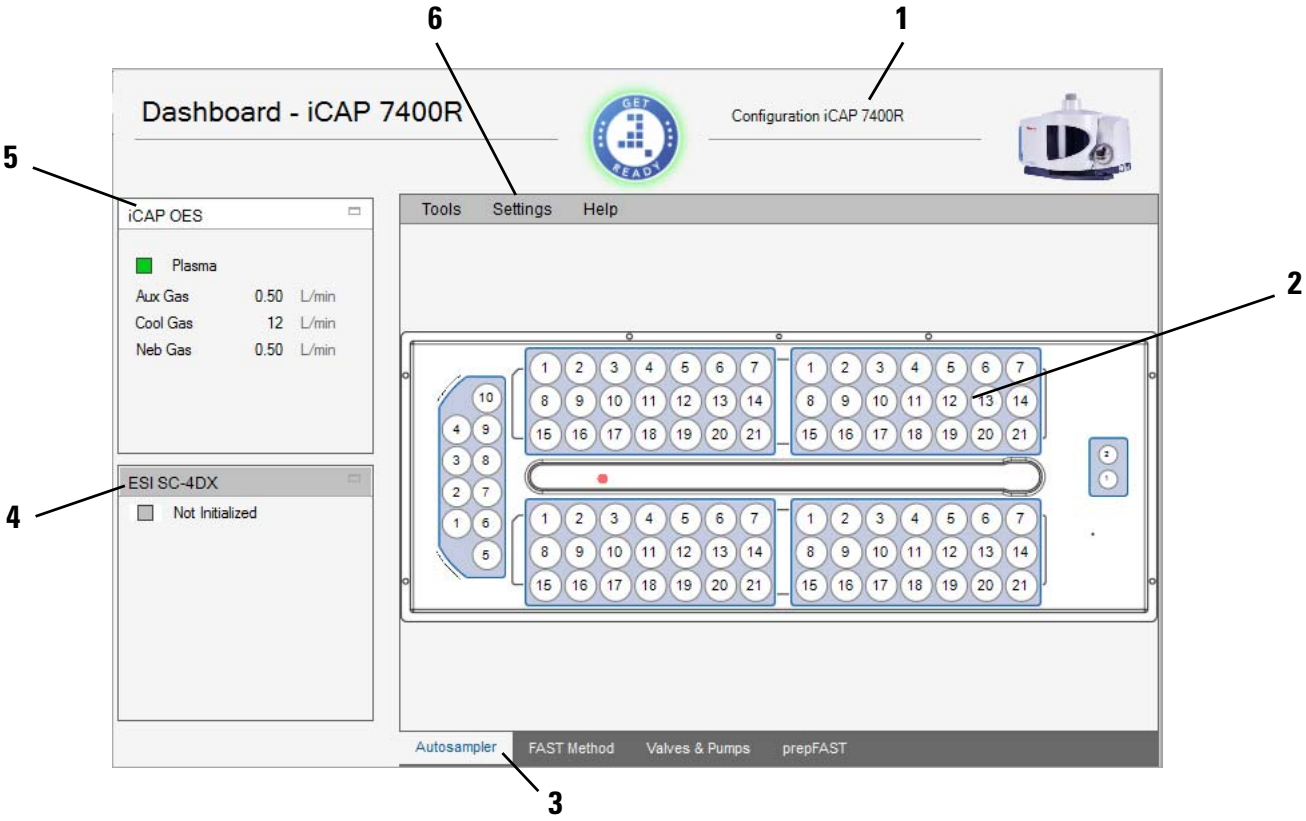
2. To navigate to the Reports folder, click **Open Report**.

   Qtegra shows the **File Manager** page and opens the tree to select the desired Report. You will see three subfolders **PerformanceReport**, **AutotuneReport** and **DetectorSetup**.

   Select a subfolder and open the desired Report. For working with the File Manager page, see "File Manager Page" on page 4-51.

Peripheral Settings on the Dashboard

The Dashboard shows the hardware configuration as loaded. Select the instrument or the peripheral to display a symbolic view of the settings, see Figure 4-19.



Labeled Components: 1=Configuration loaded, 2=data view region of instrument/peripheral, 3=tabs for specific settings of peripheral, 4=peripheral selector, 5=instrument selector, 6=data view menu

Figure 4-19. ESI autosampler on Dashboard

❖ **To open the peripheral settings page**

1. Open the **Dashboard** page of Qtegra.
2. Depending on your Configuration, a peripheral is shown below the instrument iCAP OES. Click the peripheral, for example, ESI SC-4DX (**4** in Figure 4-19) to display its setting.
3. On the lower part, find additional tabs (**3** in Figure 4-19) to change the data view of the autosampler ESI SC-4DX.
4. Select **Tools** > **Initialize** (**6** in Figure 4-19) to start the communication with the autosampler.
   Select **Calibrate** to start the calibration wizard.
5. Select **Settings** > **Racks** to define the tray layout and to specify the autotune position.
   Select **Settings** > **Rinse** to define the wash, pump and flush

parameters.
Select **Settings > Motors** to set the horizontal, rotational and vertical speed and accelerator parameters, see Figure 4-20.

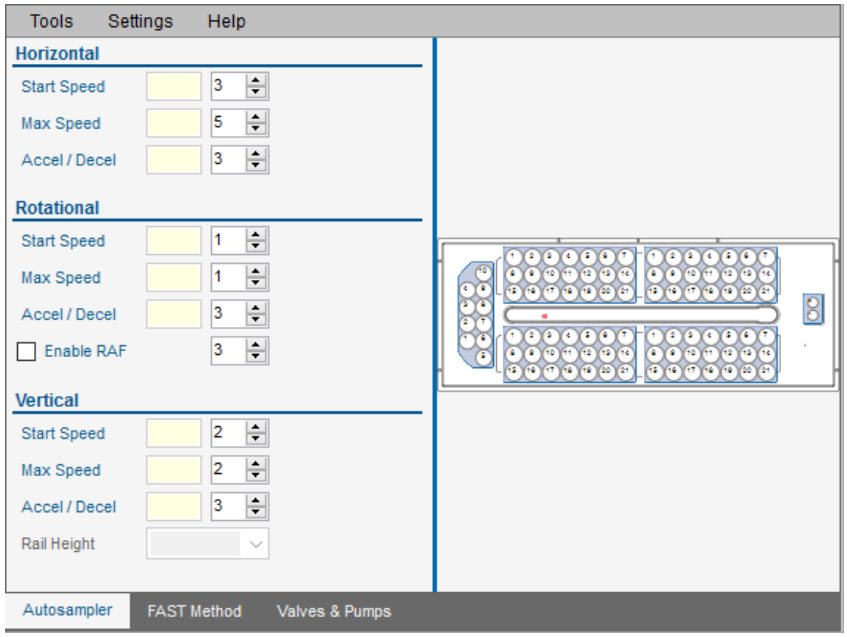


Figure 4-20. Motors setting of the ESI autosampler data view

6. Select the **Valves & Pumps** tab (**3** in Figure 4-19) to switch the FAST Pump on or off.

7. Select the **FAST Method** tab (**3** in Figure 4-19) to display the initial view, see Figure 14-32.

8. From the **User Methods** list box, select the desired method,
-or-
Click the browse buttons to select the method from the **File Open** dialog.

The FAST method is displayed under a new tab close to the initial + tab, see Figure 4-21.

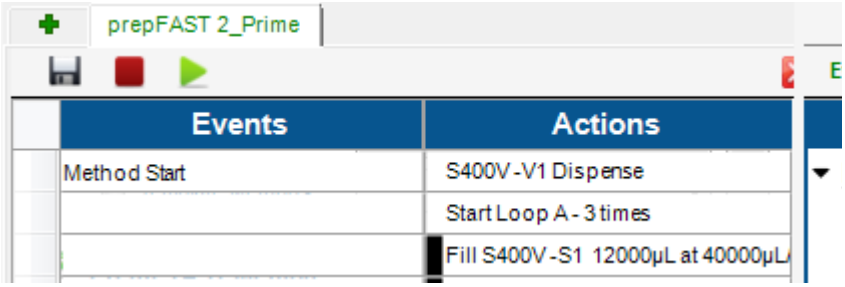


Figure 4-21. ESI FAST: Method tab showing Events and Actions

Tip See "Autodilution Using the ESI prepFAST II Method" on page 14-24 for details on how to create a prepFAST configuration and a prepFAST template.

Tip Refer to the Installation Manual of your peripheral.

Changing the Configuration

It is frequently necessary to change the Configuration of the iCAP 7000 Plus Series ICP-OES instrument.

With the **Change Configuration** function on the **Dashboard** page of Qtegra you can easily change the Configuration.

❖ **To change the Configuration**

1. On the Dashboard page, click **Change Configuration**.
   The **Select Configuration** dialog opens.

2. Select the Configuration you wish to load, see Figure 4-22.

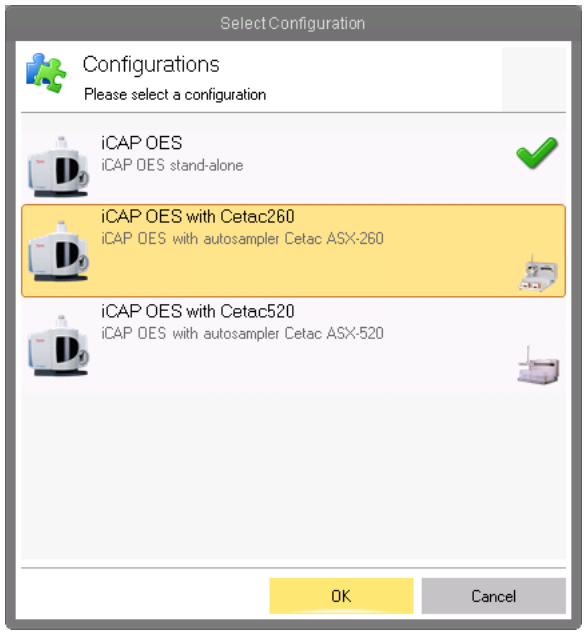


Figure 4-22. Select Configuration window

3. Click **OK**.
The selected Configuration is loaded and shown in the header of the Dashboard page.

Checking the System Status

Before starting a measurement, the system status should be checked on the Dashboard of Qtegra.

❖ **To check the system status**

1. On the Dashboard page, check the values and indicators of each subsystem, see Figure 4-23.

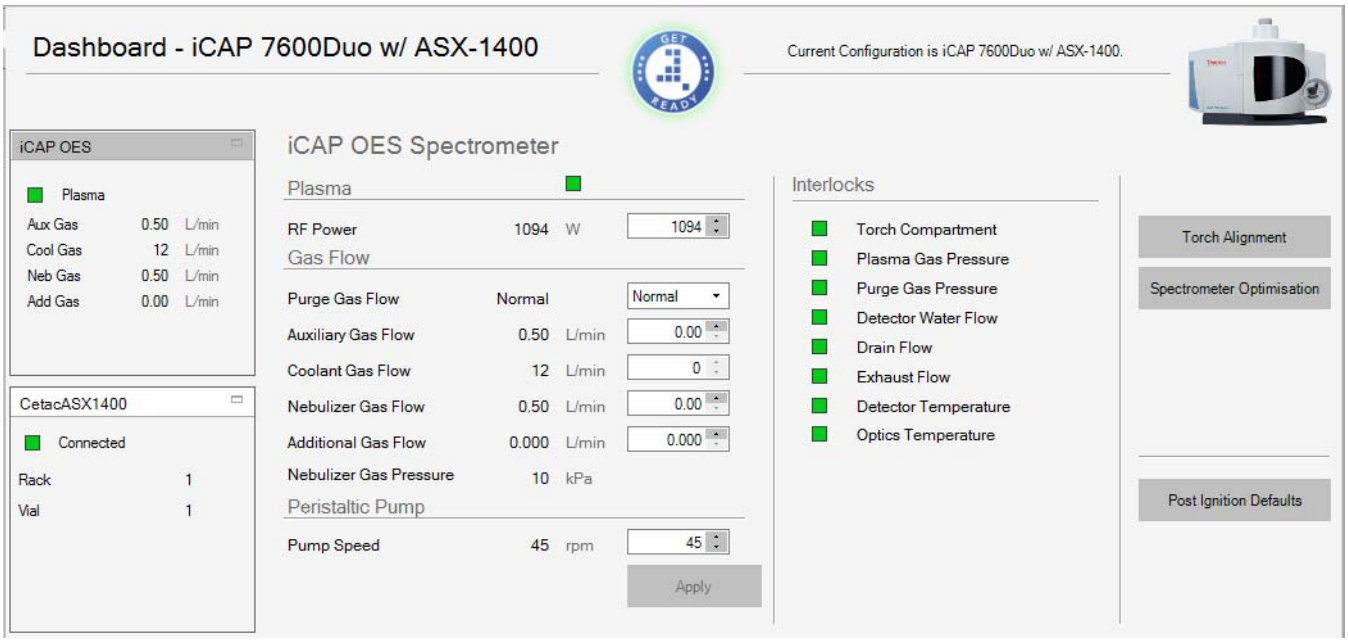


Figure 4-23. System Statuses on Dashboard

A green Get Ready indicator signals the system is ready for operation.

Adjusting System Parameters

The system parameters can be adjusted on the **Dashboard** page of Qtegra.

❖ **To adjust the system parameters**

1. On the Dashboard page, enter new values for an **iCAP OES Spectrometer** parameter, for example, *Pump Speed*, see Figure 4-24.

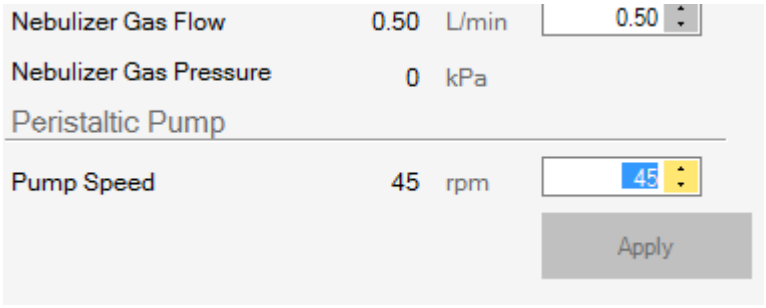


Figure 4-24. Adjusting system value on the Dashboard

2. Click inside any other edit box.
   The **Apply** button becomes available, see Figure 4-25.

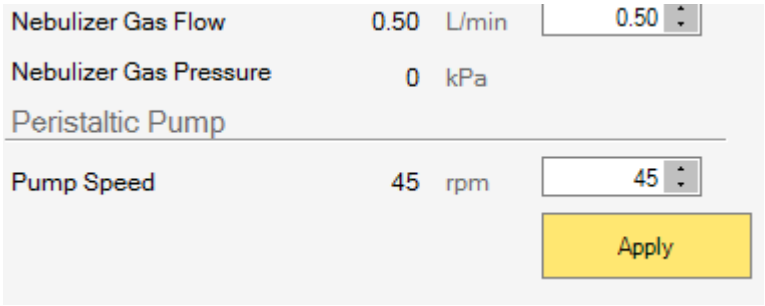


Figure 4-25. Applying values on Dashboard

3. Click **Apply**.
   The values are applied immediately.

LabBooks Page

On the **LabBooks** page of Qtegra, see Figure 4-26, LabBooks are created and opened.

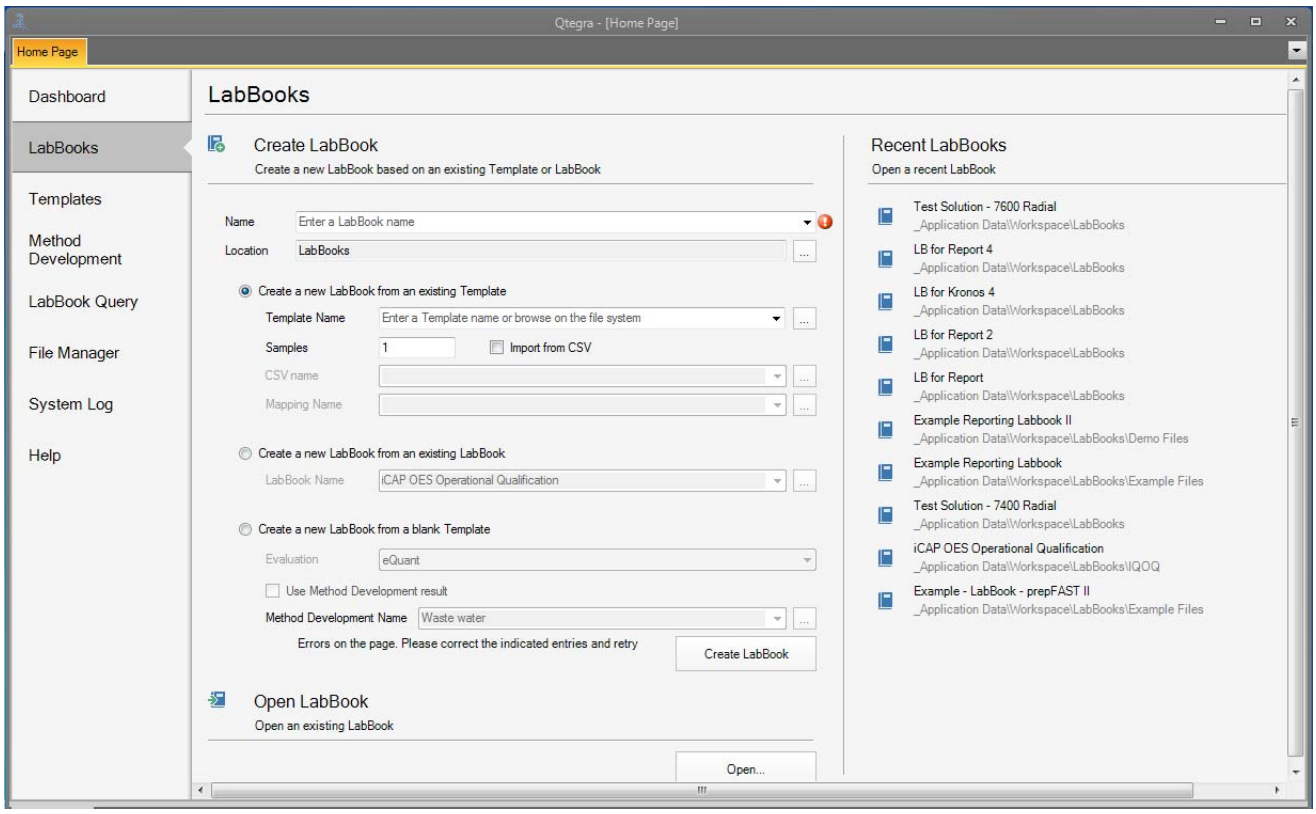


Figure 4-26. LabBooks Page of Qtegra

A LabBook that has not been scheduled includes the Method Parameters, the Sample List for the measurement, and Automatic Export settings. LabBooks created from a Template inherit the Method Parameters from the Template. The Sample List for the measurement is in this case generated from the Sample Definition of that Template.

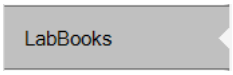
Data of analytical concentrations, raw intensities and other data formats can be defined to be automatically exported from a LabBook, either to an associated LIMS system or as Report documentation.

Once a LabBook is running, an Evaluation Results view allows you to see the results in real time. Upon completion of a scheduled LabBook, all raw intensities and concentrations are stored within the LabBook.

Additionally, for LabBooks that have finished acquiring data and have exited the Scheduler, there are Reports, Log Messages, Query and Signing views. See "LabBooks" on page 6-1 for details on LabBooks.

Tip Any values entered that are not within the given range are marked with an exclamation mark.

❖ **To open the LabBooks page of Qtegra**



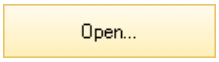
1. On the **Qtegra - [Home Page]** navigation pane, click **LabBooks**.
   The LabBooks page of Qtegra opens.

Opening a LabBook

LabBooks are opened either from the LabBooks page of Qtegra, which is described here, or from the File Manager page, see "File Manager Page" on page 4-51.

❖ **To open a LabBook in Qtegra**

1. Open the LabBooks page of Qtegra.



2. Below , click **Open**.

   The **Browse for LabBook** window opens, see Figure 4-27.

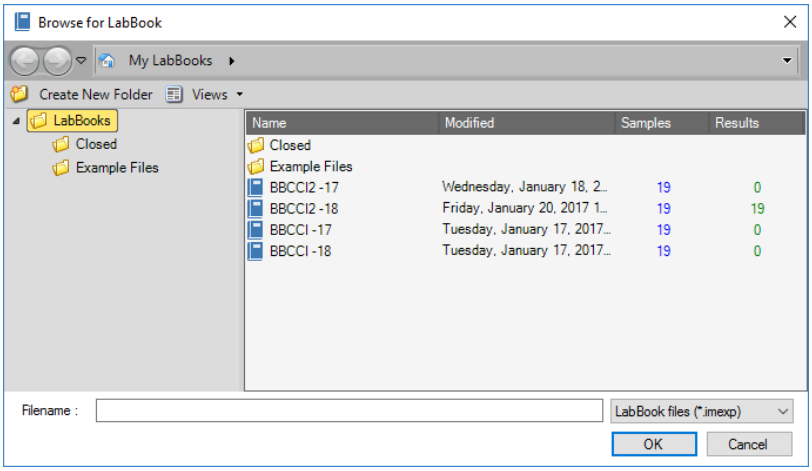


Figure 4-27. Browse for LabBook window

3. Select a LabBook.

4. Click **OK** to open the LabBook.
   The LabBook opens in a new tab in the Qtegra tool.

❖ **To open a Recent LabBook**

1. On the LabBooks page, click a LabBook in the **Recent LabBooks** section, see Figure 4-28.

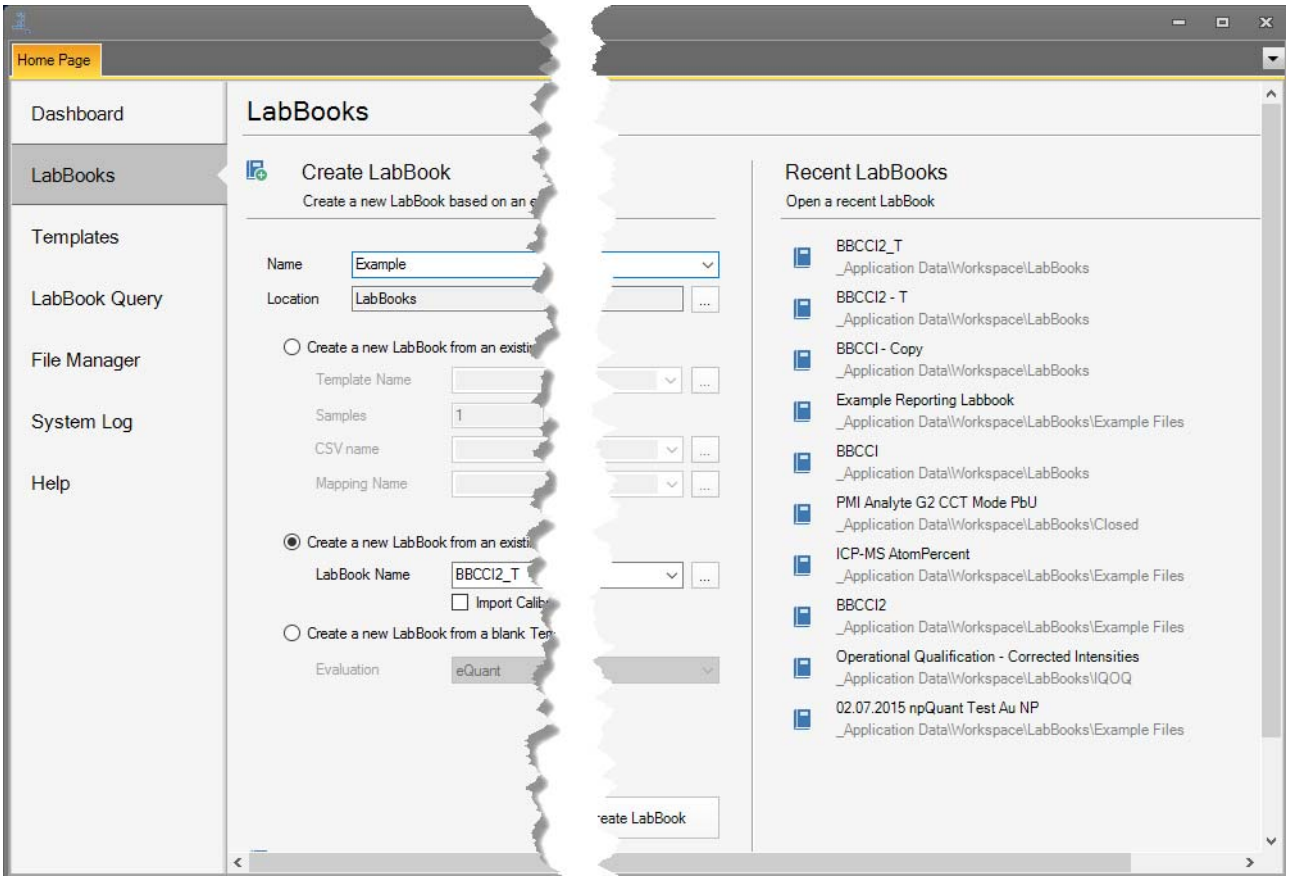


Figure 4-28. Recent LabBooks

The selected LabBook opens in a separate tab.

Creating LabBooks

Selecting the Desired Configuration

Every measurement is controlled by a LabBook. This means that you must create LabBooks as often as you run an experiment. To optimize this creation process, a LabBook is created by use of existing data and defined actions. A Template consists of three sections that describe **Initial Actions**, **Continuing Actions** and **End Actions**. See "Defining QC Settings in Sample Definition (eQuant only)" on page 9-43 for details. Every LabBook is based on a Template that provides the experiment structure and individual sample data that define your experiment.

As Qtegra User, make sure to create a LabBook that uses the desired Configuration.

❖ **To create a pre-configured LabBook**

1. On the Dashboard page, click the thumbnail of your instrument in the top right corner.
   The **Select Configuration** window opens.
2. From the Configurations list, double-click the desired item to load this Configuration. The headline changes to “Dashboard - <Name of Configuration>”.

LabBooks are created from blank Templates, existing Templates or from existing LabBooks on the LabBooks page of Qtegra.

There are 2 ways of filling the Template with sample data:

- Type the amount of samples.

  -or-

- Import samples from a CSV file, for example, from a LIMS system.

After loading your specified number of samples into your LabBook you must enter additional data for all these samples, i.e., the columns of the Sample List are actually left blank. You need to add the *Label*, the position inside the autosampler (*Rack*, *Vial*), the *Amount* and *Dilution*. As your LabBook may contain a large number of samples, you can use a CSV file and a CSV Import (page 4-25) to directly import all these sample data into your LabBook. See the following steps when using the import method.

CSV Import

If you find sample definition headers, for example, used in your LIMS system, that do not match with the Sample List headers used in Qtegra, an Administrator can create a file providing the CSV structure. The CSV structure is controlled by a mapping file that can be edited with a standard text editor. Save this file in UTF-8 encoding with “.xml” as file extension under
`C:\ProgramData\Thermo\Qtegra\_Application Data\SampleLists\TranslationTable`.

For a typical mapping file, see left-hand image in Figure 4-29.

```
<TranslationTable>
    <Delimiter>;</Delimiter>
    <Item>
        <Name>Label</Name>
        <Translation>Label</Translation>
    </Item>
    <Item>
        <Name>Amount</Name>
        <Translation>Amount</Translation>
    </Item>
    <Item>
        <Name>Qty</Name>
        <Translation>Final Quantity</Translation>
    </Item>
    <Item>
        <Name>Factor</Name>
        <Translation>Dilution Factor</Translation
    </Item>
    <Item>
        <Name>Vial</Name>
        <Translation>Vial</Translation>
    </Item>
```

```
<TranslationTable>
  <Delimiter>;</Delimiter>
  <Item>
    <Name>Label</Name>
    <Translation>Label</Translation>
  </Item>
  <Item>
    <Name>Repeats</Name>
    <Translation>R&#233;p&#233;titions</Tra
  </Item>
  <Item>
    <Name>S_Type</Name>
    <Translation>Type d'Echantillon</Transl
  </Item>
  <Item>
    <Name>Standard</Name>
    <Translation>Etalon</Translation>
  </Item>
```

Figure 4-29. Example of XML mapping file for use of CSV import; right-hand image shows use of special characters

The mapping file corresponds to an Excel sheet that contains the item name as header in the first row. All recurring <Item> tags must apply to the number of columns in your Excel sheet.

For example, <Name>*Name*</Name> from the LIMS is translated to <Translation>*Label*</Translation> for Qtegra.

Tip Ensure that you use the exact column header as used in Qtegra. For example, Qtegra recognizes *ml* for milliliter and not *mL*.

A typical translation of LIMS import is shown in Table 4-1.

Table 4-1. Example of LIMS import

Qtegra Sample List <Translation>	What the LIMS supplies <Name>
Label	Name
Dilution factor	DF
Amount	Sample Weight
Final Quantity	Final Volume
Rack Number	AS Rack
Vial Numbers	Vial

Tip The use of special characters, such as "é" is not supported by the XML standard. To be able to enter special characters in the XML mapping the appropriate numeric reference must be used. To use a numeric character reference, enter an ampersand "&" followed by the pound sign "#", the decimal code number and a semicolon, for example, "é" will generate "é" (see right-hand image in Figure 4-29).

For details on using the character reference, refer to https://en.wikipedia.org/wiki/Numeric_character_reference.

❖ To import LabBook data from CSV

1. Save your Excel file with the sample data as "CSV (comma delimited)" to create the CSV file for the import of sample data into your LabBook. Check the delimiter in the CSV file and adapt the <Delimiter> entry inside the mapping file if necessary.

	A	B	C	D	E	F
1	Label	Amount	Qty	Factor	Vial	Rack
2	S-1	3	50	1	1	1
3	S-2	3	50	1	2	1
4	S-3	3	50	1	3	1
5	S-4	3	50	1	4	1
6	S-5	3	50	1	5	1
7	S-6	3	50	1	6	1
8	S-7	3	50	1	7	1
9	S-8	3	50	1	8	1
10	S-9	3	50	1	9	1

```
Label;Amount;Qty;Factor;Vial;Rack
S-1;3;50;1;1;1
S-2;3;50;1;2;1
S-3;3;50;1;3;1
S-4;3;50;1;4;1
S-5;3;50;1;5;1
S-6;3;50;1;6;1
S-7;3;50;1;7;1
S-8;3;50;1;8;1
S-9;3;50;1;9;1
```

Figure 4-30. Excel file and corresponding CSV file with sample data

Leave the samples file on a network drive, a shared folder, or a local drive before continuing.

2. Open the LabBooks page, type a name for your LabBook and select a **Location**.

Tip The name must be unique, otherwise Qtegra displays a red exclamation mark and the creation process is interrupted.

3. From the Template Name list, select the desired Template.
4. Check **Import from CSV** to enable the following list boxes.
5. Click **[...]** to search for your CSV file. Next time you may only select the CSV file from the list.
6. Click **[...]** to search for your mapping file with ".xml" extension. Next time you may only select the XML file from the list.
7. Click **Create LabBook** to generate the LabBook table with all specified contents. Qtegra switches to display the Sample List, see Figure 4-31.

	Label	Status	Rack	Vial	Survey Ru
1	S-1		1	1	
2	S-2		1	2	
3	S-3		1	3	
4	S-4		1	4	
5	S-5		1	5	
6	S-6		1	6	
7	S-7		1	7	
8	S-8		1	8	

Figure 4-31. Sample List filled with sample data

Creating a LabBook

You can either create a LabBook from the LabBooks page or from an already opened Template.

❖ **To create a LabBook from an opened Template**

1. The Template toolbar offers a button to create a LabBook. See "Template Toolbar" on page 5-2.

❖ **To create a LabBook in Qtegra**

1. Open the LabBooks page of Qtegra. On first run, no *Recent LabBooks* is shown. Perform step 2 to step 4 to create your LabBook.

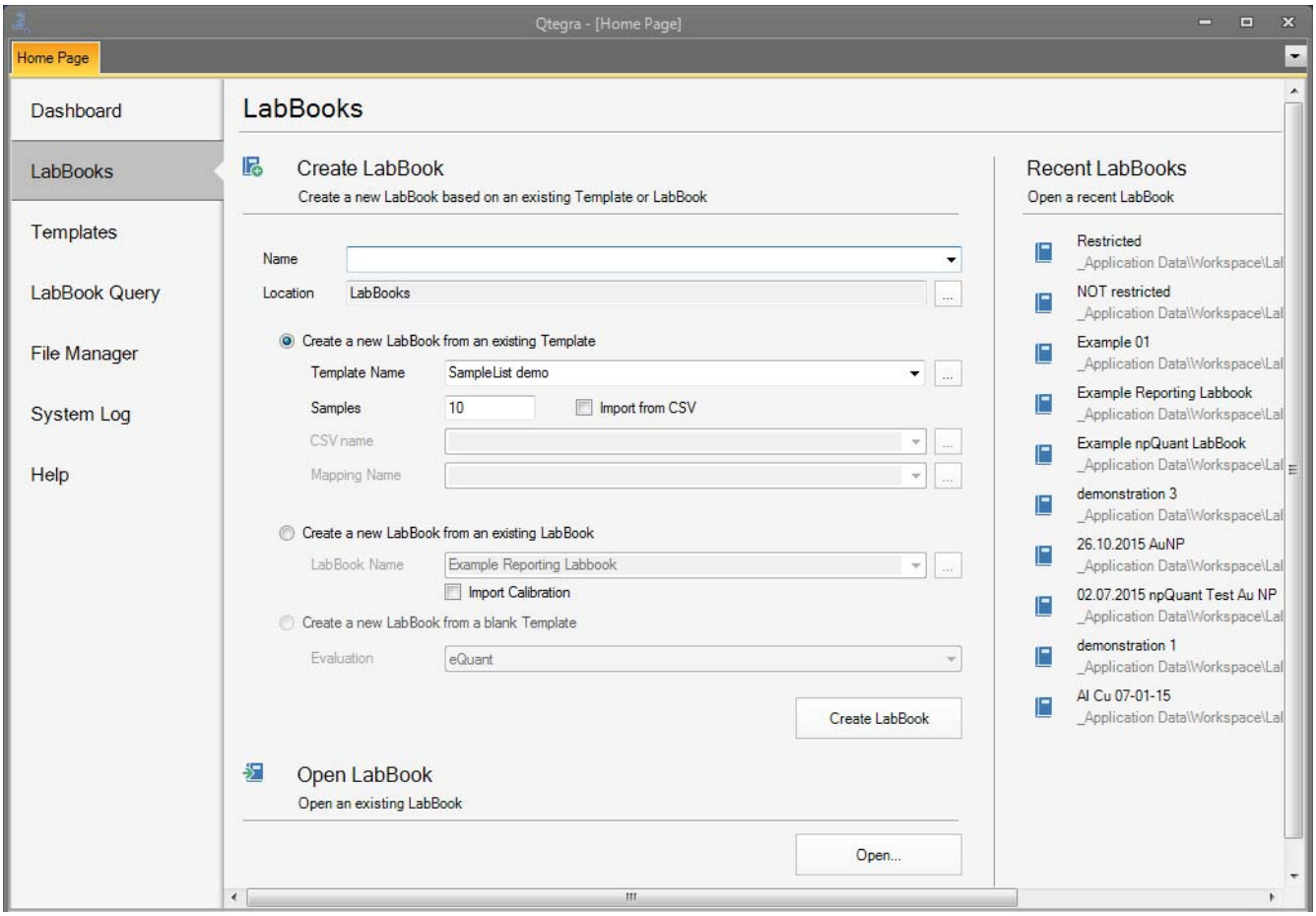


Figure 4-32. Typing the Name for a new LabBook

2. Type a **Name** for the LabBook.
3. Select a **Location** (see Figure 4-32) for your desired folder. Qtegra starts with “LabBooks” as default location. We recommend

individual folders per user, “Toms Files”, for example. See Figure 4-33.

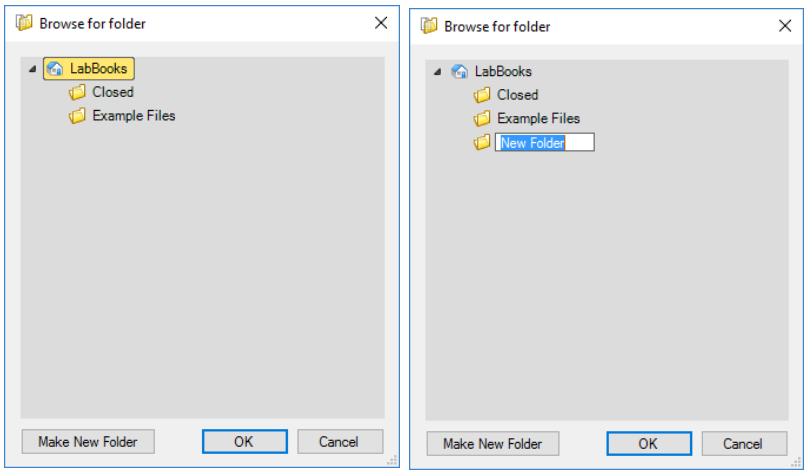


Figure 4-33. Creating new LabBooks folder

4. To create a new LabBook select one of the following options:

   a. **Create a new LabBook from an existing Template**
   Choose this option, when your LabBook shall base on a template that is shipped with this software or that was created in the past. Templates are stored on your system. This option may be used generally to compile the LabBook from an unmodified Template and a Sample List from a CSV file (see “CSV Import” on page 4-25).
   Select a **Template Name** from the drop-down list. Type a number for **Samples**. If a Sample List is available, select **Import from CSV**, and select a **CSV name** and a **Mapping Name** from the drop-down list to run the import.

   b. **Create a new LabBook from an existing LabBook**
   Choose this option, when your LabBook shall base on a formerly used LabBook that is selected from the **LabBook Name** drop-down list. All sample lines are set back to initial values. This option is used, when a measurement failed and needs to be scheduled once again.

   Tick the **Import Calibration** check box to use the calibration curves from the existing LabBook. See “Importing Calibration Data from an Existing LabBook” on page 4-32 for details.

   Alternatively, open a LabBook and copy it to create a new LabBook. See “Copying an existing LabBook” on page 4-31 for details.

   c. **Create a new LabBook from a blank Template**
   Choose this option, when you want to create a LabBook for a new analysis method without having Method Parameters (see “Method Parameters Settings” on page 9-3 for defining). You

may develop analytes, Measurement Modes and Sample Lists. Select an **Evaluation** from the drop-down list.

5. Click **Create LabBook** to display your new LabBook. During this procedure the message “Loading Workspace, please wait” is displayed.

6. On the **Content** pane, click **Sample List** to check the Sample List parameters.

   The final Sample List is defined by the number of samples selected when creating a LabBook. The Sample List in the LabBook is created from the parameters defined in “Sample Definition for a Template” on page 5-5.

7. Click **Automated Export** to define the data for export.
   See “Automatic Export - Template” on page 5-10 for details.

8. On the toolbar of the **LabBook** page, click **Save** to save your LabBook.

Copying an existing LabBook

A common method to create a LabBook uses existing LabBooks that ran already. You have the choice to exclude desired entries before creating a new LabBook. The advantage of this method is the reliability of your source LabBook that ran successfully.

❖ To copy an existing LabBook

1. Open the File Manager page of Qtegra, and select your source LabBook.
   The LabBook opens as its own tab.

2. Optionally, exclude unwanted values as follows:

   a. In the **Concentrations** table, select the concentration of elements that are unwanted to calculate the calibration curve, see Figure 4-34.

   b. To remove unwanted concentration values resulting from the last calibration, right-click to open the shortcut menu and select **Exclude entry**, see Figure 10-36.
   Point to another cell. The entry is displayed light-gray to

indicate the exclusion. The calibration curve is calculated without the excluded value.

27Al (STD) [ppb]
0.279
-0.001
5.265 (5.000)
10.426 (10.000)
20.260 (20.000)
185.325 (200.000)
N/A
22,770.647 (25,000.

27Al (STD) [ppb]
0.278
0.000
5.247 (5.000)
10.389 (10.000)
20.189 (20.000)
184.674 (200.000)
N/A
22,690.697 (25,000.

Figure 4-34. Included and excluded concentration

c. In case of accidental exclusion, click the light-gray cell and select **Include entry** from the shortcut menu.

3. **Save** the modified LabBook.
4. Finally, select **Create > New LabBook** to generate a new LabBook.

The new LabBook is based on all source data except the following:

- All suspended entries
- All excluded entries
- Samples that where added during QC

All entries are set to be evaluated, that means all entries in the Evaluate column are checked and used in the Evaluation Results, Exports, Queries, and Reports.

Importing Calibration Data from an Existing LabBook

When you wish to create a new LabBook from an existing LabBook, you can copy the calibration curves to skip the time-consuming calibration lines, which shortens the overall runtime. Another advantage of this method is the reliability of your source LabBook that ran successfully and contains a sufficient calibration.

❖ **To import calibration data from an existing LabBook**

1. Open the LabBooks page of Qtegra, and select the **Create a new LabBook from an existing LabBook** option based on your source LabBook.

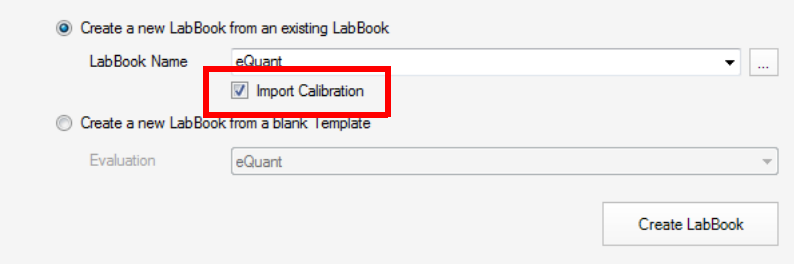


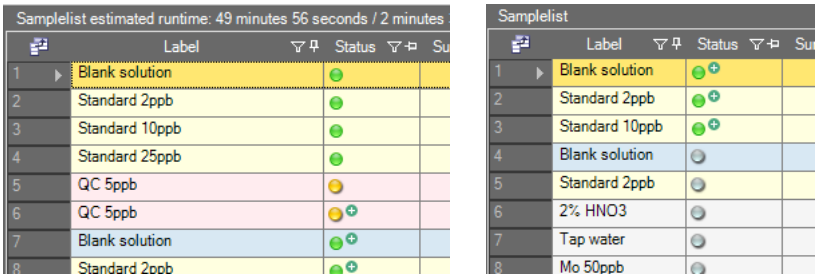
Figure 4-35. Import Calibration check box

2. Tick **Import Calibration** to import the calibration data into the new LabBook.
The calibration data will then be shown in your LabBook and in the evaluation results.

Tip This check box is only available if the existing LabBook contains a calibration.

Tip Only successful analyses from the calibration block are imported. If, for example, one of the analyses in the calibration block fails due to a QC failure, then this failing analysis is not copied across into the created LabBook.

3. Click **Create LabBook**.
The new LabBook opens as its own tab. The Sample List is created according to the existing LabBook and shows the status of the initial BLK and STD samples already green indicated.



Labeled Components: left-hand=finished LabBook, right-hand=new LabBook

Figure 4-36. Sample list with imported calibration data

4. When you schedule this LabBook, the measurement starts with the first sample line that is not already finished, that means, it does not show a green indicator. In the example (see Figure 4-36, right-hand image) the measurement is starting with sample line 4 *Blank solution*.

Editing a LabBook

LabBooks are edited in Qtegra. Editing a LabBook involves a number of parameters, see "LabBooks" on page 6-1 for a complete description of LabBooks.

❖ **To edit a LabBook**

1. From the LabBooks page, open your LabBook.
2. Edit your LabBook.
   See also "Method Parameters Settings" on page 9-3 and "Sample List of LabBook" on page 6-13.
3. On the toolbar of your LabBook page, click **Save** to save your LabBook.

Deleting a LabBook

LabBooks are deleted on the **File Manager** page of Qtegra.

❖ **To delete a LabBook**

1. On the File Manager page, click the **LabBooks** folder (or the subfolder for the LabBook you wish to delete), see Figure 4-37.

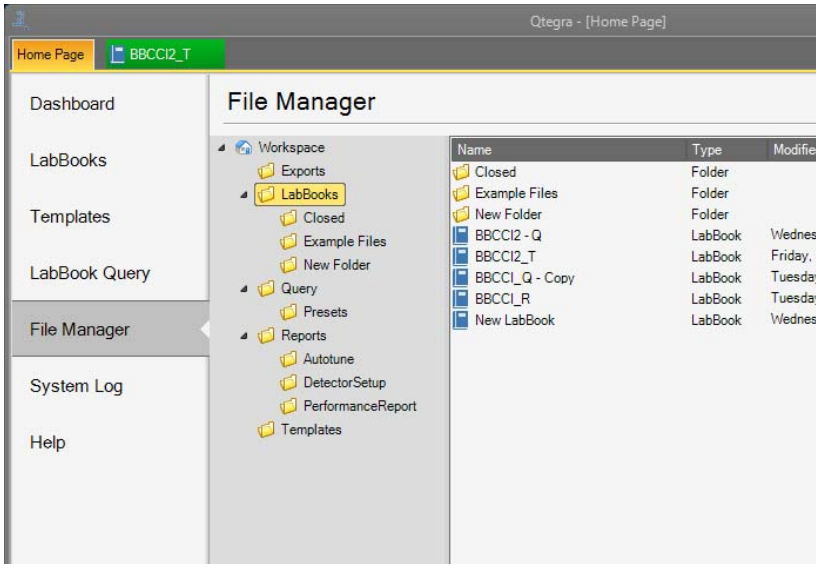


Figure 4-37. File Manager - LabBooks

2. Right-click the LabBook you wish to delete in the right-hand list.
A shortcut menu opens, see Figure 4-38.

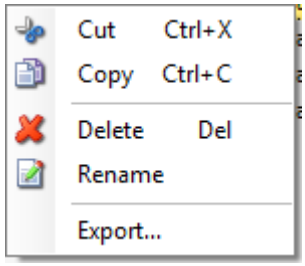


Figure 4-38. Shortcut menu of the File Manager

3. Select **Delete** from the shortcut menu.
The LabBook is deleted.

Closing a LabBook

LabBooks are closed in Qtegra by clicking the appropriate button on the toolbar of the LabBook or by simply closing the tab of the LabBook.

❖ **To close a LabBook**

1. On the toolbar of your LabBook page, click **Close** to close your LabBook.

-or-

Click **Close** in the tab of the LabBook.

Templates Page

On the **Templates** page of Qtegra, see Figure 4-39, Templates for your methods are created and opened.

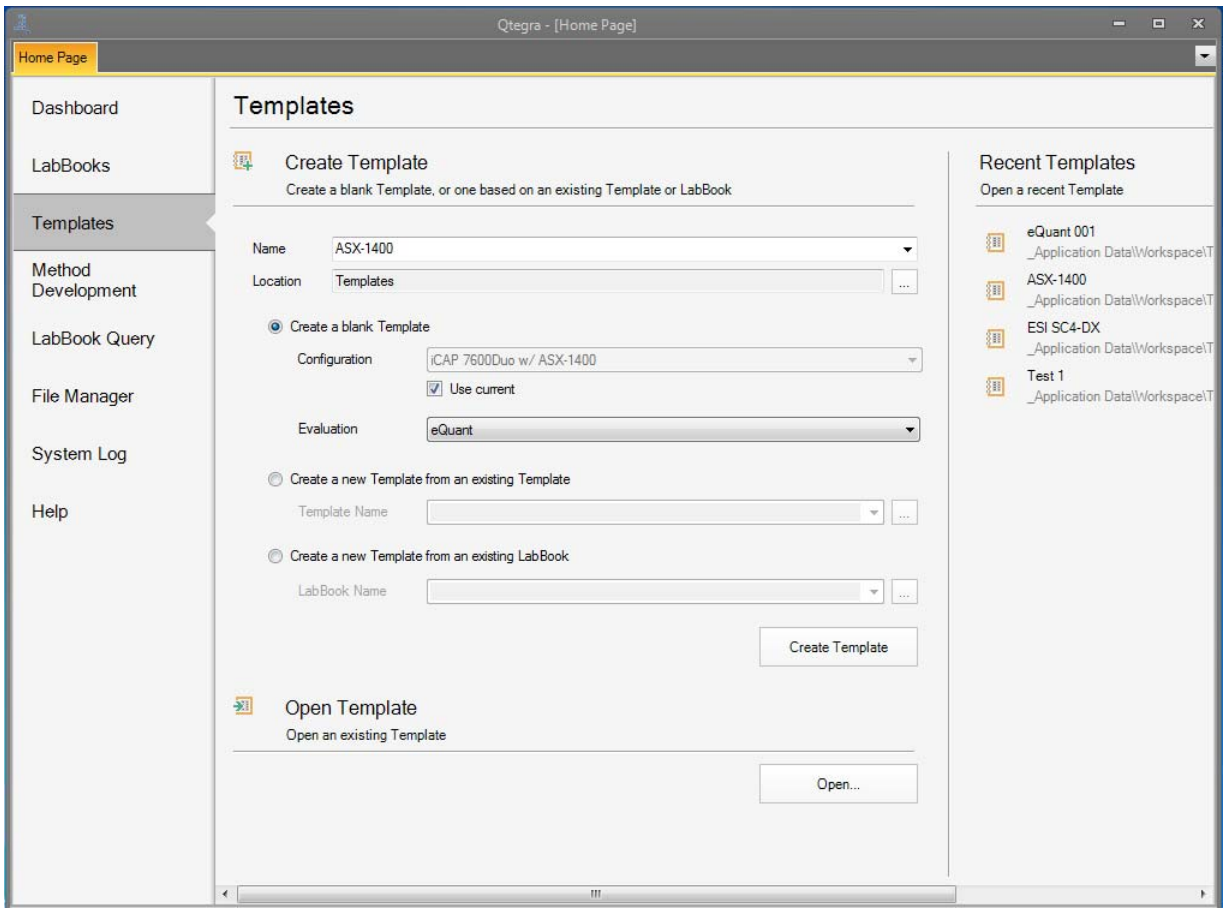
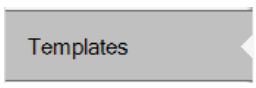


Figure 4-39. Templates Page of Qtegra

A **Template** contains all basic information on analytes, acquisition parameters, standards and sample definitions as well as Automatic Export settings. Templates are generally created by the Administrator for different types of applications. Once a Template is created and saved, it can serve as the basis for different analytical measurements (LabBooks).

Tip Any values entered that are not within the given range are marked with an exclamation mark.

❖ To open the Templates page of Qtegra



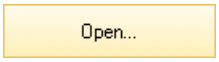
1. On the **Qtegra - [Home Page]** navigation pane, click **Templates**. The Templates page of Qtegra opens.

Opening a Template

Templates are opened either from the Templates page of Qtegra, which is described here, or from the File Manager page, see "File Manager Page" on page 4-51.

❖ **To open a Template in Qtegra**

1. Open the Templates page.
2. Below  , click **Open**.



The **Browse for Template** dialog opens, see Figure 4-40.

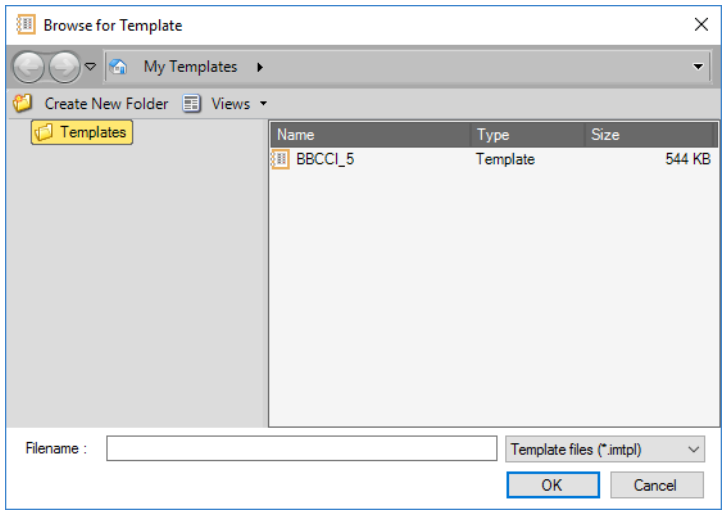


Figure 4-40. Browse for Template dialog

3. Select a Template.
4. Click **OK** to open the Template.
The Template opens in a new tab of the Qtegra tool.

❖ **To open a Recent Template**

1. From the Templates page, select a Template in the **Recent Templates** section, see Figure 4-41.

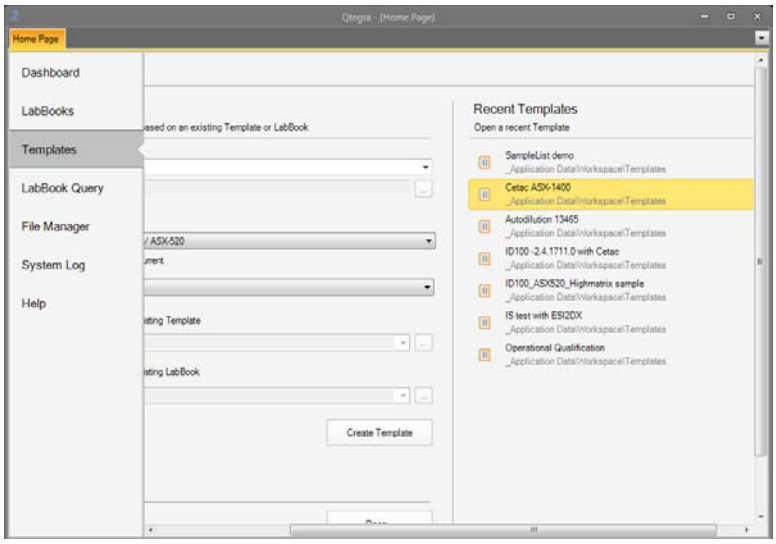


Figure 4-41. Recent Templates

The selected Template opens in a separate tab.

Creating a Template

Templates are created from blank Templates, existing Templates or existing LabBooks in Qtegra. For blank Templates, you need to select a system **Configuration**. Configurations, including peripherals (**Instruments**), are defined by your Administrator in the **Experiment Configurator** applet of the Configurator tool (see "Experiment Configurator" on page 3-15).

❖ **To create a new Template in Qtegra**

1. On the Templates page, type a **Name** for the Template and select a **Location**, see Figure 4-42.

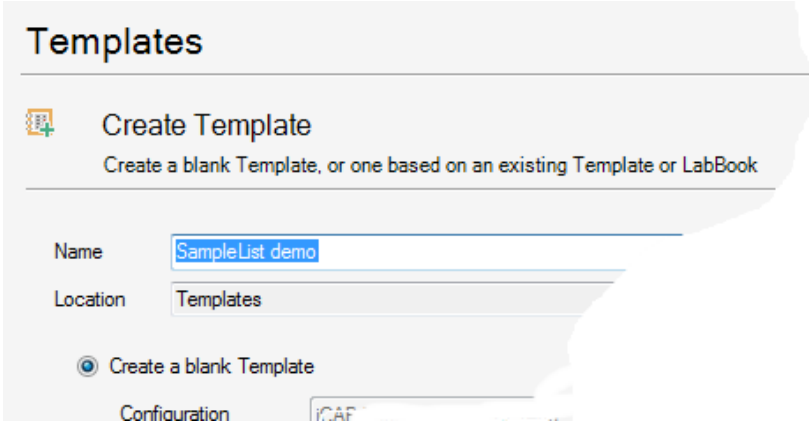


Figure 4-42. Typing the Name for a Template

2. Select the first option if you wish to **Create a blank Template**, and select a **Configuration** and an **Evaluation** from the drop-down lists. With the selected **Configuration** a number of predefined sets of parameters for the Template, for example, instrument and peripheral settings, are automatically loaded.

3. Select the second option if you wish to **Create a new Template from an existing Template** and select a **Template Name** from the drop-down list.
   -or-
   Type the Template name or browse ... to choose it.

4. Select the third option if you wish to **Create a new Template from an existing LabBook** and select a **LabBook Name** from the drop-down list.
   -or-
   Type the LabBook name or browse ... to choose it.

Create Template

5. Click **Create Template** to create the new Template.
   A new tab opens for the new Template.

6. In the tab of your Template, define the **Method Parameters**.
   See "Method Parameters Settings" on page 9-3 for details.

7. Click **Sample Definition** to set up the Sample List parameters.
   See "Sample Definition for a Template" on page 5-5 for details.

   The final Sample List is defined by the number of samples selected when creating a LabBook. The Sample List in the LabBook is created from the parameters in Sample Definition in the Template.

8. Click **Automated Export** to define the data for export. See "Automatic Export - Template" on page 5-10 for details.

9. On the toolbar of your **Template** page, click **Save** to save your Template.

Editing a Template

Templates are edited in Qtegra. See "Templates" on page 5-1 for a complete description of the parameters involved.

❖ **To edit a Template in Qtegra**

1. From the Templates page, open your Template.
2. Edit the **Method Parameter** settings.
   See "Method Parameters Settings" on page 9-3 for details.
3. Edit the **Sample Definition** settings.
   See "Sample Definition for a Template" on page 5-5 for details.

4. On the toolbar of your Template, click **Save** to save your Template.

Closing a Template

Templates are closed by clicking the appropriate button on the toolbar of the Template or by simply closing the tab of the Template.

❖ **To close a Template**

1. On the toolbar of your Template, click **Close** to close your Template.

   -or-

   Click **Close** in the tab of the Template.

LabBook Query Page

On the **LabBook Query** page of Qtegra, you define the location of the LabBooks and the period of time measurements were done, see Figure 4-43, and parse through the available results.

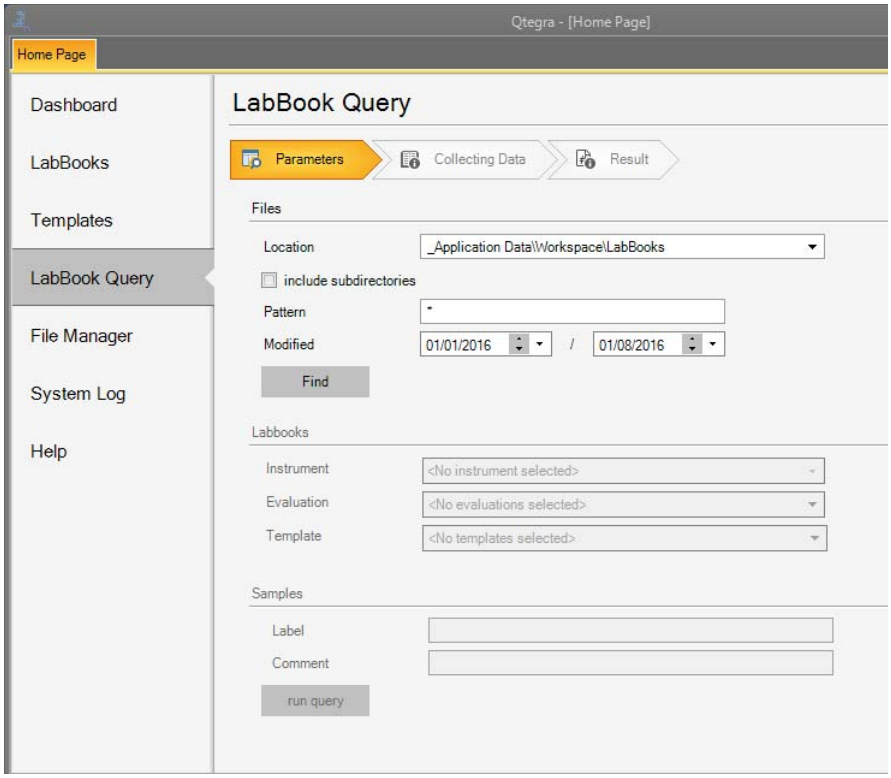


Figure 4-43. LabBook Query Page of Qtegra

You can then narrow down the query for the LabBooks meeting these criteria by further defining Instrument, Evaluation type and Template.

On the resulting **Query** page, you select the data you wish to view, see Figure 4-44.

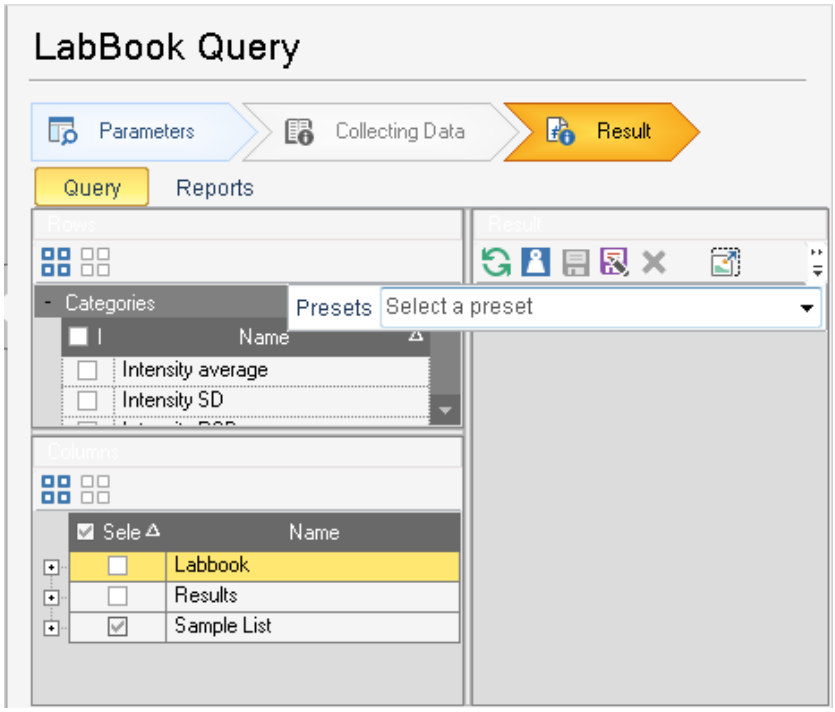


Figure 4-44. LabBook Query Page of Qtegra Query view

For details, see "Displaying Result Data" on page 4-43 and "Managing Results Data Presets" on page 4-46.

Reports of the selected data are created on the **Reports** view of a LabBook Query Result page, see Figure 4-45.

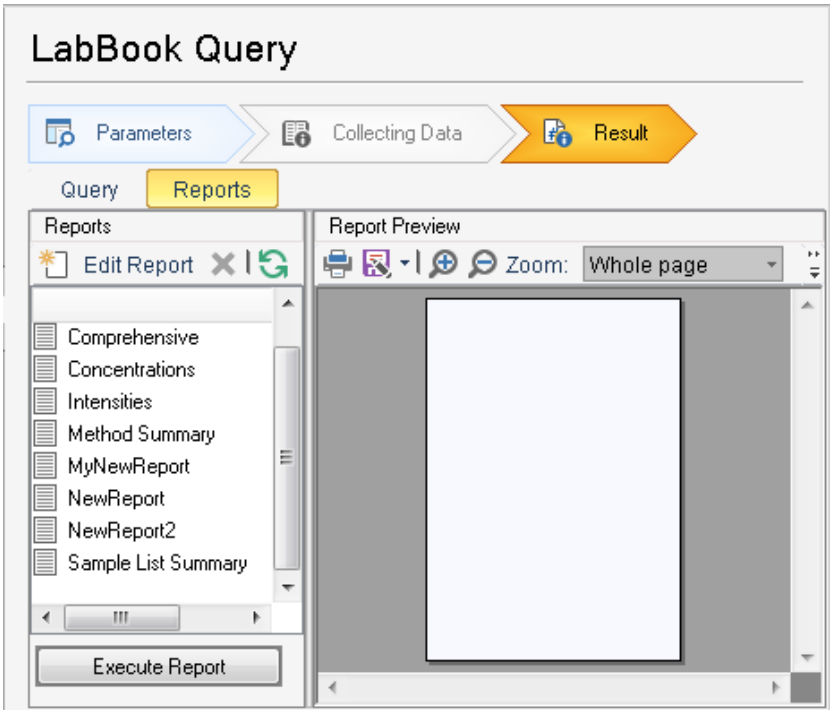
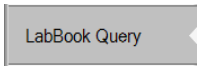


Figure 4-45. LabBook Query Page of Qtegra Reports view

For details, see "Generating Reports" on page 4-47 and "Getting Started with Qtegra Reports" on page 8-2.

❖ **To open the LabBook Query page of Qtegra**



1. From the **Qtegra - [Home Page]** navigation pane, click **LabBook Query**.
   The LabBook Query page of Qtegra opens.

Displaying Result Data

The parameters of a measurement are set to be displayed on the LabBook Query page of Qtegra.

❖ **To display the result data on the Result page of Qtegra**

1. Open the LabBook Query page.
2. In the **Parameters** view of the LabBook Query page, select the **Location** from the drop-down list.

3. Type the **Pattern** and select the date for **Modified** when the LabBooks were acquired, see Figure 4-46.

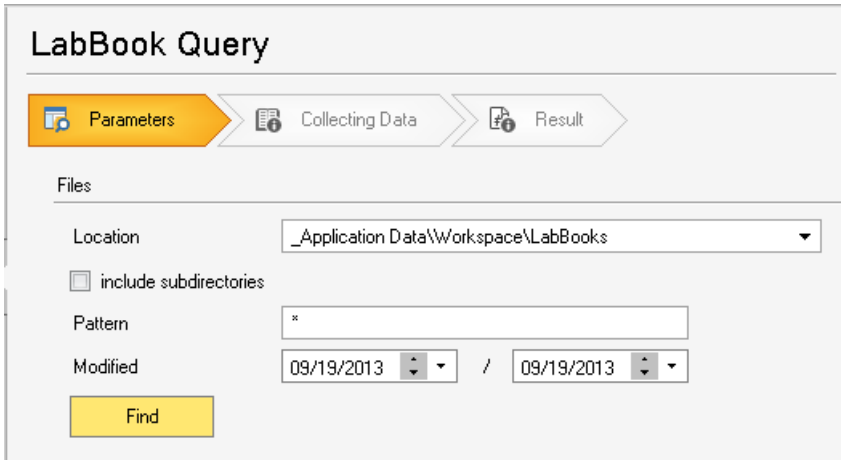


Figure 4-46. Files section in LabBook Query page

If you type `* (asterisk)` in the **Pattern** field, all LabBooks in the folder are searched. Type an asterisk followed by a fixed string and another asterisk (for example, `*fast*`) to return all LabBooks with the string "fast" in the name, which may refer to all prep*FAST* LabBooks. The search string is not case-sensitive. As an alternative, type `wrk37*` to collect all LabBooks with a name starting with "wrk37" to indicate, for example, the employee number 37.

4. Click **Find** to start the search for LabBooks that match the defined values.
The **LabBooks** field displays the first entries in the list of results, see Figure 4-47.

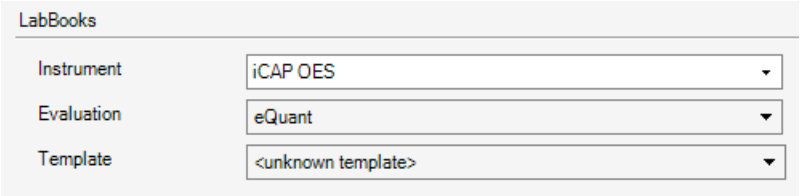


Figure 4-47. LabBooks found in LabBook Query page

5. Select **Instrument**, **Evaluation** and **Template** from the drop-down lists.

6. For **Samples**, type the **Label** as in the Sample List, for example, *Sample 1*.

run query

7. Click **run query** to start the query.
Qtegra collects the data, see Figure 4-48.

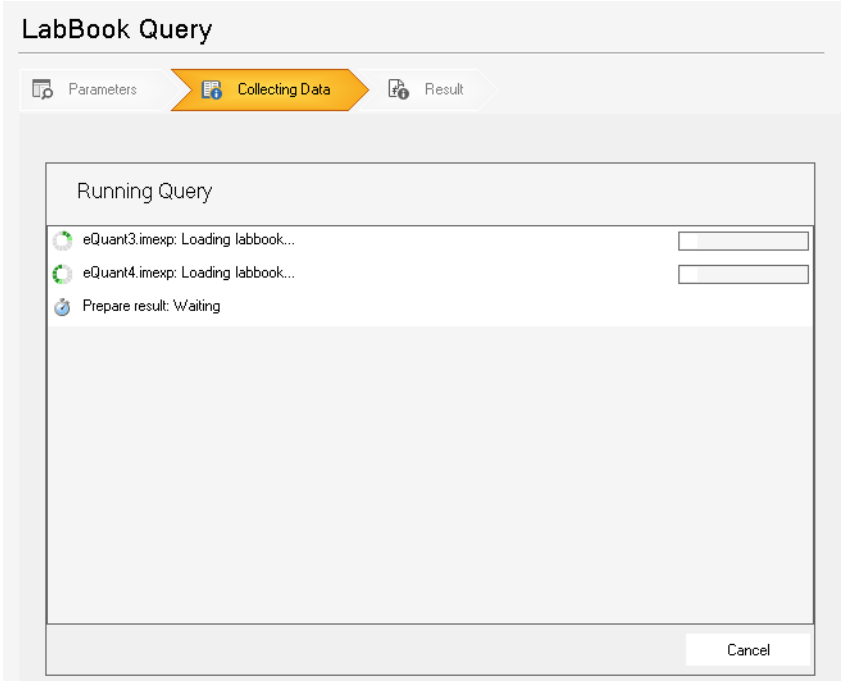


Figure 4-48. LabBook Query page collecting data in Qtegra

8. In the left pane, select the check boxes for the data you wish to display.

The results are displayed when the query has been executed, see Figure 4-49.

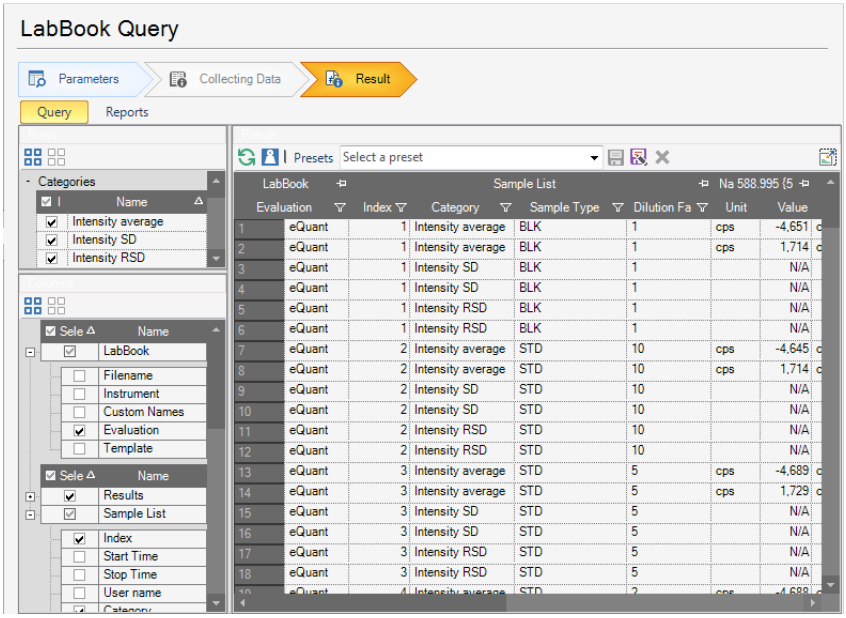


Figure 4-49. LabBook Query page displaying results in Qtegra

9. Click **Refresh** to refresh the display.

10. Click **Hide** if you wish to hide the units.
    The columns **Unit** are hidden. Repeat to display the units again.

Managing Results Data Presets

In Qtegra, the display options for result data of a measurement can be saved as presets, see Figure 4-50.

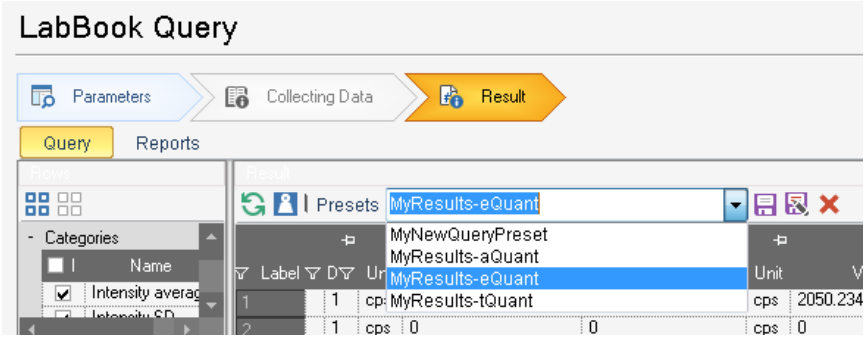


Figure 4-50. Results display presets on LabBook Query Page of Qtegra

❖ **To save a result data preset**

1. From the LabBook Query page, select the results you wish to display as described in "Displaying Result Data" on page 4-43.

2. Above the results table, click **Save as** to save the preset as new preset.
   The **Save New Preset** dialog is displayed, see Figure 4-51.

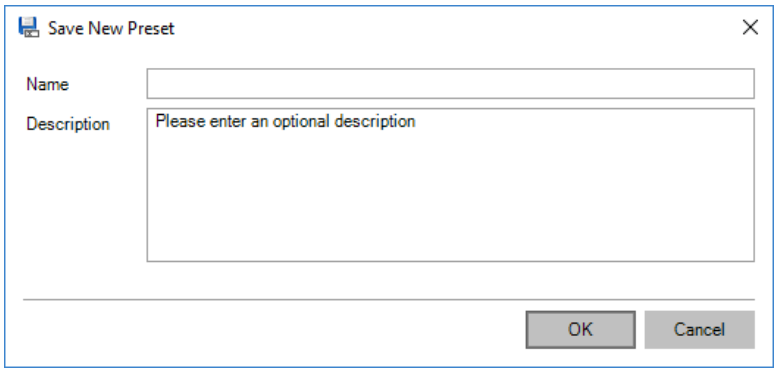


Figure 4-51. Save New Preset dialog in Qtegra

Tip Result data presets saved here will be available as well in the Query view of a completed LabBook.

3. Type a **Name** for the preset.

4. Type a **Description**.

5. Click **OK**.
   The preset is added to the list.

❖ **To save a preset**

1. From the LabBook Query page, select the results you wish to display as described in "Displaying Result Data" on page 4-43.
2. Select a preset from the drop-down list.
   The data is displayed according to the selected preset.
3. Change column widths or select different check boxes on the left to change the presented data.
4. Click **Refresh** to refresh the display.
5. Click **Save** to save the result data preset.

❖ **To delete presets**

1. From the LabBook Query page, select the results you wish to display as described in "Displaying Result Data" on page 4-43.
2. From the **Preset** list, select the preset you wish to delete.
3. Click **Delete** to delete the result data preset.
   The **Delete Preset** dialog is displayed, see Figure 4-52.

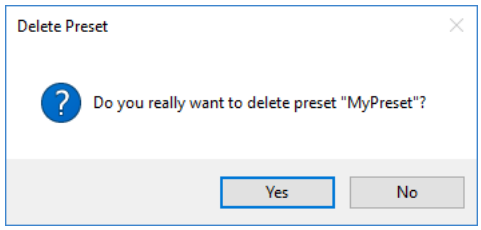


Figure 4-52. Delete Preset dialog in Qtegra

4. Click **Yes**.
   The preset is deleted from the list.

Generating Reports

In the **Reports** view of the LabBook Query page of Qtegra, you generate result data Reports from presets.

Generally, you can structure your Report to your needs, add headings, tables and graphs to specify the presentation of the result data.

Tip For details on creating Report presets, see "Getting Started with Qtegra Reports" on page 8-2.

❖ **To open the Reports view on the LabBook Query page**

1. From the LabBook Query page, display your result as described in "Displaying Result Data" on page 4-43.

2. In the LabBook Query Result view, select the **Reports** tab. The **Reports** page opens, see Figure 4-53.

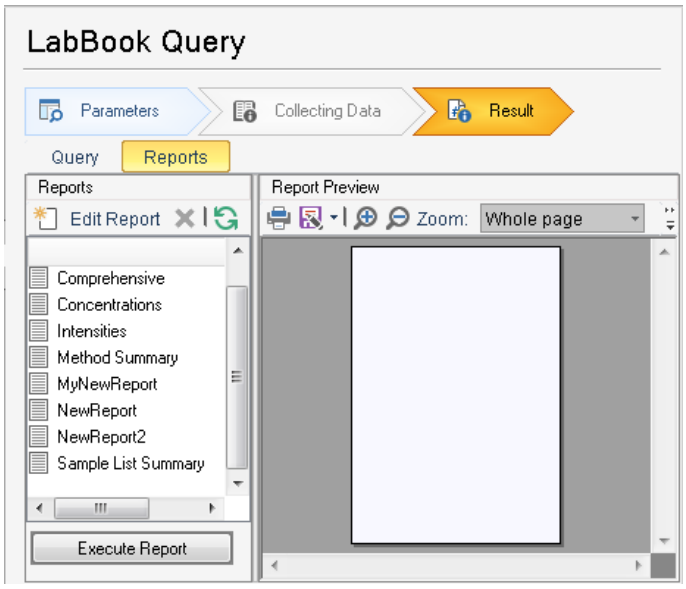


Figure 4-53. LabBook Query Reports page

❖ To generate a Report

1. From the LabBook Query page, display your result as described in "Displaying Result Data" on page 4-43.

2. In the LabBook Query Result view, select the **Reports** tab. Previously defined Reports are listed on the left pane, see Figure 4-54.

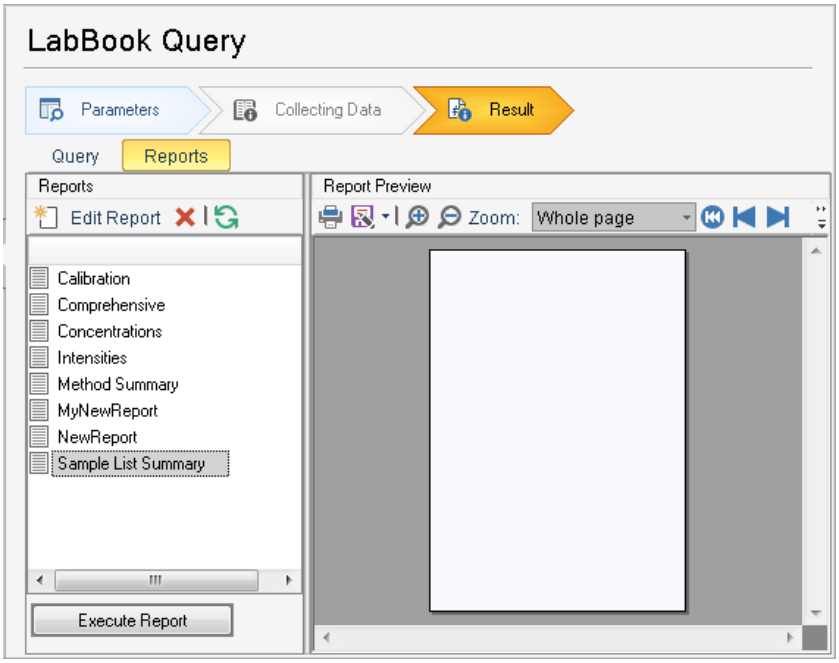


Figure 4-54. LabBook Query Reports page showing defined Reports

Tip In a completed LabBook, this is the **Reports** page of the **Query** view.

3. From the left pane, select a Report from the list and then

   Click **Execute Report**.

   -or-

   Click **Update** above the list.

The Report is generated as defined in the Report layout selected and displayed in the **Report Preview** on the right pane, see Figure 4-55.

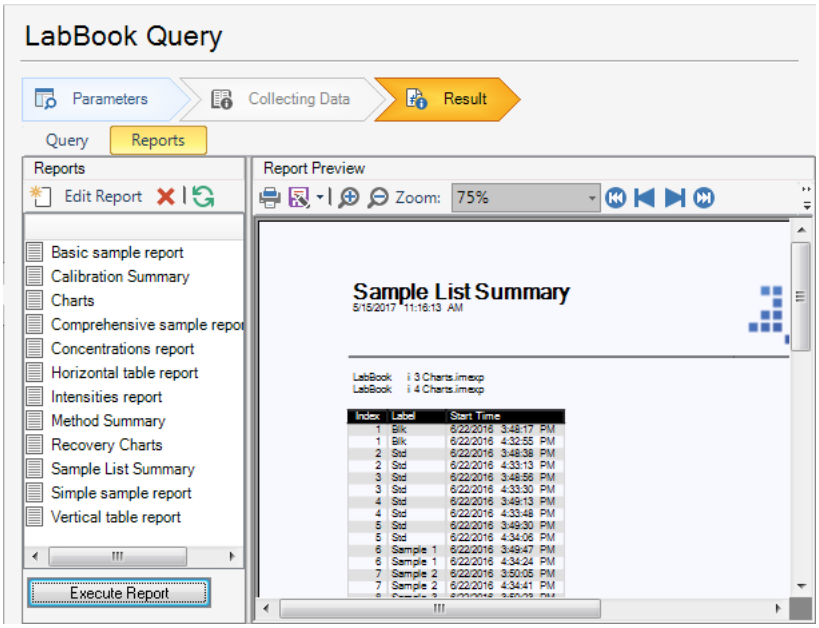


Figure 4-55. LabBook Query Reports page showing an executed Report

4. **Print** the Report.

-or-

Save the Report if desired.

File Manager Page

On the **File Manager** page of Qtegra, see Figure 4-56, you organize your Template and LabBook files as well as the Reports generated by the Get Ready process.

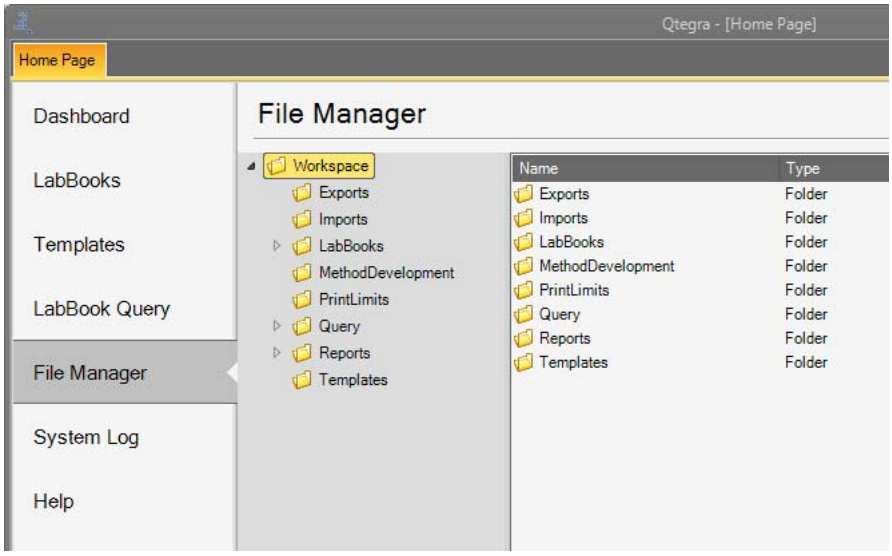
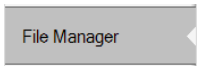


Figure 4-56. File Manager Page of Qtegra

❖ **To open the File Manager page of Qtegra**



1. From the **Qtegra - [Home Page]** navigation pane, click **File Manager**.
   The File Manager page of Qtegra opens.

❖ **To open a Template from the File Manager page of Qtegra**

1. From the File Manager page, select the **Templates** directory.
2. Double-click the Template you wish to open.
   The Template is opened in a new tab.

❖ **To open a LabBook from the File Manager page of Qtegra**

1. From the File Manager page, select the **LabBooks** directory.
2. Double-click the LabBook you wish to open.
   The LabBook is opened in a new tab.

❖ To create a new folder in the Workspace

1. From the File Manager page, right-click **Workspace** to create a new folder, see Figure 4-57.

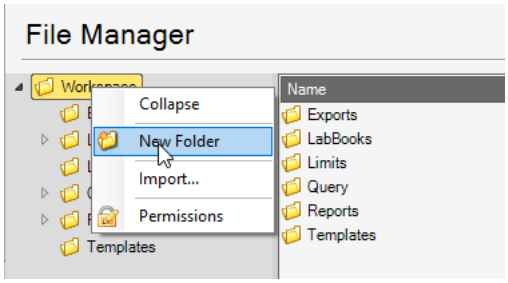
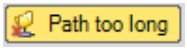


Figure 4-57. Shortcut menu File Manager Workspace

2. Select **New Folder** from the shortcut menu.
3. Type a name for the new folder.
4. Click anywhere in the folder.
   -or-
   Press **<Enter>**.
   The new folder is accepted.



Tip When you have created a very long path to a folder under Windows, Qtegra cannot use this path to read or save files. To indicate this behavior, *Path too long* is displayed in the folder tree of the File Manager.

❖ To create a new folder in LabBooks or Templates

1. From the File Manager page, right-click the **LabBooks** or **Templates** folder to create a new folder, see Figure 4-58.

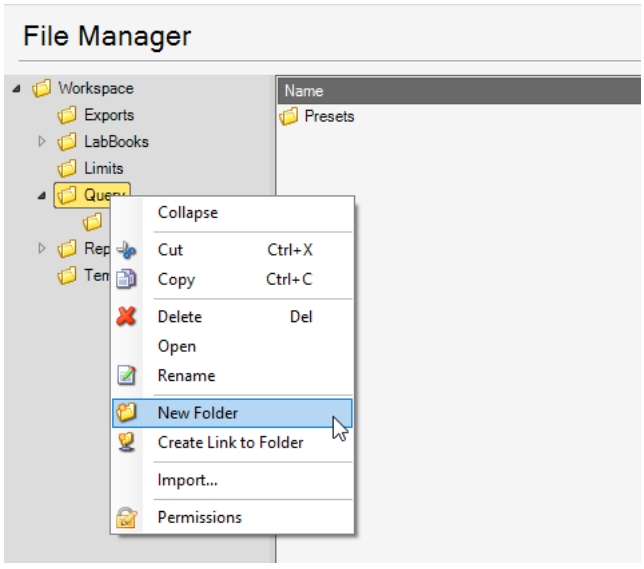


Figure 4-58. Shortcut menu File Manager subfolder

2. Select **New Folder** from the shortcut menu.

3. Type a name for the new subfolder.
The first subfolder is shown on the right.

4. Click anywhere in the **Workspace**.
-or-
Press **<Enter>**.
The new subfolder is accepted.

❖ **To create a network link to a folder in LabBooks or Templates**

1. From the File Manager page, right-click the **LabBooks** or **Templates** folder for which you wish to create a link to a network folder.

2. Select **Create Link to Folder** from the shortcut menu, see Figure 4-59.

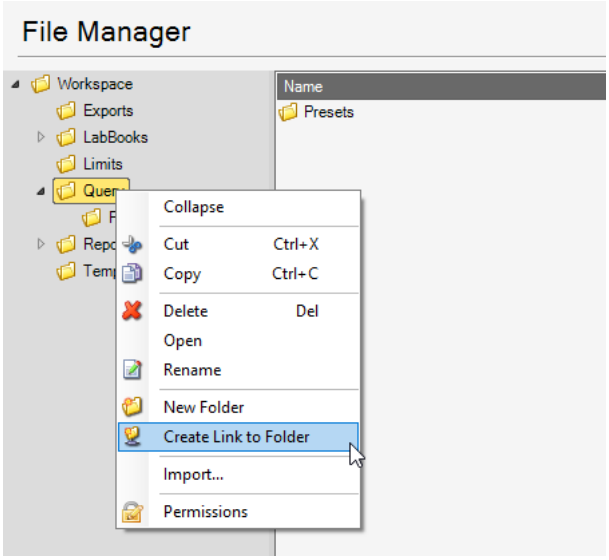


Figure 4-59. Shortcut menu File Manager subfolder showing Create Link to Folder

3. In the **Select Folder** dialog, select the folder you wish to create the network link to.

Tip Your Administrator must have prepared the Windows system, refer to Central Data Storage.

4. Click **Select Folder**.

5. Enter a name for the new folder, see Figure 4-60.

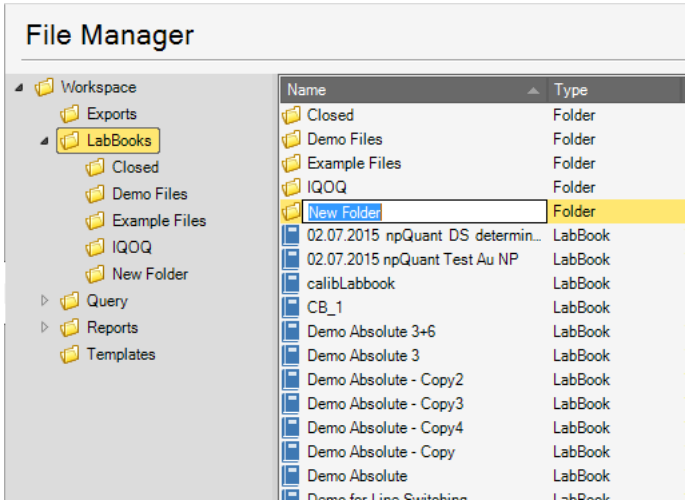


Figure 4-60. Naming new network link to folder

Tip Be careful when you store data to the network location. LabBooks should not be opened in several locations at the same time.

6. Enter a name for the new folder.

7. Click anywhere in the folder.
   -or-
   Press **<Enter>**.
   The new name is accepted.

Managing Files

On the **File Manager** page of Qtegra, you can explore, cut, copy, delete, rename, or export your Templates and LabBook files.

❖ To cut a Template or LabBook file

1. From the File Manager page, select the folder, for example, *LabBooks* to show the file you wish to cut.

2. Right-click the file you wish to cut, see Figure 4-61.

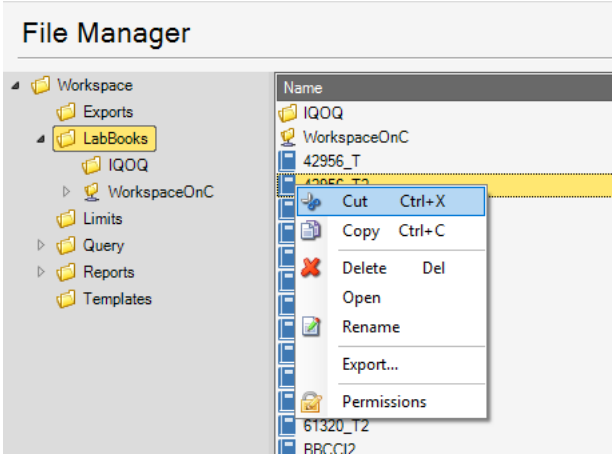


Figure 4-61. Shortcut menu of file for cut

3. Select **Cut** from the shortcut menu.
4. Select the new folder.
5. Right-click in the new folder, see Figure 4-62.

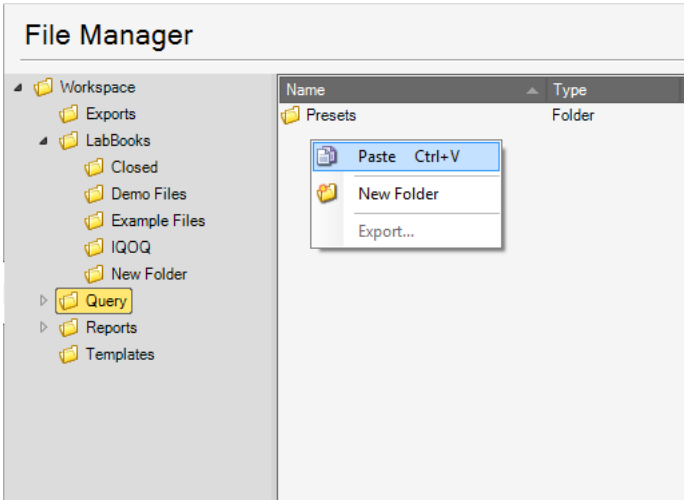


Figure 4-62. Shortcut menu of file for paste

6. Select **Paste** from the shortcut menu.
   The file you cut is moved to the selected folder.

❖ **To copy and paste a Template or LabBook file**

1. From the File Manager page, select the folder, for example, *LabBooks* to show the file you wish to copy.

2. Right-click the file you wish to copy, see Figure 4-63.

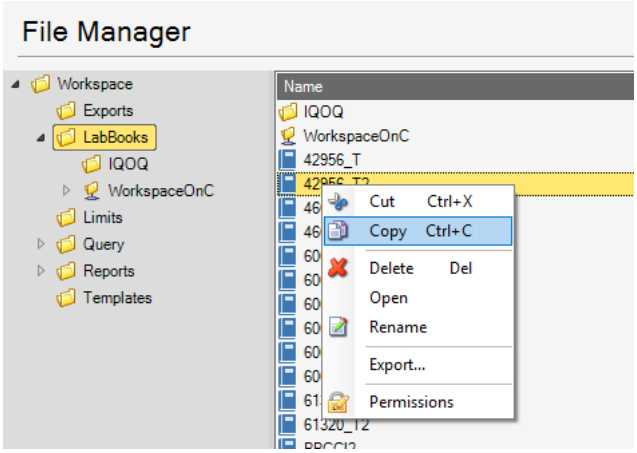


Figure 4-63. Shortcut menu of file for copy

3. Select **Copy** from the shortcut menu.
4. Select the location for the file.
5. Right-click and select **Paste** from the shortcut menu. The file is copied to the selected location.

❖ To delete a Template or LabBook file

1. From the File Manager page, select the folder to show the file you wish to delete.
2. Right-click the file you wish to delete, see Figure 4-64.

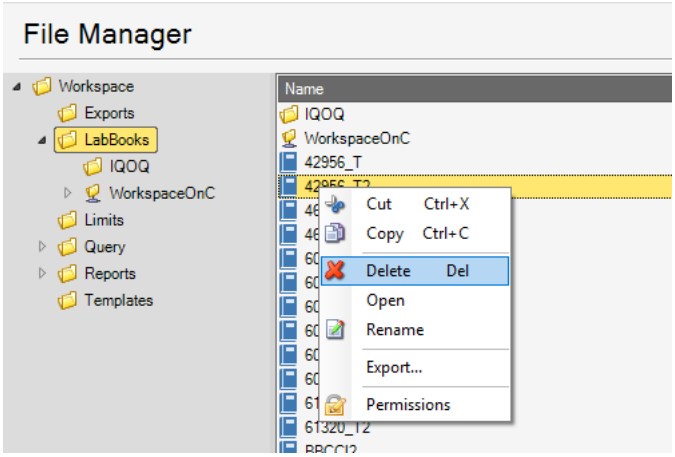


Figure 4-64. Shortcut menu of file for delete

3. Select **Delete** from the shortcut menu.
   A confirmation dialog opens, see Figure 4-65.

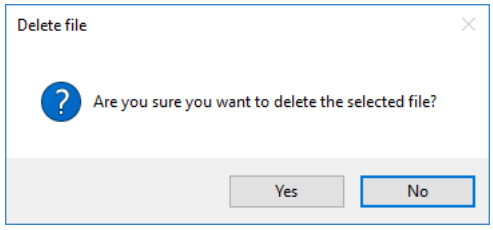


Figure 4-65. Confirmation dialog to delete file

4. Click **Yes**.
   The file is deleted.

❖ **To rename a Template or LabBook file**

1. From the File Manager page, select the folder to show the file you wish to rename.
2. Right-click the file you wish to rename, see Figure 4-66.

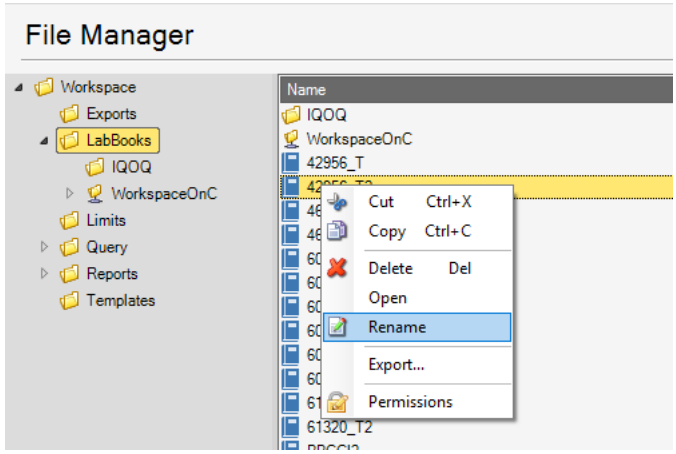


Figure 4-66. Shortcut menu of file for rename

3. Select **Rename** from the shortcut menu.
4. Type the new name for the file.
5. Click anywhere in the folder.
   -or-
   Press **<Enter>**.
   The new name is accepted.

❖ **To export a Template or LabBook file**

From the File Manager page, you can export files from the Qtegra ISDS Workspace by generating a copy of the original file.

1. From the File Manager page, select the folder to show the file you wish to export.
2. Right-click the file you wish to export, see Figure 4-67.

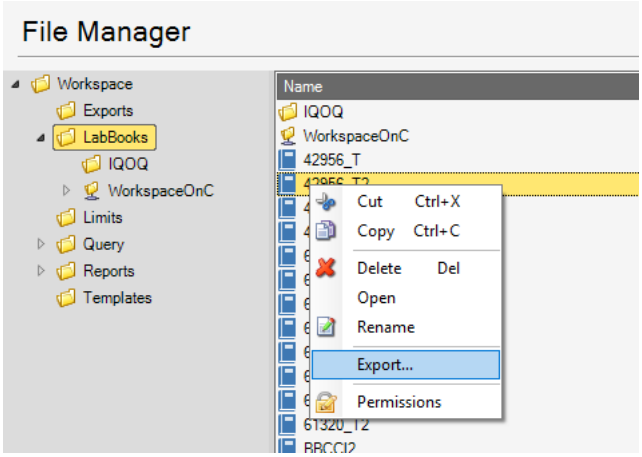


Figure 4-67. Shortcut menu of file for export

3. Select **Export** from the shortcut menu.
The **Browse For Folder** dialog opens, see Figure 4-68.

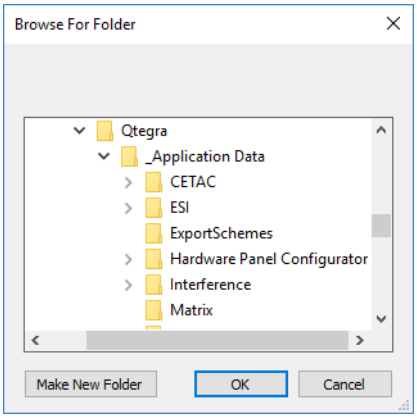


Figure 4-68. Browse For Folder dialog

4. Select a folder and click **OK**.
The selected file is copied to the selected destination.

Displaying additional File Information

The columns shown in the File Manager can be manually selected to show additional information as required. The choice of columns displayed is defined from a shortcut menu.

❖ To display additional file information

1. From the File Manager page, select a folder to define the columns displayed.

   Tip The column choice defined is then displayed to all folders.

2. Right-click the table header to show a shortcut menu.

3. The choices provided in the shortcut menu are described in Table 4-2.

Table 4-2. File Manager page - shortcut menu commands

Menu Command	Description
Size Column To Fit	Resizes the width of the currently selected column to display all its contents.
Size All Columns To Fit	Resizes the width of all columns to fully display their contents.
Name	The file name.
Type	The *Folder, LabBook, Report*, or *Template* to specify the file type.
Created	The original creation date of this file. Do not mix with File Created.
Type	Specifies the file as *Folder, LabBook* or *Template*.
Modified	The date of last modification.
Size	The file size in KB (kilo bytes).
Configuration	The name of the Configuration used (LabBooks only).
Configuration Description	The description for the Configuration used for a LabBook.
Created By	The user name of the Windows user account who created the file.
Template	The Template the LabBook was created from (LabBooks only).
Last Changed By	The user name of the last Windows user account to save the LabBook.
Samples	The number of samples in the LabBook.
Results	The number of measured samples.
Acquired By	The user name of the Windows user account who measured the LabBook.
Started At	The date and time when LabBook measurement started.

Table 4-2. File Manager page - shortcut menu commands, continued

Menu Command	Description
File Created	The date and time when the LabBook or Template was created in the displayed folder. Do not mix with Created.
Finished At	The date and time when LabBook measurement finished.
File Modified	The date and time when the file was last modified.
More...	Opens the **Choose Columns** dialog to select the desired columns and to arrange the columns sort order.

Setting File Permissions

With Qtegra ISDS Software 2.8 SR3, the file access may be managed by permissions. The **Permissions** dialogs appear like original Windows dialogs but the file service controls its own permissions inside Qtegra.

Defining Permissions

With access to the **Permissions** dialogs, you define the Access rights by selecting a principal and setting the permissions respectively at the file or folder level you currently have selected.

Tip To be compatible with earlier Qtegra versions, no changes in the Configurator lead to the same behavior as before. Without permissions, the file access is only controlled by the settings under User Actions > File Manager > Files, Folders, LabBook, Report, and Template.

❖ **To enable the Permissions feature**

1. In the Configurator tool, select the **Access Control** applet.
2. Expand User Actions > File Manager > All Items to select the Permissions item.
3. The right pane shows the Access mode for 6 default User Groups. Initially, only the Administrator group has *Full access* to the Permissions feature. All other groups have restricted *Read only* rights.
4. Select the User Group and switch to *Full access* to grant the members of the group full access to the Permissions feature.
5. Restart Qtegra to apply the new settings.
   The Permissions shortcut menu item is then available (see

Figure 4-69). User Groups with Read only rights see the inactive menu item and can not open the Permissions dialogs.

As an example on how to grant permissions, a member of Qtegra Users shall get *Read only* permissions on the LabBooks > Example Files folder.

❖ **To set Read only permission for a LabBook folder**

1. As an Administrator open Qtegra ISDS and select the File Manager page.
2. Expand the folder tree and select the folder, which access shall be restricted for Qtegra Users or Qtegra User Groups, for example, the *QtegraAnalyst*.
3. Right-click the folder and select **Permissions**.

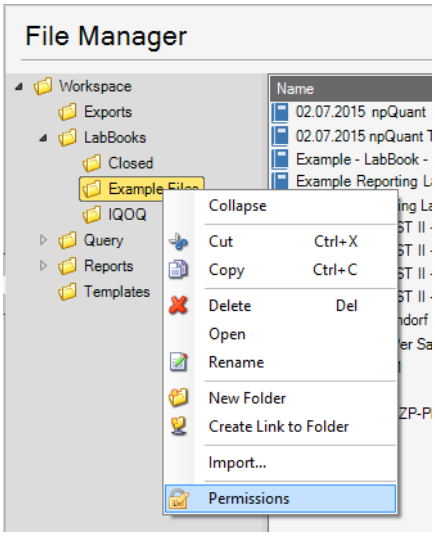


Figure 4-69. Shortcut menu of folder for Permissions

The **Permissions** dialog opens and initially shows no entry.

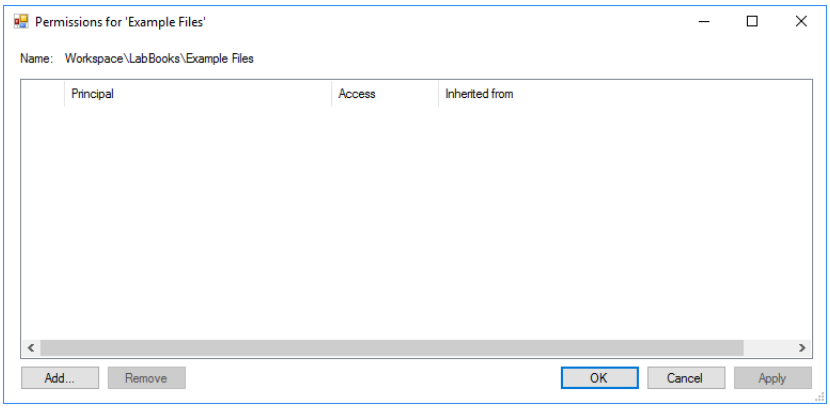


Figure 4-70. Empty Permissions dialog

4. Click **Add** to add a principal and to set the permissions in the initial Permissions dialog.

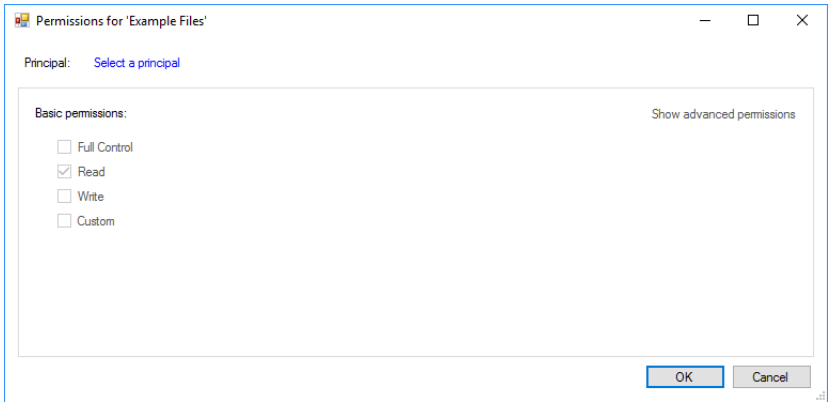


Figure 4-71. Initial Permissions dialog

5. Click **Select a principal** to select a user or a group.

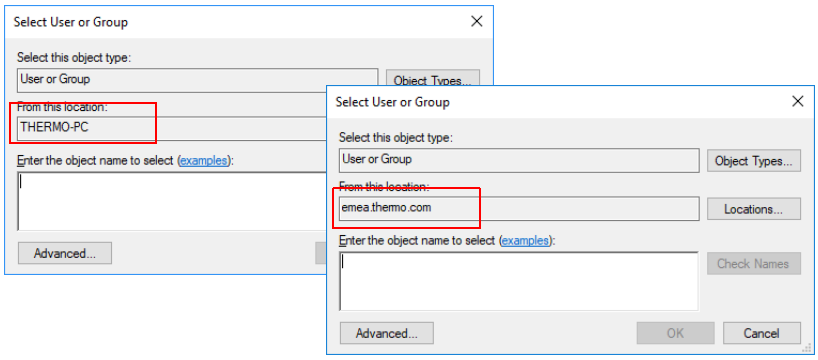


Figure 4-72. Select User or Group dialog - left: local user group, right: domain account

a. Depending on the user management, the Location shows your *Windows computer name* or *domain*. Click **Locations** to select another location.

b. In the lower box, enter the object name for the principal.

   In case of **Windows user management**, the name appears as "Location\Username". Enter, for example, `thermo` and click **Check Names** to autofill the box, resulting in "THERMO-PC\Thermo". See left image of Figure 4-72.

   -or-

   In case of a domain using an Active Directory, the name appears as used company-wide. Enter, for example, `thermo` and click **Check Names**. In most cases, the **Multiple Names Found** dialog opens to show all matching names. Select the desired name and click **OK** to fill the **Object Name** box. See right image of Figure 4-72.

c. If you do not know the exact object name, click **Advanced** to open the **Select User or Group** dialog where you can search for the object.

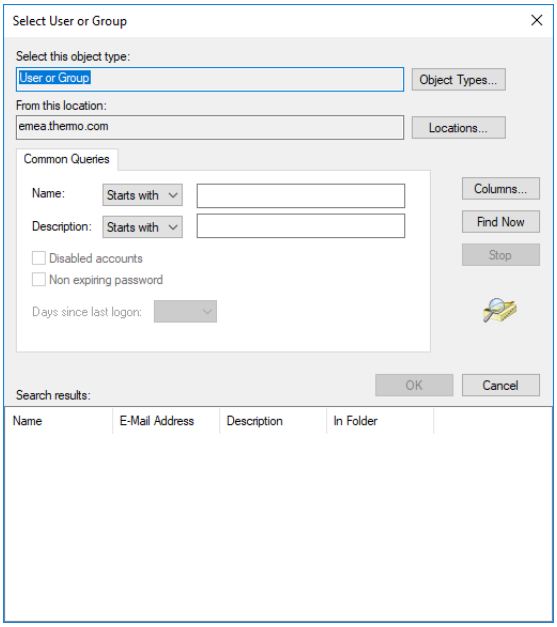


Figure 4-73. Advanced Select User or Group dialog

d. Enter all known parts of the object and click **Find Now** to show the results.
-or-
Leave the **Name** and **Description** empty and click **Find Now** to show the entire list with all available objects.
Double-click the desired entry to fill the **Object Name** box.

e. If your PC is connected to the Internet, click examples to show the explanations from the *Microsoft TechNet webpage*.

f. To remove objects that have been added by accident, just select the object and press **<Del>** on your keyboard.

6. The selected principal is displayed on top of the initial **Permissions** dialog.

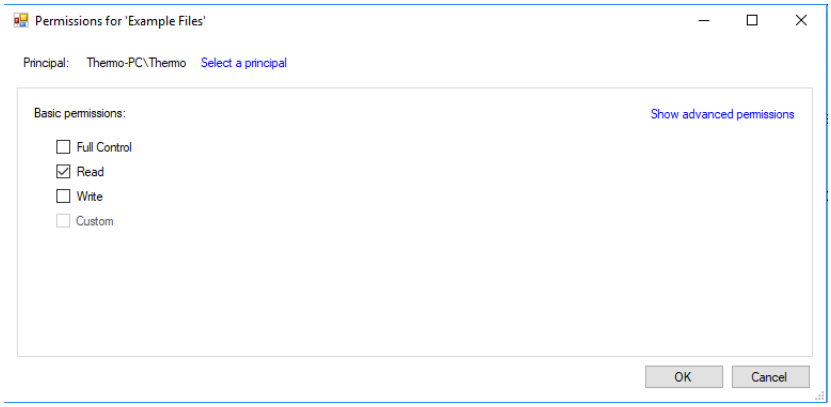


Figure 4-74. Permissions dialog with principal

7. To define the permission, tick the desired box under **Basic permissions**.
-or-
Click **Show advanced permissions** to define detailed permissions.

Tip All changes in the file structure, like creation, renaming or deletion of a folder, affect only the subfolders of the Qtegra Workspace. As soon as a file or folder is copied to another directory, the permission is lost.

See Table 4-3 for a description of basic permissions.

Table 4-3. Basic permissions description

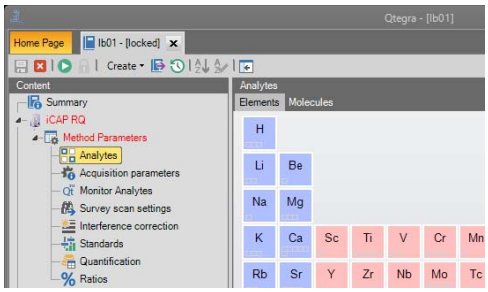
Permission	Description
Full Control	Allows all operations to be performed by the principal and equals the sum of *Read* and *Write*.
Read	The principal can read the Template or LabBook file, that means, the file can be opened but not modified. The principal can create a new Template or LabBook based on a file with *Read* permission. Note that the file is locked if no *Modify* permission is set, see the following example: 

Table 4-3. Basic permissions description, continued

Permission	Description
Write	With this permission all advanced permissions are included. Note that *Read* is not included.
Custom	This permission is always disabled and only activated if an advanced permission is set.

See Table 4-4 for a description of advanced permissions.

Table 4-4. Advanced permissions description

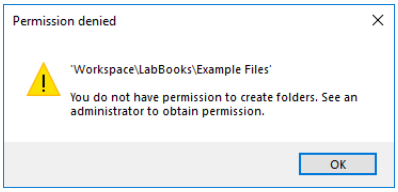
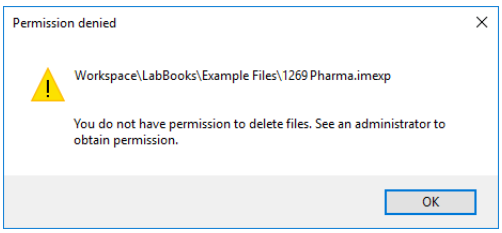
Permission	Description
Create files	The principal can create a Template or LabBook. Note that creation does not include the *Read, Modify* or *Execute* permission.
Create folders	Allows the principal in the File Manager to create a folder below the currently selected folder. With missing permission, the following dialog opens: 
Rename files	Allows the principal in the File Manager to rename a file.
Rename folders	Allows the principal in the File Manager to rename a folder.
Modify files	This permission is necessary to modify the Template or LabBook. If the principal is granted with additional *Read* permissions, it also includes the initial steps after creation like setting up the analytes and standards. The file is locked if no *Modify* permission is set.
Delete files	Allows the principal in the File Manager to delete a file. With missing permission, the following dialog opens: 

Table 4-4. Advanced permissions description, continued

Permission	Description
Delete folders	Allows the principal in the File Manager to delete a folder.
Execute	The principal can schedule the LabBook.

❖ **To view or edit permissions**

1. Select the File Manager page.
2. Expand the folder tree and select the folder, which permissions shall be viewed for Qtegra Users.
3. Right-click the folder and select **Permissions**. The Permissions dialog (see Figure 4-75) shows the currently defined access rights and optionally where the permissions are inherited from.

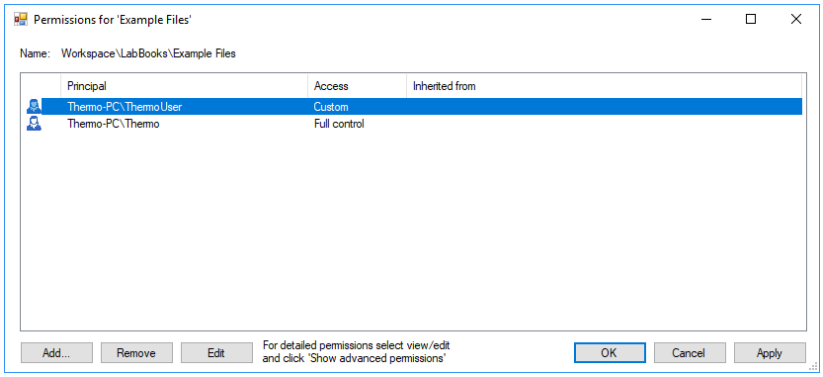


Figure 4-75. Permissions dialog with list of principals

4. Select the principal entry and then click **View** (if inherited) or **Edit** to show the detailed permissions.

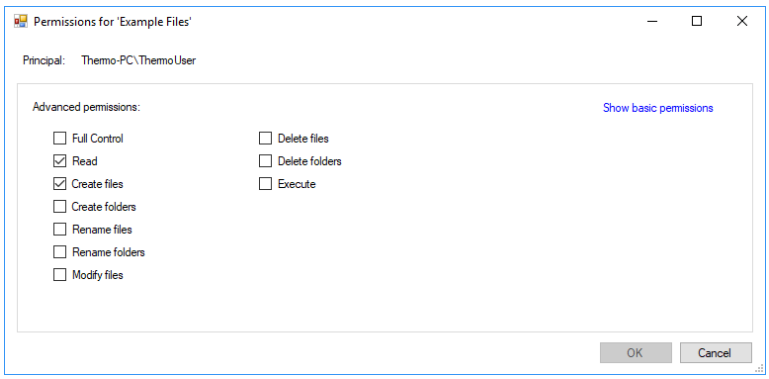


Figure 4-76. Permissions dialog with advanced permission view

5. Click **Show advanced permissions** and clear or tick a check box to update the permissions as required.

Tip Any permission granted on a folder affects all files and folders below this file structure. All properties are inherited. If you define additional permissions on a lower file or folder level, the resulting permission is a combination of both settings.

Using Permissions

The following example explains how to use permissions. Imagine, your company analyses food and environmental samples.

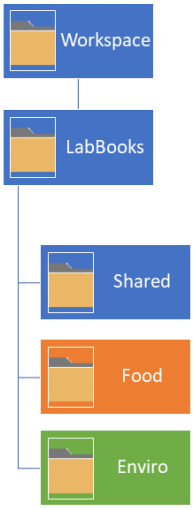


Figure 4-77. Example for a folder hierarchy

In the example, 'LabBooks' is set up with *Read* permission for all principles using Qtegra. The 'Shared' folder has *Write* permission for both groups. The 'Food' folder has *Write* permission for the food group, and the 'Enviro' folder has *Write* permission for the environmental group.

This isolates the group folders 'Food' and 'Enviro' from being modified by the other domain group.

If your company uses Active Directory groups, this kind of restricting access to folders is the easiest and best way of administering Qtegra permissions.

If not, and you use local PC accounts, you will have to repeat setting up the permissions on every instrument PC.

If your company uses domain groups to allow or deny access to another user, you only add or remove the user to or from that group, and all instrument PCs will see the change.

For new group members, simply add them to the respective domain group, ‘Food’ or ‘Enviro’, and they will automatically have the correct desired access on all instruments.

Displaying Reports

Once the performance check and tuning of the instrument is executed, the resulting data is generated and provided under File Manager > Workspace > Reports.

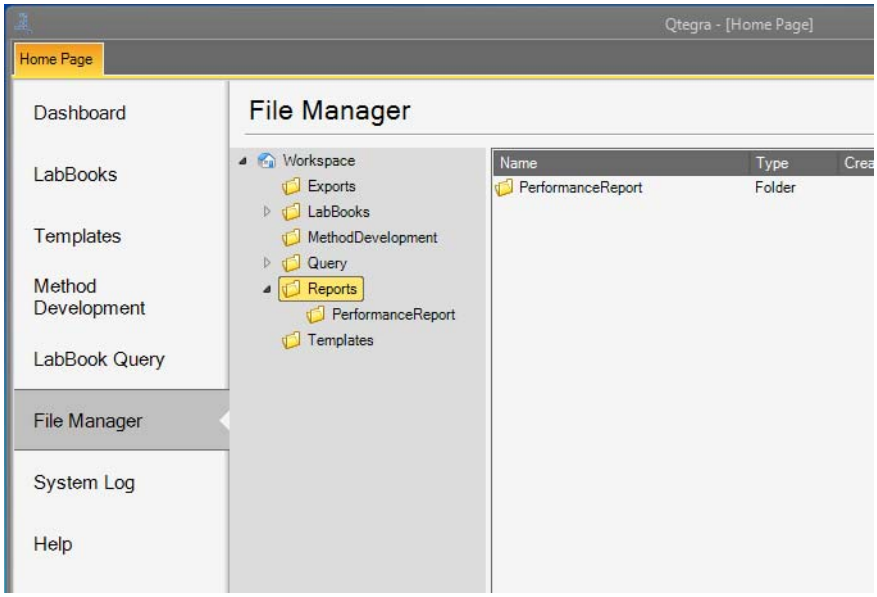


Figure 4-78. Reports tree on File Manager view

Expand the Reports item and select the subfolder as desired.

System Log Page

The **System Log** page, see Figure 4-79, provides information about changes to the system as it may be required by your SOP. For details, for example, to enable compliance settings via **Enable global compliance**, refer to "Compliance with your SOP" on page 2-37.

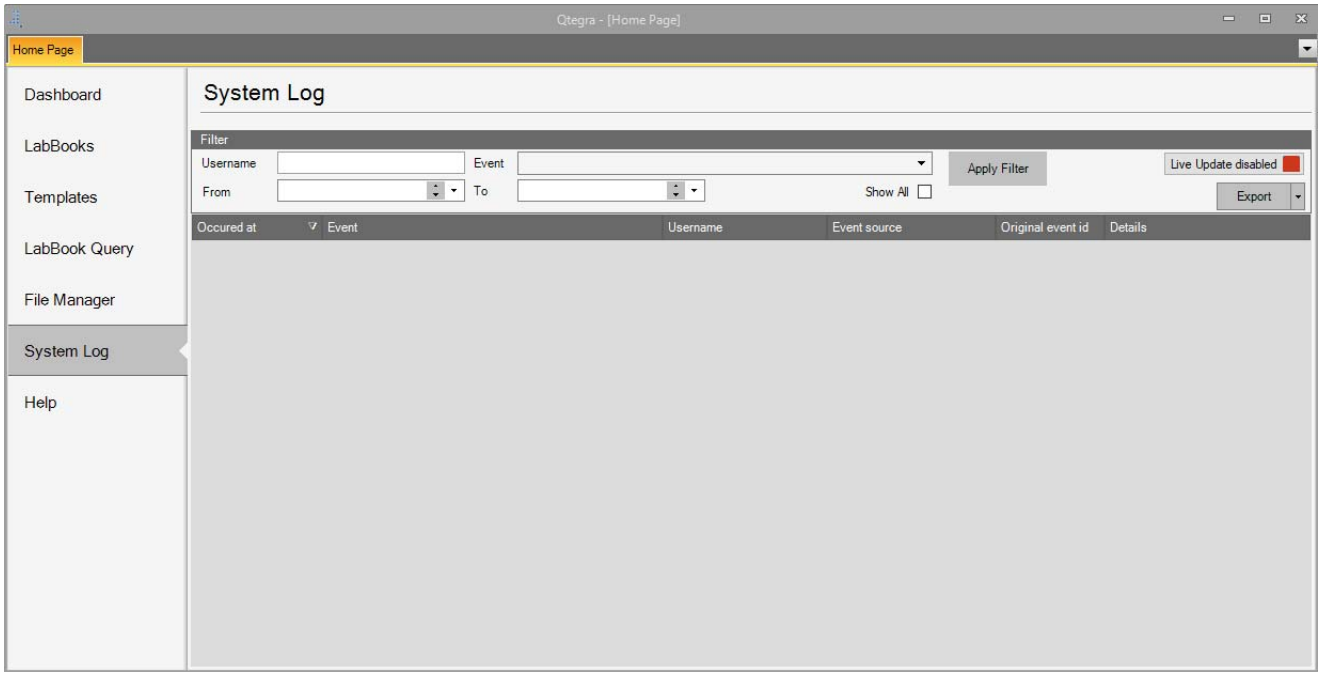
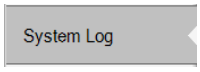


Figure 4-79. System Log Page of Qtegra

Many customers, for example, pharmaceutic companies, want to set up the environment that it complies with 21 CFR Part 11. This page of the Qtegra ISDS Software allows to check your system regarding changes in special settings. The System Log keeps all system data. Qtegra ISDS extracts the relevant part and displays this part as a table that may be configured by the user.

❖ **To open the System Log page of Qtegra**



1. From the **Qtegra - [Home Page]** navigation pane, click **System Log**.
   The System Log page opens.

   Tip System logs must be activated by setting the **Enable compliant system log** value in the Configurator to *True*. When set to *False*, no further events are collected but the existing entries may be displayed.

   The System Log displays a collection of compliant events initiated by Windows and Qtegra. The events are displayed as a list, which provides several functions to focus on the desired data. All information is collected from the Operating System and therefore displayed in more or less internal descriptors.

By default, the list shows 6 columns that are explained in Table 4-5.

Table 4-5. System Log columns

Column	Content
Occurred at	Date and time stamp of the logged event.
Event	Description of the event that is logged. Open the Category listbox above the list to see all possible events.
Username	Name of the originator, who initiated the event. Examples are the current Windows computer shown as *machine name*, Windows user shown by the *login name*, Windows services shown as *System*, *network service*, *local service*, and others.
Event source	*Windows security eventlog* to display Windows as originator. *Qtegra* to display this application as originator.
Original event id	The Windows events are internally stored with an identifier. This id may help to get detailed information about the event.
Details	If possible, Qtegra displays details about the event to show precise logged events, like setting values.

Filters are set on top of the System Log page, see Figure 4-80.

Figure 4-80. Filter settings on top of System Log page

Initially, no entries are shown as no filter is active and Show All is not ticked. 

is set by default to reduce the system load, that means, no further log entries are appended to the list but are collected in the background. With **Show All** enabled, events initiated by all users including, for example, *System, Computer name, Network Service*, and *Local Service* are shown.

❖ To filter the System Log

1. To reduce the amount of list entries and to focus on desired items, you may set a filter.

   Tip Every filter affects the complete System Log database. The displayed list nevertheless reduces the amount of items to 100 rows per page.

2. To filter by **Username**, type at least a part of the desired name into the edit box. Qtegra does not distinguish between upper and lower case letters.

   Click **Apply Filter** to update the list view accordingly.

3. To filter by a **date** or **time range**, click the triangle that opens a calendar sheet to select the begin in the **From** box and the end in the **To** box, see Figure 4-81.

   Click **Apply Filter** to update the list view accordingly.

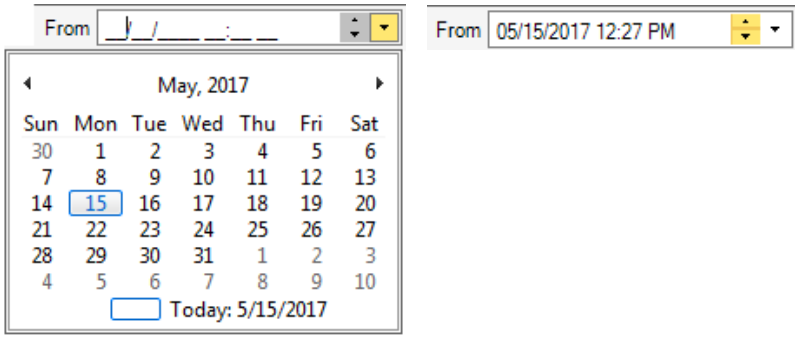


Figure 4-81. Date selection and Time justification on System Log page

4. To filter by **Event**, open the **Category** list box and select the item(s) you want to focus. The list box always contains all possible events independent from the events listed in the System Log.

   The selected categories are shown below this list box.
   Click **Apply Filter** to update the list view accordingly.

Tip Use the Category filter to focus on events that may contradict the rules from your SOP. In the filtered list, check the Details column to estimate the impact, see Table 4-6.

Table 4-6. Events with critical impact on 21 CFR Part 11

Category/Event [a]	Impact/Action
A windows system audit policy was changed	This event is written whenever a Windows setting relevant for auditing is changed. This can happen either by Qtegra itself when global compliance is established but also when the settings are changed manually or through a potentially existing Windows domain. Changes by Qtegra can be identified when looking at the other events surrounding the audit policy change: Qtegra itself will write events that it is now going to change audit policy settings. If no such context is found, this event indicates modifications originated from some other source. In that case, further investigation is necessary. **Tip** Qtegra will only try to reapply the settings for global compliance on system restart.
Windows audit policies could not be applied as configured	Qtegra was not able to activate the Windows settings necessary for full auditing. After this event, the system is not in a compliant state. The reason for this has to be further investigated in the Windows system event log and may require modification of the Windows system or domain settings.
System log auditing stopped	This event is written when the Windows system services belonging to Qtegra are stopped either explicitly or during system shutdown. System modifications are not audited until those services are started again.
System log auditing is now permanently turned off	The setting for global compliance has been explicitly set to *false* and all auditing is now turned off until the setting is manually activated again.
* A windows user account was changed	The credentials of the user account were changed, for example, if the user was added to or removed from a user group.

Table 4-6. Events with critical impact on 21 CFR Part 11, continued

Category/Event [a]	Impact/Action
* A windows audit policy setting differs from configuration	This event indicates differences in settings. Check both the Windows audit settings and the Qtegra configuration.
* A windows audit policy setting has been modified to match configuration	This security policy setting determines whether the operating system generates audit events when changes are made to authentication policy.
* System resources for auditing are exhausted	This event indicates an extremely high period of activity prevented Windows from logging a number of security events.
* A windows logon was attempted using explicit credentials	This event tracks different situations: • A user connects to a server or runs a program locally using alternate credentials. • This event is also logged when a process logs on as a different account such as when the Scheduled Tasks service starts a task as the specified user. • With User Account Control enabled, an end user runs a program requiring admin authority.

[a] Events marked with an asterisk are not critical regarding to your SOP settings but may appear in the System Log.

5. To remove a filter, click into the box on top of the System Log view and delete the entry.

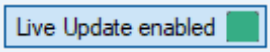
   Click **Apply Filter** to update the list view accordingly.

❖ **To navigate through the results**

1. After you clicked **Apply Filter**, the resulting system log events are listed.

2. Below the list, click the navigation buttons to leaf one page forward or backward or to scroll to the beginning or end.

3. Drag the slider on the right edge to scroll through the 100 items that are shown per page.

   Tip When 

is selected, the list is updated every minute. After update, the slider jumps to the first page. Therefore, you may lose your current view. The filter values remain active.

4. To suppress continuous updates, set 

.

❖ To arrange the System Log view

1. To move a column to another position, click the column header you want to move, and drag this selection horizontally to the desired position.
   Arrows indicate the target position. Release the mouse button to move the column to the desired position.

❖ To export the System Log

The exported files always contain only the filtered data. To export a longer list, reset the filters and the max. rows value before you start to export.

1. Expand the **Export** button and select the file format for the Report.
2. Select **Save as HTML** to generate a Report that is displayed in the Browser.
   The Browse For Folder dialog is opened to select the folder where you want to save the HTML output.
3. Select **Save as PDF** to compile a PDF Report that shows the (filtered) System Log.
   The PDF is shown in your PDF viewer.
   The Save As dialog is opened to select the folder and to type the file name of the PDF file.
4. Select **Save as RTF** to generate a Report that is displayed in Microsoft Word or your alternative RTF viewer.
   The Save As dialog is opened to select the folder and to type the file name of the RTF file.
5. Select **Save as XML** to generate a Report that is displayed in the Browser.
   The Browse For Folder dialog is opened to select the folder where you want to save the XML output.

Help Page

The **Help** page of Qtegra, see Figure 4-82, provides information about Qtegra, support and tools.

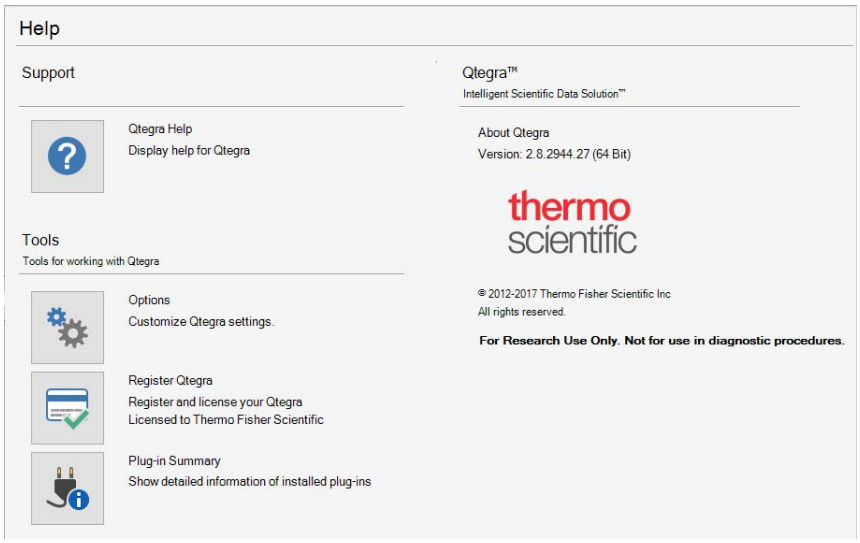


Figure 4-82. Help Page of Qtegra

❖ **To open the Help page of Qtegra**

1. From the **Qtegra - [Home Page]** navigation pane, click **Help**. The **Help** page of Qtegra opens.

Support on the Help Page

The **Support** section on the **Help** page of Qtegra offers access to the Qtegra Help.

❖ **To open the Qtegra Online Help**

1. On the Help page of Qtegra, click **Qtegra Help**. The *Software Manual* opens in your PDF Viewer tool.

Customizing Home Page Settings

In the **Tools** section on the **Help** page of Qtegra, you can customize your **Home Page** settings.

❖ **To customize the Home Page settings**

1. On the Help page of Qtegra, click **Options**.

2. Under **Available** on the left pane, select **Home Page**, see Figure 4-83.

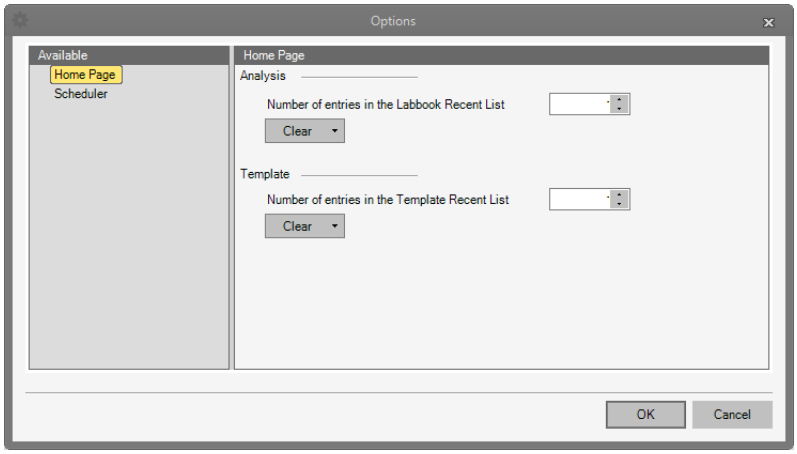


Figure 4-83. Home Page settings in Options dialog of Help page

3. For **Analysis** on the right, select the number of entries for **LabBook Recent List**.
4. From the **Clear** drop-down list, select **All entries** or **Unpinned entries** if you wish to clear the list.
5. For **Template** on the right, select the number of entries for **Template Recent List**.
6. From the **Clear** drop-down list, select **All entries** or **Unpinned entries** if you wish to clear the list.
7. Click **OK**.

Customizing Scheduler Settings

In the **Tools** section on the **Help** page of Qtegra, you can define your **Scheduler** settings.

Tip To customize the Scheduler, you can also click on the toolbar of the Scheduler.

❖ **To customize the Scheduler settings**

1. On the Help page of Qtegra, click **Options**.

2. Under **Available** on the left pane, select **Scheduler** to define the settings, see Figure 4-84.

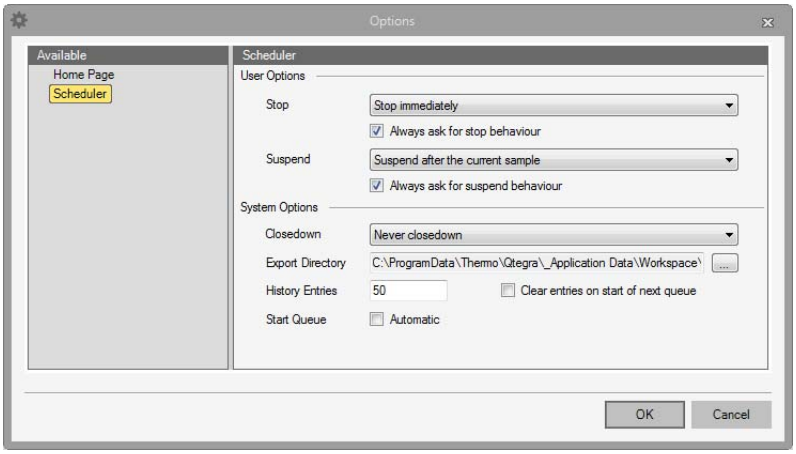


Figure 4-84. Scheduler settings in Options dialog of Help page

3. For **User Options** on the right, select the stop behavior of the Scheduler from the drop-down list **Stop**.
4. Select the **Always ask for stop behavior** check box if you wish to be asked every time.
5. Select the suspend behavior from the drop-down list **Suspend**.
6. Select the **Always ask for suspend behavior** check box if you wish to be asked every time.
7. For **System Options**, select the close-down options from the **Closedown** drop-down list.
8. Click ... to choose the **Export Directory**. After installation, this directory is set to C:\ProgramData\Thermo\Qtegra_Application Data\Workspace\Exports.
9. Type a number for **History Entries** to specify the maximum entries of completed LabBooks (refer to “Completed LabBooks”).
10. Select the **Clear entries on start of next queue** check box to clear the list of completed LabBooks with every start of the Scheduler.
11. For **Start Queue**, select **Automatic** if you want the measurement to start immediately when a LabBook is added to the Scheduler.
12. Click **OK**.

Registering Qtegra

The **Tools** section on the **Help** page of Qtegra offers access to the license manager of Qtegra.

❖ **To show details of registration information**

1. On the Help page of Qtegra, click **Register Qtegra**.
2. The Qtegra Registration Manager opens with the Registration Overview about the license type, activation type, licensed optional features and modules.
3. In the Qtegra Registration Manager window, click **Update Registration** to add additional license keys or to update your address data.

For details on registering Qtegra, refer to the *Installation Guide*.

Information about Plug-ins

When solving problems with the plug-ins or to get information about the last changes of the plug-ins used in your instrument environment, you can get information about the installed version on this page. This may help the support staff or Thermo Fisher Scientific field service engineers.

❖ **To show detailed information of installed plug-ins**

1. On the Help page of Qtegra, click **Plug-in summary**.
   A dialog opens and displays a list of available plug-ins, see Figure 4-85.

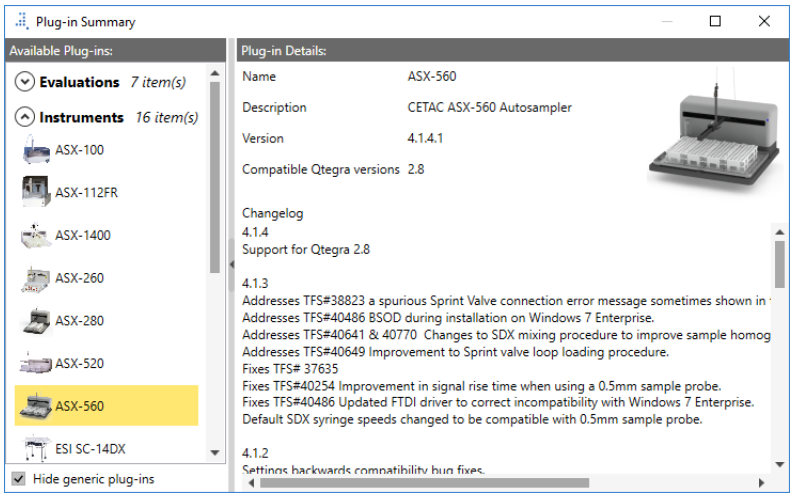


Figure 4-85. plug-in Summary window

2. To display the plug-in details, select the desired plug-in on the left pane.
   The right pane then shows a preview thumbnail of the selected item and its full name, description, version number, and the compatible Qtegra ISDS Software version number.
   The changelog shows the history of changes.

The Plug-in Summary dialog provides the following options.

- Collapse and expand the **Instruments** and **Evaluations** plug-ins if desired.
- To show generic plug-ins, remove the tick from **Hide generic plug-ins**. A *GenericInstrument* is a user defined virtual instrument for advanced customers.

3. To close this summary view, click **Close [×]** in the upper right corner of the window.

Scheduler

In the **Scheduler** tool of Qtegra, the measurement for a scheduled LabBook is executed. The completed LabBook is automatically deleted from the Scheduler and added to the list of Completed LabBooks.

Tip The Scheduler tab can be moved within Qtegra to change to a separate window.

The buttons to control the Scheduler are summarized in the toolbar of the **Scheduler**, see Table 4-7.

Table 4-7. Control buttons for the Scheduler

Icon	Meaning	Description
	Run	Begins scheduling the LabBooks waiting in the ready queue.
	Suspend	Suspends the scheduling of LabBooks waiting in the ready queue.
	Stop	Stops the scheduling of LabBooks waiting in the ready queue.
	Move to Top	Moves the selected LabBooks to the head of the Scheduler waiting queue.
	Move Up	Moves the selected LabBook up one position in the Scheduler waiting queue.
	Move Down	Moves the selected LabBook down one position in the Scheduler waiting queue.
	Move to Bottom	Moves the selected LabBooks to the foot of the Scheduler waiting queue.
	Remove	Removes the selected LabBooks from the Scheduler waiting queue.
	Remove All	Removes all LabBooks from the Scheduler waiting queue.
	Options	Displays the Scheduler Options dialog to define stop and suspend behavior and system options regarding the close-down behavior, the export directory, number of history entries, and start queue behavior.

Table 4-7. Control buttons for the Scheduler, continued

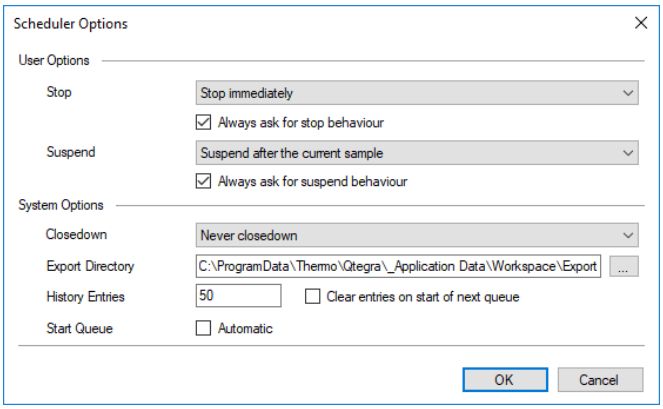
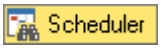
Icon	Meaning	Description
		
		The Scheduler settings can be customized via the Options button in the Scheduler toolbar, or in the **Tools** section on the **Help** page of Qtegra.

Figure 4-86. Scheduler Options dialog

Tip The Scheduler region can be moved within Qtegra to change to a separate window.

❖ **To open the Scheduler of Qtegra**



1. From the **Qtegra - [Home Page]**, click **Scheduler** to open the **Scheduler** tab, see Figure 4-87.

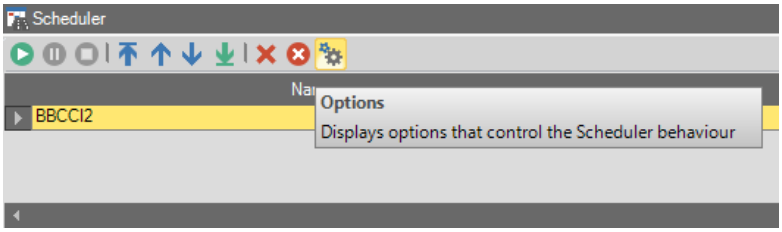


Figure 4-87. Scheduler tool

❖ **To add a LabBook to the Scheduler and run it**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook.

2. On the toolbar of the LabBook, click **Schedule** to schedule the LabBook for execution.
   -or-

Press **<Ctrl> + <R>**.
The LabBook is added to the Scheduler.

Tip If the **Automatic** check box has been selected for **Start Queue** in the **Options** settings of the Scheduler, the measurement starts immediately.

3. In the Scheduler, select the LabBook and click **Start** to start the measurement.
The LabBook measurement starts, see Figure 4-88.

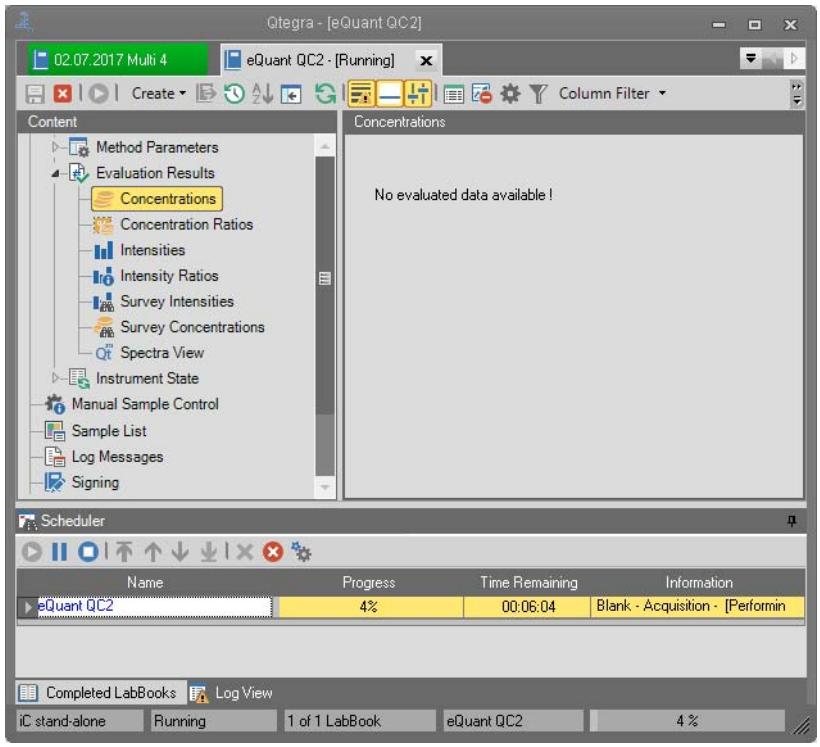


Figure 4-88. Scheduler tool

Tip The Configuration of this LabBook must match the currently loaded Configuration on the Dashboard. If an error message is displayed in the Log View indicating an incompatibility between the configuration saved in the LabBook and the current configuration, the LabBook is not added to the Scheduler. In this case, open the original LabBook and check the Summary page for the instruments configured and change your Configuration accordingly.

In the Scheduler, the **Progress** column shows the progress of the execution in percent.

❖ To stop the execution of a LabBook in the Scheduler

1. Check the progress of the execution to make sure a LabBook is currently running and the Scheduler toolbar buttons are enabled.

2. On the Scheduler toolbar, click **Stop**.
   The **Stop Behavior** dialog opens, see Figure 4-89.

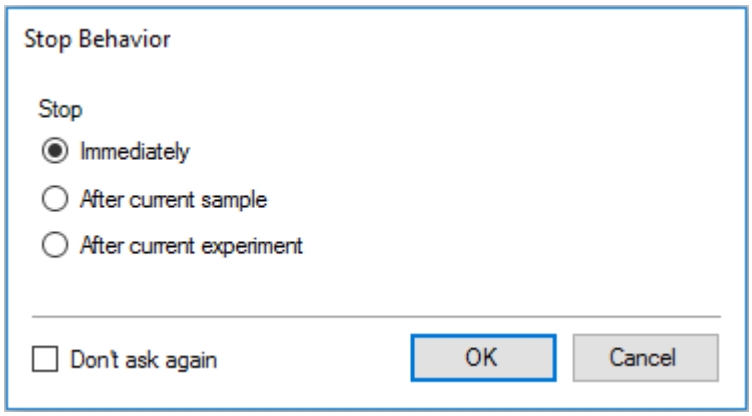


Figure 4-89. Stop Behavior dialog

3. Select **Immediately** to stop the execution of the LabBook and to remove it from the Scheduler queue.

   Select **After current sample** to keep measuring the current sample and then stop the LabBook and remove it from the Scheduler queue.

   Select **After current experiment** to perform the measurement of the current LabBook until its end. Then stop the Scheduler and keep all following LabBooks in their scheduled position. Click **Start** to start the next LabBook.

4. Tick **Don't ask again** to keep your selection for all scheduled LabBooks. In case the **Stop** button is clicked no Stop Behavior dialog is displayed. Open the **Scheduler Options** dialog (see Figure 4-86) to clear this setting.

❖ **To pause the execution of a LabBook in the Scheduler**

Beside the option to pause a LabBook automatically, you may interrupt the execution in the Scheduler as follows:

1. Check the progress of the execution to make sure a LabBook is currently running and the buttons of the Scheduler toolbar are enabled.

2. On the Scheduler toolbar, click **Pause**.
The **Suspend Behavior** dialog opens, see Figure 4-90.

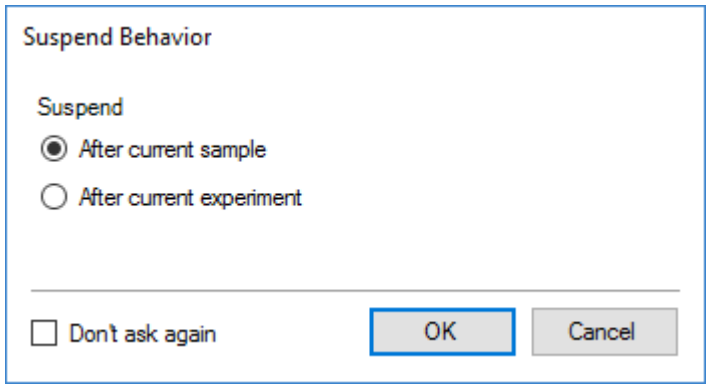


Figure 4-90. Suspend Behavior dialog

3. Select **After current sample** or **After current experiment** to define the suspend behavior.

4. Click **OK**.
The execution of the LabBook is paused after the selected action has been completed.

5. On the Scheduler toolbar, click **Start** again to resume the execution of the LabBook.

❖ **To change the order of LabBooks in the Scheduler**

1. Check the progress of the execution to make sure some LabBook are added to the Scheduler, and the buttons of the Scheduler toolbar are enabled.

2. In the Scheduler, select the LabBook you wish to move up or down in the queue.

3. Click one of the arrow buttons to move the LabBook to the desired position in the queue, for example, to the top of the queue, see Figure 4-91.

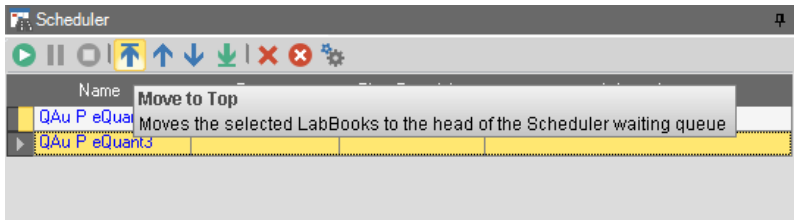


Figure 4-91. Moving LabBook in Scheduler queue

4. Click **Delete** to delete the selected LabBook.

5. Click **Remove all** to remove all entries of the queue.

❖ **To set additional options of the Scheduler**

1. On the Scheduler toolbar, select **Options** to display the Scheduler Options dialog.
2. Refer to “Customizing Scheduler Settings” for additional User and System Options.

Completed LabBooks

Upon completion of a LabBook, the LabBook is automatically deleted from Scheduler and added to the **Completed LabBooks** tab in Qtegra, see Figure 4-92.

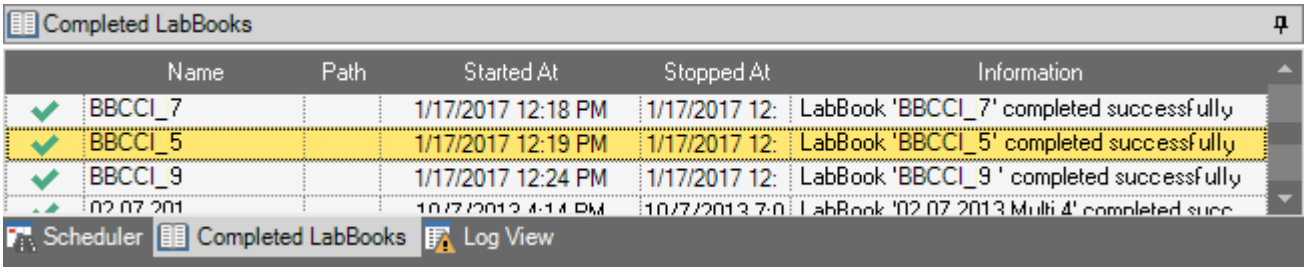


Figure 4-92. Completed LabBooks

Tip The Completed LabBooks tab can be moved within Qtegra to change to a separate window.

To reduce the number of entries in this list of completed LabBooks, set a value for History Entries in the Options dialog. Tick the desired check box in the Options dialog to clear this list of completed LabBooks upon every start of the Scheduler.

❖ **To open the Completed LabBooks tab**

1. From the **Qtegra - [Home Page]**, click **Completed LabBooks** to open the **Completed LabBooks** tab.
   All LabBooks that have already been executed are listed.

❖ **To open a LabBook from the Completed LabBooks**

1. In the Completed LabBooks list, click the LabBook you wish to open.
   The completed LabBook is opened in a new tab.

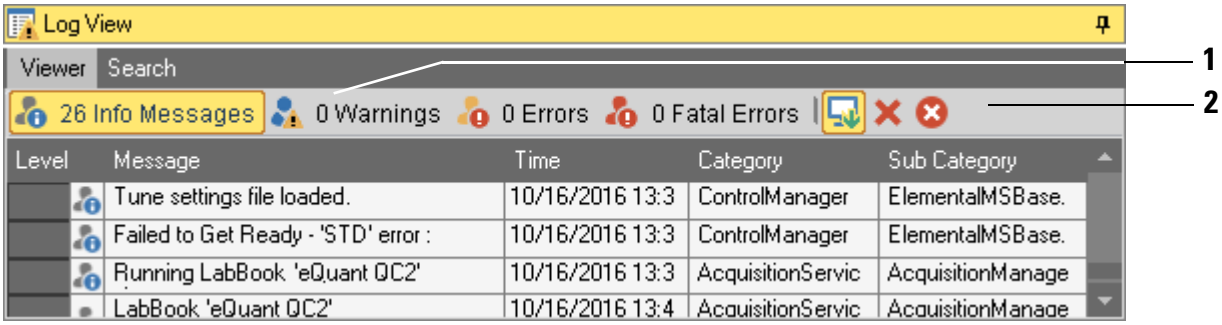
Log View

The **Log View** region of Qtegra displays a list of messages, such as errors and warnings. By default, different levels of messages are displayed. The Viewer tab is also shown in the Configurator tool.

Tip The Log View region can be moved within Qtegra to change to a separate window.

❖ **To open the Log View region**

1. From the **Qtegra - [Home Page]**, click **Log View** to open the **Log View** region, see Figure 4-93.



Labeled Components: 1=Message level selectors, 2=Viewer toolbar

Figure 4-93. Log View region in Qtegra

❖ **To scroll directly to incoming messages in the Viewer**

1. In the Log View region, select the **Viewer** tab.

2. On the toolbar, click **Scroll to message**.
The Viewer scrolls directly to new incoming messages.

❖ **To delete rows in the Viewer**

1. In the Log View region, select the **Viewer** tab.
2. Select the row or rows you wish to delete.

3. On the toolbar, click **Delete**.
The selected row or rows are deleted from the Viewer tab.

❖ **To clear all in the Viewer**

1. In the Log View region, select the **Viewer** tab.

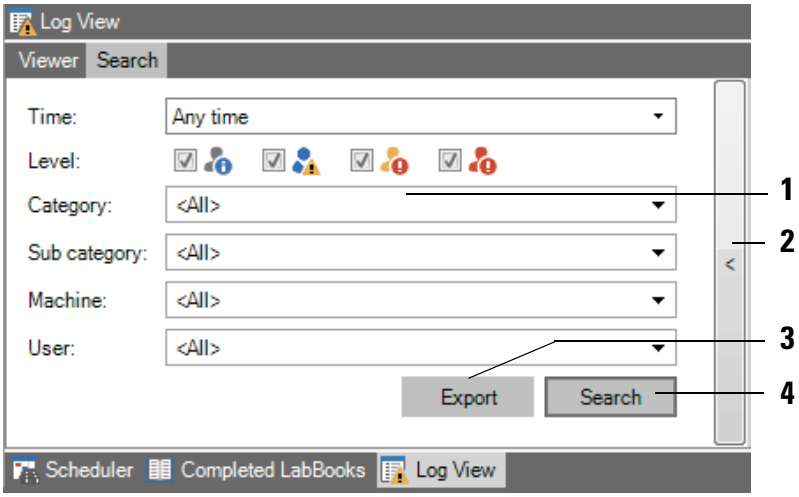
2. On the toolbar, click **Clear all**.
All entries are deleted from the Viewer tab, but all logged messages remain in the internal Qtegra ISDS Software database.

Tip The row deletion and clear all actions in this Viewer do not change the permanently stored information in the internal Qtegra ISDS Software logs.

To query the permanent logs, open the Search tab in the Log View region.

❖ **To search all logged events**

1. In the Log View region, select the **Search** tab.
   A pane opens to enter search data, see Figure 4-94.



Labeled Components: 1= Filter settings area, 2=Collapse/Expand button, 3=Export button, 4=Search button

Figure 4-94. Log View Search window

Initially, no filter is set and all search levels are selected (**1** in Figure 4-94).

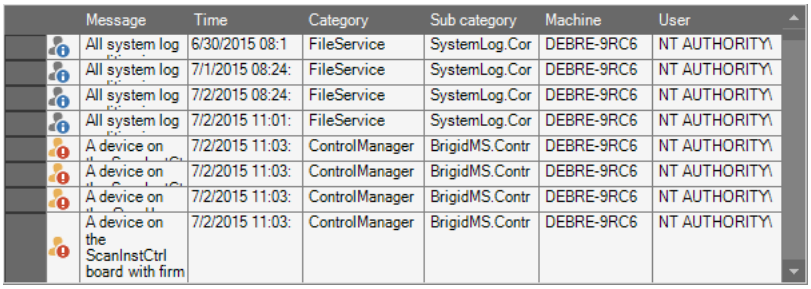
2. To reduce the list of log messages displayed, use the drop-down menus to filter the items as per Table 4-8.

Table 4-8. Search filter settings

Filter	Description
Time	Provides a list of time ranges (**Last hour**, **Last 12 hours**, **Last 24 hours**, **Last 7 days**). Select **Custom range** to set the begin and end of the period in a dialog. Select **Any time** to reset the filter.
Level	Tick the check boxes  to set the filter for **Info Messages**, **Warnings**, **Errors**, or **Fatal Errors**. Select all check boxes to reset the filter. For details refer to “Message levels”. Depending on the value of Configurator > Settings > Logging > ShowAll an additional filter icon  is displayed to show all messages including debug messages.
Category	Provides a list of software modules and services to select the category, which is responsible for the logged message. **AcquisitionService**, **Configurator**, **ControlManagerService**, **FileService**, **HardwareService**, **HubService**, **Qtegra**, **ServiceStatus** are available.
Sub category	Provides a list of all sub categories used in Qtegra ISDS Software. Select the sub category if you need to focus the Log View on this level. Remove all selections to reset the filter.
Machine	Provides a list of computer names, where this log file was created and updated. Remove all selections to reset the filter.
User	Provides a list of Qtegra users including the **NT AUTHORITY \ SYSTEM** user that represents automated Qtegra actions. Select the user to show log messages created by his/her activity. Remove all selections to reset the filter.

Search

3. Click **Search** (**4** in Figure 4-94) to display the search result. On the right, the filtered log file shows the result list with the Level, Message, Time, Category, Sub category, Machine, and User.



Message	Time	Category	Sub category	Machine	User
All system log	6/30/2015 08:1	FileService	SystemLog.Cor	DEBRE-9RC6	NT AUTHORITY\
All system log	7/1/2015 08:24:	FileService	SystemLog.Cor	DEBRE-9RC6	NT AUTHORITY\
All system log	7/2/2015 08:24:	FileService	SystemLog.Cor	DEBRE-9RC6	NT AUTHORITY\
All system log	7/2/2015 11:01:	FileService	SystemLog.Cor	DEBRE-9RC6	NT AUTHORITY\
A device on	7/2/2015 11:03:	ControlManager	BrigidMS.Contr	DEBRE-9RC6	NT AUTHORITY\
A device on	7/2/2015 11:03:	ControlManager	BrigidMS.Contr	DEBRE-9RC6	NT AUTHORITY\
A device on	7/2/2015 11:03:	ControlManager	BrigidMS.Contr	DEBRE-9RC6	NT AUTHORITY\
A device on the ScanInstCtrl board with firm	7/2/2015 11:03:	ControlManager	BrigidMS.Contr	DEBRE-9RC6	NT AUTHORITY\

Figure 4-95. Search result list

4. Click the arrow button (**2** in Figure 4-94) to collapse the Filter pane and to expand the search result list.

5. In the search result list, click the leftmost cell to select the appropriate rows. Right-click to open the shortcut menu where you may copy the selection to your Windows clipboard.

Export

6. Click **Export** (**3** in Figure 4-94) to save the search result list as a CSV file that may be opened with the associated program. The exported file is named *LogViewMessages.csv*, by default.

Message levels

Qtegra displays four levels of error messages.

Table 4-9. Message levels

Level	Description
Info 	**Information message** This is the lowest level of message shown in the Log View. An information message is generated for informational purposes in Qtegra ISDS Software. It does not reflect any issue with the actual measurement. Example messages are: “Igniting the plasma”, “Rinsing autosampler”, Drain Sensor Enabled”, etc.
Warnings 	**Warning message** This is the next highest level of message shown in the Log View. A warning message indicates an event in Qtegra ISDS Software that might possibly lead to an error. Example messages are: “Moving to rinse failed”, “Unable to move motors.”, “Export was incomplete”, etc.

Table 4-9. Message levels, continued

Level	Description
Errors 	**Error message** This is the next highest level of message. An error message indicates possibly recoverable errors in Qtegra ISDS Software. Example messages are: “Failed to run exposure”, “Error during Nebulizer Optimization”, etc.
Fatal errors 	**Fatal error messages** This is the highest level of message shown in the Log View. A fatal error messages indicates a severe error that may prevent Qtegra ISDS Software from continuing working properly. Example messages are: “Could not load calibration data, please ensure the file CidSpectrum.bin is available.”, “GetParameter for {0} failed”, etc. It is recommended to call the Thermo Fisher Scientific field service engineer to solve the problem.

Unexpected Errors

Under rare circumstances, it can happen that Qtegra needs to be restarted. In this case, Qtegra opens a message to inform the user.

The message depends on the current status of Qtegra applet or LabBooks. In case Templates, LabBooks or applets are saved, an automatic restart is initiated. A count down is displayed, see Figure 4-96.

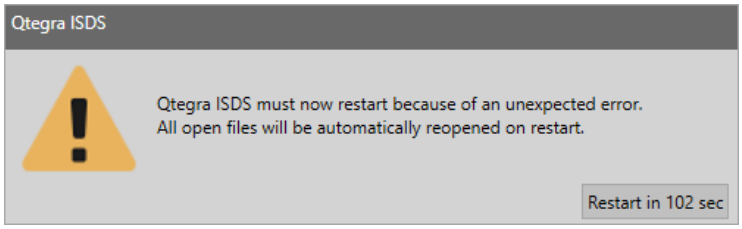


Figure 4-96. Qtegra restart message with count down

In case files are changed but not saved, a slightly different message is shown, see Figure 4-97.

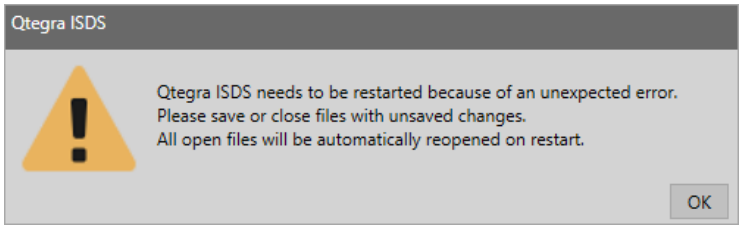


Figure 4-97. Qtegra restart message with OK button

When this message is shown, click **OK**. Further messages will open and ask to save or close each Template, LabBook or applet with changes. Then Qtegra closes and restarts automatically.

All open files will be automatically reopened on restart.

5

Templates

The analytical workflow for sample measurement is defined in a Template. A Template ideally suited when one or more analytical methods are run on a routine basis with fixed method parameters but varying sample numbers, for example, provided through a Laboratory Information Management System (LIMS). Templates are created as shown in "Templates Page" on page 4-36.

Templates are based on a particular Configuration, which is usually defined by the Administrator or Thermo Fisher Scientific field service engineer (see "Configurator" on page 3-1) and reflects your system setup. Each Template consists of a Method Parameters section, a Sample Definition section, an Automatic Export section, and a section for the Peripherals if so configured for this Configuration.

The Method Parameters within a Template are dependent on the evaluation method assigned to the Template (see "Evaluation Methods" on page 9-2). For every application an appropriate Template can be created.

Contents

❖ **To open the Templates page in Qtegra ISDS Software**

1. From the **Qtegra** - [**Home Page**] navigation pane, click **Templates**. The Templates page of Qtegra opens.
2. Create or open a Template as shown in "Templates Page" on page 4-36.

   The Template opens in a new tab with the following items.

Template Toolbar

The Template tab offers buttons to save, close or run a Template, see Figure 5-1.

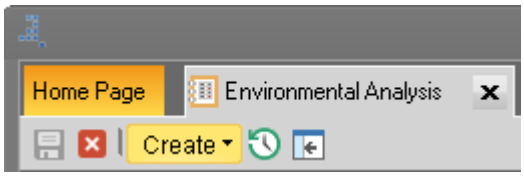


Figure 5-1. Template toolbar

Additionally, you can create a new LabBook or Template from the current Template, view the history of the current Template or hide the Content pane.

❖ **To save a Template**

1. Change the settings as appropriate.

2. Click **Save** to save the changes.
   -or-
   Press **<Ctrl> + <S>** to save your Template.
   The **Save Template** dialog opens, see Figure 5-2.

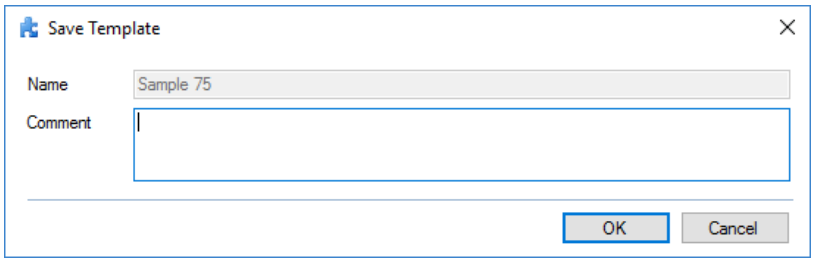


Figure 5-2. Save Template dialog

3. Enter a **Comment** for the Template.
   The comment will be shown in the History view.
4. Click **OK**.
   The Template is saved.

❖ **To close a Template**

1. Click **Close** on the Template toolbar.

   -or-

   Click **Close** in the tab of the Template to close the Template.

❖ **To create a LabBook or Template from an existing Template**

1. In the Templates view, click **Create**.
   The **Create** drop-down menu opens, see Figure 5-3.

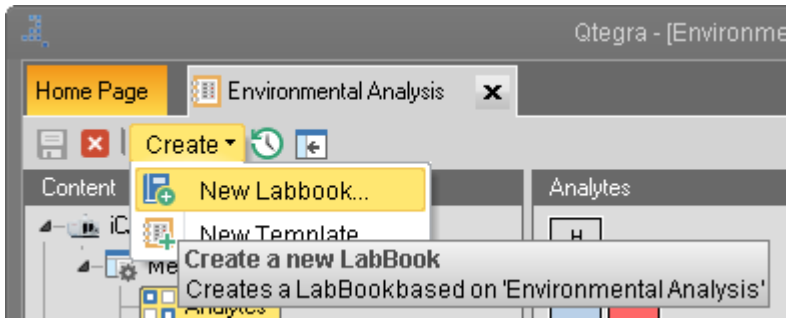


Figure 5-3. Create drop-down in Templates toolbar

2. Click **New LabBook** if you wish to create a new LabBook from the existing current Template.
   The **LabBooks** view of the **Home Page** opens. See "Creating LabBooks" on page 4-24 for further details.

3. If you wish to create a new Template from the existing current Template, click **New Template**.
   The **Templates** view of the **Home Page** opens. See "Creating a Template" on page 4-38 for further details.

❖ **To view, compare and export the history of a Template**

For details, refer to "To view, compare and export the history of a LabBook" on page 6-5 as your action is the same.

❖ **To hide the Content pane**

1. In the Templates view, the **Content** pane is shown on the left, see Figure 5-4.

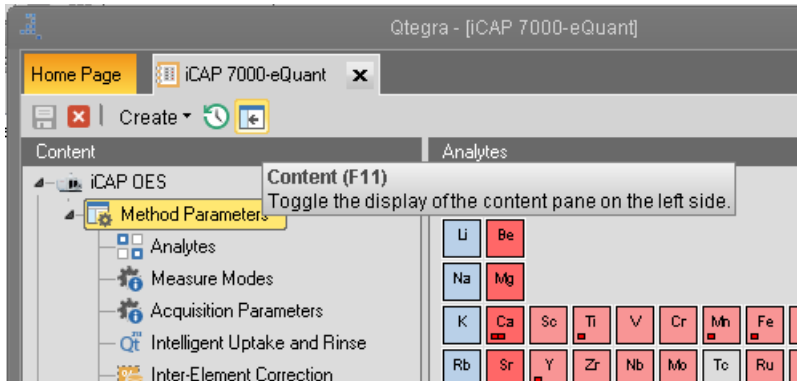


Figure 5-4. Content pane of Template visible

2. Click **Toggle**.
   -or-
   Press <F11>.

The **Content** pane is hidden, see Figure 5-5. The main window area may be used to display the selected Method Parameter in a maximum size.

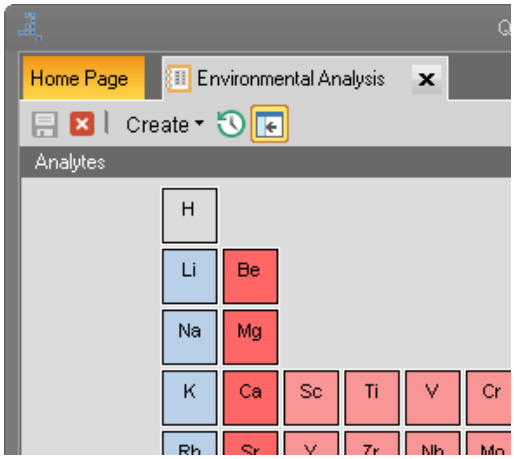


Figure 5-5. Content pane of Template hidden

3. Click **Toggle**.
   -or-
   Press <**F11**> to show the **Content** pane again.

Sample Definition for a Template

In the Sample Definition view of a Template (see Figure 5-6) you define the sample type and actions inserted in the LabBook that you create from this Template.

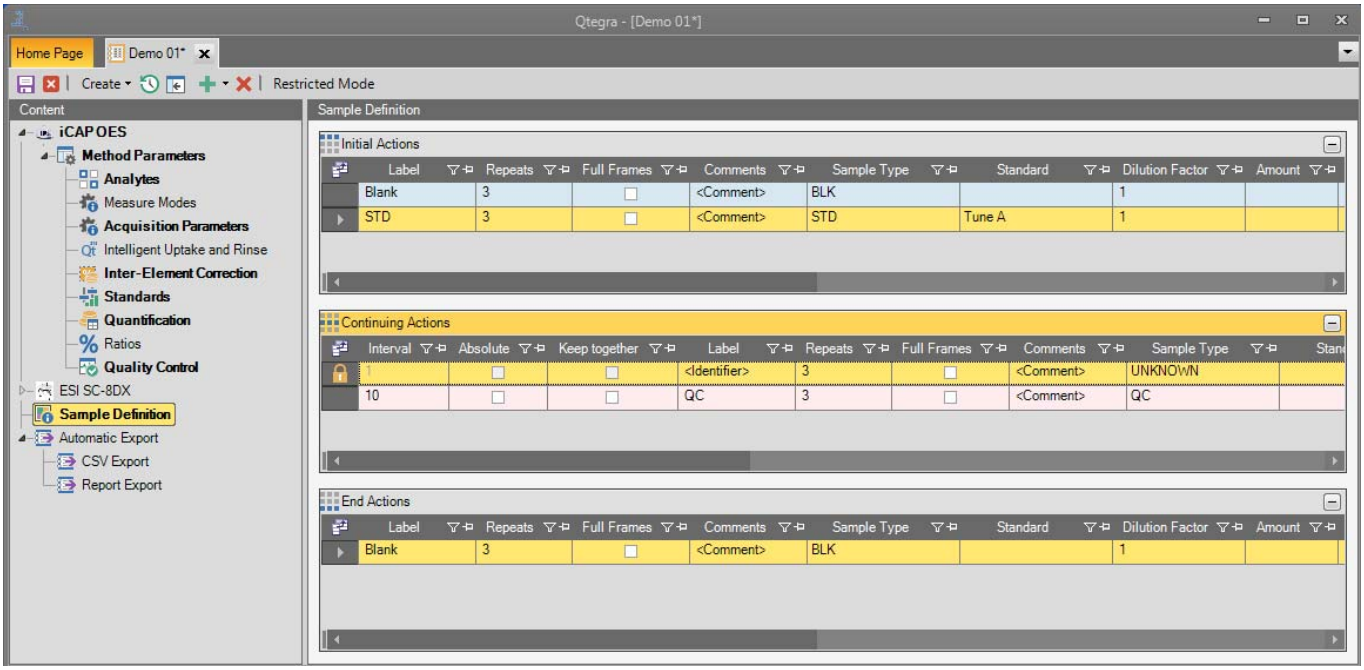


Figure 5-6. Sample Definition view

Tip For Sample Definition, the Restricted Mode button is added to the toolbar of the Template. Activated, this option restricts editing of the Sample List for the LabBook created from this Template. Samples can then only be added or deleted at the end of the Sample List.

The Sample Definition consists of three sections in your Template to be populated with Blanks, Standards, QCs, and Unknown samples.

In the **Initial Actions** you enter samples to be inserted once at the start of the Sample List. Usually, samples of type BLK, STD, and initial QC are defined here. Click the green Plus sign on the toolbar to add a line, where you can specify the initial action, for example, select *BLK* from the Sample Type drop-down menu and double-click the Label and type *Blank*. Add another line and specify at least one standard, for example, select *STD* from the Sample Type drop-down menu, select the standard solution *Tune A* from the Standard drop-down menu, and type *STD* as the Label.

The **Continuing Actions** lines make up a repeating unit of the Sample List when creating a LabBook. Typically, standard and unknown sample types are defined here, see Table 5-1. The Continuing Actions rows unit is repeated with the number of samples desired for the LabBook. If, for

example, the Interval is set to *10*, the QC sample will be inserted after each 10 samples. If the Interval is set to *5*, the QC sample will be inserted after each 5 samples.

The **End Actions** rows are for samples (such as QC samples) to be inserted at the end of the Sample List.

Table 5-1. Columns of Sample Definition > Continuing Actions

Column	Description
Interval	Amount of UNKNOWN samples to be added to your LabBook, until the next line is run. The first line always is locked and the Interval is set to *1*. This line acts as a place holder for UNKNOWN samples to be added during creation of a LabBook.
Absolute	Part of continuing actions in your Template. This option is only relevant for QC entries to become compliant with US EPA. When you tick this check box, the sample is latest inserted as the sample line defined by the *Interval*. If, for example, due to other repetitions sample measurements are added and would therefore block the desired line, this option ensures QC at least to appear at the specified line.
Keep together	Part of continuing actions in your Template. This option is only relevant for QC entries to become compliant with US EPA. When you tick this check box, the sample is kept together with the following line. If, for example, a QC entry is inserted by its definition, both lines that are kept together will never be split. Instead, the other action (QC) is set above.

Depending on the evaluation method selected for the Template, the columns of the components may differ. Columns that may be shown in Sample Definition and Sample List are explained in Table 14-5.

After creating a LabBook from the Template (see "Template Toolbar" on page 5-2 and "Creating LabBooks" on page 4-24), the column **Special Blank** is added to the Sample List (see Figure 6-15).

❖ **To open the Sample Definition view of a Template**

1. On the Templates view, click **Sample Definition** to open the Sample Definition view.

Customizing the Columns for Sample Definition

You can show or hide the columns for **Initial Actions, Continuing Actions** and **End Actions** of the Sample Definition view and change the order in the table.

❖ **To customize the appearance of columns**

1. Open the Sample Definition view.

2. In the **Initial Actions, Continuing Actions** and **End Actions** section you wish to change, click the **Field Chooser** icon.
   -or-
   Open the shortcut menu on the table header and select Columns > More.

   The **Choose Columns** window opens, see Figure 5-7.

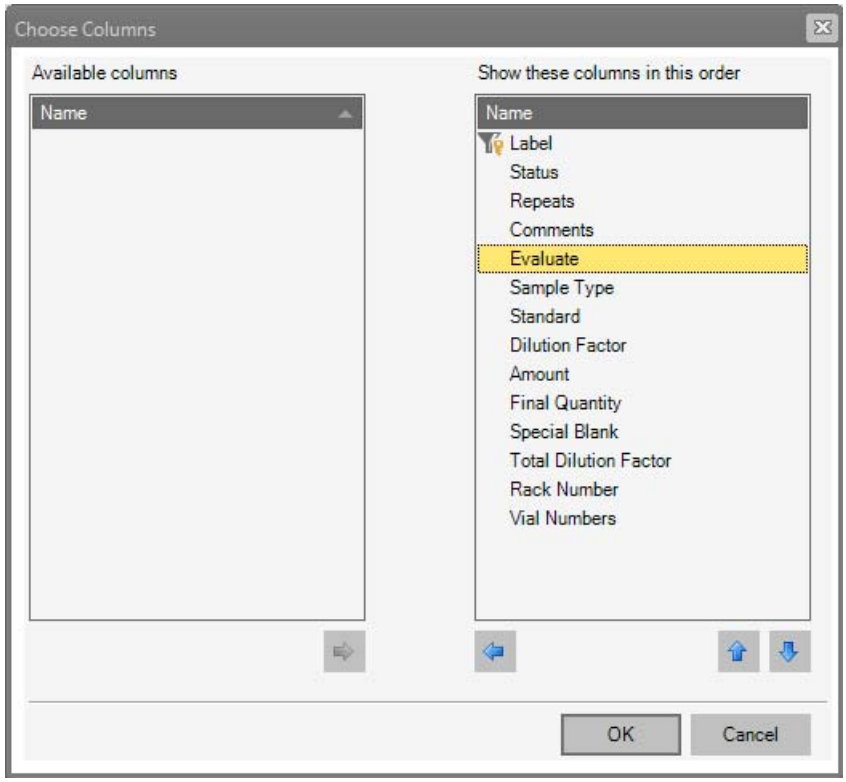


Figure 5-7. Choose Columns window of Sample Definition

3. Click the up/down arrow to move the column headings up or down.

4. Select a column in the right list and click the left arrow.
   -or-
   Double-click a column heading in the right list to move it to the list of available columns.
   This column is hidden in the Sample Definition view.

5. Click **OK**.
   The columns are arranged accordingly.

Defining the Initial, Continuing and End Actions

In the Sample Definition view of Qtegra, Initial, Continuing and End Actions items are defined. Additional lines can be added and values can be defined.

❖ **To define Initial, Continuing and End Actions**

1. Open the Sample Definition view.

2. On the toolbar of the Template, open the Actions drop-down menu, see Figure 5-8.

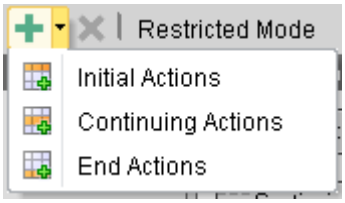


Figure 5-8. Add lines for Sample Definition

3. Select the item you wish to add a line for.
A line is added to the selected item.

4. Type the values in each column to your needs.
-or-
Select an item from the drop-down menu, if available.
For details on the columns, see "Sample Definition for a Template" on page 5-5.

5. Click **Save** to save the changes to your Template.

Defining the Settings in Sample Definition

The settings for your experiment are defined in the Sample Definition section of your Template.

❖ **To define the settings of your experiment**

1. On the Template view, define **Initial Actions, Continuing Actions** and **End Actions** as appropriate.

2. Add as many rows as you need for your experiment.

3. Type a **Label** for each row.

4. Select a **Sample Type** from the drop-down list, see Figure 5-9.

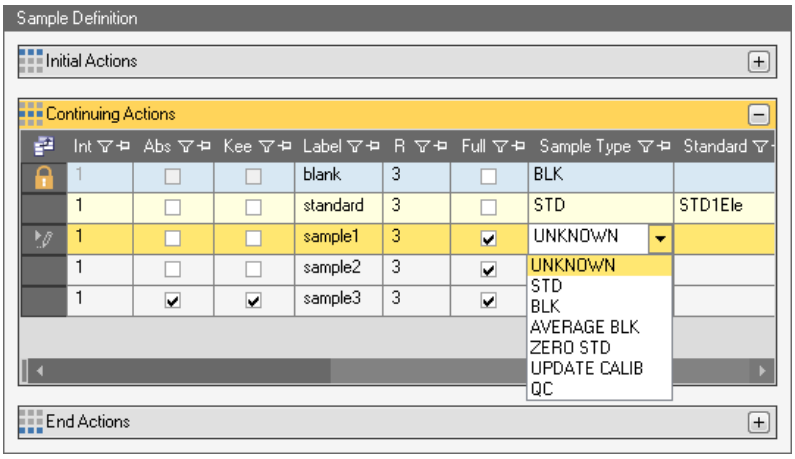


Figure 5-9. Sample Type drop-down in Template Sample Definition

For example, select **STD** for the calibration solution **UNKNOWN** for the samples, and **BLK** or **AVERAGE BLK** for blanks.

5. Type a value for each column.
-or-
Select an item from the drop-down list, as appropriate.

Tip For details on the columns, see "Sample Definition for a Template" on page 5-5.

6. Click **Save** to save the changes to your Template.

Automatic Export - Template

In the **Automatic Export** view of a Template in Qtegra, you define the export settings for your data as CSV or XML file and for Reports, see Figure 5-10.

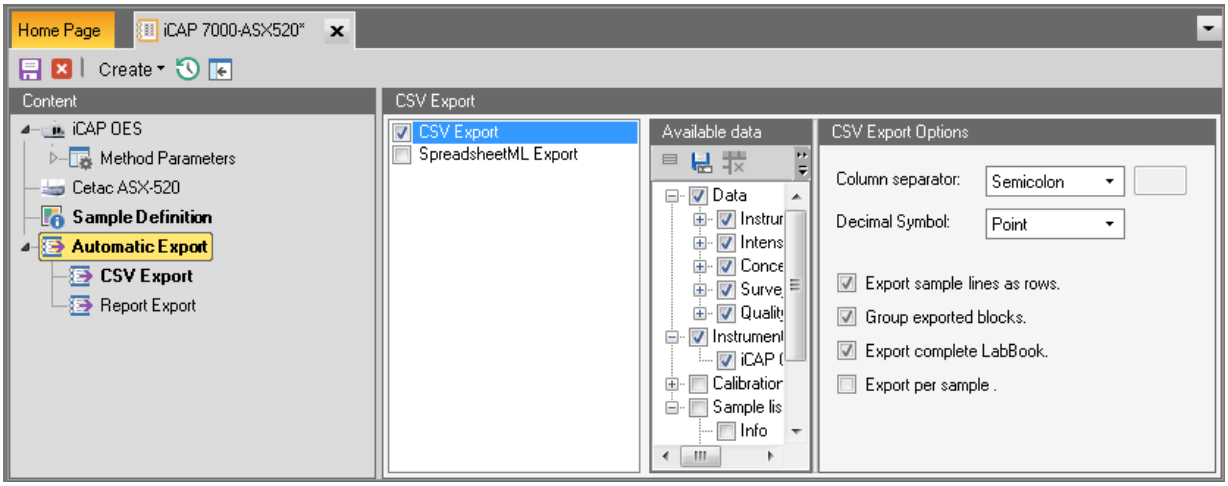


Figure 5-10. Template Automatic Export settings

Tip The following description is demonstrated on a Template but does also refer to a LabBook.

Upon completion of the LabBook, the data are automatically exported as defined.

The export directory is defined under System Options in the Scheduler settings, see "Customizing Scheduler Settings" on page 4-76.

❖ **To define automatic export settings**

1. On the Templates view, expand Automatic Export and click CSV Export to select the Automatic Export view.

2. Select the **CSV Export** check box to define these export settings, see Figure 5-11.

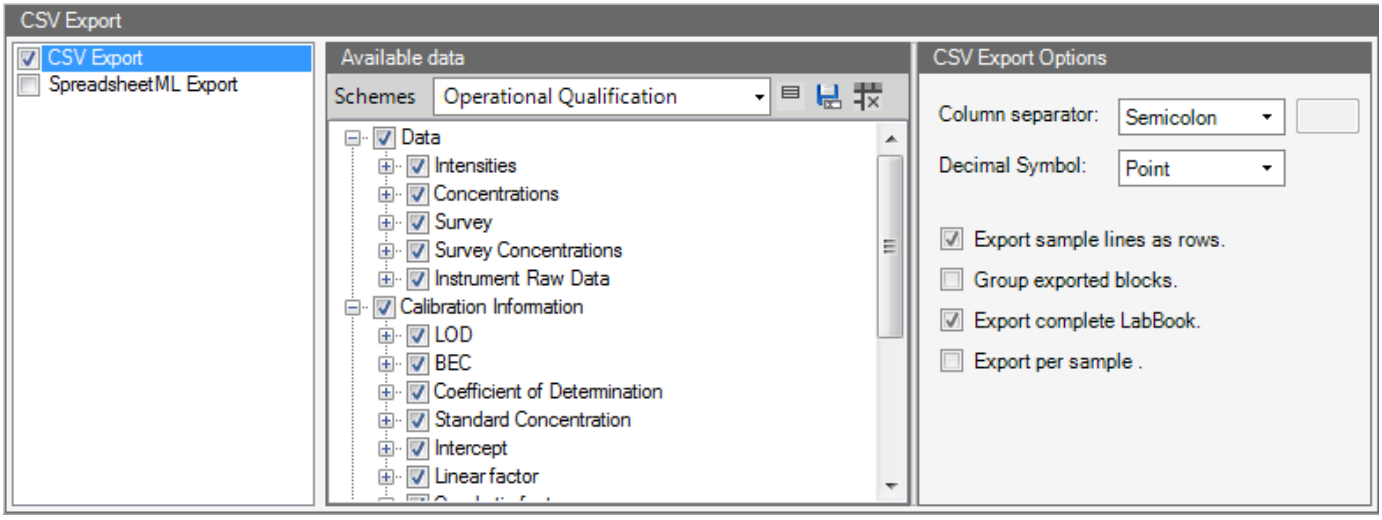


Figure 5-11. Automatic Export, CSV Export settings

3. For **Available data**, select the check boxes for the data you wish to export.
   -or-
   Select one of the pre-defined **Schemes** from the list box.

4. From **CSV Export Options**, select a **Column separator** from the drop-down list.
   Usually, a *Semicolon* is used to separate singular items within one data set. You may select *Tab* instead or *Custom* for a user defined symbol. In this case, be aware of incompatibility, when you read the exported file with another application.

5. To keep decimal values in singular item, select a **Decimal symbol** that must be different from the Column separator.
   Usually, a *Point* is used in most of the English speaking countries, and a *Comma* is used, e.g., in Central Europe.

6. Select the **Export sample lines as rows** check box to show the sample lines as rows.
   If you do not select this check box, the sample lines are exported as columns.

7. Select the **Group exported blocks** check box to group the data output.

8. Select the **Export complete LabBook** check box if you wish to export one file for one LabBook.

9. Select the **Export per sample** check box if you wish to export one file per sample.

10. Click **Save As** on the toolbar of Available data to save the setting to a scheme.
    The **Save Export Scheme** dialog opens, see Figure 5-12.

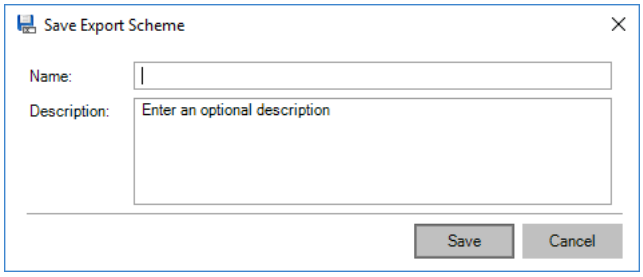
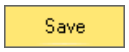


Figure 5-12. Save Export Scheme dialog

11. Type a **Name** and **Description**.



12. Click **Save**.
    The settings for **CSV Export** are saved to this scheme.

13. Select **SpreadsheetML Export** to define these export settings, see Figure 5-13.

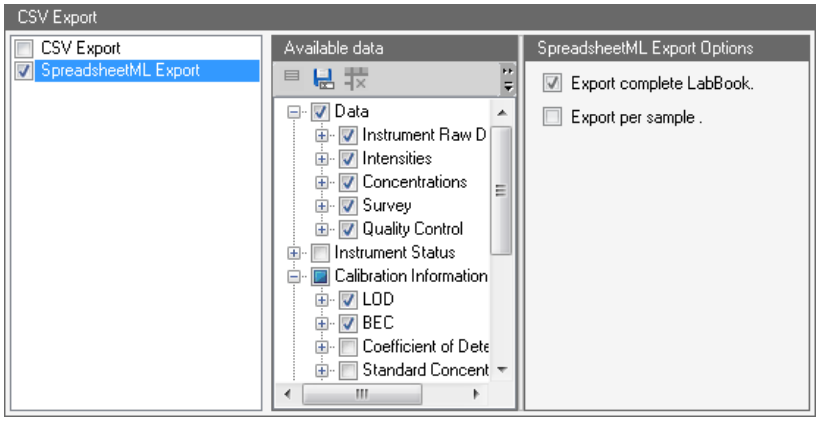


Figure 5-13. Automatic Export, XML settings

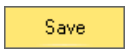
14. From **Available data**, select the data you wish to export.

15. From **SpreadsheetML Export Options**, select the **Export complete LabBook** check box if you wish to export one file for one LabBook.

16. Select the **Export per sample** check box if you wish to export one file per sample.

17. Click **Save As** on the toolbar of Available data to save the setting to a scheme.
    The **Save Export Scheme** dialog opens, see Figure 5-12.

18. Type a **Name** and **Description**.



19. Click **Save**.
    The settings for **SpreadsheetML Export** are saved to this scheme.

20. Click **Save** to save the changes to your Template.

❖ **To load a scheme for automatic export settings**

1. On the Templates view, click Automatic Export to open the **Automatic Export** view.

2. From the toolbar of Available data, open the **Schemes** listbox to select a scheme, see Figure 5-14.

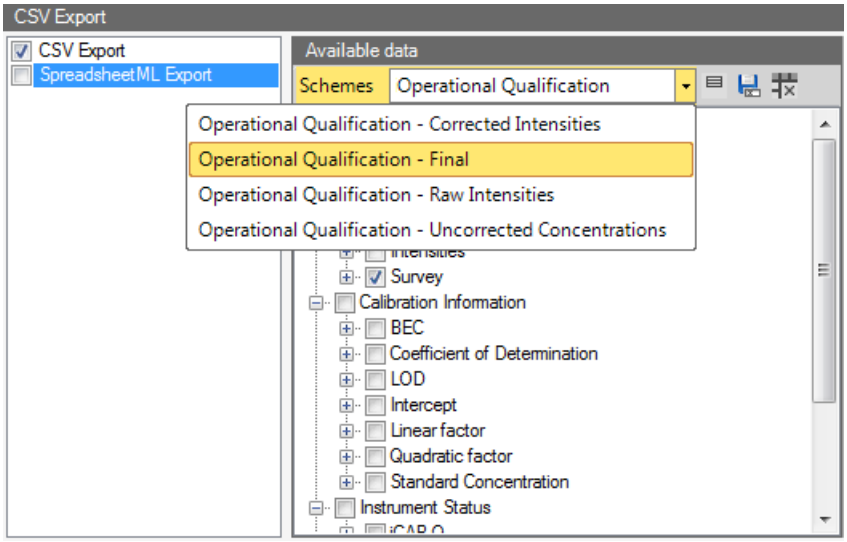


Figure 5-14. Load Export Scheme list box

3. Select the desired scheme to load this scheme.
The check boxes in the Available data pane are selected.

Tip Your selection of a scheme is independent from the export data format. This means, you can select a scheme for CSV Export as well as for SpreadsheetML Export.

❖ **To define Report export settings**

1. On the Templates view, expand Automatic Export and click Report Export to open the Report Export view.

2. Click **Add** to add a row to the table.

3. For **Report name**, expand the drop-down list, see Figure 5-15.

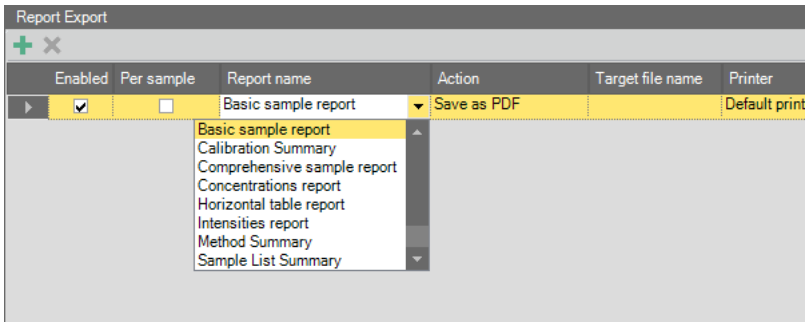


Figure 5-15. Report name drop-down

4. Select the Report, you wish to add.

5. For **Action**, expand the drop-down list and select the file format for the Report, see Figure 5-16.

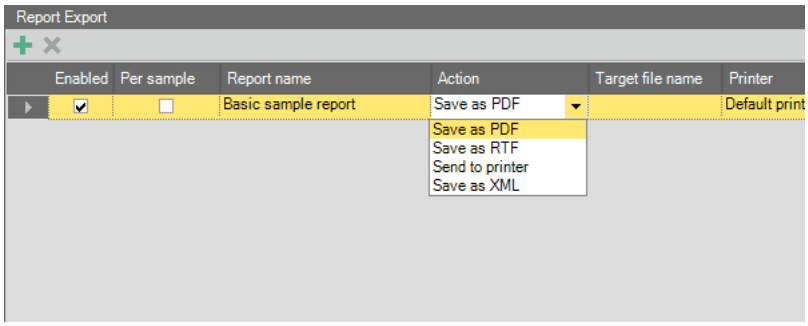


Figure 5-16. Action drop-down

   a. Select **Save as PDF** to compile a PDF Report that is shown in your PDF viewer.
   The Save As dialog (see Figure 6-7) is opened to select the folder and to type the file name of the PDF file.

   b. Select **Save as RTF** to generate a Report that is displayed in Microsoft Word or your alternative RTF viewer.
   The Save As dialog is opened to select the folder and to type the file name of the RTF file.

   c. Select **Save as XML** to generate a Report that is displayed in the Internet Explorer.
   The Browse For Folder dialog (see Figure 6-8) is opened to select the folder where you want to save the XML output.

6. Select **Enabled** for the Reports you wish to automatically export.

7. Select **Per sample** if you wish to create Reports per sample.

8. Double-click the field and type a name for your Report for **Target file name**.

9. Select a **Printer** from the drop-down list. The list offers all printers that are configured on your Windows system.
   Default printer sends the LabBook or samples directly to the default printer of your Windows environment.

10. Repeat to add other Reports.

11. If you wish to delete a row in the table, click the gray field in front of the row or rows you wish to delete.

    Click **Delete** and confirm the message dialog to delete the rows.

12. Click **Save** to save the changes to your Template.

6

LabBooks

LabBooks are based on the settings specified in the "Templates" on page 5-1 in Qtegra. These setting can still be adjusted in the LabBook before the measurements is run.

Contents

❖ To open or create a LabBook in Qtegra

- From the **Qtegra - [Home Page]** navigation pane, open a LabBook as described in "Opening a LabBook" on page 4-23.
- From the **Qtegra - [Home Page]** navigation pane, create a LabBook as described in "Creating LabBooks" on page 4-24.

LabBook Toolbar

In the LabBook tab, Qtegra offers buttons to save, close, run, export a LabBook, to view the history, and to sort items, see Figure 6-1.

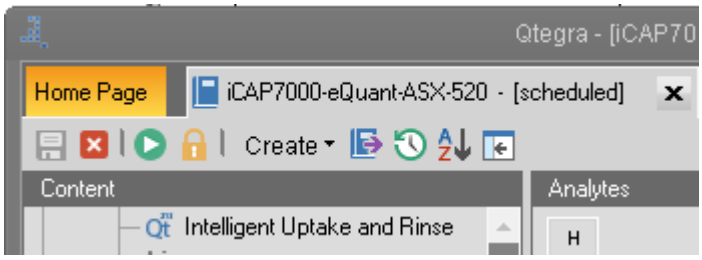


Figure 6-1. LabBook toolbar

Additionally, you can create a new LabBook or Template from the existing LabBook, view the History of the current LabBook or hide the Content pane.

Once the LabBook has been executed, new functions become available on the toolbar. For the Sample List, buttons to add and change Sample List rows are offered, see "Sample List of LabBook" on page 6-13. Buttons to recalculate data are added to the toolbar for "Evaluation Results" on page 6-33.

❖ To save a LabBook

1. Change the LabBook settings as appropriate.
2. Click **Save** to save the LabBook.
   The **Save LabBook** dialog opens.
3. Enter a **Comment** for the LabBook.
   The comment will be shown in the History view.
4. Click **OK** to save the LabBook.

Tip During the saving process you can not edit or modify any LabBook entries. Wait until the saving process is closed and the menu items are enabled.

❖ To close a LabBook

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook as described in "Opening a LabBook" on page 4-23.
2. Click **Close** on the toolbar.

   -or-

   Click **Close** in the tab of the LabBook to close the LabBook.

❖ **To run a LabBook**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook as described in "Opening a LabBook" on page 4-23.

2. On the toolbar of the LabBook, click **Schedule** to schedule the LabBook.
The LabBook is added to the queue in the Scheduler and the LabBook is locked.

Tip If the **Automatic** check box has been selected for **Start Queue** in the **Options** settings of the Scheduler (see "Customizing Scheduler Settings" on page 4-76), the measurement starts immediately.

3. In the Scheduler, select the LabBook and click **Run**.
The LabBook measurement is executed.

❖ **To create a LabBook or Template from an existing LabBook**

1. In the LabBook view, click **Create**.
The **Create** drop-down menu opens, see Figure 6-2.

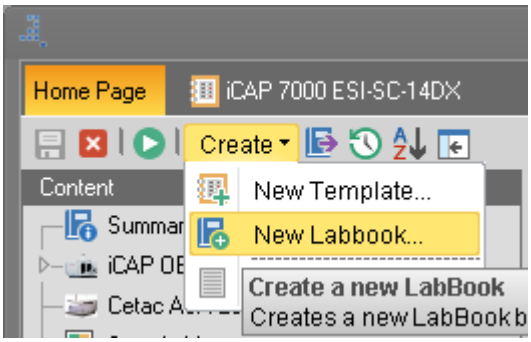


Figure 6-2. Create button in LabBook toolbar

2. Click **New Template** if you wish to create a new Template from the current LabBook.
The **Template** view of the **Home Page** opens. See "Creating a Template" on page 4-38 for further details.

3. If you wish to create a new LabBook from the current LabBook, click **New LabBook**.
The **LabBook** view of the **Home Page** opens. See "Creating LabBooks" on page 4-24 for further details.

❖ **To export LabBook data**

1. On the toolbar of the LabBook, click **Export**.
-or-
Press **<Ctrl> + <E>**.

The **Export data** dialog opens, see Figure 6-3.

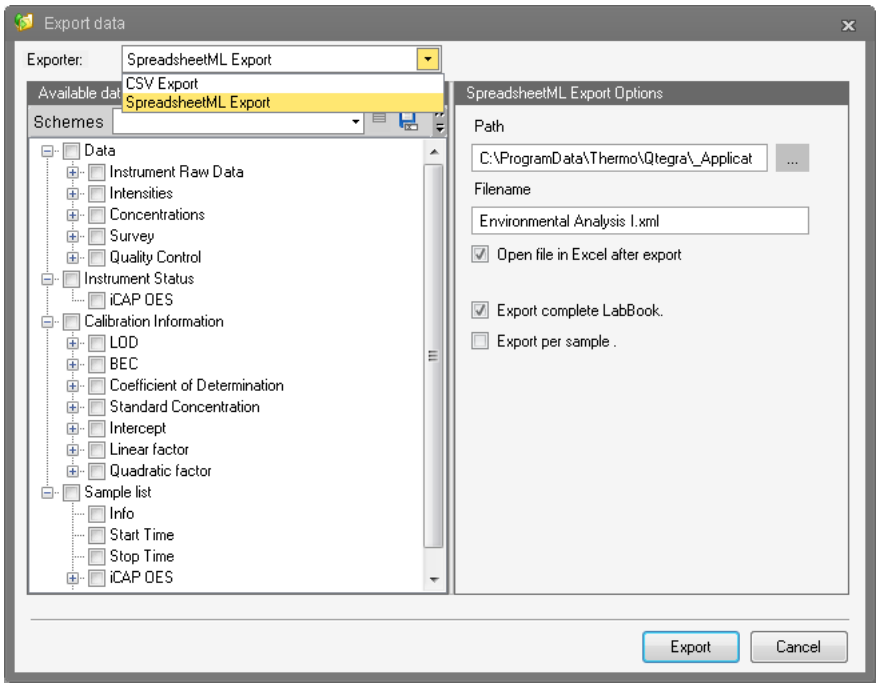


Figure 6-3. Export data dialog of LabBook

2. For **Exporter**, select **CSV Export** or **SpreadsheetML Export**.
3. In the Export Options section on the right pane, select the items as follows:
   a. For the **SpreadsheetML Export**, select a **Path** and type a **Filename**.
   b. For **CSV Export**, also select the **Column separator**, a **Decimal Symbol**, and select the check boxes for **Export sample lines as rows**, **Group exported blocks**, **Export complete LabBook** and **Export per sample**, as appropriate.
4. Click the browse buttons next to the **Path** entry to select another path where the exported LabBook will be saved.
   The standard **Save As** dialog is opened to select the desired path.
5. Click **Save** to copy this selected path into the **Export data** dialog.
   The file is not yet exported.
   The Save As dialog is closed.
6. If desired, select the check box **Open file in Excel after export** or **Open containing folder after export**.
7. From the **Available data** list, select the check boxes for the data you wish to export, or
   Open a **Scheme** to select pre-defined data.

a. Click **Save As** to save the settings as your scheme.
The **Save Export Scheme** dialog opens, see Figure 6-4.

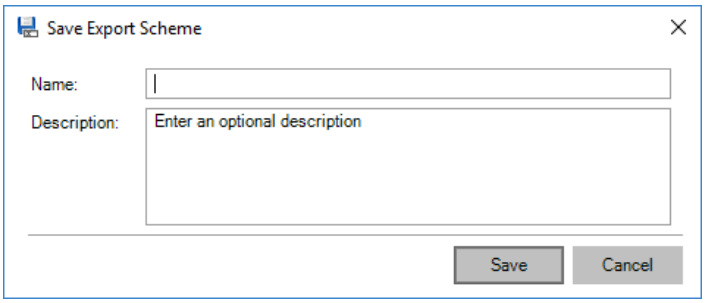


Figure 6-4. Export scheme of LabBook

b. Type a **Name** and a **Description**.

c. Click **Save**.

8. In the Export data dialog, click Export.

❖ **To view, compare and export the history of a LabBook**

1. On the toolbar of the LabBook, click **View History**.
The **History** dialog for this LabBook opens, see Figure 6-5.

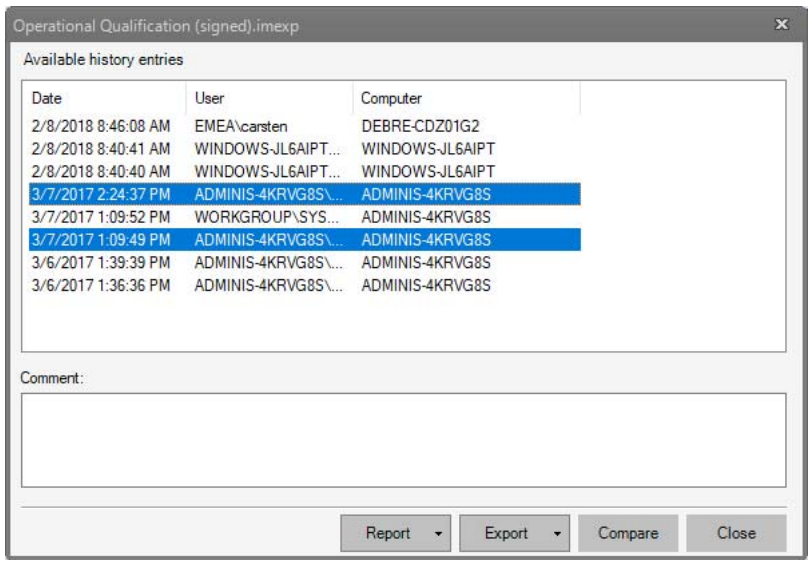


Figure 6-5. History dialog for LabBooks

Tip According to SOP compliance viewing and exporting the history is only allowed for specified user groups.

2. To compare the history entries, press **<Ctrl>** or **<Shift>** and select the range of history entries you wish to compare.

3. Qtegra allows to select more than two entries for comparison purposes.

4. Click **Compare** to compare the selected entries.
The **Comparison** dialog opens and shows all selected entries column by column, see Figure 6-6.

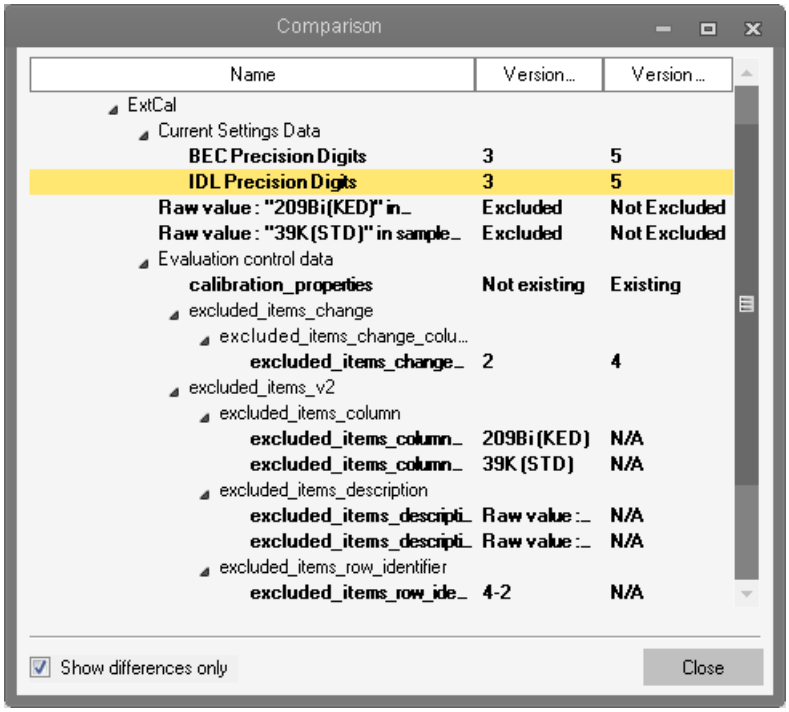
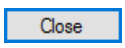


Figure 6-6. History Comparison dialog for LabBook

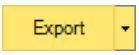
5. Resize or maximize the Comparison window to make all entries visible. The column header shows the date of selected entry with the oldest version left and the newest version right.

6. Click the triangle in front of the items to collapse and expand the items to focus on the interesting parts.

7. Select **Show differences only** if you wish to view only the differences, which is the default setting.
When removing the tick, Qtegra needs a few seconds to update the list and to show all history entries. Differences then are shown in bold letters.



8. **Close** the **Comparison** dialog.



9. Expand **Export** and select the file format for the history export.

   a. Select **Save as HTML** to compile a HTML history.
   The Browse For Folder dialog (see Figure 6-8) is opened to select the folder where you want to save the HtmlReport folder with the *index.html* file and all images used. The Browser opens to display the HistoryReport.

   b. Select **Save as PDF** to compile a PDF history that is shown in your PDF viewer.

The Save As dialog (see Figure 6-7) is opened to select the folder and to type the file name of the PDF file.

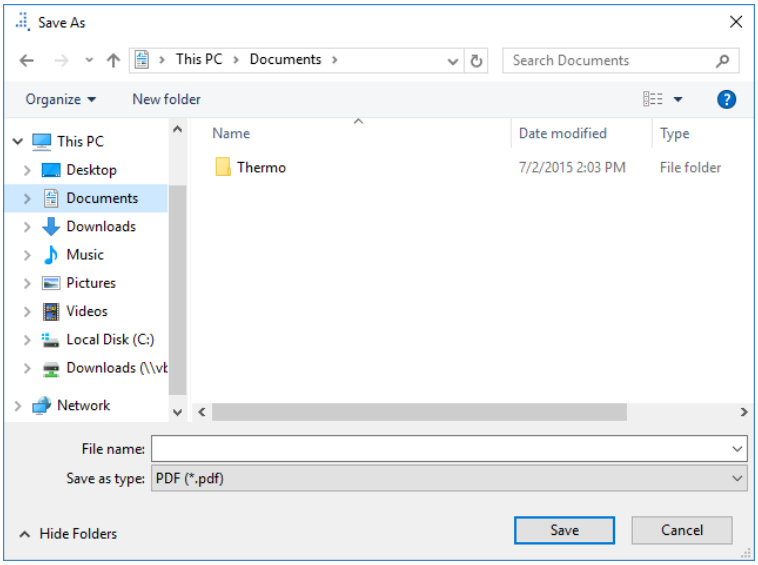


Figure 6-7. Save As dialog for export as PDF

c. Select **Save as RTF** to generate a history that is displayed in Microsoft Word or your alternative RTF viewer.
The Save As dialog is opened to select the folder and to type the file name of the RTF file.

d. Select **Save as XML** to generate a history that is displayed in the Internet Explorer.
The Browse For Folder dialog (see Figure 6-8) is opened to select the folder where you want to save the XML output.

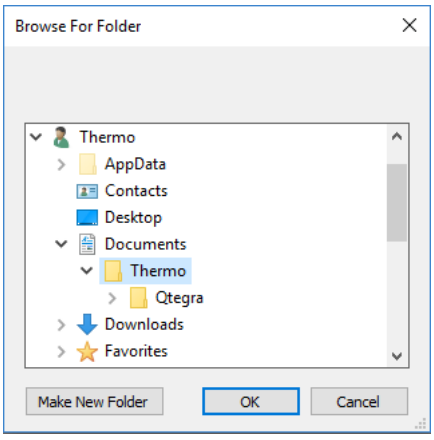
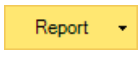


Figure 6-8. Browse For Folder dialog for export as XML

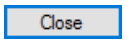
Once the folder is selected, click **OK** to open the XML file in your browser.



10. Expand **Report** and select History entries or History comparison.

a. With **History entries**, the History entries Report is opened to show the available history entries as on the initial dialog, see Figure 6-5.

b. With **History comparison**, the History Compare Result Report is opened to show the selected history entries similar to Figure 6-6.



11. **Close** the **History** dialog for this LabBook.

❖ **To hide the Content pane**

1. In the LabBook view, the **Content** pane is shown on the left, see Figure 6-9.

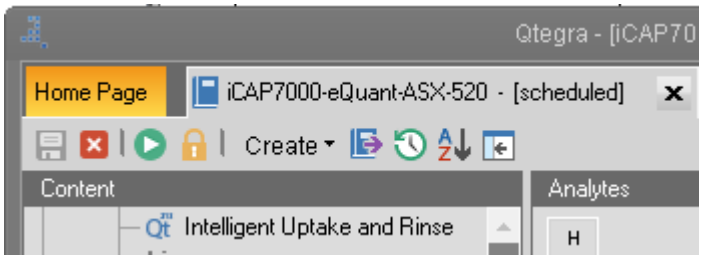


Figure 6-9. Content pane of LabBook visible

2. Click **Toggle**.
-or-
Press <F11>.
The **Content** pane is hidden, see Figure 6-10.

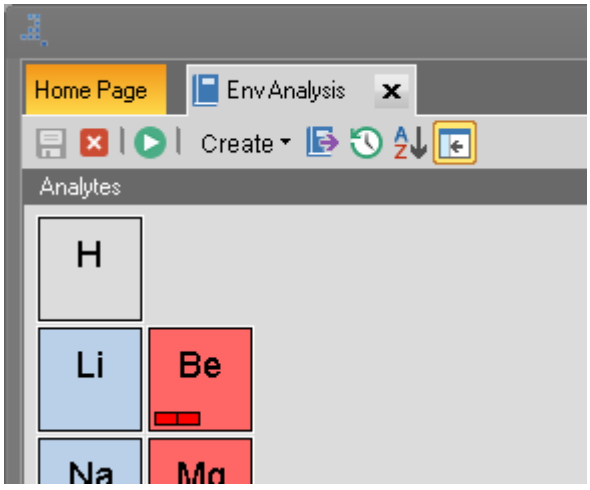


Figure 6-10. Content pane of LabBook hidden

3. Click **Toggle**.
-or-
Press <F11> to show the **Content** pane again.

Sorting the Analytes

In several cases it is helpful to get the views of Method Parameters and Evaluation Results in a comparable layout. Qtegra provides a mechanism to sort the analytes according to your needs.

Once defined, the sort order is applied to the LabBook. An option allows to apply the selected sort order to the LabBook when it opens. The arrangement is valid for several views but, for example, not for the Reports that have their own sorting routine.

The sorting that you arranged in the Sort window is applied to the following views of your LabBook:

- Method Parameters
  - Acquisition Parameters
  - Interference Correction
  - Quantification
  - Quality Control
- Evaluation Results
  - Concentrations
  - Intensities
- Query

See the description below to understand the sort function.

❖ **To arrange the analytes**

1. On the toolbar of the LabBook, click **Sort**.
   The Qtegra **Sort** window opens, see Figure 6-11.

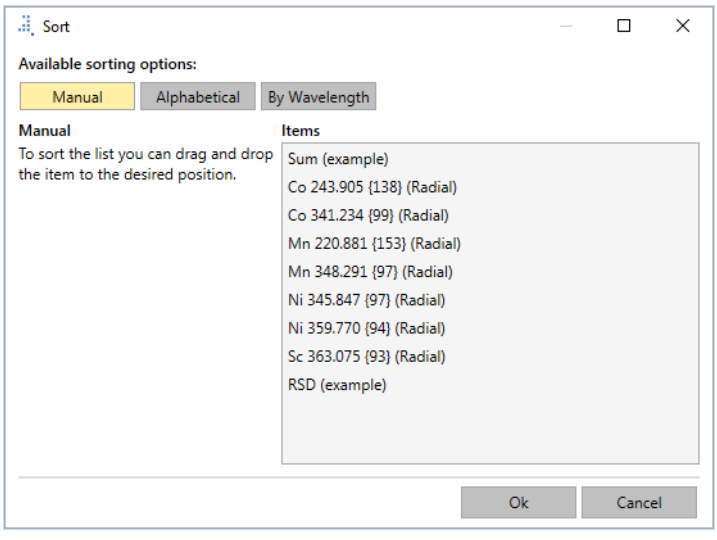


Figure 6-11. Sort window

2. The highlighted button above the list indicates the former arranged sort order. Click the desired button to sort the list according to your needs.

   a. Click **Manual** and drag the list items to the desired position to sort the analytes.

   b. Click **Alphabetical** to sort the analytes in alphabetical order. *Alphabetical* sort order includes the wavelength of the analyte, ratios and calculation traces .

   c. Click **By Wavelength** to sort the analytes by their wavelength. Ratios and calculation traces are appended to this list.

   For *Alphabetical* and *By Wavelength*, click **Ascending** or **Descending** to revert the sort order.

   As soon as you drag items to another position, the sorting option changes to *Manual*.

3. Click **OK** to apply the sort order to the currently opened LabBook. Note that this sort order is only saved permanently with the LabBook if **Apply sort order** is active.

4. Click **Cancel** to leave the open LabBook unchanged.

❖ **To apply the sort order to your LabBook**

1. On the LabBook toolbar, click **Apply sort order**.

2. The button changes yellow  to indicate the status for the sort function.

   When you change the sorting of analytes, the sort order is applied to the LabBook. The sort order will be saved when the LabBook is saved. Once you open this LabBook again, the last specified sort order is used in the views, see "Sorting the Analytes" on page 6-9.

Method Parameters of LabBook

Method Parameters differ for each LabBook and are inherited from the Template from which the LabBook is created in Qtegra. The type of **Evaluation** selected for the Template also controls the availability of the Method Parameters for the LabBook.

An example of the Method Parameters available for a LabBook based on an eQuant evaluation is shown in Figure 6-12.

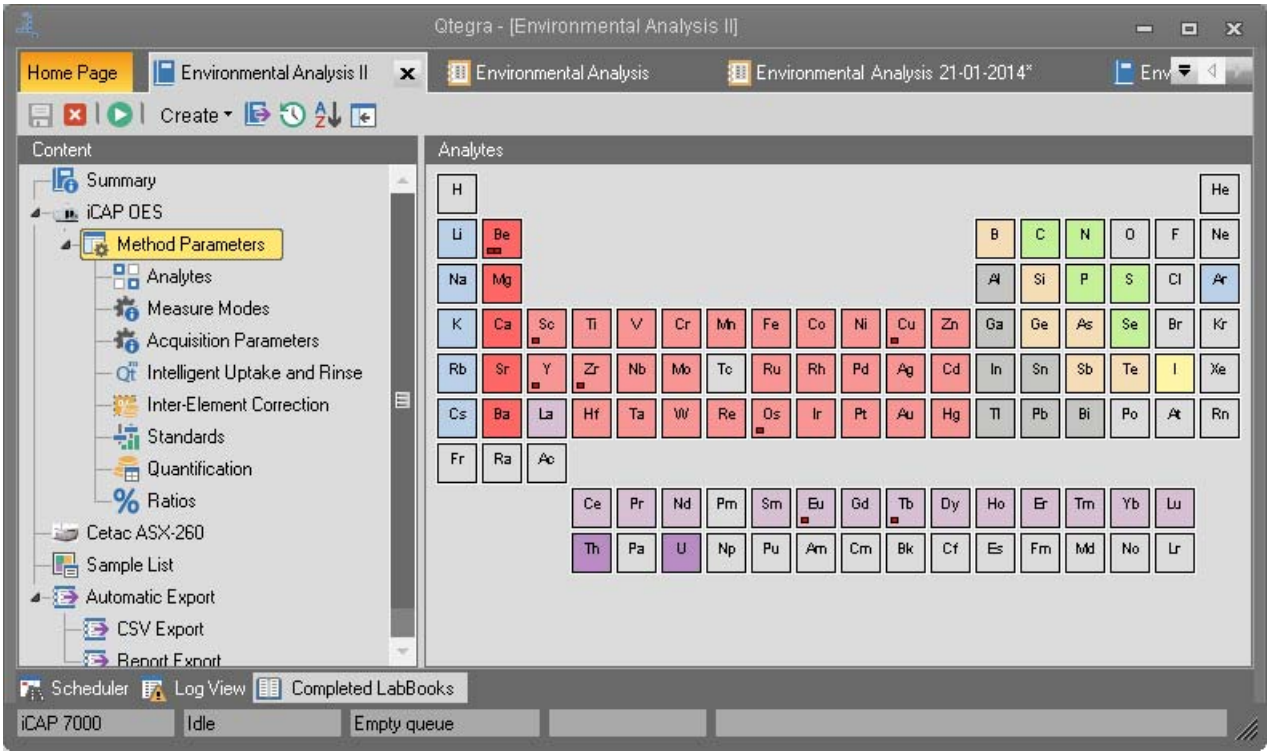


Figure 6-12. LabBook Method Parameters

All settings of the Method Parameters can be still be changed in the LabBook. For details, see "Method Parameters Settings" on page 9-3.

Tip The Sample List of a LabBook is generated from the settings in Sample Definition of a Template, see "Sample Definition for a Template" on page 5-5.

The color scheme of the periodic table of the LabBook is inherited from the definitions in the Template, see "Color Scheme of the Periodic Table" on page 14-62.

Summary of LabBook

A summary page is added to each LabBook in Qtegra. This page shows the Filename, information about Properties, Dates, People, and Instrument Plug-in Versions for the LabBook, see Figure 6-13.

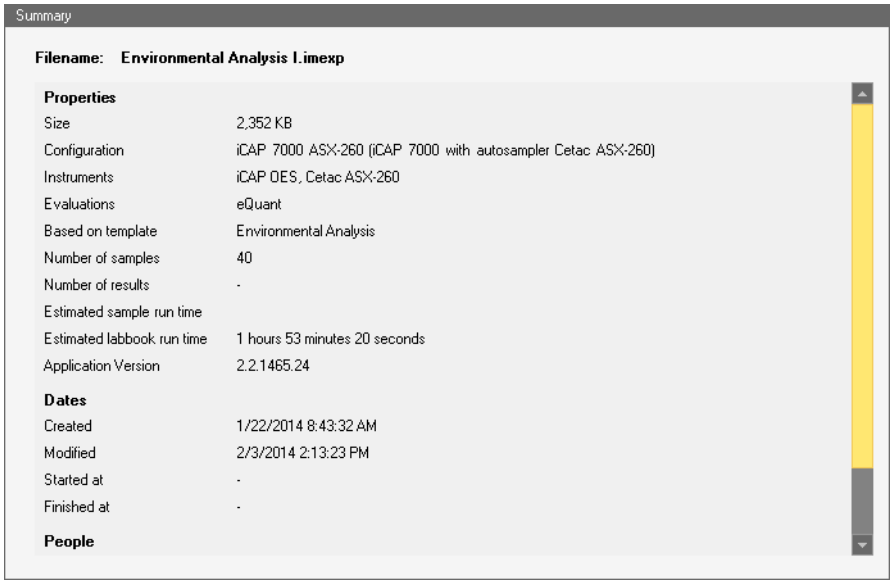


Figure 6-13. Summary of LabBook

❖ To show the summary of a LabBook

1. In the LabBook view, click **Summary** to view the summary of the LabBook.
2. The **Instrument Plug-in Versions** may help in case of problems when contacting the Qtegra ISDS Software support.

Sample List of LabBook

The Sample List of a LabBook is based on the number of samples selected for analysis, and on the structure of the Initial Actions, Continuing Actions and End Actions items defined in the section of the Templates (see "Sample Definition for a Template" on page 5-5).

An example of a Sample List in a LabBook created from an eQuant Template is shown in Figure 6-14.

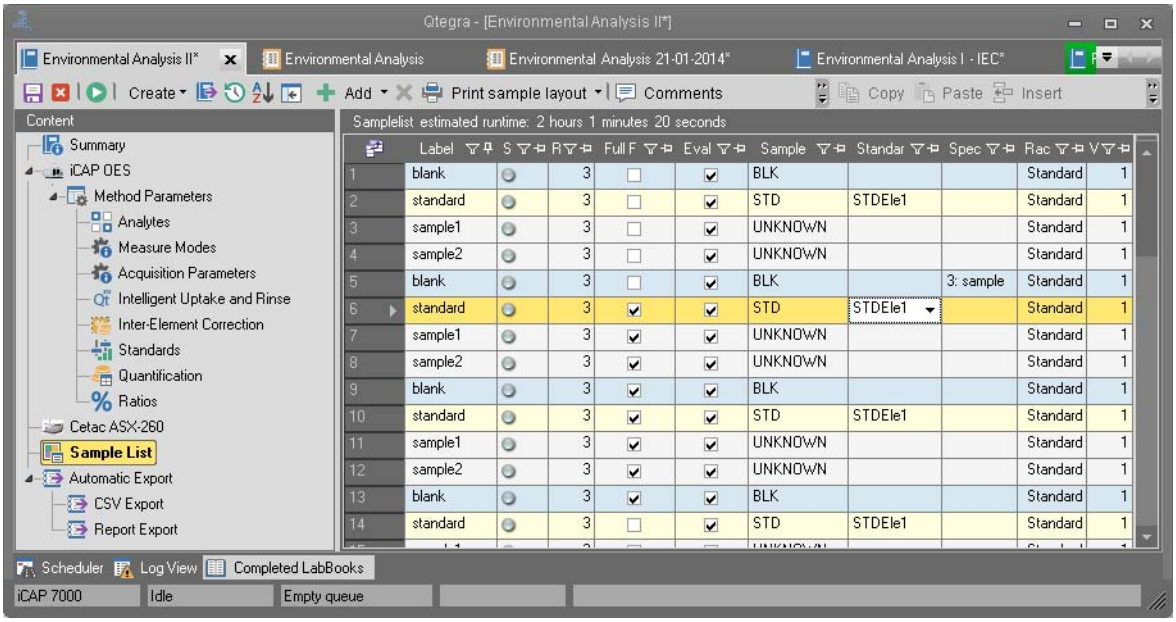


Figure 6-14. Sample list of LabBook

Depending on the evaluation method of the LabBook, the columns of the components may differ. All columns that may be shown in Sample List are explained in Table 14-5.

With **Special Blank**, see Sample List example in Figure 6-15, it is possible to subtract the calculated concentrations of a sample from those of one or more others.

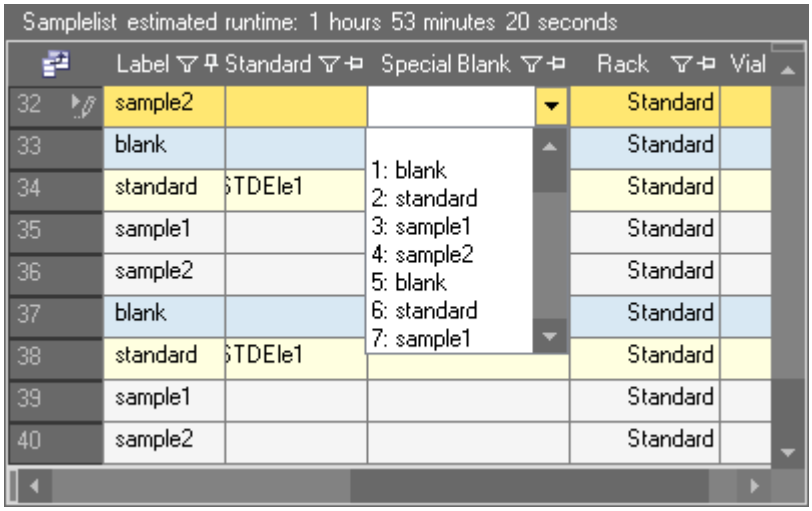


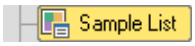
Figure 6-15. Sample List view with Special Blank

Any values entered that are not within the given range are marked with an .

Special Functions of the Sample List

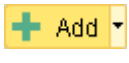
Tip Some functions are only available, when your LabBook is not finished.

❖ **To view the Sample List**



1. In the LabBook view, click **Sample List** to view the **Sample List** of the LabBook.

❖ **To add rows to the Sample List**



1. In the **Sample List** of the LabBook, click **Add** to add a row at the end of the Sample List.

   -or-

2. Click the arrow next to **Add** and select **Add Rows** from the drop-down menu.
   The **Number of rows** dialog opens, see Figure 6-16.

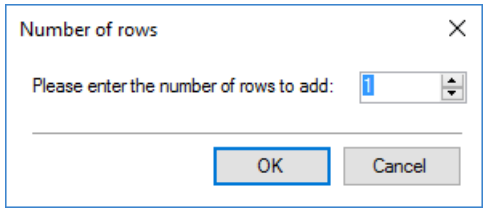


Figure 6-16. Define the number of rows to be added to the Sample List

3. Enter the number of rows to be added to the Sample List.
4. Click **OK**.
   The rows are added at the end of the Sample List.

❖ **To paste values from Excel**

1. Open the **Sample List** of the LabBook.
2. From your Excel sheet, select a range of cells and press **<Ctrl> + <C>** to copy the desired range using the Windows clipboard.
3. In the Sample List, select the upper left target cell of the range you want to paste. Then right-click to open the shortcut menu and select **Paste**.
   -or-
   Press **<Ctrl> + <V>** to paste the values into your Sample List.

Tip If the Excel cells contain a value including the unit, both parts are separated by a blank.
You may only copy valid units that are supported by Qtegra ISDS Software. Units are always written with small letters. On errors, the tooltip of a red indicator shown next to the cell helps to understand the error.

❖ **To delete a row from the Sample List**

1. In the **Sample List** of the LabBook, click the gray field in front of the row you wish to delete.
   The row is selected.

2. Click **Delete** to delete the selected row.

❖ **To show comments of the Sample List**

1. In the **Sample List** of the LabBook. click **Comments** to show the comment for the selected row.
   The list of comments opens below the Sample List.

❖ **To add comments of the Sample List**

1. In the **Sample List** of the LabBook, show the comment for the selected row below the Sample List.

2. Click **Add Comment** to add a comment for the selected row.
The **User Comment** window opens, see Figure 6-17.

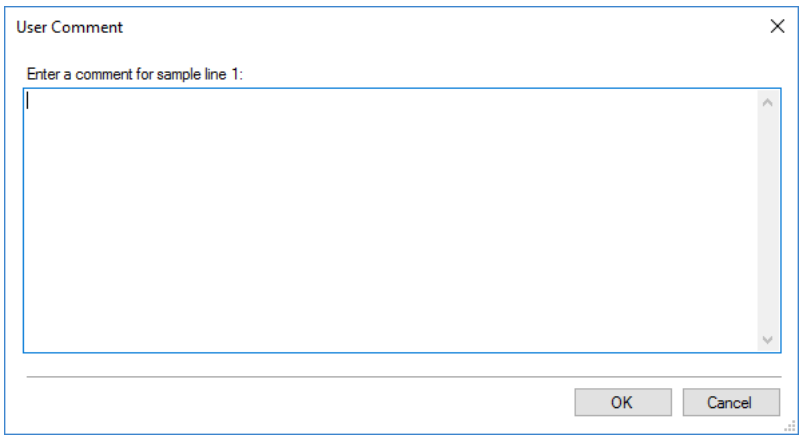


Figure 6-17. Add user comment to Sample List row

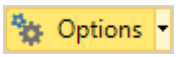
3. Type your comment.
4. Click **OK**.
The comment is added and the User Comment window closes.

❖ **To hide comments of the Sample List**

1. In the **Sample List** of the LabBook with opened list of comments, click **Comments** to hide the comment for the selected row.
The list of comments is hidden.

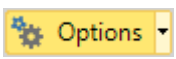
❖ **To save user settings for the Sample List**

1. In the **Sample List** of the LabBook, arrange the columns according to your needs as described in the chapter "Designing the LabBook Table" on page 14-48.



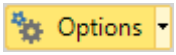
2. Click the arrow next to Options to show the menu items.
3. Click **Save User Default** to save the current column order of your Sample List.
The menu is collapsed and your setting is saved.

❖ **To load user settings for the Sample List**



1. In the **Sample List** of the LabBook, click the arrow next to **Options** to show the menu items.
2. Click **Load User Default** to load the column order that has been saved before.
The menu is collapsed and the setting is applied to the Sample List.

❖ **To specify user options for the Sample List**



1. In the **Sample List** of the LabBook, click **Options** to show the Options dialog, see Figure 6-18.

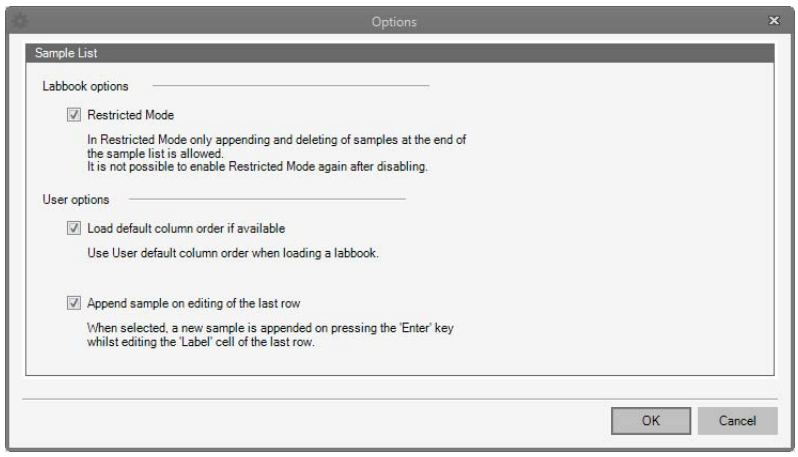


Figure 6-18. Options dialog of Sample List with enabled Restricted Mode

The **Restricted Mode** functionality depends on the activation in the Sample Definition of a Template. This mode does only affect the composition of the Sample List in the LabBook according to the predefined repetition rules. See "Sample Definition for a Template" on page 5-5.
Once you removed the tick mark from this option, the restricted mode is turned off, which then allows you to modify all samples of the LabBook.
Click **OK** to make your changes available. A confirmation dialog opens, see Figure 6-19.

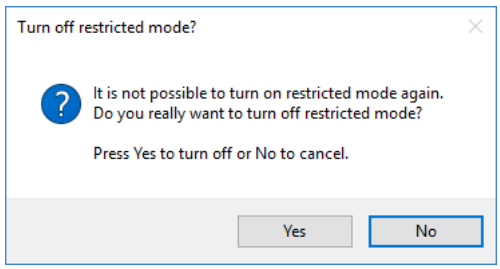


Figure 6-19. Confirmation dialog when turning off the restricted mode

2. Click **Yes** to turn off the restricted mode.
   -or-
   Click **No** to cancel and to show the Options dialog.

3. In the User options section, tick **Load default column order if available** to use your defaults as default column order.

4. Tick **Append sample on editing of the last row** to automatically append a new sample row when editing the Label.
   In the **Label** field, press **<Enter>** to close the edit mode and to

append a new sample row.
If this check box is not ticked, click **Add** on the Sample List toolbar to append a sample row to the Sample List.

Automatic Export of LabBook

Before measurement, you can define **Automatic Export** settings for a LabBook. Upon completion of the LabBook, the data are automatically exported.

Tip Automatic Export settings are not available for Completed LabBooks since they have already been exported if so defined. For export functions of Completed LabBooks, see "LabBook Toolbar" on page 6-2.

You define the export settings for your data as CSV or XML file and for Reports, see Figure 6-20.

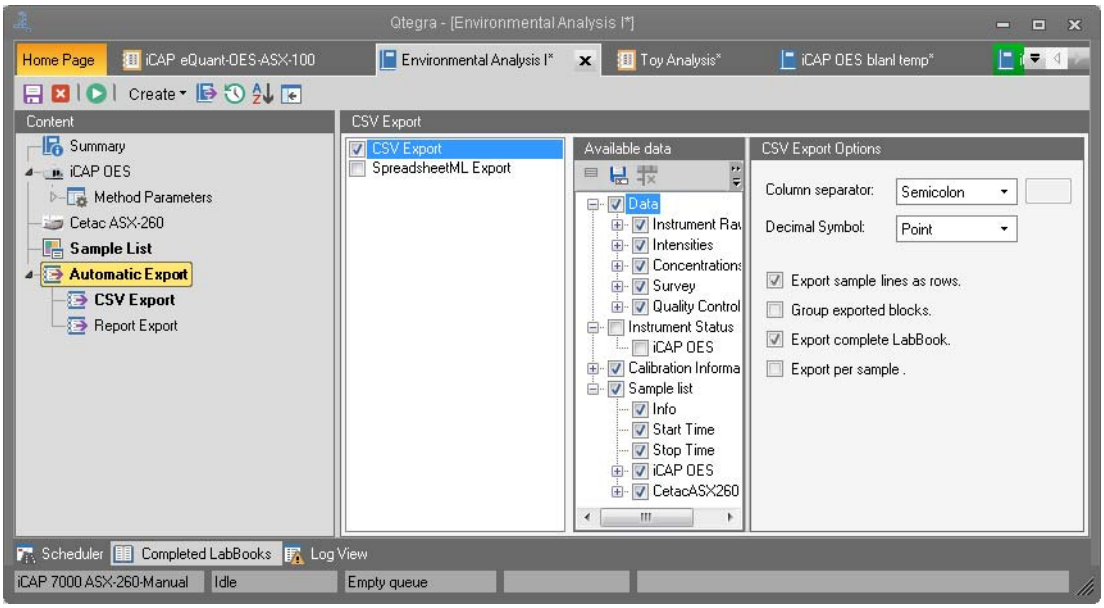


Figure 6-20. LabBook Automatic Export settings

LabBooks inherit the Automatic Export settings from the Template. See "Automatic Export - Template" on page 5-10 for details.

Flags and Limits

The functionality provided by Flags and Limits allows the user to replace (or reformat) values based on a series of defined criteria. The modified values are then displayed inside the Qtegra evaluation views and used for export or reporting. Flags and Limits is only enabled for LabBooks measured using the eQuant evaluation type. Flags is enabled for LabBooks using the aQuant or rQuant evaluation types.

Tip The raw, original data is not affected and is never lost. The use of Flags and Limits is an optional feature. Access to Flags and Limits can be controlled by User Access Rights.

Flags

In Flags you define changes made by replacement or reformatting of data according to a series of criteria or 'flags'. For example, changing the color of values in QC analyses that lie outside of defined limits to make them easier to identify in the data set, see Figure 6-21.

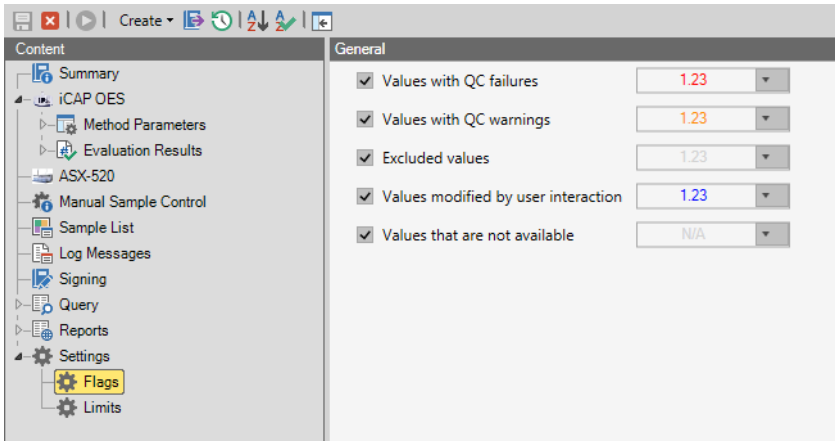


Figure 6-21. LabBook Flags

To activate a Flag, select the check box for the corresponding Flag type. See Table 6-1 for an explanation of each General Flag.

The decisions made in Flags and Limits control the display of data in the Intensities and Concentrations views of Evaluation Results as well as data exported via Query Excel Export, SpreadsheetML Export or shown in Reports. Data export using CSV Export or Query CSV Export is also affected by the changes made in Flags and Values but ignores the color coding.

Table 6-1. General Flags

Flag	Impacts
Values with QC failures	Values outside defined QC failure limits. For details on QC failures, see "Quality Control Failure Rules" on page 10-6.
Values with QC warnings	Values outside defined QC warning limits. For details on QC warnings, see "Quality Control Failure Rules" on page 10-6.
Excluded values	Values manually excluded in Evaluation Results views.
Values modified by user interaction	Displayed for average values to indicate that one or more value in that block has been manually excluded.
Values that are not available	Displayed when no value is available. For a complete list of potential reasons for "N/A", see "N/A Indicator in Concentrations List" on page 14-33.

Tip The flags are applied with the priority displayed in Table 6-1. For example (based on the default formatting), the average concentration value for QC failure value will be displayed with red text even if one or more value has been excluded.

Once a Flag check box has been selected, the formatting controls for that Flag become accessible. See "Setting the Format Options for Flagged Values" on page 6-24 for a detailed description on how to set the display options.

Limits (eQuant only)

The Limits page allows for Flags to be displayed based on values in the Qtegra ISDS LabBook. Values can be flagged against global criteria or per analyte for increased flexibility, see Figure 6-22.

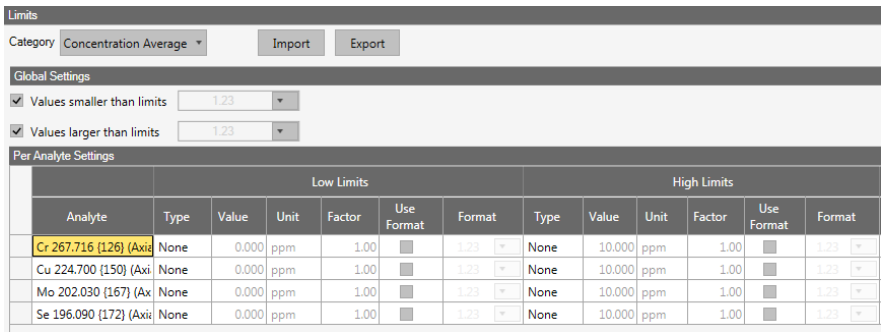


Figure 6-22. Limits window

The **Limits Category** drop-down box defines the data type that should be assessed. Currently only *Concentration Average* is supported. The Low and High Limits settings of the Per Analyte settings section can be saved to (or recalled from) a template for use in multiple LabBooks.

To load a previously saved set of Limits, click **Import**. The Import Limits dialog opens the Limits folder in the Qtegra Workspace to show any previously created template files (.qtpl). The template files don't save the limits set in the Global Settings sections. Select the desired template and click **OK** to apply the defined Flags and Limits settings to the analytes in the currently opened LabBook. Limits are evaluation mode dependent.

To save your definition of Limits, click **Export** to open the Export Limits dialogs, enter a name, and click **OK**.

Global low and high limits can be applied to all values in the LabBook by selecting one of the tick marks in the **Global Settings** section, see Figure 6-23.

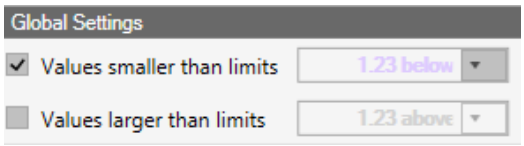


Figure 6-23. Global Settings section

See "Setting the Format Options for Flagged Values" on page 6-24 for a detailed description on how to set the formatting options for values flagged by the limits defined in Global Settings. Analyte specific limits can be defined individually for more flexibility.

The relevant tick mark in Global Settings however must first be activated to allow access to the per analyte settings.

❖ **To specify Low and High Limits per analyte**

1. To set the **Low Limits**, select the required limit **Type**: *None, LOD (Limit of Detection), MQL (Method Quantification Limit), User defined*.

The cells to the right become active depending on the choice made.

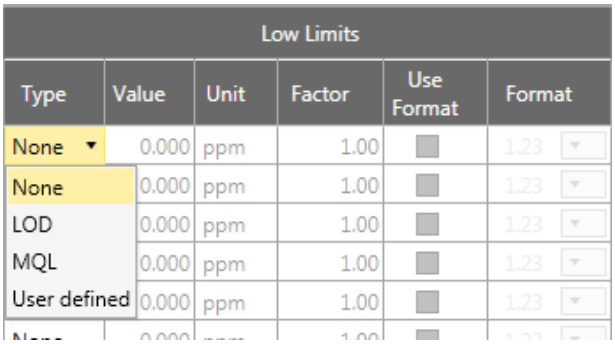


Figure 6-24. Choices for Low Limits

2. For a limit based on LOD or MQL, a **Factor** can be entered to adjust the Low Limit by a multiple of the LOD or MQL value.

3. For User defined, enter a value and unit to be used for the Low Limit.

4. Select **Use Format** to enable analyte specific choice of text, text position, font weight, and font color. See "Setting the Format Options for Flagged Values" on page 6-24 for a detailed description on how to set the display options.

5. To set the **High Limits**, select the required limit **Type**: *None, Calibration Range, User defined*.

   The cells to the right become active depending on the choice made.

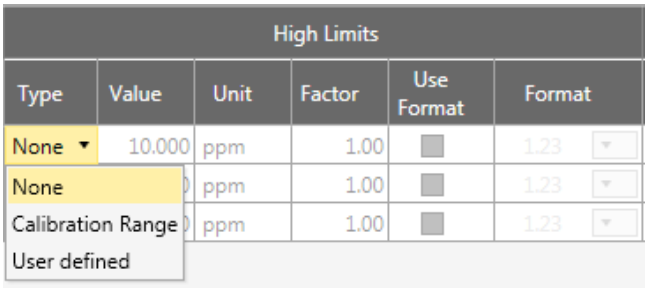


Figure 6-25. Choices for High Limits

6. For a limit based on Calibration Range, a **Factor** can be entered to adjust the High Limit by a multiple of the value.

7. For User defined, enter a value and unit to be used for the High Limit.

8. Select **Use Format** to enable analyte specific choice of text, text position, font weight, and font color. See "Setting the Format Options for Flagged Values" on page 6-24 for a detailed description on how to set the display options.

Setting the Format Options for Flagged Values

The same formatting dialog is used in both Flags and Limits sections.

❖ **To define Flag formatting**

1. Select the **Enabled** check box in front of the item you want to flag. The settings drop-down becomes active.
2. Click the **Settings** arrow to display the list of formatting and text options.

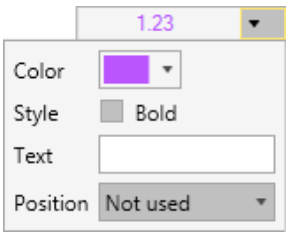


Figure 6-26. Formatting choices for Flags

3. Expand the **Color** box to select a color from the **Main palette** or from the **More colors** option.
4. Select **Bold** if the values shall be displayed in bold style.
5. Type a **Text** if any additional or replacement text should be displayed as specified in the Position drop-down.
6. From the **Position** drop-down, select one of the following options:

   - *Not used*: No text replacement takes place.
     Default option to display the originally measured value.
   - *Left*: The text is displayed left of the value.
     Select this option to display the text as a prefix to the value. The value itself remains unchanged. Extend the text with a blank space to separate out your text and the value.
   - *Right*: The text is displayed right of the value.
     Select this option to display the text as a suffix to the value. The value itself remains unchanged. Start the text with a blank space to separate out the value and your text.
   - *Replace*: The text is displayed instead of the value.
     Select this option to display the desired text instead of the value. As noted above, the value itself is not affected and never lost, but is not displayed.

Once your choices are made, a preview of any changes is displayed.

Figure 6-27. Example of values modified by Flags

The data display settings defined in Flags and Limits are then applied in the Evaluation Results views, Query, Data Export, and Reports. In the following examples, sample results with concentrations higher than the Calibration Range are shown with a bold violet font, see Figure 6-28.

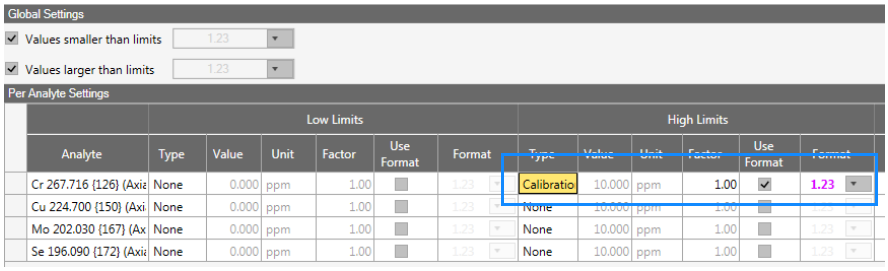


Figure 6-28. Example of Per Analyte Flag Settings

Flags and Limits - Evaluation Results view

Concentrations

Sample results with concentrations higher than the Calibration Range are indicated with bold violet values, as shown in Figure 6-29.

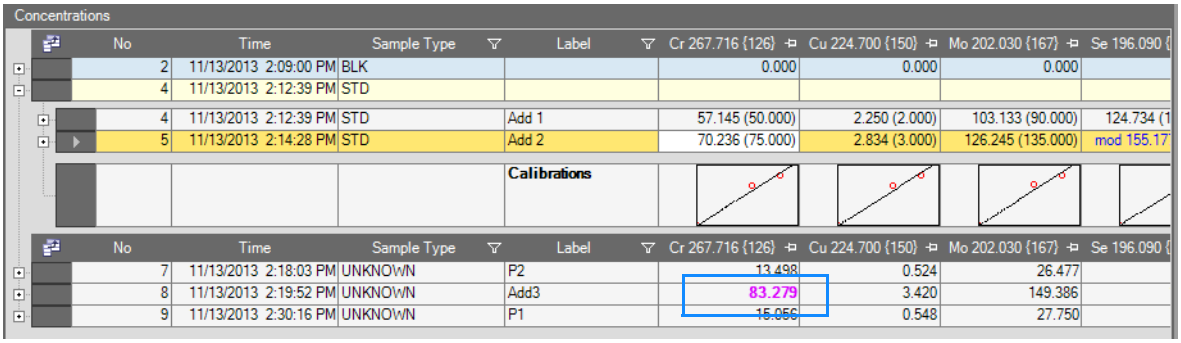


Figure 6-29. Example Concentrations view displaying a Calibration Range Flag for Cr267.716

Intensities

Values outside a specified range are highlighted as set under Flags. As an example, see blue values with prefixed “mod” in Figure 6-30 that were modified by user interaction.

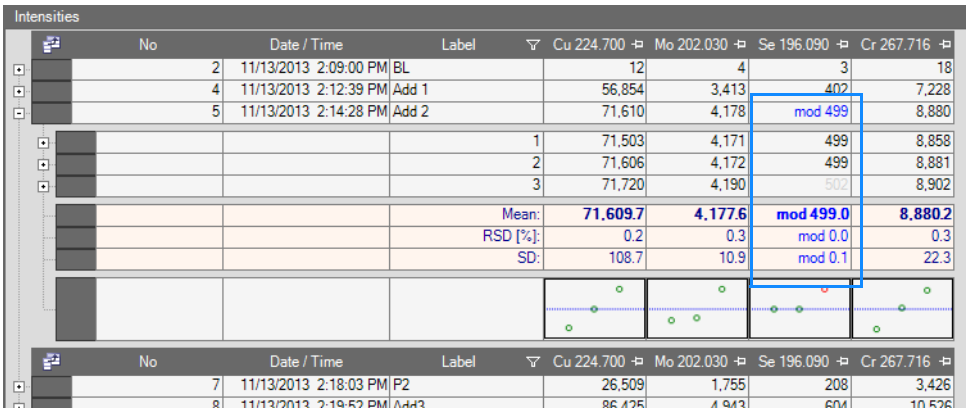


Figure 6-30. Example Intensities view displaying values of Se 196.090 modified by user interaction

Flags and Limits - Query

The following screenshots are based on the same examples shown above for the Concentrations and Intensities views. Sample results with a concentration higher than the Calibration Range are shown in bold violet, values modified by user interaction are shown in blue with the prefix “mod”.

In the Query, values outside the specified ranges are highlighted as set under Flags and Limits, see Figure 6-31.

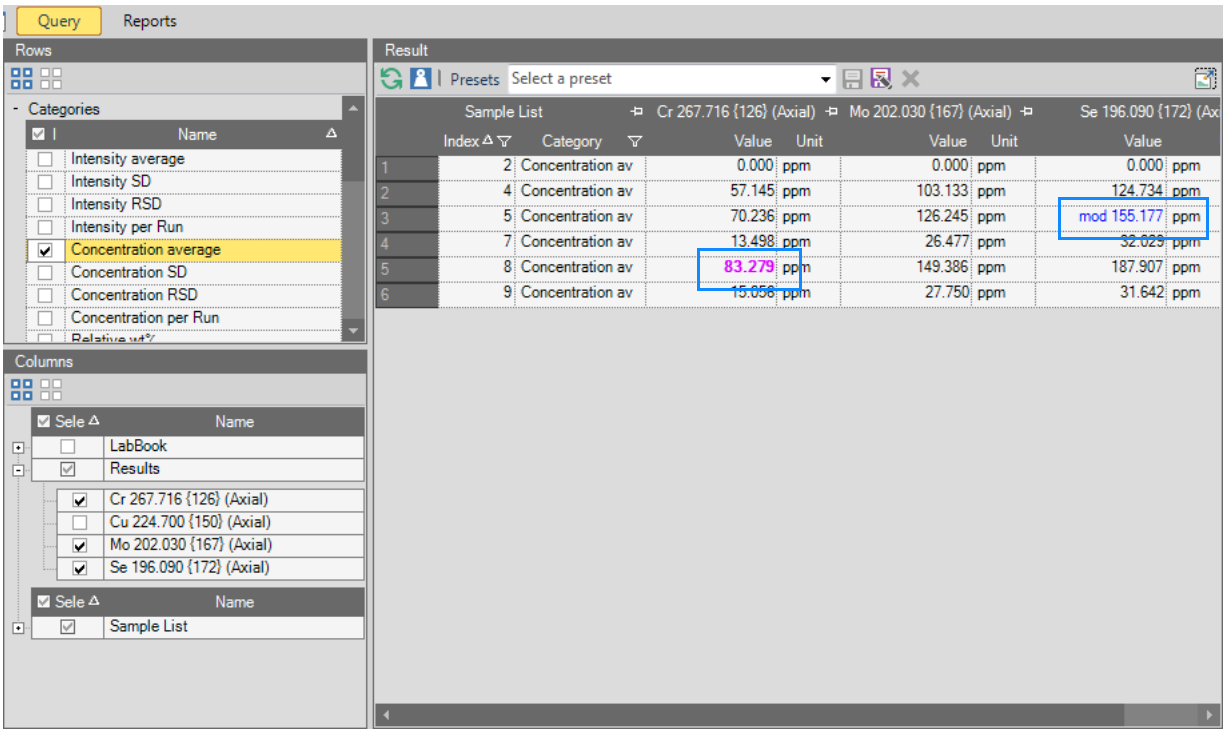


Figure 6-31. Example Query displaying a Calibration Range Flag (Cr) and user modified values (Se)

Flags and Limits - Reports

All Reports containing the Concentration average can be selected to show the Flags and Limits settings.

Vertical Table Report

See the following example for a *Vertical table report* made from the Query, see Figure 6-32.

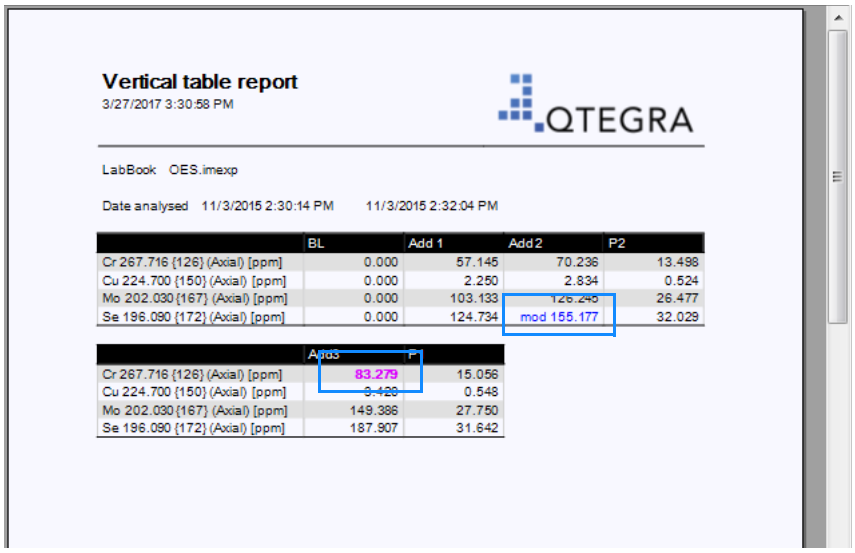
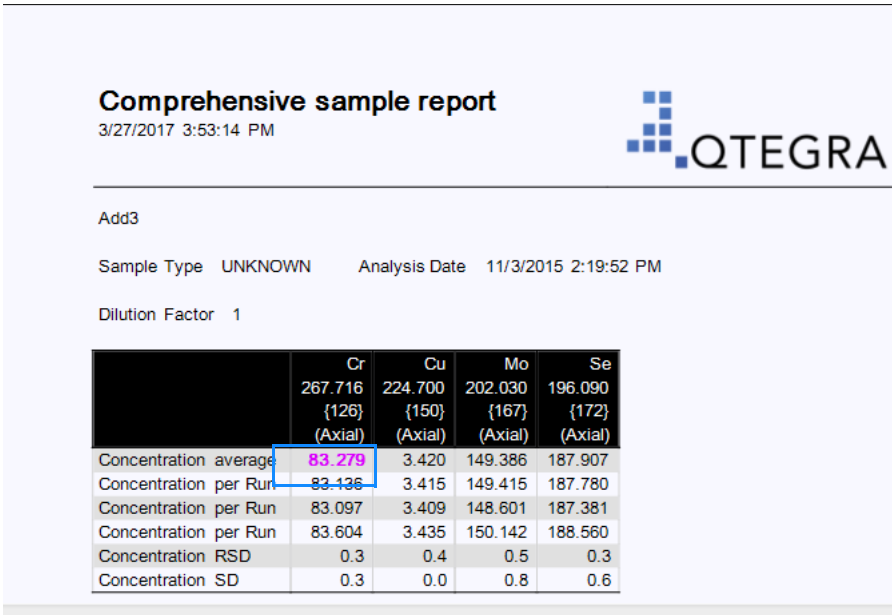


Figure 6-32. Vertical Table Report displaying a Calibration Range Flag (Cr) and user modified values (Se)

Comprehensive Sample Report

See the following example for a *Comprehensive sample report* made from the Query, see Figure 6-33.



Comprehensive sample report
3/27/2017 3:53:14 PM

QTEGRA

Add3

Sample Type UNKNOWN Analysis Date 11/3/2015 2:19:52 PM

Dilution Factor 1

	Cr 267.716 {126} (Axial)	Cu 224.700 {150} (Axial)	Mo 202.030 {167} (Axial)	Se 196.090 {172} (Axial)
Concentration average	83.279	3.420	149.386	187.907
Concentration per Run	83.136	3.415	149.415	187.780
Concentration per Run	83.097	3.409	148.601	187.381
Concentration per Run	83.604	3.435	150.142	188.560
Concentration RSD	0.3	0.4	0.5	0.3
Concentration SD	0.3	0.0	0.8	0.6

Figure 6-33. Comprehensive Sample Report displaying a Calibration Range Flag (Cr)

Scheduling a LabBook

To schedule a measurement, open a LabBook and run it. Or, select the desired LabBook in the File Manager and drag it to the Scheduler pane.

Evaluation results can be accessed in a running LabBook so results can be viewed in real time, see "Evaluation Results" on page 6-33.

In the **Tools** section on the **Help** page of Qtegra, you define your **Scheduler** settings, see "Customizing Scheduler Settings" on page 4-76.

Tip To customize the Options of the Scheduler, you can also click **Options** on the toolbar of the "Scheduler" on page 4-80.

❖ To run a LabBook

1. On the toolbar of the LabBook, click **Schedule** to schedule the LabBook for execution.
   -or-
   Press **<Ctrl> + <R>**.

   The LabBook is added to the Scheduler. A **Locker** icon is shown in the LabBook toolbar to indicate that changes in the LabBook are unavailable. See Figure 6-34.

2. Depending on your Scheduler settings, the LabBook starts automatically. Alternatively, in the Scheduler toolbar, select the LabBook and click **Run** to start the measurement.

   The LabBook measurement starts, see Figure 6-34. The LabBook tab indicates "[scheduled]" or "[Running]".

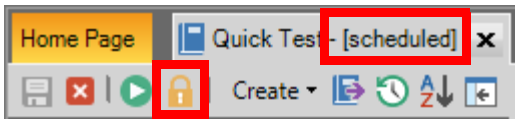


Figure 6-34. LabBook scheduled indicators

❖ To modify a scheduled LabBook

1. As long as the measurement of your LabBook has not started, you can remove it from the Scheduler. In the Scheduler, select your LabBook and click the **Locker** icon.

2. In the confirmation message, click **Yes**.
   Your LabBook is removed from the Scheduler.

3. Make your changes and save your LabBook.

4. Click **Run.**
   -or-
   Press **<Ctrl> + <R>** to schedule your LabBook.

Tip Your LabBook now is appended to the Scheduler list. Use the Up and Down buttons to move your modified LabBook to the desired position.

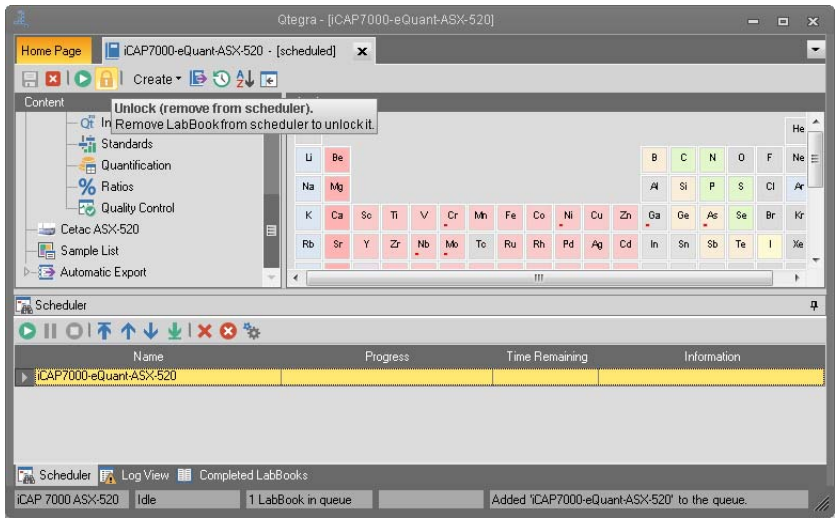


Figure 6-35. Measurement started for scheduled LabBook

Tip If the **Automatic** mode has been selected for **Start Queue** in the **Options** settings of the Scheduler (see "Customizing Scheduler Settings" on page 4-76), the measurement starts immediately.

When the measurement has started the LabBook tab indicates "[Running]".

The completed LabBook is automatically deleted from the Scheduler and added to **Completed LabBooks**, see "Completed LabBooks" on page 4-87. The LabBook tab changes to green and indicates "[Completed]". If an error occurred during the acquisition, the LabBook tab changes to red.

Viewing the Results of a Measurement

After acquisition, the results of the measurement are added to the completed LabBook and can be viewed in Qtegra. Log Messages can be viewed, the results can be electronically signed, different sets of queries can be placed and Reports can be printed.

❖ **To view the results of a measurement**

1. From the **Qtegra - [Home Page]**, click **Completed LabBooks**.
2. In the **Completed LabBooks** tab, click the LabBook you wish to view.
   The completed LabBook opens in a separate tab, see Figure 6-36.

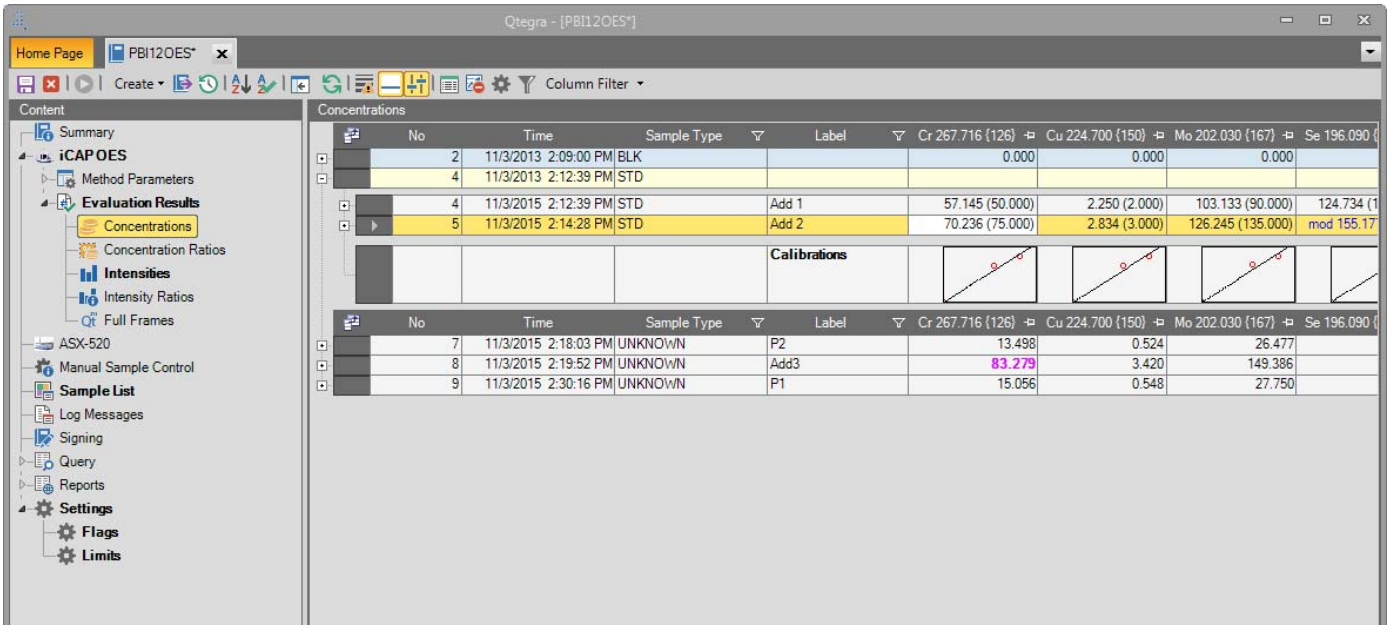


Figure 6-36. Completed LabBook

3. Expand **iCAP OES** to show the items added to the LabBook after measurement, see Figure 6-37.

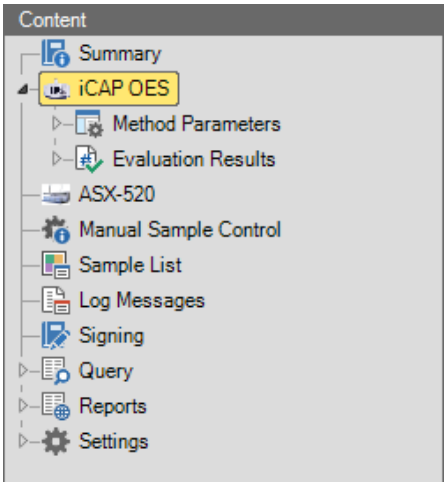


Figure 6-37. Added items of a completed LabBook

The items **Evaluation Results** and **Instrument State**, and the menus **Log Messages**, **Signing**, **Query** and **Reports** have been added to the LabBook.

Evaluation Results

The **Evaluation Results** view displays the data acquired within a LabBook and can be viewed during the actual acquisition of a LabBook in Qtegra.

The presentation of the evaluation results differs, according to the "Method Parameters Settings" on page 9-3 defined.

❖ **To open the Evaluation Results view**

1. In the **Completed LabBooks** list, select the LabBook you wish to view.
   The completed LabBook is opened in a new tab.

2. Expand **Evaluation Results** to open the **Evaluation Results** view, for example, see Figure 6-38.

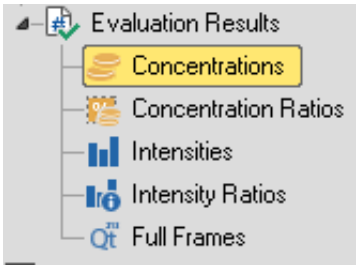


Figure 6-38. Evaluation Results sub-menus in completed LabBook

The toolbar of the completed LabBook shows several additional buttons for Evaluation Results, see Figure 6-39.

Figure 6-39. Toolbar of completed LabBook

The function of the additional buttons is explained in Table 6-2.

Table 6-2. Additional buttons in toolbar for Evaluation Results

Button	Icon	Meaning
Recalculate		Qtegra updates the data automatically whenever you make changes. For some applications, however, the update is not performed automatically. The button then flashes to advise you there are some updates to be performed.
Inter-Element Correction		Switches the mathematical interference correction on and off.
Blank Correction		Switches the Blank correction on and off.
Use Internal Standard		Switches the use of an internal standard on and off.
Display Details		Displays an enlarged graph of the calibration curve including the calculated values for the background equivalent concentration (BEC), the instrumental detection limit (IDL) and the most common statistical data.
Hide Thumbnails		Hides or shows the thumbnails (small graphical display) of the evaluation results.
Display Settings		Opens the **Display Settings** dialog (see Figure 6-40) where you can set the digits to be displayed for evaluation results, set the **Internal Standard Ratio** display to **True** or **False** and enter a customized name for **General**.
Column Filter	Column Filter	Switches the columns to be displayed for the selected result view.

Display Settings can be set for any LabBook. Set parameters for the Calibration view, the Concentrations view, the Intensities view, the Ratios view, and general and quantification parameters according to your needs.

❖ To open the Display Settings dialog

1. On the LabBook toolbar, click **Display Settings** to open the Display Settings dialog, see Figure 6-40.

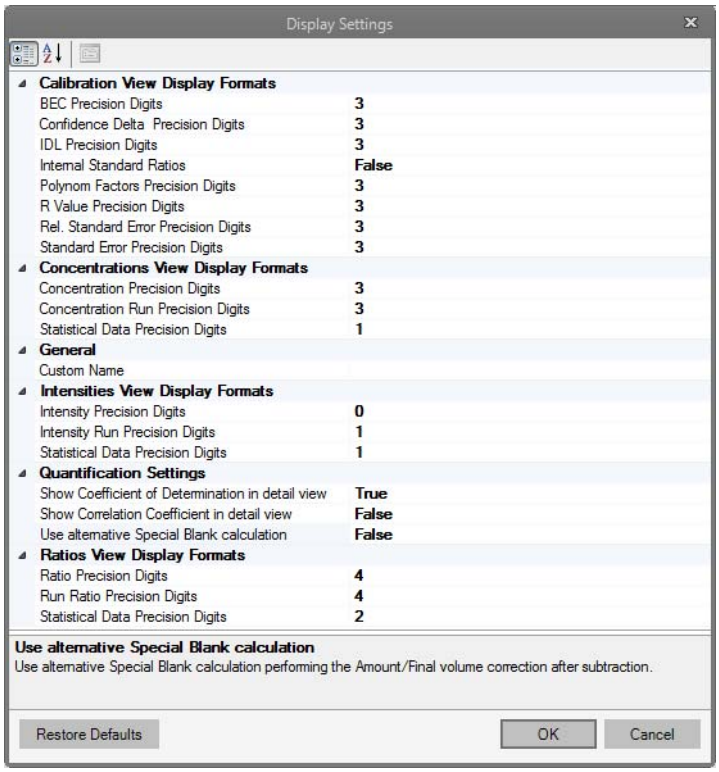


Figure 6-40. Display Settings dialog showing the default values

2. Select the item you want to change. A short description is shown below the list to explain the item. Thus you can see that, for example, the Correlation Coefficient is also known as R, and the Coefficient of Determination as R^2.

Tip Changes are only valid for the currently selected LabBook. To use your settings in general, create your LabBooks from this modified LabBook.

Log Messages

The **Log Messages** view of a LabBook is added to the LabBook after a measurement has been run for this LabBook.

The table in **Log Messages** contains all events with appropriate time stamps which occur throughout the manipulation of the LabBook. All information, warning and error messages are logged here including information about the service concerned.

❖ **To open the Log Messages view**

1. In the **Completed LabBooks** list, select the LabBook you wish to view.
   The completed LabBook is opened in a new tab.

2. Click **Log Messages** to view the **Log Messages** of the completed LabBook, see Figure 6-41.

Log Messages

Logged at	Level	Message	Time	Category	Sub Catego
Line no. 2: standard		Total evaluation time [msec] : 16, Data loading time [msec] : 1, Peak detection time [msec] : 0	7/25/2013 11:04:00.	Qtegra	ChromBase.E
Experiment scheduling		Total evaluation time [msec] : 21, Data loading time [msec] : 0, Peak detection time [msec] : 0	7/25/2013 11:04:48.	Qtegra	ChromBase.E
Line no. 4: standard		Total evaluation time [msec] : 17, Data loading time [msec] : 0, Peak detection time [msec] : 1	7/25/2013 11:05:37.	Qtegra	ChromBase.E
Line no. 5: sample		Total evaluation time [msec] : 24, Data	7/25/2013 11:06:25.	Qtegra	ChromBase.E

Figure 6-41. Log Messages in completed LabBook

❖ **To filter Log Messages**

1. In the **Log Messages** view, click  in the header of the column you wish to filter the display of.

A drop-down menu opens, see Figure 6-42.

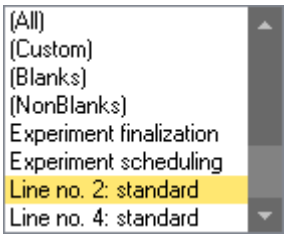


Figure 6-42. Log Messages filter drop-down menu in completed LabBook

2. Select an item from the drop-down menu.
The column shows only the selected values.

❖ **To customize filters in Log Messages**

1. In the **Log Messages** view, click  in the header of the column you wish to filter the display of.

2. From the drop-down menu, see Figure 6-42, select **(Custom)**.
The **Custom Filter** dialog opens, see Figure 6-43.

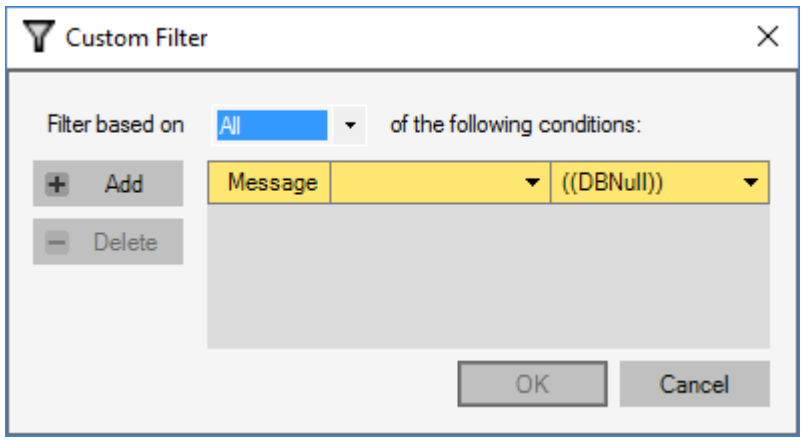


Figure 6-43. Custom Filter dialog of Log Messages in completed LabBook

3. From the **Filter based on** drop-down menu, select **Any** or **All**.

4. Click ▼ of the left column to open the **Rule** drop-down menu, see Figure 6-44.

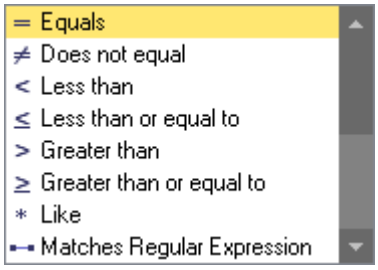


Figure 6-44. Rule drop-down menu of Custom Filter dialog

5. Select a rule from the drop-down menu.
6. Click ▼ of the right column to open the **Argument** drop-down menu, see Figure 6-45.

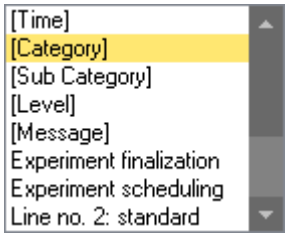


Figure 6-45. Argument drop-down menu of Custom Filter dialog

7. Select an argument from the drop-down menu.
8. Click **OK**.
The specified rules are immediately applied to the table.

Signing

The **Signing** view of a LabBook is added to the LabBook after a measurement is completed.

Signing is used to protect the acquired data and to verify the operator. Certificates are required to activate the signing feature. These Digital SSL certificates are issued by Trusted CA Certificate Authorities (for example, VariSign, GlobalSign, Thawte and CAcert) and must be purchased separately. They are applied by your Administrator.

Tip Large companies will usually have their own certificates. Ask your Administrator. See "Qtegra LabBook Signing" on page 2-19 on how to make certificates available.

❖ To open the Signing view

1. In the **Completed LabBooks** list, select the LabBook you wish to view.
   The completed LabBook is opened in a new tab.

2. Click **Signing** to open the **Signing** view, see Figure 6-46.

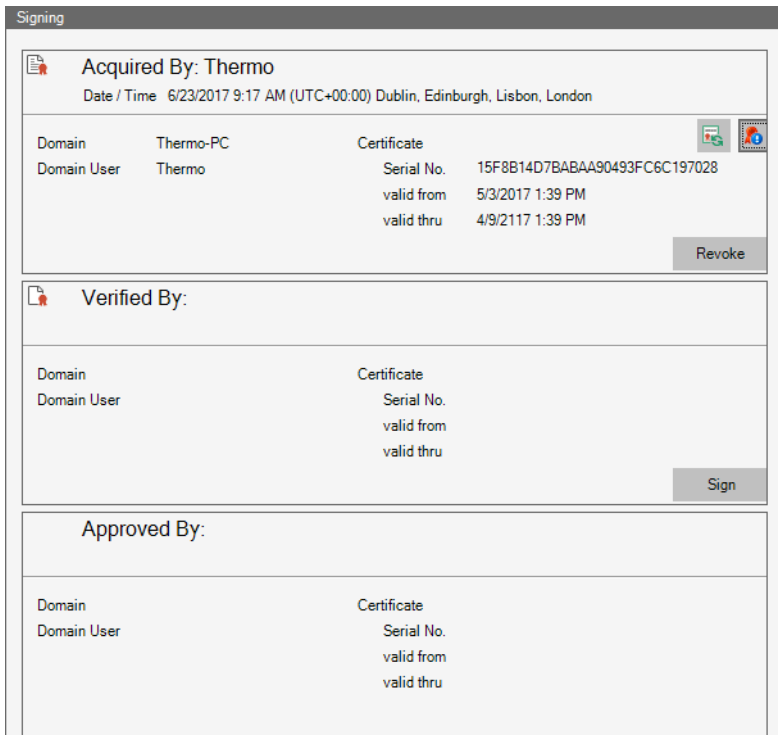


Figure 6-46. Signing in completed LabBook

The LabBook may be signed in multiple steps, for example *Acquired, Verified* and *Approved*. All steps are defined and named in the Configurator (see "Signature Workflow" on page 3-28). After signing, every step can be revoked if sufficient user rights are set under Configurator > Access Control > User Actions > LabBooks > Electronic Signatures.

After the first step has been signed, the **Sign** button switches to **Revoke** and the next step gets a **Sign** button. With a signature on the final step, the LabBook is approved and you therefore may not directly revoke the signature of the initial steps.

❖ To sign the LabBook

1. Open the **Signing** view of your LabBook.

2. In the pane representing the actual step, click **Sign**.
   The **Select certificate for signature** dialog opens, see Figure 6-47.

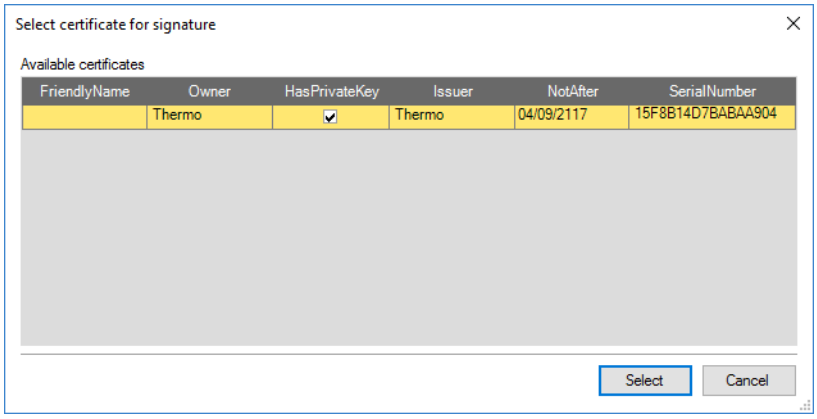


Figure 6-47. Select certificate for signature dialog

   A list of valid certificates which contain a private key necessary for signing is shown.

3. Select your certificate from the list and click **Select**.

4. Follow the instructions.
   Any further step subsequently must be signed by the user as defined in the Configurator.

❖ To open a signed or locked LabBook

1. Every signed LabBook can be opened with a compatible version of Qtegra ISDS Software.

2. If a LabBook was locked (see page 3-28 for locking with signing) and then opened, the LabBook tab indicates the lock state.

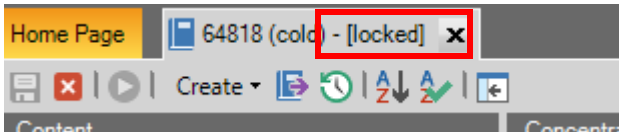


Figure 6-48. "locked" hint for signed LabBook

   This state shows that no changes can be made with this LabBook, for example, no data can be excluded in the Concentrations view, Standards are grayed out in the Standards view.

3. If a LabBook was signed and then opened with a later version of Qtegra ISDS Software, the LabBook is indicated with a yellow hint in the toolbar.

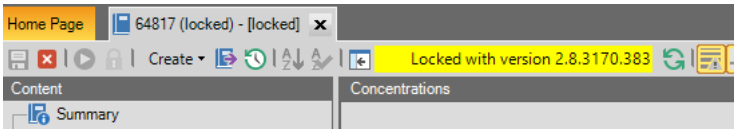


Figure 6-49. Toolbar hint for signed LabBook

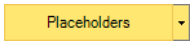
The signed LabBook is protected and verified by the operator and can therefore not be modified.

Electronic signatures can be added to the Report to document the signing level.

❖ **To add the Signature to the Report**

1. Open the **Reports** view of your signed LabBook. At least the first level must be signed.
2. Expand the Reports tree and select one item.
   The Report Preview is shown.
3. Click **Edit Report** on the Preview toolbar.
4. To place the signature in the page footer, select the Page footer from the Report Settings tree.
   By default, "$(PageNumber) / $(PageCount)" is shown as placeholders.

   a. Click **Add** to add a new placeholder.



   b. Expand the **Placeholders** button and select *Signature*.
   "$(Signature)" is shown in the Text box.

   c. Click **Execute Report** to check the new footer in the Report.

d. Finally, close and reopen your LabBook to see the signature(s) in the Report's footer, see Figure 6-50.

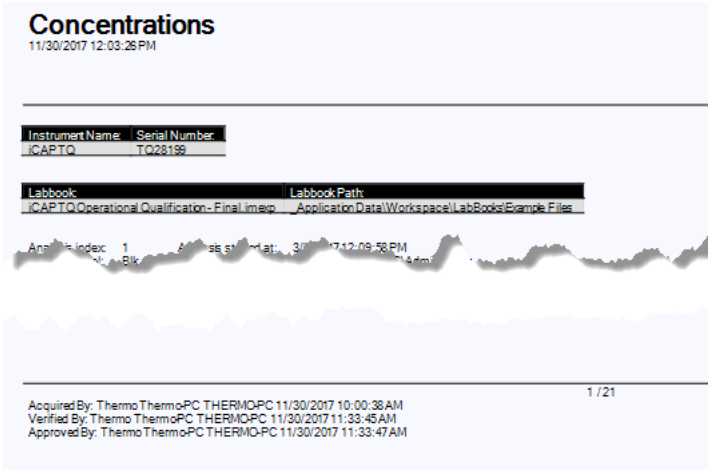


Figure 6-50. Signatures in the Concentrations Report footer

e. If you select *XML Renderer* as Output Format, the signature is appended to the code, see Figure 6-51.

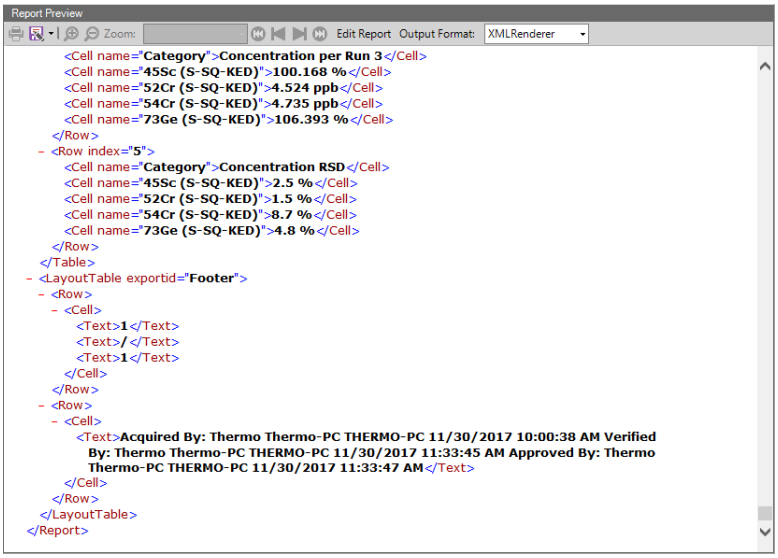


Figure 6-51. Signatures in the Concentrations Report (XML Renderer)

5. As an alternative, the signature can also be placed in the Content area with Data Tables from the *Signatures* source, see Figure 6-52.

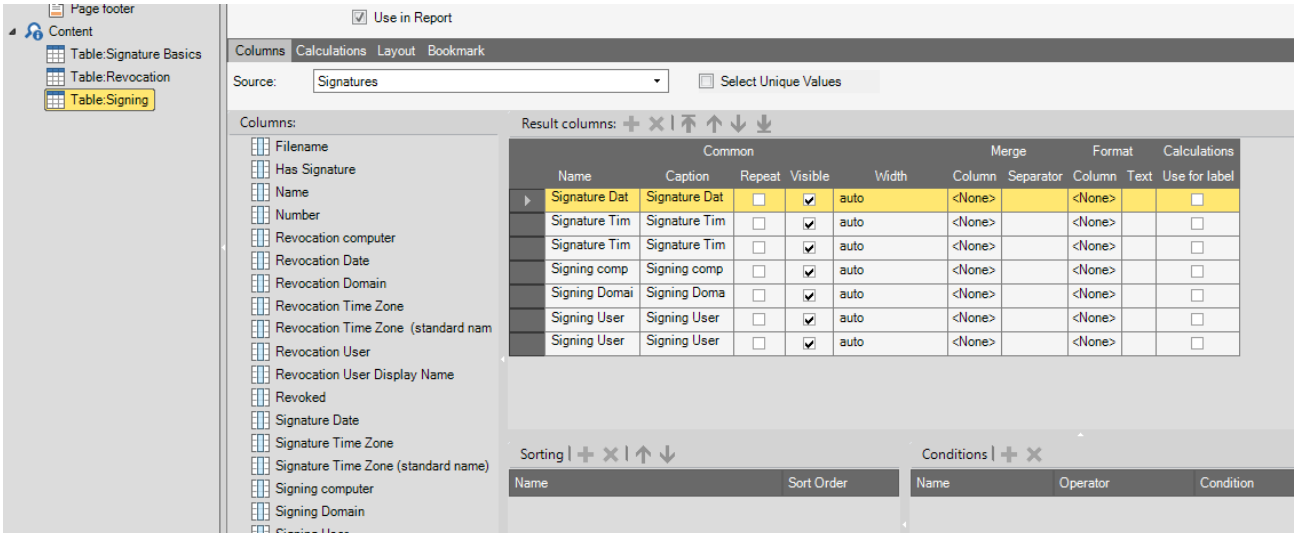


Figure 6-52. Signatures Table in the Report Editor

6. Click **Execute Report** to show the current output.
The Report shows the Signature columns as specified. Based on the example in Figure 6-52, the *Date* and *Time Zone* (UTC based and with standard name), the name of the *Signing computer* and *Domain*, and the login name and display name of the *Signing User* are shown.

Query

Query is used to gather and arrange LabBook data for export into third party packages (such as Excel) and for printing or saving as a Report (that allows for additional formatting changes, additional calculations etc.) The **Query** view of a LabBook is only available once data is acquired.

For **Query**, the toolbar of the completed LabBook adds the **Query** and **Reports** buttons, and the **Create** drop-down item **New Report** is activated, see Figure 6-53.

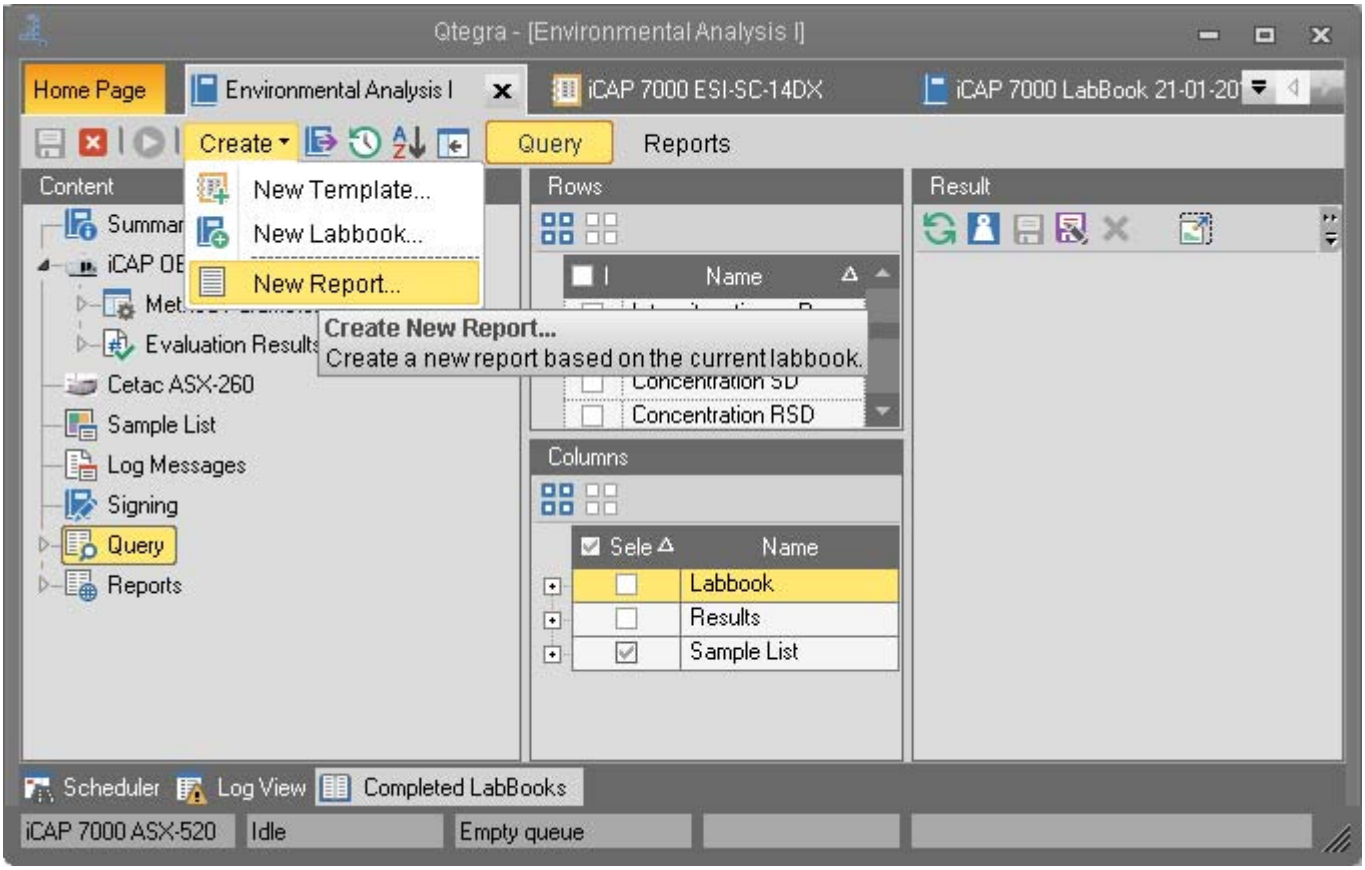
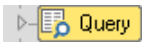


Figure 6-53. LabBook toolbar of a completed LabBook in Query

Data is gathered for export as a Query by selection from a series of data sources.

❖ **To open the Query view**

1. Open a LabBook that contains results. It will be displayed in its own tab.



2. Click **Query** in the content pane of the LabBook.

Query

3. On the toolbar of the LabBook, open the **Query** view to open the screen as shown in Figure 6-54.

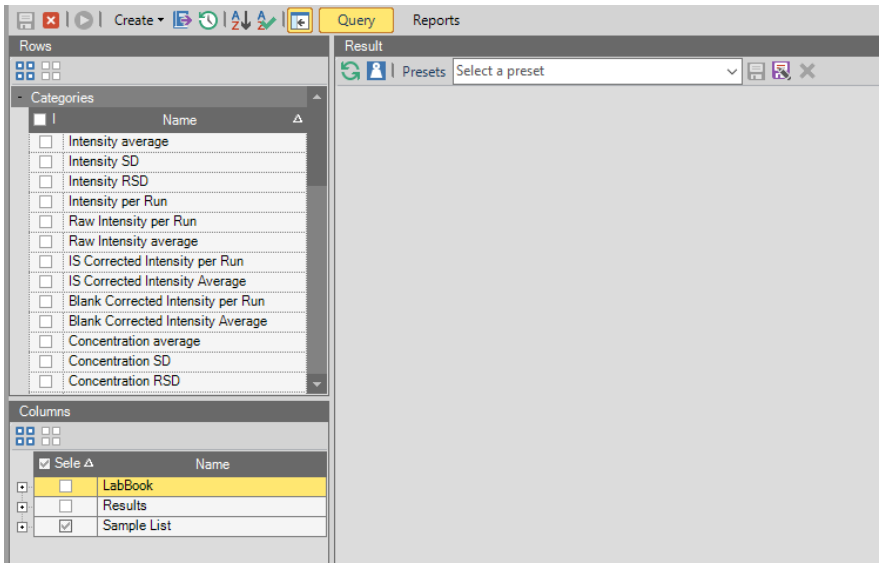


Figure 6-54. Initial Query view of a completed LabBook

The result data display of a query is defined by the selection of individual data categories and LabBook, Sample List or Results parameters. Perform at least step 1 to step 3 of the procedure as follows.

❖ **To define result data display of a Query**

1. In the **Rows** section of the Query view, select the individual data **Categories** you wish to display.

   -or-

   Click **All** to select all data categories.

   For details on the individual data categories, see page 6-49.

2. In the **Columns** section, click **Expand** to view all parameters, and select the **LabBook**, **Sample List**, and **Results** parameters you wish to display.

   -or-

   Click **All** to select all parameters.

3. In the **Result** section, click **Update** to display the selected result values, see Figure 6-55.

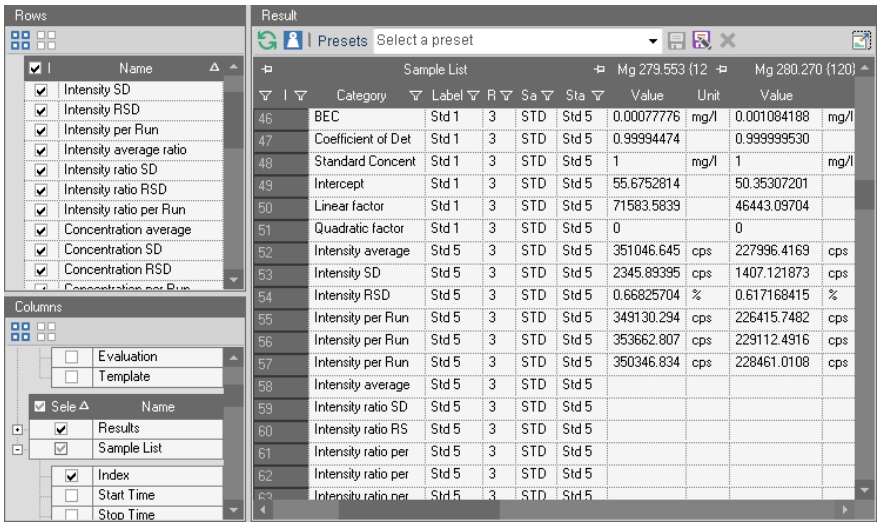


Figure 6-55. Query view with results in completed LabBook

4. Click **Hide Units** to hide or show the units.

❖ **To save a Query preset**

1. Open a LabBook that contains results. It will be displayed in its own tab.

2. Open the Query view and define the result data.

3. On the toolbar of the Result pane, click **Refresh** or press **<F5>** to display the selected result values.

4. From the **Presets** drop-down list, click **Save Preset As**.
The **Save New Preset** dialog is displayed, see Figure 6-56.

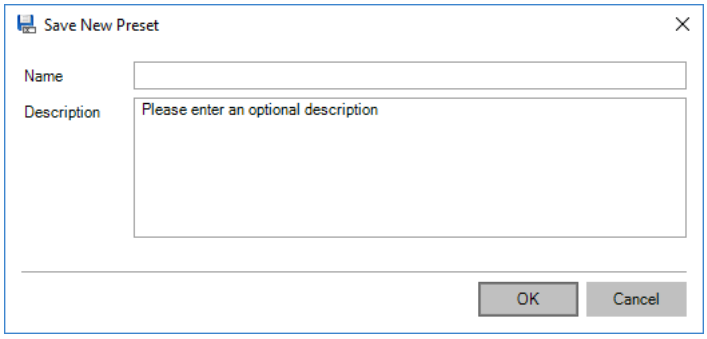


Figure 6-56. Save New Preset dialog in Query view

Tip Result data presets saved here will be available as well in the Query view of the **LabBook Query** page, see "LabBook Query Page" on page 4-41.

5. Type a **Name** for the preset.

6. Type a **Description**.

7. Click **OK**.
The preset is added to the list.

❖ To export Query result data

1. Open a LabBook that contains results. It will be displayed in its own tab.

2. Open the Query view and define the result data.

3. On the toolbar of the Result pane, click **Refresh** or press **<F5>** to display the selected result values.

4. On the toolbar of your LabBook, click **Export**.
-or-
Press **<Ctrl> + <E>** to open the **Export data** dialog, see Figure 6-57.

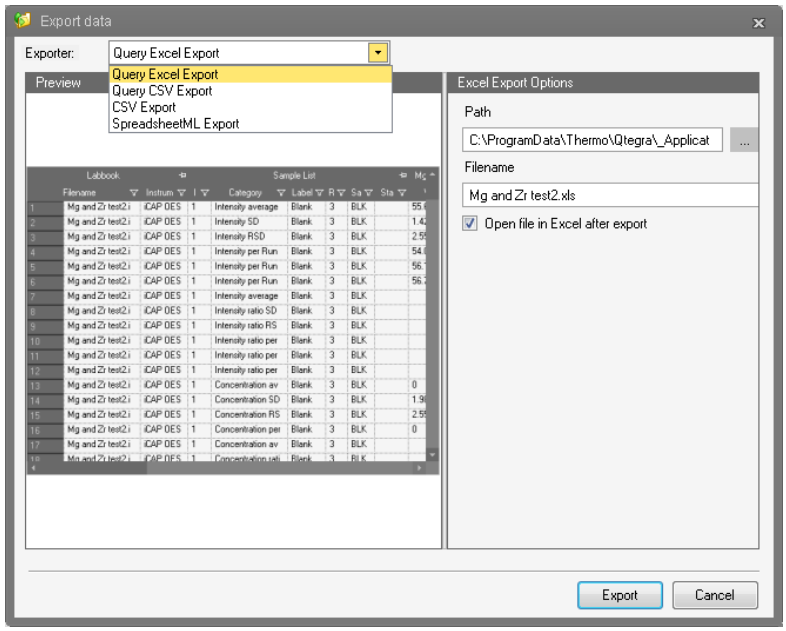


Figure 6-57. Export data dialog

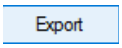
Tip For tQuant and trQuant LabBooks, additionally **Laser Data Reduction Export** (compatible with both Iolite and GLITTER v 4.4.4 and above) is available to define the analytes results to be exported.

5. Select your export format from the **Exporter** drop-down menu.
Query Excel Export will generate an XML file that is opened with Excel, by default.
Query CSV Export will generate a comma separated file (*.csv) that is opened with a text editor, for example, Notepad.

CSV Export and *SpreadsheetML Export* are not valid for Query tables and may therefore be ignored.

Tip Query based exports are not suited for LIMS ("N/A" values are exported as "0", zero, which may be imported into LIMS systems without forcing format errors). Best to use *CSV Export* and *SpreadsheetML Export* for laser.

6. Type the **Path** for the export file,
   -or-
   Click the browse button to open the standard dialog to navigate to the desired folder.
7. Edit the **Filename** for the export file, or keep the proposal.
8. Depending on your selection from the Exporter, the right pane of the Export data dialog varies.
   a. For *Query Excel Export*, select **Open file in Excel after export** to automatically run the associated program displaying your exported file.
   b. For *Query CSV Export*, select **Open file in Notepad after export** to automatically run the associated program displaying your exported file. Select the **Column separator** and **Decimal Symbol** from the list boxes.



9. Click **Export**. When the file name already exists, a message is displayed to confirm or deny overwriting.
   The file is exported and opened immediately if so defined.

❖ **To delete Query presets**

1. Open a LabBook that contains results. It will be displayed in its own tab.
2. Open the Query view.
3. In the Results section on the right, select the preset you wish to delete from the **Presets** list.

4. Click **Delete** to delete the result data preset.
   The **Delete Preset** dialog is displayed, see Figure 6-58.

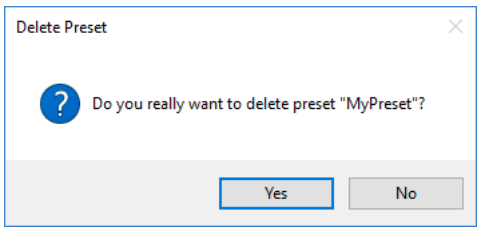
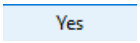


Figure 6-58. Delete Preset dialog in Qtegra



5. Click **Yes**.
   The preset is deleted from the list.

Categories

The Categories section in the Query view of a LabBook lists the data types that can be added as rows in the exported data set. See Table 6-3 for a description of the supplied categories. For additional information on each data type, see "Basic Mathematical Methods" on page 11-1 and "Data Processing Algorithms for eQuant" on page 13-1.

Table 6-3. Categories with reference to detailed description

Name	Description
BEC	The background equivalent concentration is defined as the analyte concentration that produces a net signal (peak minus background) equal to the background. See "Background Equivalent Concentration (BEC)" on page 13-5.
Blank Corrected Intensity Average	Calculated from the IS Corrected Intensity Average minus the intercept. See "Blank Corrected Intensity" on page 13-15.
Blank Corrected Intensity per Run	Calculated from the IS Corrected Intensity per Run minus the intercept. See "Blank Corrected Intensity" on page 13-15.
Coefficient of Determination	See "Coefficient of Determination (R^2)" on page 11-4.
Concentration Average	Arithmetic mean of Concentration per Run values. See "Average" on page 11-2. Note that the Concentration Average from standard addition measurements (aQuant) shows the concentration of the individual sample ("STD" or "ZERO STD"). To get the result concentration of a "STD" or "ZERO STD" block in the Query and Reports, select *Zero Standard Concentration*.
Concentration per Run	Concentration value per run, corrected for any dilution or special blank.
Concentration RSD	Relative standard deviation of Concentration per Run values. See "Relative Standard Deviation (RSD)" on page 11-2.
Concentration SD	Standard deviation of Concentration per Run values. See "Standard Deviation (SD)" on page 11-2.
Correlation Coefficient	The Pearson correlation coefficient is calculated from the Coefficient of Determination. See "Correlation Coefficient (R)" on page 11-4.
Intensity Average	Arithmetic mean of Intensity per Run values. See "Average" on page 11-2.
Intensity per Run	Intensity value per run, corrected for interference.
Intensity RSD	Relative standard deviation of Intensity per Run values. See "Relative Standard Deviation (RSD)" on page 11-2.

Table 6-3. Categories with reference to detailed description, continued

Name	Description
Intensity SD	Standard deviation of Intensity per Run values. See "Standard Deviation (SD)" on page 11-2.
Intercept (a)	Intercept of linear and 2nd order calibration curves. $f(x) = bx + a$ $f(x) = cx^2 + bx + a$
IS Corrected Intensity Average	Arithmetic mean of IS Corrected Intensity per Run values.
IS Corrected Intensity per Run	Intensity per Run values, corrected by Internal Standard.
Linear Factor (b)	Factor used in calibration curve $f(x) = bx + a$
LOD	See "Limit of Detection (LOD)" on page 13-4.
Measured Concentration Average	Arithmetic mean of Measured Concentration per Run values.
Measured Concentration per Run	Concentration measured per run, without correction for dilution or special blank.
MQL	See "Method Quantification Limit (MQL)" on page 13-4.
Quadratic Factor (c)	Factor used in calibration curve $f(x) = cx^2 + bx + a$
Raw Intensity Average	Arithmetic mean of Raw Intensity per Run values.
Raw Intensity per Run	Intensities per run without any correction for interference.
Relative at%	Arithmetic mean of Relative Atom Percent per Run values. See "Relative Atom Percent (RelAt%) and Relative Weight Percent (RelWt%)" on page 13-16.
Relative at% per Run	Relative Atom Percent per Run.
Relative wt%	Arithmetic mean of Relative Weight Percent per Run values. See "Relative Atom Percent (RelAt%) and Relative Weight Percent (RelWt%)" on page 13-16.
Relative wt% per Run	Relative Weight Percent per Run.
RSE	See "Relative Standard Error (RSE)" on page 11-2.
Standard Concentration	Concentration value for the standard referred to for that analysis.
TuneSettings	Tune Settings for a couple of instrument specific parameters, for example, Additional Gas Flow, Peristaltic Pump Speed, Plasma Power, Nebulizer Flow.
Zero Standard Concentration	Concentration of the zero standard using in Standard Addition calibration routines.

Query Reports

❖ **To open the Reports view of a query**

1. Open a LabBook that contains results. It will be displayed in its own tab.
2. Open the Query view and define the result data.
3. 

On the toolbar of the LabBook, click **Reports** to open the Reports view (see also "Qtegra Report Preview" on page 8-66).
For details on creating Reports, see "Using the Qtegra Report Editor" on page 8-15.
4. From the list of Reports, select one item.
5. 
On the toolbar of the Reports pane, click **Display Report** or click **Execute Report** below the list to display the selected Report.

   The Report can be modified, printed or exported as described in "Qtegra Reports" on page 8-1.

Reports

The **Reports** view of a completed LabBook displays the results of a measurement in Report formats previously created.

For creation of Reports, see "Using the Qtegra Report Editor" on page 8-15.

❖ **To show a Report**

1. Open a LabBook that contains results. It will be displayed in its own tab.

2. Click **Reports** to open the Report Preview, see Figure 6-59.

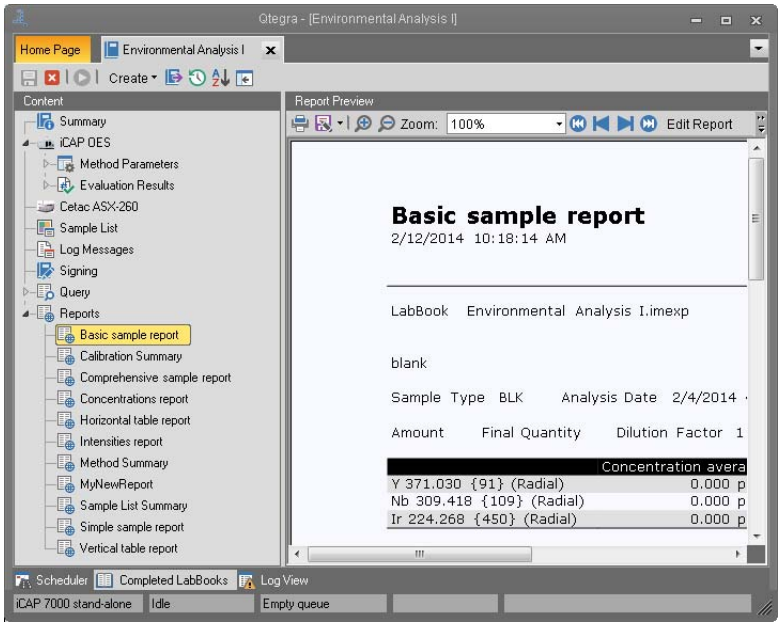


Figure 6-59. Report Preview of a completed LabBook

The results of the measurement are displayed using the layout of the first Report in the list on the left.

3. Select a Report layout to change the Report layout accordingly.

Reports Editor

In the Report Preview of a completed LabBook in Qtegra, you generate result data Reports from presets.

You can structure your Report to your needs, add headings, tables and graphs to specify the presentation of the result data. For details on creating Report presets, see "Report Settings Items" on page 8-25.

7

Method Development

General Remarks

The Method Development tool of Qtegra ISDS Software provides two routines to support users in the method development process. The first routine, Element Finder, suggests wavelengths for the user's measurement based on the selection of elements from the Periodic Table and by optionally performing a series of measurements on the sample of interest.

In the second routine, Plasma Optimization, plasma parameters are optimized in a multivariate manner. Only important parameters are optimized to reduce the time required to perform the optimization process. The routine allows the user to optimize the plasma parameters for highest average intensity, for best signal to background ration, or for best signal to square root of background ratio.

Contents

The Method View

Start Page for Method Development

The Start Page for Method Development provides options to create a new method or to open a previously completed.

❖ **To create a new method**

1. From the **Qtegra - [Home Page]**, click **Method Development**. The **Method Development** page of Qtegra opens, see Figure 7-1.

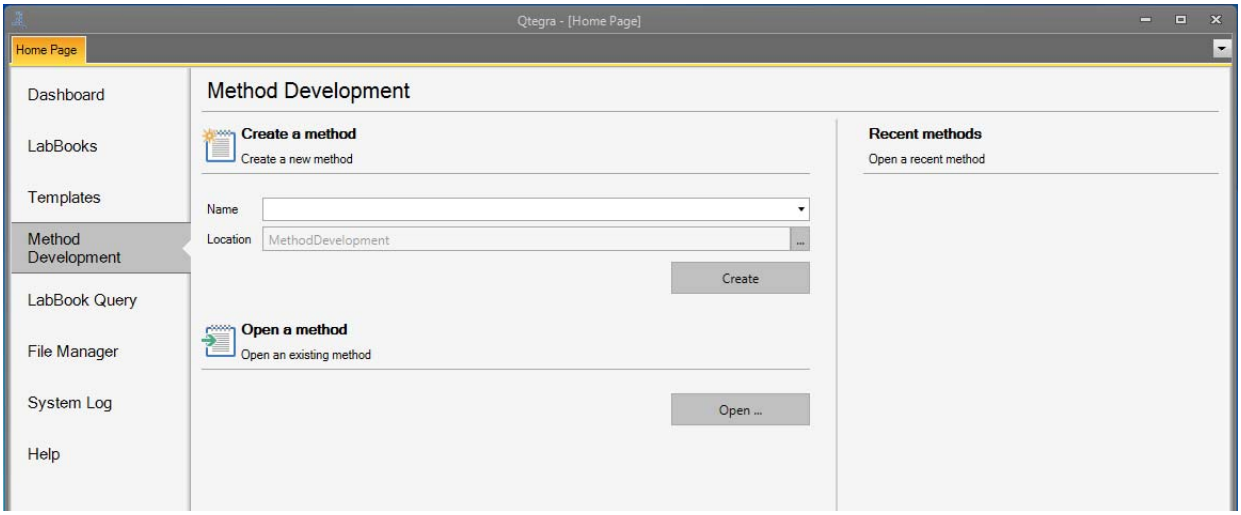


Figure 7-1. Method Development page

2. Enter a unique **Name** for the method and select a **Location** if desired. A red frame around the **Name** box indicates that the name already exists. Enter a unique name to proceed to the next step.
3. Click Create to create the new method.
   A tab opens for the newly created method with two tiles shown. Once methods have been created and completed, they are shown in the History list located on the right hand side of the page, see "The Method View" on page 7-2.
4. Select either **Element Finder** or **Plasma Optimization**.

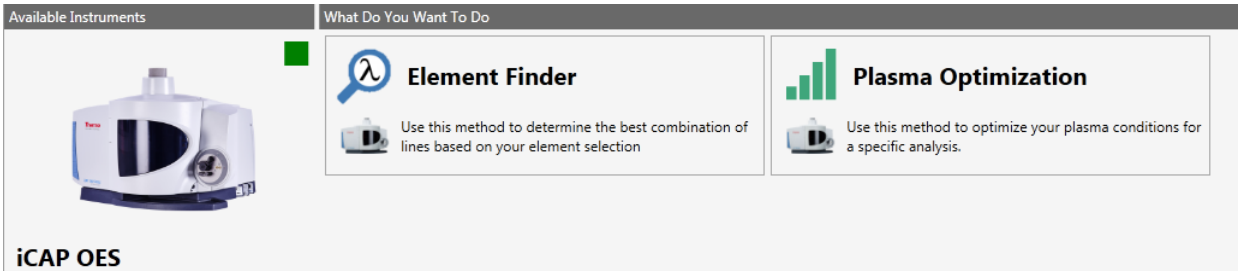


Figure 7-2. Initial view for creating a new method

Tip In Method Development the status indicator for the current configuration only indicates if the instrument is connected or not. To see if the Status is *Ready* or *Not Ready* return to the Dashboard on the Qtegra [Home Page].

5. For **Element Finder**, the method view changes to the first step of the Method Creation wizard. See "The Element Finder" on page 7-4.
   -or-
   For **Plasma Optimization**, see "Plasma Optimization" on page 7-12.

The Element Finder

This routine is used to determine a list of wavelengths that is best suited for analysis. The workflow does not explicitly require knowledge of the matrix or analyte elements that are present in the sample. If these are known, they can be selected on the appropriate screens.

The wavelengths found by the algorithm can then be used to create a pre-filled method. Alternatively, it is possible to determine elements contained in the sample by making a Fullframe measurement within Element Finder. Input from the user can be compared with or added to the Element Finder result.

Elements found by the Element Finder routine are marked as Matrix by default. This means that they are used by the algorithm to determine which wavelengths are best suited to the analysis but they will not be measured. Changing their type to Analyte Element will mean that they are measured when exported to a LabBook.

Creating a Method

The creation of a method is easy to execute. The Method Creation wizard provides all steps for user input.

Tip Select the Configuration that you want to use to perform Element Finder. If a Configuration is changed before the Element Finder result has been saved, all progress will be lost and the Method View page will be shown.

Selecting Analyte Elements

❖ To select the analytes of your sample

1. In the step **Select Analyte Elements**, select the elements from the Periodic Table that you want to analyze. These elements are referred to as Analyte Elements within an Element Finder routine.
   As in a normal LabBook, elements outside the instrument's detection capability can not be selected, see Figure 7-3.

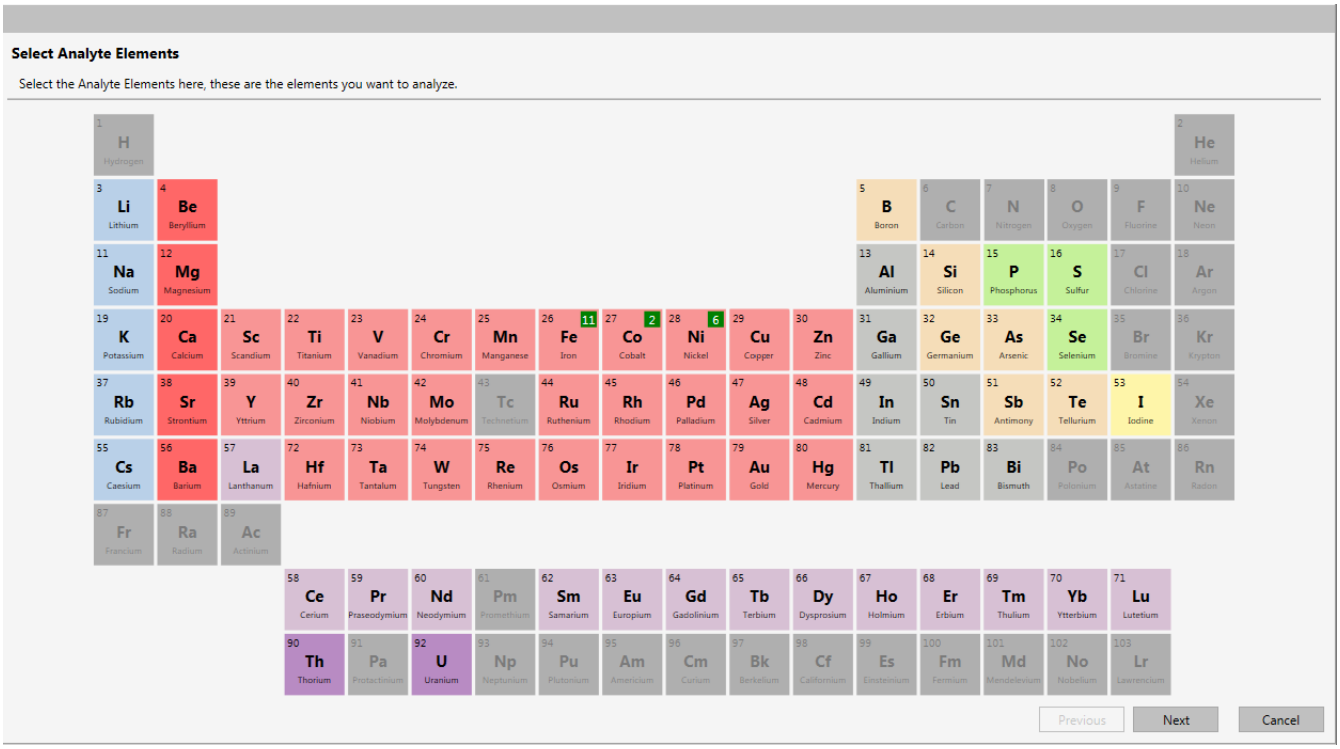


Figure 7-3. Selection of Analyte Elements

Selected Analyte Elements are indicated by a green box in the top right hand corner of the element tile. The number within the tile denotes the amount of wavelengths that could be suitable for analysis and is updated with each subsequent element selection. If an element has been selected by error, it can be removed by clicking on it again. The box in the top right hand corner will be removed.

Tip If you do not know what is in your sample, you can skip this step without selecting any element and clicking Next. For iCAP 6200 and 7200 this step must take place.

2. Click **Next** to open the next page of the wizard.

Selecting Matrix Elements

❖ To select the Matrix Elements

1. In the step **Select Matrix Elements**, click to select the elements which are in your matrix from the Periodic Table. Matrix Elements are elements you do not want to analyze but are contained in your sample, see Figure 7-4.

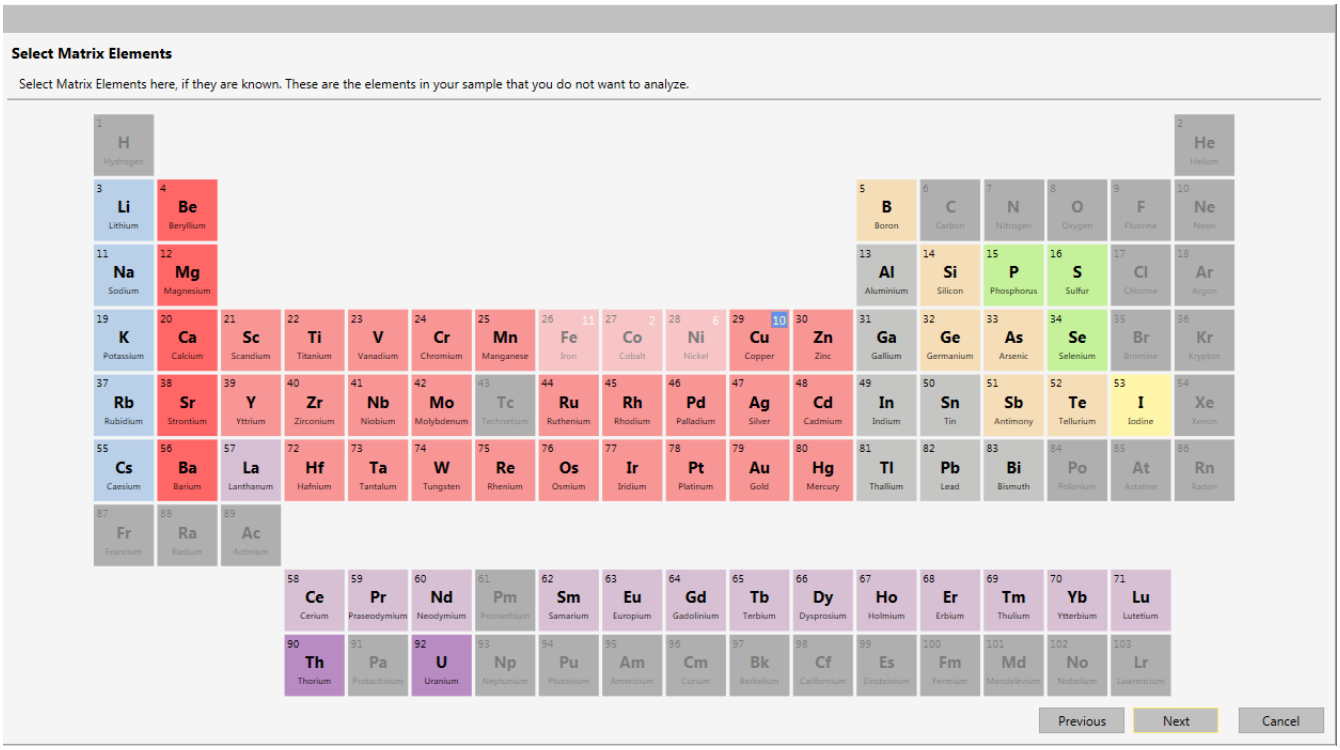
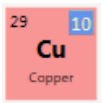


Figure 7-4. Selection of Matrix Elements



Selected Matrix Elements are indicated by a blue box in the top right hand corner of the element tile. The number within the tile denotes the amount of wavelengths that could be suitable for analysis and is updated with each subsequent element selection.

Selected Analyte Elements are indicated by a light-colored tile, see Fe, Co, Ni in Figure 7-4. These elements therefore can not be selected as Matrix Elements. To change the Analyte and Matrix status, see "Viewing the Result" on page 7-9.

If an element has been selected by error, it can be removed by clicking on it again. The box in the top right hand corner will be removed.

Tip If you do not know which Matrix Elements are in your sample, you can skip this step without selecting any element and clicking Next. For iCAP 6200 and 7200 this step must take place.

2. Click **Next** to open the next page of the wizard.

Element Finder

1. In this step, Qtegra shows the view to perform Element Finder, see Figure 7-5.

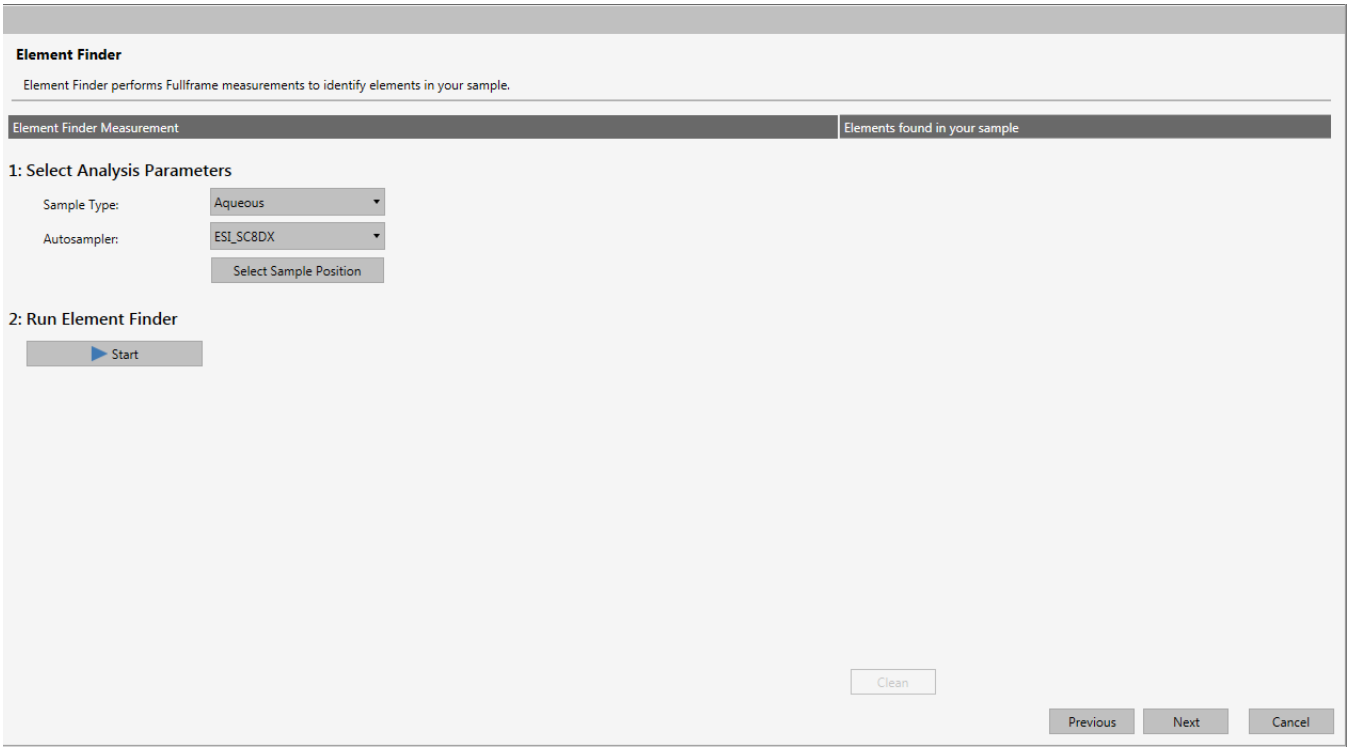


Figure 7-5. Perform Fullframe page after execution

2. Under **Parameters**, from the **Sample Type** listbox, select *Aqueous* or *Organic* according to your sample.
3. From the **Autosampler** listbox, select either *Manual sampler* or *<Autosampler>* according to your instrument Configuration. For details on autosampler settings, see "Autosampler Settings" on page 7-18.
4. Click Start to execute the Element Finder measurement.

   The Element Finder performs a series of Fullframe measurements starting with the visible spectrum followed by the ultraviolet spectrum.

   Tip Fullframe measurements in Element Finder can not be performed using an iCAP 7200 Duo instrument. A typical sample should be used at this point.

   The Run Element Finder area shows the progress and result of the Fullframe measurements.

After the Fullframe measurements are complete, they are analyzed and the elements that are found are displayed, see Figure 7-6.

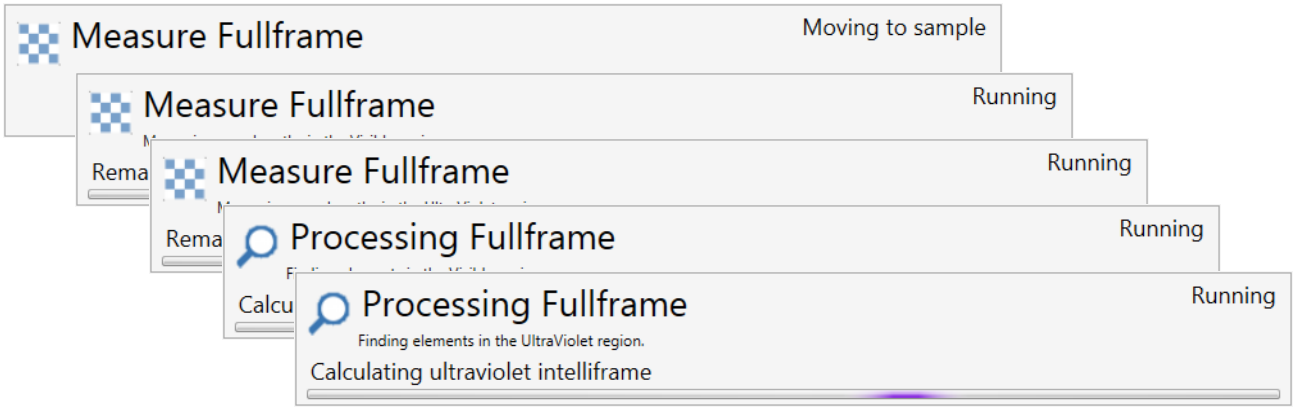


Figure 7-6. Executing a Fullframe measurement

5. In the **Element Finder Result** area, the number of analyzed elements and number of additional elements found are shown, see Figure 7-7.

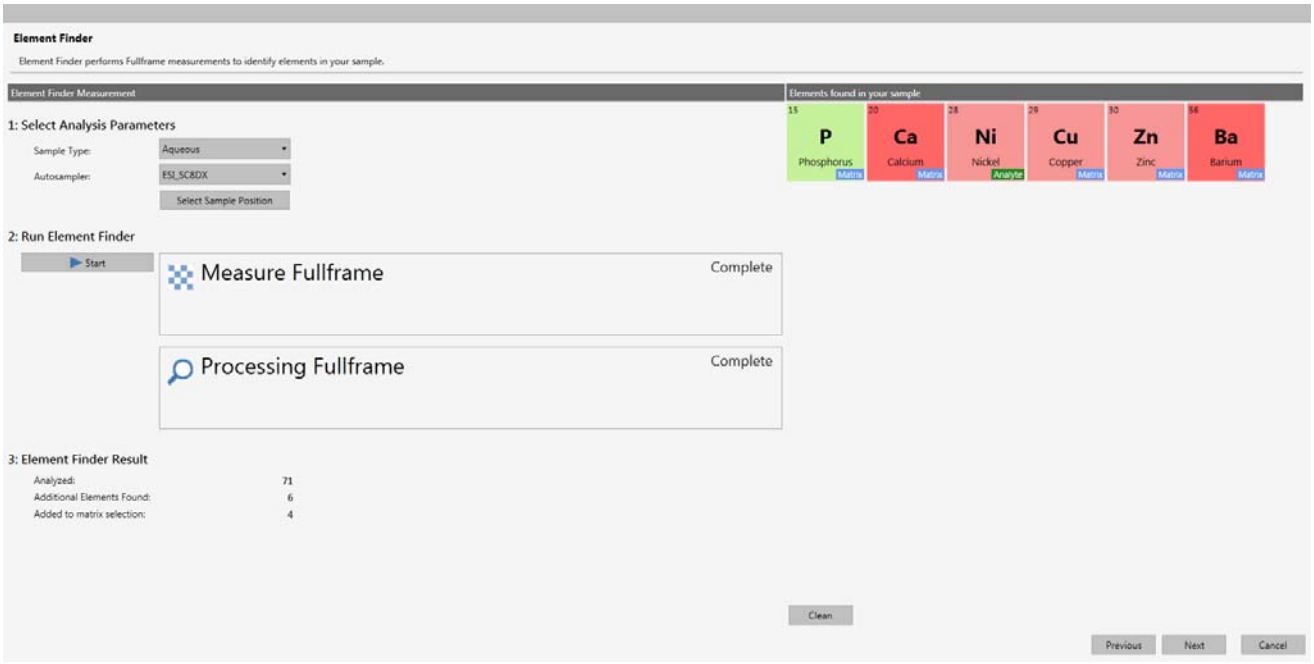


Figure 7-7. Element Finder view for a completed measurement

6. If you would like to perform another Element Finder Measurement, click Clean, and then Start.
7. Click **Next** to open the next page of the wizard.

Viewing the Result

In this step, the **Result** screen shows the wavelengths that are best suited to your analysis according to selections made on previous screens (if any) and output of the Element Finder measurement. By default, elements that are found by the Element Finder measurement are marked as Matrix Elements. Each element will automatically have a wavelength that is best suited to the analysis selected.

It is possible to change their type from Matrix to Analyte Elements, and if desired, modify the wavelengths that have been suggested by Qtegra.

Buttons below the suggested wavelength pane allow these changes to be made.

❖ **To change the Analyte and Matrix type**

1. Hover over the element tile and click the **Toggle** button (see Figure 7-8) to change the element from or to Analyte or Matrix as desired.

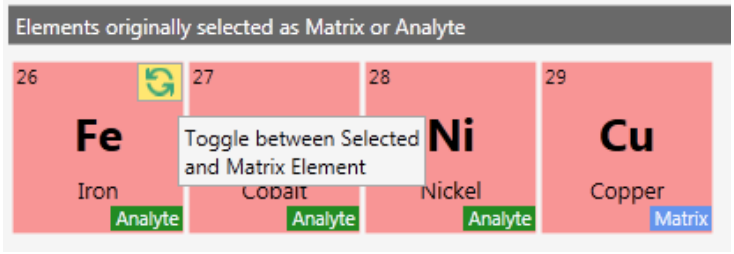


Figure 7-8. Analyte/Matrix Toggle button

   The Matrix indicator (blue) changes to the Analyte indicator (green).

2. Click Apply Changes to update the view.

❖ **To change suggested wavelengths**

1. Click the row of the wavelength of the Analyte Element to display the spectrum view for the selected wavelength. Wavelengths of the visible spectrum are displayed in light yellow, wavelengths of the ultraviolet spectrum are displayed in violet.

The spectrum of only one Analyte Element wavelength can be shown at a time, see Figure 7-9.

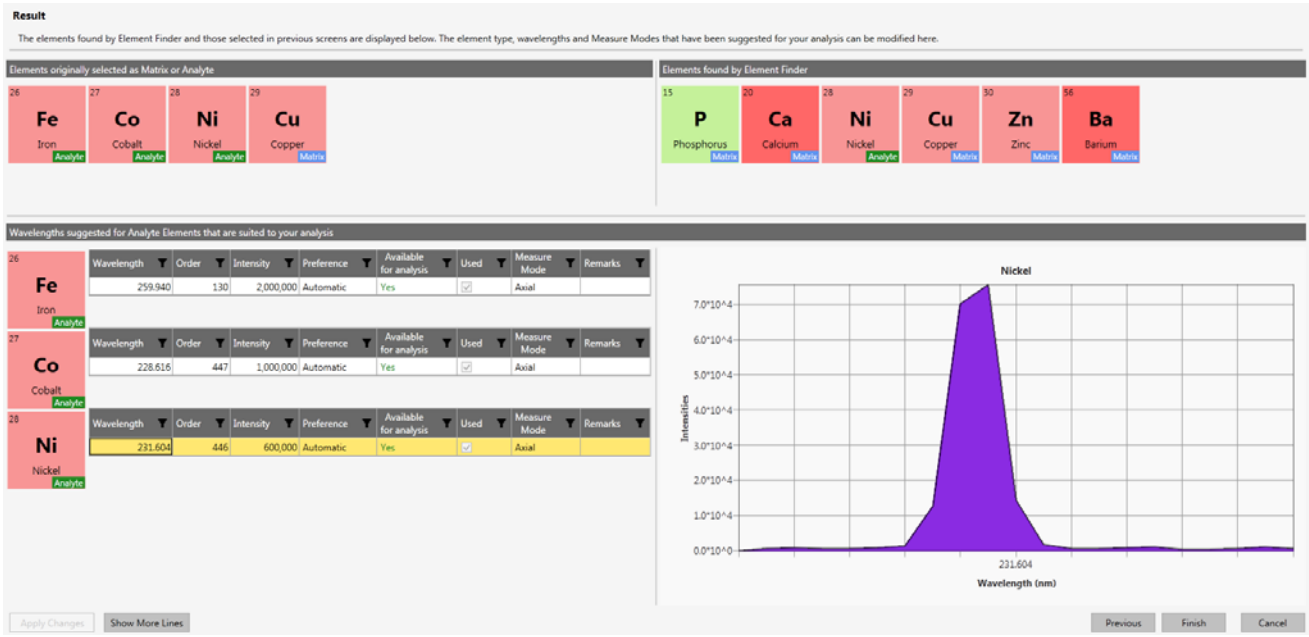


Figure 7-9. Element Finder Result view

Tip If no Fullframe measurements have been performed then no spectra are displayed.

2. By default, the list of elements shows 1 wavelength per element. To view all wavelengths available for the element, click

   Show More Lines.

   The list is expanded. By default all wavelengths have a Preference of Automatic. The Preference of the wavelengths can be modified as desired.

3. From the listbox of the **Preference** column, select either *Automatic*, *Exclude*, or *Include* to specify the use of the specific wavelength.
   Automatic means that the algorithms within Element Finder will determine if the wavelength should be used.
   The most intense wavelength that is suitable for analysis will be marked as **Available for Analysis**.
   Include means that this wavelength must be used and will be included in the wavelengths used for analysis.
   Exclude means that the wavelength will not be **Available for Analysis**.

   Tip If a change is made to the Preference column the wavelength originally suggested by Element Finder as Available for Analysis will then change its state to No. To keep the original wavelength as Available for Analysis change the Preference of that wavelength to Include.

Entries in the **Remarks** column explain reasons for the wavelength **Preference**, for example, interferences with other wavelengths and corresponding elements.

4. From the listbox of the **Measure Mode** column, select either *Axial* or *Radial*. The possible **Measure Modes** will depend on the instrument Configuration.
5. Click Show Less Lines to show 1 wavelength per element.
   The list is collapsed and shows the default view.
6. If any modifications have been made or if you have changed the element type from either Analyte or Matrix, Apply Changes toggles its color. Click the button to update the view after your changes.

❖ **To save the current method**

1. After all changes are done, make sure that Apply Changes is not highlighted.
2. Click Finish to save the current method.
   A confirmation dialog opens to enter a comment.
3. The initial page is shown with the tiles to run the Element Finder or to perform the Plasma Optimization. The completed Element Finder routine is saved to the History entries, see Figure 7-10.

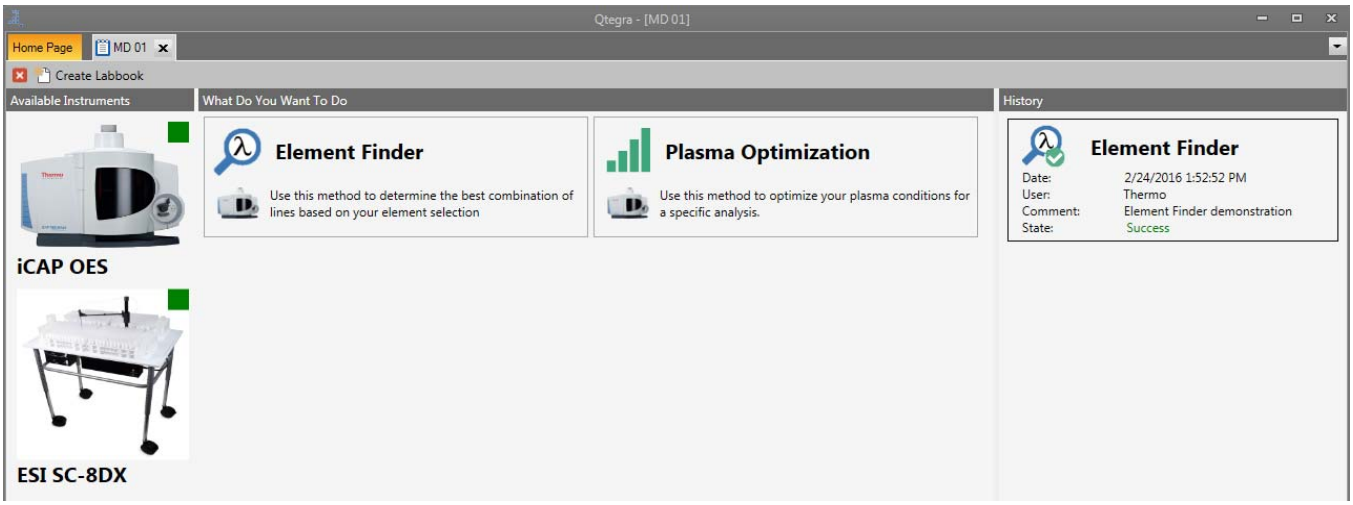


Figure 7-10. Method Development page with completed Element Finder result in the History pane

Plasma Optimization

This routine is used to optimize the plasma parameters for your method.

Plasma optimization can be performed on the output of the Element Finder tool or on a custom selection of elements and wavelengths. The starting parameters are determined by the selected sample type, aqueous or organic.

The following parameters are optimized in a multivariate manner:

- Plasma power
- Plasma gas
- Nebulizer gas
- Radial viewing height (Radial instruments only)

During the optimization process the parameters are shown in real time. Once the optimization is complete it is possible to apply these parameters to a LabBook.

Tip If you have an iCAP 7200 Duo instrument, the plasma optimization is limited. Only plasma power is optimized, either 1150 or 1300 W.

Optimizing the Plasma Parameters

Plasma parameters can be optimized for a previously completed Element Finder method or by selecting wavelengths through the wizard. In the following, both ways are described.

Plasma Optimization on Element Finder Result

❖ **To optimize the plasma parameters using the output of the Element Finder**

1. From the initial view of your method (see Figure 7-10), hover over the Element Finder method in the History pane to show additional buttons.

2. Select **Create Plasma Optimization**.
The Periodic Table is shown with all Analyte Elements already selected, see Figure 7-11.

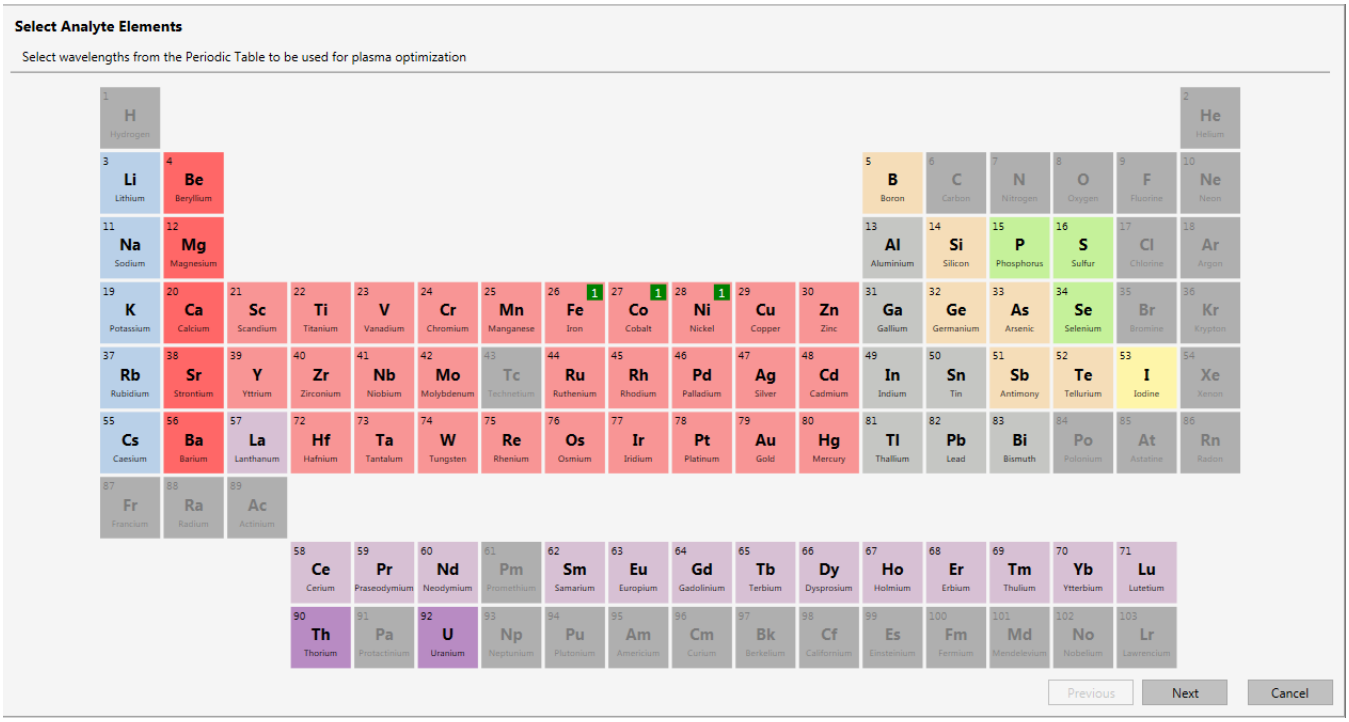


Figure 7-11. Selected elements for plasma optimization

To use the pre-selection, perform the next step.

-or-

Deselect the Analyte Elements you do not wish to use for plasma optimization.
Select additional Analyte Elements you wish to use for plasma optimization.

Tip Modifying the wavelengths from the output of the Element Finder in this way, may lead to an incorrectly optimized set of plasma parameters.

3. Click **Next** to open the Perform Optimization page of the wizard, see Figure 7-12.

Plasma Optimization Wizard

❖ **To optimize the plasma parameters by using the wizard**

1. From the initial view of your method (see Figure 7-2), click **Plasma Optimization** to run the wizard.

2. Select the elements and wavelengths from the Periodic Table that you want to optimize plasma parameters for.

   Elements outside the instrument's detection capability can not be selected, see Figure 7-12.

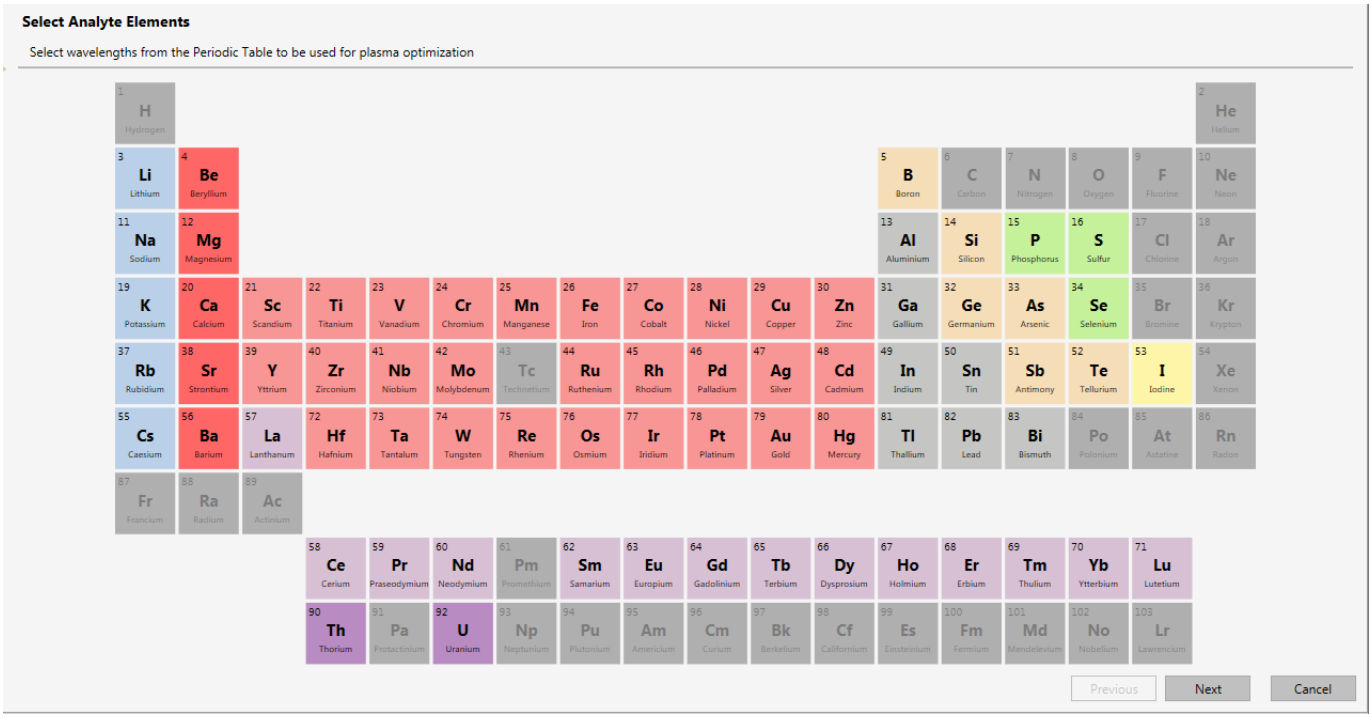
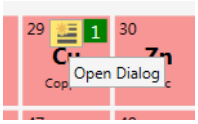


Figure 7-12. Selection of elements for Plasma Optimization

Selected elements are indicated by a green box in the top right hand corner of the element tile. By default, optimization is performed on the most intense wavelength of the selected element.

If an element has been selected by error, it can be removed by clicking it again. The box in the top right hand corner will be removed.



To select specific wavelengths hover over the tile and select **Open Dialog**.
-or-
Right-click the element tile.

The **Wavelength Selection** dialog opens, see Figure 7-13.

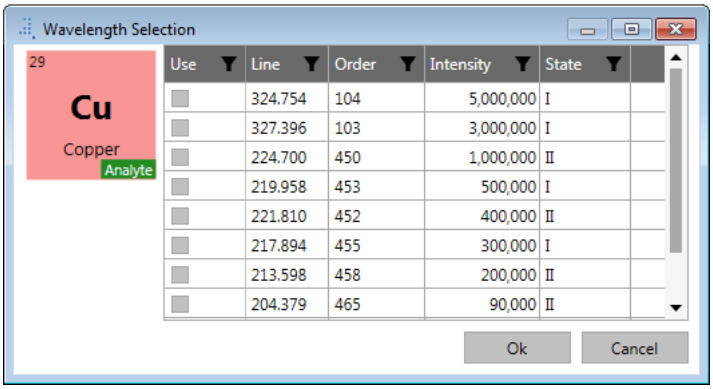


Figure 7-13. Wavelength Selection dialog

Tick the wavelengths as desired. Close this dialog with **OK**.

3. Click **Next** to open the Perform Optimization page of the wizard, see Figure 7-14.

Figure 7-14. Selection of optimization parameters

4. From the **Sample Type** listbox, select either *Aqueous* or *Organic* according to the composition of your sample.

5. From the **Optimize for** listbox, select *Intensity*, *Signal to Background Ratio*, or *Signal to Square Root of Background Ratio*.
   Select **Intensity** to find the parameters that give the highest average intensity for the selected wavelengths. The optimized parameters will not give plasma parameters that will lead to the highest intensity for each individual wavelength.
   Select **Signal to Background Ratio** to optimize plasma parameters to give the best average signal to background ratio for the wavelengths selected. As with Intensity the optimized parameters will not give plasma parameters that will lead to the best signal to background ratio for each individual wavelength. The signal to background ratio is a rough indicator of detection limit.
   Select **Signal to Square Root of Background Ratio** to optimize plasma parameters to give the best signal to square root of background ratio for the wavelengths selected. As with **Intensity** and **Signal to Background Ratio** the optimized parameters will not give plasma parameters that will lead to the best signal to background ratio for each individual wavelength. The signal to square root of background is a better approximation of the detection limit than the signal to background ratio, however the optimization routine using this metric is likely to take longer than selecting any other metric.

6. From the **Autosampler** listbox, select either *Manual sampler* or *<Autosampler>* according to your instrument Configuration.
   For details on autosampler settings, see "Autosampler Settings" on page 7-18.

7. Click Start to perform the plasma optimization based on your selections.
   The button changes to Stop.

   The **Perform Plasma Optimization** area shows the progress of the optimization process, see Figure 7-15.

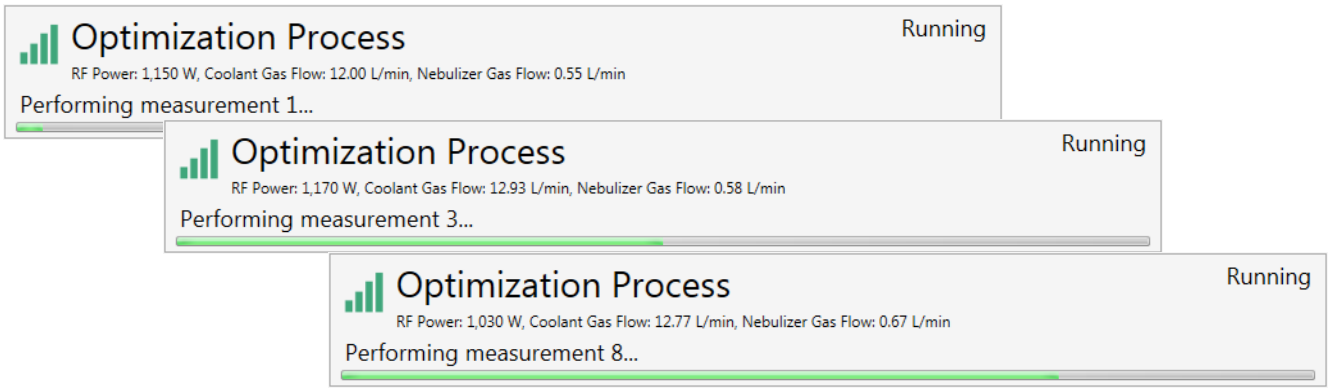


Figure 7-15. Performing the plasma optimization

Tip A typical sample should be used to carry out the plasma optimization.

8. If desired, click Stop to abort the optimization process. A message is displayed in the Result area.

   After the optimization process has successfully finished the **Result** area shows the optimized RF Power, Coolant Gas Flow, Nebulizer Gas Flow, and - depending on the instrument Configuration - Radial View Height values, see Figure 7-16.

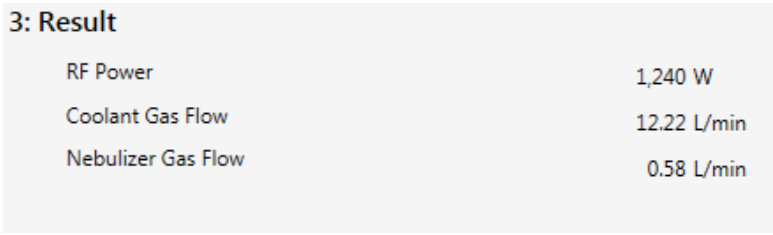


Figure 7-16. Viewing the optimization result values

9. Click Finish and enter a comment to save the plasma optimization file to the History.

   The Method View page is shown with the tiles to run the Element Finder or to perform the Plasma Optimization. The completed Plasma Optimization routine is saved to the History entries, see Figure 7-17.

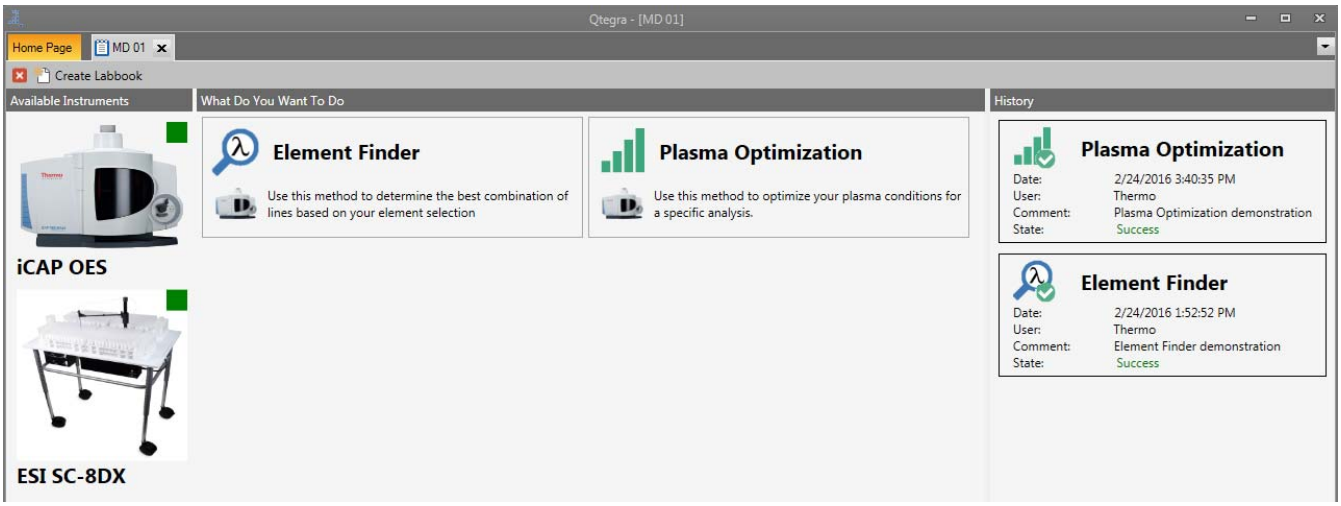


Figure 7-17. Method page after successful Plasma Optimization

Autosampler Settings

The Element Finder and Plasma Optimization wizards provide an option to specify autosampler parameters.

❖ **To specify autosampler values**

1. If an Autosampler, for example, *CetacASX520* or *ESI SC8DX* is selected, Select Sample Position is shown. When this button is clicked, a dialog opens where it is possible to specify timings and sample positions, see Figure 7-18.

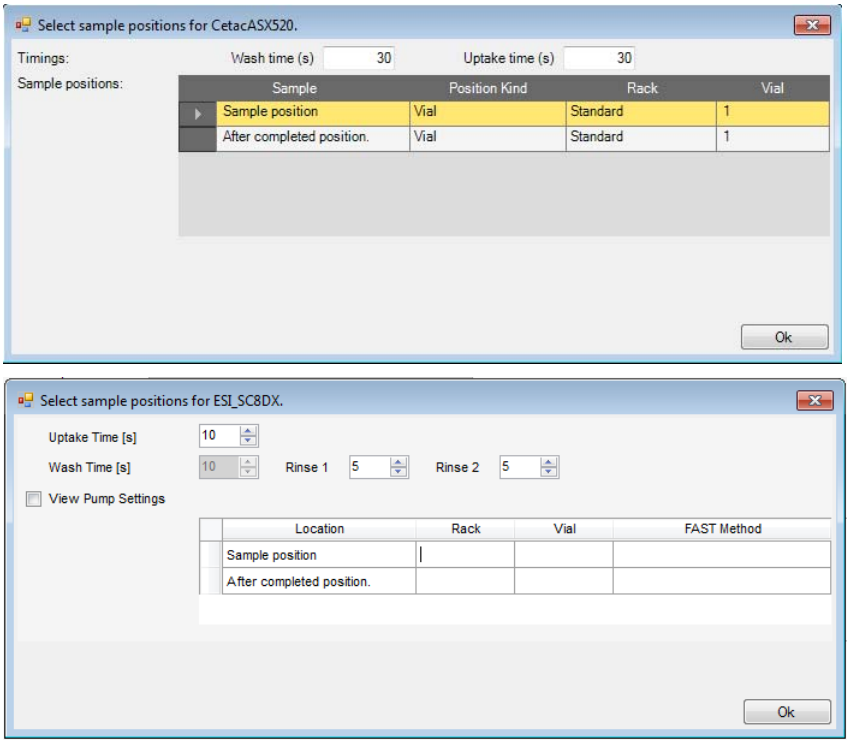


Figure 7-18. Select sample positions for autosampler dialog; top: CETAC ASX; bottom: ESI SC

2. Type **Wash time (s)** and **Uptake time (s)**.

   Tip The minimum uptake time delay is set by the instrument to help ensure that the sample has entered the plasma. If you require a longer uptake time, simply set the time desired.

3. For *ESI SC* autosamplers, set the flush time (s) for **Rinse 1** and **Rinse 2**.

4. For *ESI SC* autosamplers, tick **View Pump Settings** to show detailed pump and flush settings for Rinse 1 and Rinse 2. To close the Pump Settings view, remove the tick.

5. For *CETAC ASX*, under **Sample position**, select *Vial*, *Home* or *Rinse* for the **Position Kind**.

On errors, the tooltip of a red indicator shown next to the cell assists in understanding the error.

6. Under **Rack**, select the *Rack number* where your sample is placed.
7. Under **Vial**, type the desired *vial number*.
8. In the second row, define the position parameters for the probe after completed plasma optimization.
9. Click **OK** to apply the sample and return positions.

Working with Completed Methods

Completed methods can be used to create LabBooks or can be used to create new methods.

Creating a LabBook based on a Method

❖ **To create a LabBook based on a Method Development result**

1. From the **Qtegra - [Home Page]**, click **LabBooks**.
   -or-
   From the Method View page, click **Create LabBook**.

   The **LabBooks** page of Qtegra opens, see Figure 4-26.

2. Type a unique **Name** for the LabBook.

3. Select the option **Create a new LabBook from a blank Template**.

4. Select the **Evaluation** from the listbox.

5. Tick the **Use Method Development result** check box and select a method from the **Method Development Name** listbox.

6. Click **Create LabBook**.
   The Create LabBook from Method Development result window opens, see Figure 7-19.

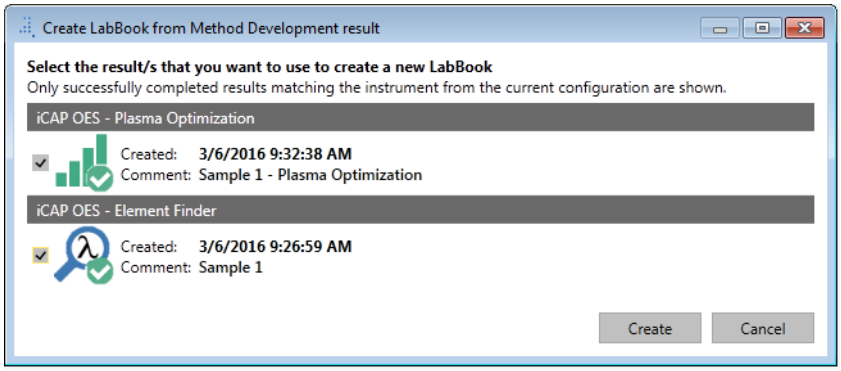


Figure 7-19. Create LabBook from Method Development result window

7. Tick the check box to select the desired Plasma Optimization and/or Element Finder result and click **Create**.

   Once the Method Development results have been processed, your new LabBook is opened. The LabBook consists of all Analyte Elements, wavelengths, Measure Modes, acquisition parameters, and instrument parameters, which are saved in the method file. It is then possible to start with the creation of the **Sample List**.

Opening an Existing Method

❖ To open an existing method

1. From the **Qtegra - [Home Page]**, click **Method Development**. The **Method Development** page of Qtegra opens, see Figure 7-1.
2. In the **Open a method** section, click Open ... to select an existing method from the **Open Method Development File** dialog.
   -or-
   In the **Recent methods** list, select an existing method.

   A new tab is opened for the selected method, see Figure 7-20.

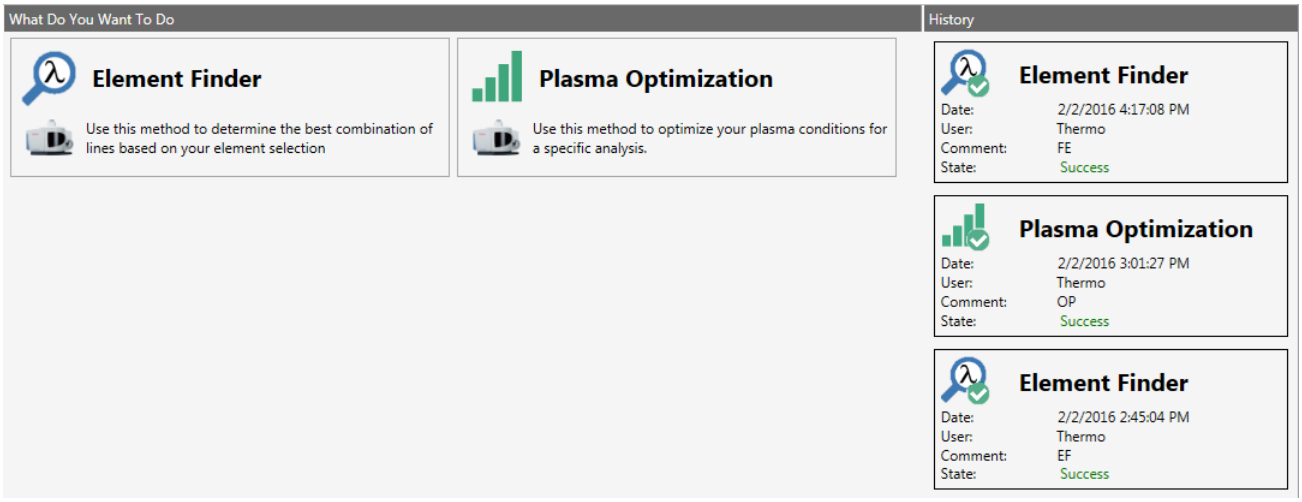


Figure 7-20. List of recent methods

Viewing Details of a Method

❖ **To view details of a completed method**

1. From the **Qtegra - [Home Page]**, click **Method Development**. The **Method Development** page of Qtegra opens, see Figure 7-1.
2. In the **Open a method** section, click Open ... to select an existing method from the **Open Method Development File** dialog.
   -or-
   In the **Recent methods** list, select an existing method to open a new tab for the selected method, see Figure 7-20.
3. When hovering a **History** tile, the following command icons are shown:

Create Plasma Optimization
This command icon is shown on Element Finder entries only. Select this icon to create a Plasma Optimization based on the result of the Element Finder method, see "Optimizing the Plasma Parameters" on page 7-12.

Create new
This command icon is shown on Element Finder entries only. Select this icon to create a new method from the previously completed Element Finder. This allows rapid modification of the original method, starting with the first page of the Element Finder wizard, see "Creating a Method" on page 7-4. The original method will remain unchanged.

Once you have made any desired modifications it is possible to click **Finish** and save the method. This will then be added to the **History** list.

Show summary (Element Finder)
The view changes to show the **Summary** overview, see Figure 7-21.

The Element Finder Summary is composed of four sections. The first shows the date that the selected Element Finder was conducted, the user who performed it, any comments and state of the routine. The second sections shows all user selected Analyte Elements, followed by Matrix and Analyte Elements found by the Element Finder. The final section shows which wavelengths have been selected for Analyte Elements.

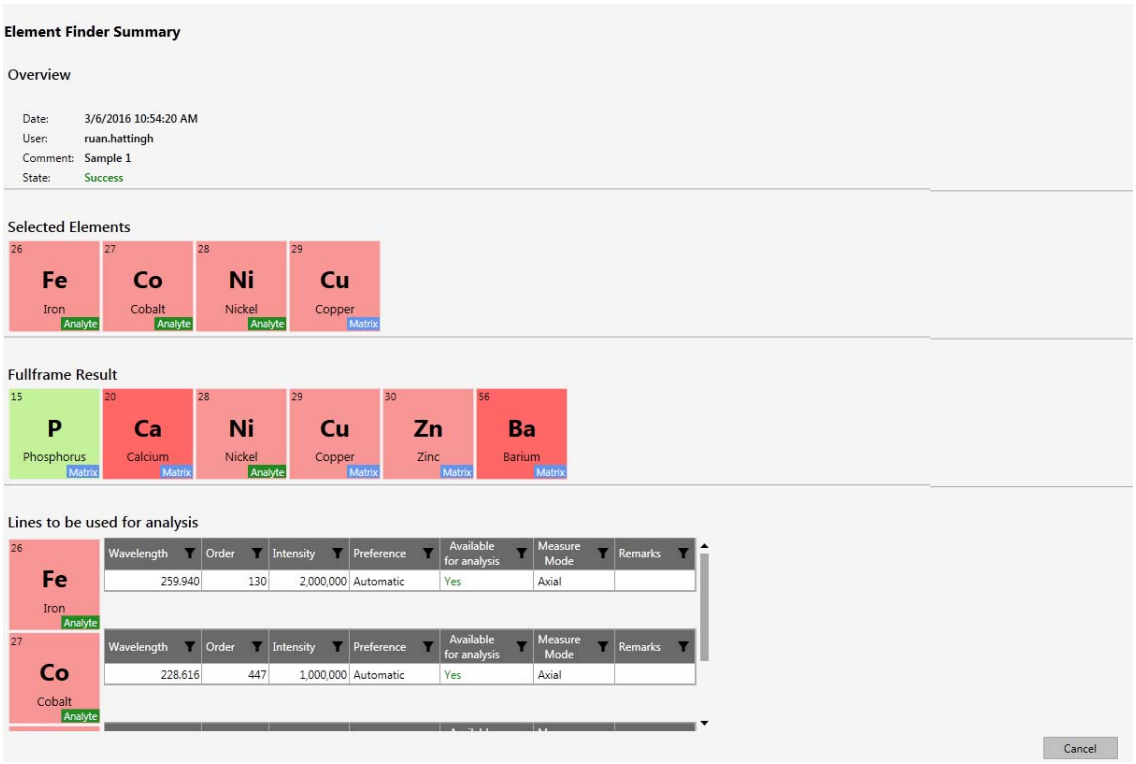


Figure 7-21. Element Finder Summary page including the Cancel button in the lower right edge

Show summary (Plasma Optimization)
The view changes to show the **Summary** overview.
The Plasma Optimization Summary is composed of two sections, see Figure 7-22. The first shows the date that the selected Plasma Optimization was conducted, the user who performed it, any comments and state of the routine. The second section shows the final optimized parameters.

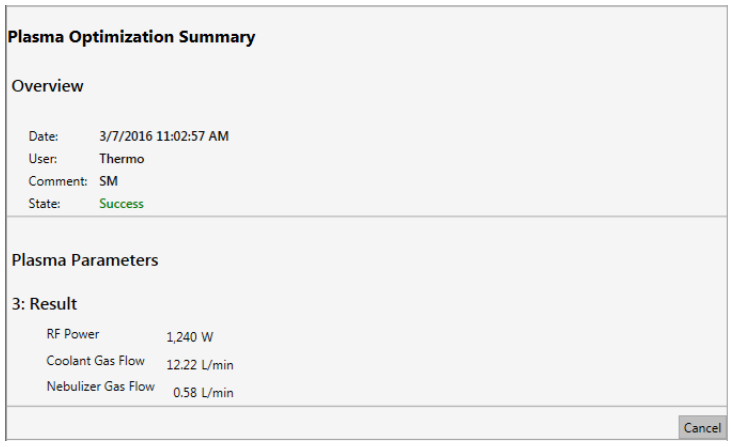


Figure 7-22. Plasma Optimization Summary page including the Cancel button in the lower right edge

4. Click Cancel to close the summary page.

8

Qtegra Reports

This chapter describes the necessary steps to create and execute Reports using the Qtegra Report Editor. All of the information was acquired with version 2.2 of the Qtegra ISDS Software.

Contents

Getting Started with Qtegra Reports

Features in Qtegra ISDS Software allow flexible Report templates to be created so that data acquired by and stored in a LabBook can be easily distributed to colleagues or customers. A wide range of features are available: from support of graphics to allow the use of company logos to sophisticated calculations to allow data from multiple LabBooks to be combined in a single Report in order to meet the requirements of USP <232>.

Reports can be printed and exported in a variety of different formats including password protected PDF. Reports can be automatically generated per analysis in a LabBook-based acquisition to allow for on the spot data evaluation with color-coded flagging of Quality Control (QC) data carried through into the final Report.

Report creation is straightforward, and a series of example Report templates are supplied to allow for modified Reports to be easily generated.

This chapter outlines basic information about Qtegra Reports.

❖ **To open the Reports view**

1. From the **Qtegra - [Home Page]**, click 

.
2. In the **Completed LabBooks** list, click the Name to open the LabBook you wish to view.
   The completed LabBook is opened in a new tab.
3. Click 

to open the **Report Preview**.

Concentrations Report

This section describes the use of a Report for one LabBook and for multiple LabBooks.

Concentrations Report for One LabBook

A Report is applied to a single LabBook by first opening a LabBook and then selecting one of the available Reports. Several example Report templates are supplied with Qtegra ISDS Software. See Figure 8-1.

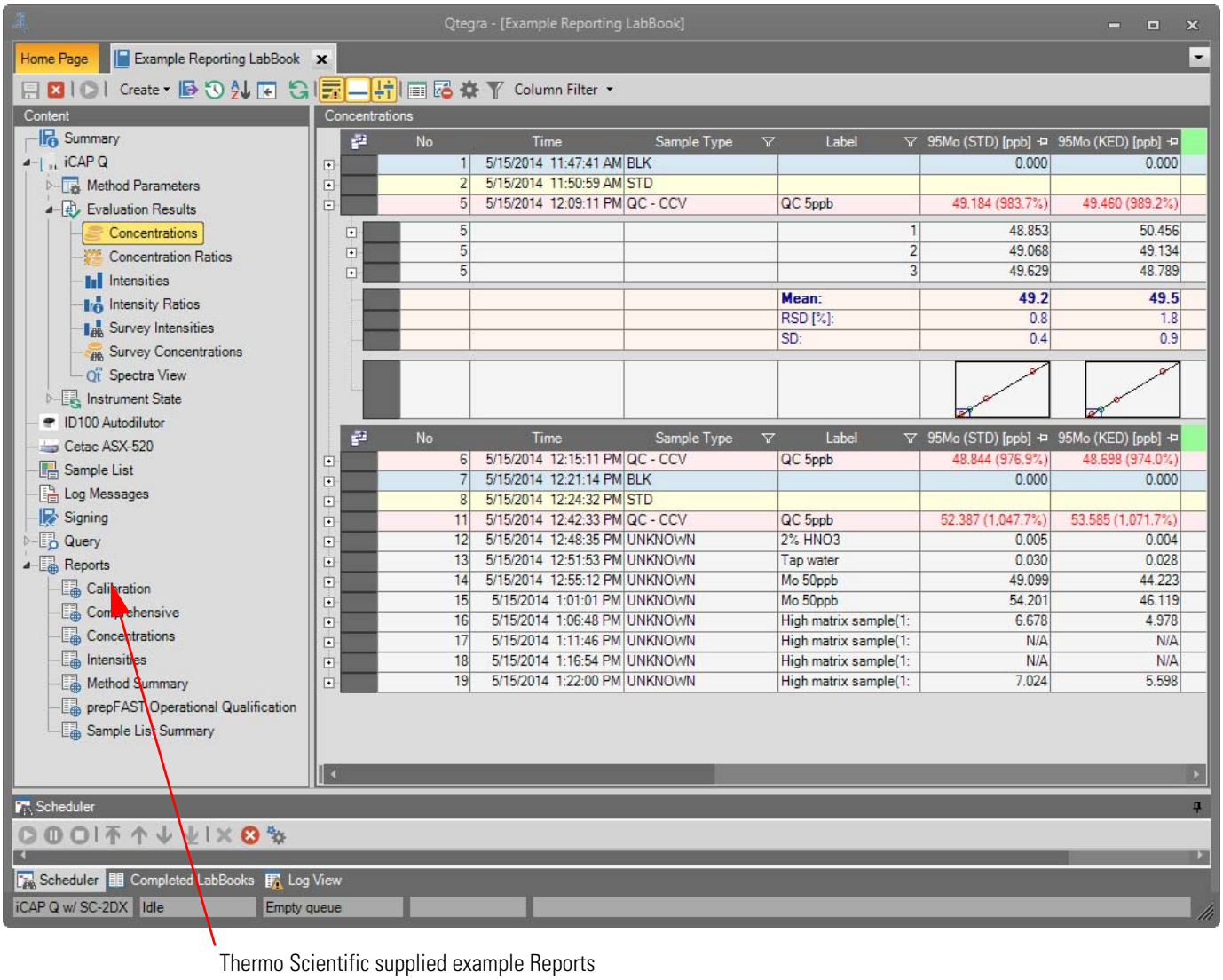


Figure 8-1. Example Report templates supplied with Qtegra ISDS Software

Tip The Reports shown here are supplied with the ICP-MS. The Reports supplied with the iCAP ICP-OES are different but are used the same way.

Once selected, the Report template is populated with data from the open LabBook and displayed. See Figure 8-2.

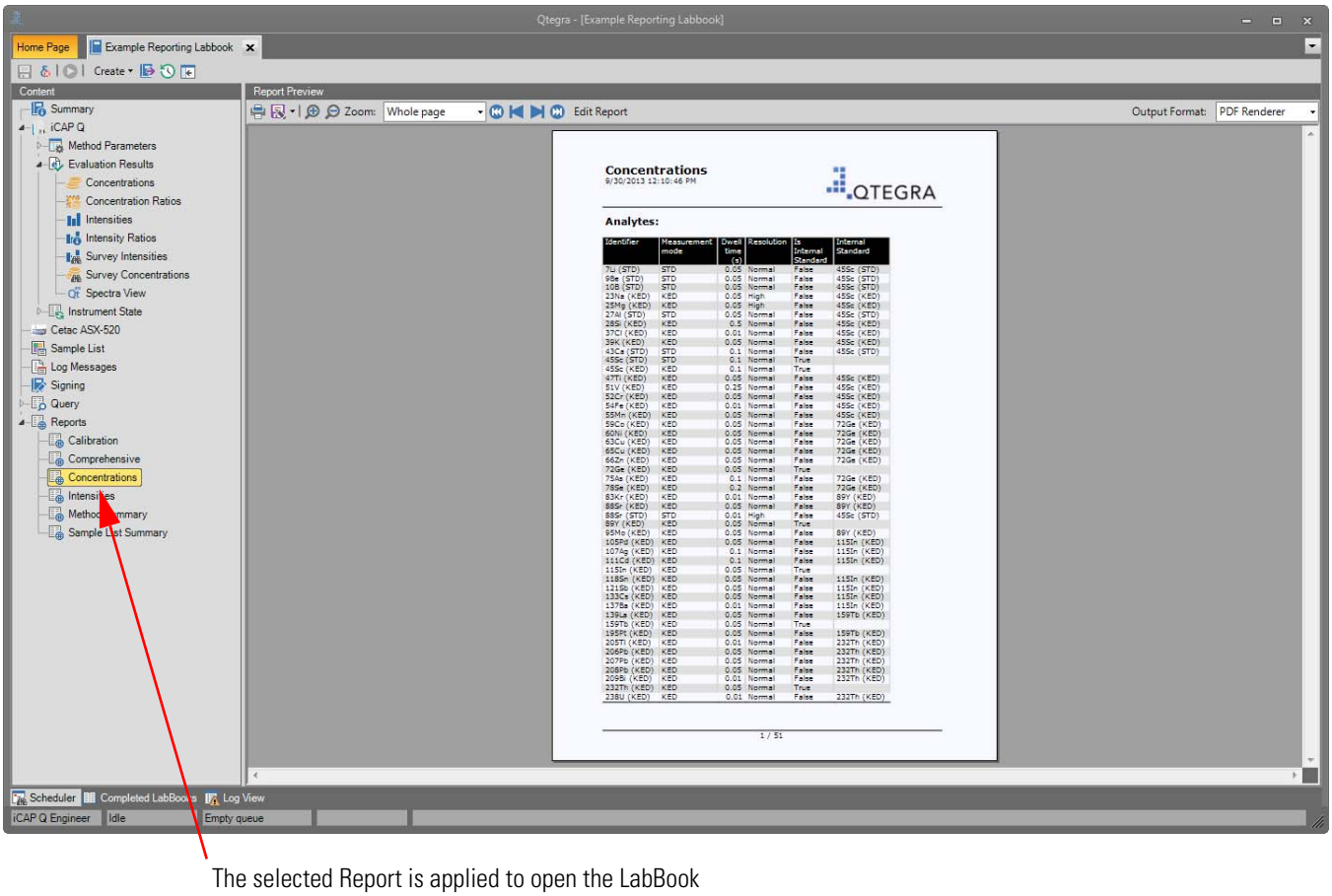


Figure 8-2. Report template populated with data from a selected LabBook

The Reports entry is always available except when a scheduled LabBook is running. Then, the Content pane shows only the Method Parameters, the Evaluation Results, the autosampler or Manual Sample Control, and the Sample List entry.

Concentrations Report for Multiple LabBooks

Once the criteria for a LabBook query have been defined and applied to multiple LabBooks, the resulting data set can be used to generate a Report, see Figure 8-3.

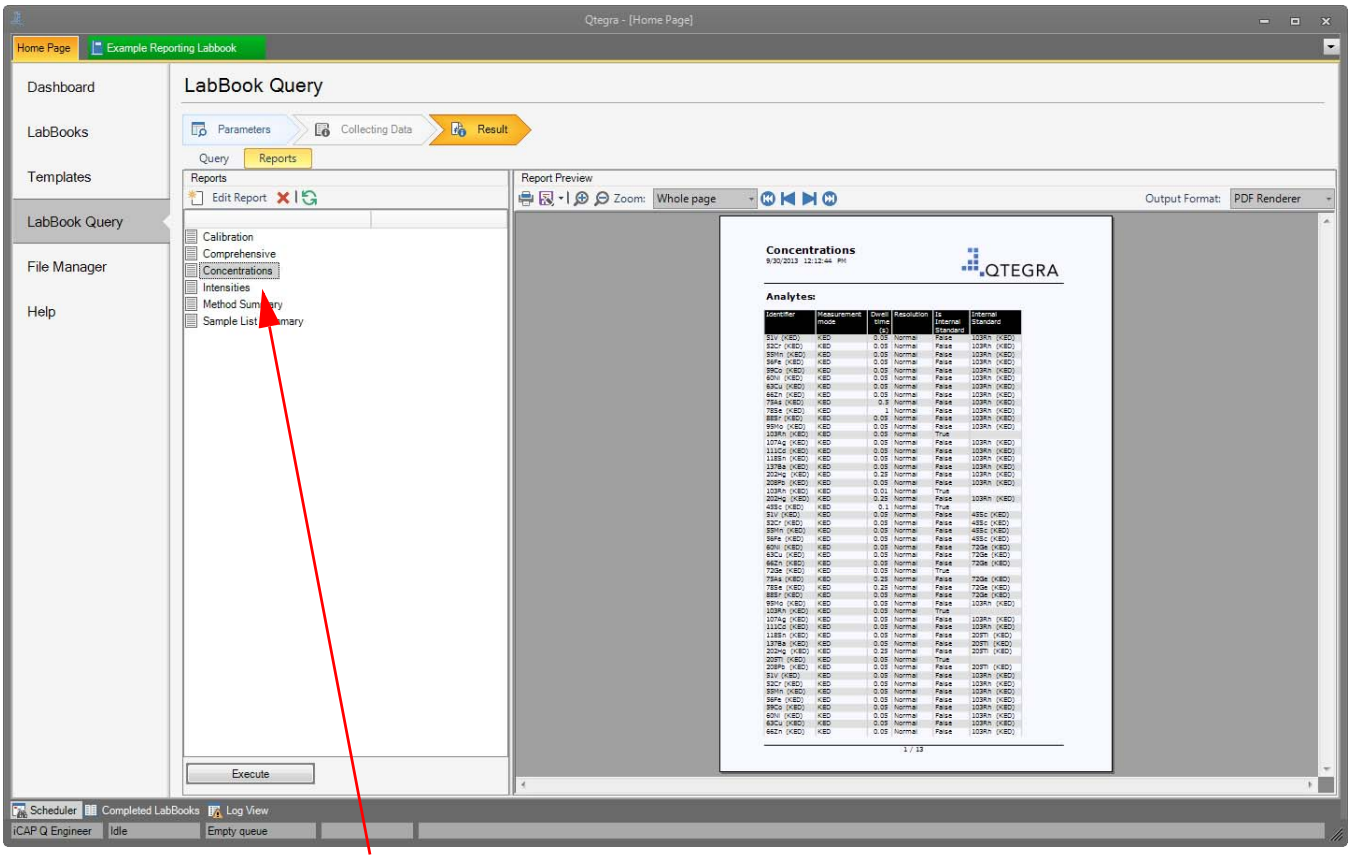


Figure 8-3. Generating a concentrations Report based on the results of a LabBook query

Creating Quantification Values for a Report

A Report can be modified in order to show quantification results in its lists. To provide the calculation traces, your Template or LabBook must be prepared accordingly.

Relative atom percent (Relative at%) and relative weight percent (Relative wt%) are calculated for analytes on the following conditions:

- A multi-calculation trace with “Sum” operator is defined.
- The analyte matches the selection defined for the multi-calculation trace.
- A concentration is available for the analyte.

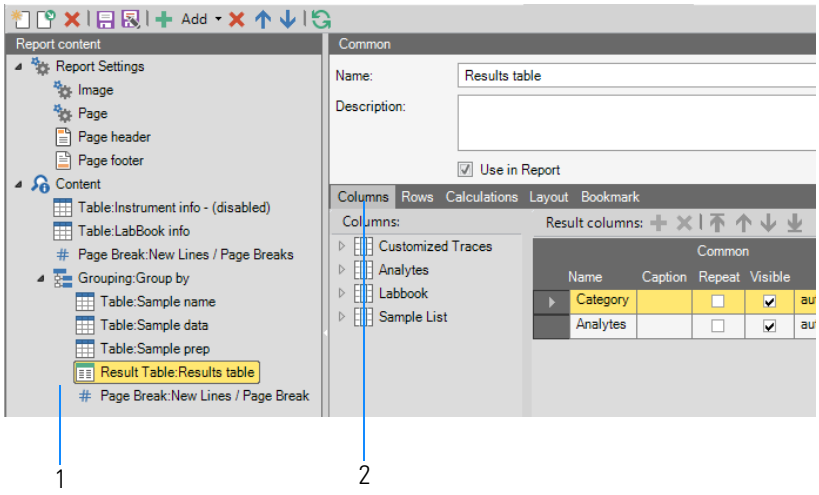
See “Quantification” on page 9-33 for details on how to define calculation traces.

Adding Calculations to a Report

Calculation traces are certain operations provided by Qtegra (*Average, Max, Min, RSD, SD, Sum*) and can be customized under Method Parameters > Quantification > Calculation Trace.

❖ To add Calculation Traces to a Report

1. Open a finished LabBook with operations defined in Method Parameters > Quantification > Calculation Trace.
2. From the Content pane, select the Report template you wish to add calculation traces to. The template is populated with data from the LabBook.
3. On the Report Preview toolbar, click **Edit Report** to open the editor.
4. In the Report Content pane, expand Content > Grouping:Group by to select **Result Table:Results table** (**1** in Figure 8-4).



Labeled Components: 1=expanded Report Content pane, 2=five category tabs

Figure 8-4. Selecting the Results table

5. From the five category tabs in the right pane (**2** in Figure 8-4), select **Columns** and expand **Customized Traces** to see all customized traces, which you defined in the LabBook.
6. Select the item(s) you want to add to the Report and click **Add** from the Result columns toolbar.
   The item(s) are appended to the list.
7. To check the result, click **Execute Report** from the main toolbar.
   The pages with the Results table show the calculated values from customized traces.
   After checking the preview click **Edit Report** to switch back to the edit mode.

❖ To add Predefined Calculation Traces to a Report

1. Select **Rows** from the category tabs (**2** in Figure 8-4). Double-click each item of interest (for example, *LOD, MQL, Relative at%, Relative wt%*) to move it from Available to Selected, see Figure 8-5.

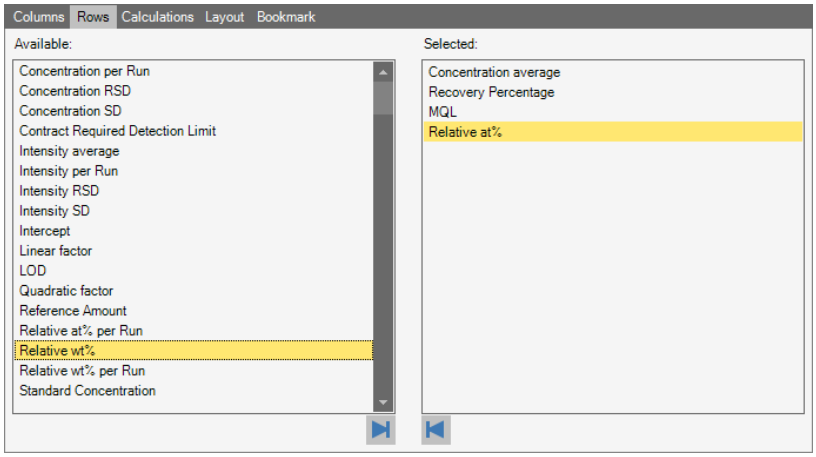


Figure 8-5. Selecting predefined calculation traces

2. The items selected in Figure 8-5 are printed in the Report as follows.

Basic sample report
11/22/2016 3:12:11 PM

QTEGRA

Dilution Factor 1

	Concentration average	Relative at%
Co 243.905 {138} (Radial)	2,200.049 µg/ml	16.792 %
Mn 348.291 {97} (Radial)	1,982.768 µg/ml	16.234 %
Ni 359.770 {94} (Radial)	2,202.269 µg/ml	16.879 %
Sc 363.075 {93} (Radial)	89.401 %	
Co 341.234 {99} (Radial)	2,209.034 µg/ml	16.860 %
Ni 345.847 {97} (Radial)	2,197.966 µg/ml	16.846 %
Mn 220.881 {153} (Radial)	2,001.870 µg/ml	16.390 %
Sum (example)	12,793.958 µg/ml	
RSD (example)	5.097 ppm	

	MQL	Recovery Percentage 1
Co 243.905 {138} (Radial)	0.360 µg/ml	100.002 %
Mn 348.291 {97} (Radial)	0.125 µg/ml	99.138 %
Ni 359.770 {94} (Radial)	0.908 µg/ml	100.103 %
Sc 363.075 {93} (Radial)		
Co 341.234 {99} (Radial)	0.073 µg/ml	100.411 %
Ni 345.847 {97} (Radial)	0.197 µg/ml	99.908 %
Mn 220.881 {153} (Radial)	3.771 µg/ml	100.094 %
Sum (example)		
RSD (example)		

Figure 8-6. Predefined calculation traces shown in the Report

3. After checking the preview, click **Edit Report** to switch back to the edit mode.

Printing a Report

A Report containing the results from a LabBook can be printed by clicking the **Print** icon from the main reporting toolbar, see Figure 8-7.

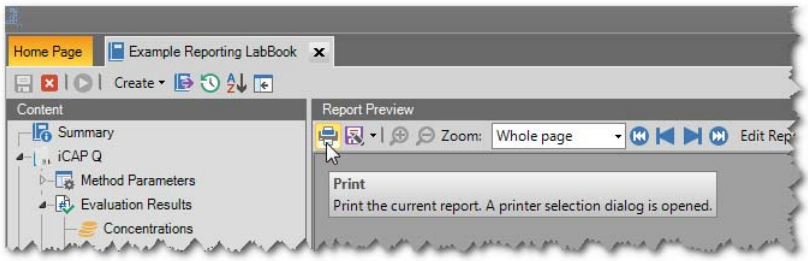


Figure 8-7. Printing a Report

❖ **To print a Report**

1. Open the **Reports** view as shown in "To open the Reports view" on page 8-2.
2. From the **Report Preview** toolbar, click **Print** to print the currently displayed Report.
   A printer selection dialog is displayed.

   Tip Printing will always create one Report that is currently selected. You may select each particular Report listed in the Reports section of the Content pane to the left and then click **Print** to print this Report.

Saving as HTML File

The populated Report can be saved as an HTML file by selecting *HTML Renderer* from the Output Format drop-down menu.

❖ **To save the Report as an HTML file**

1. Open the **Reports** view as shown in "To open the Reports view" on page 8-2.
2. From the **Report Preview** toolbar, expand the **Output Format** button to display the menu items. Select **HTML Renderer**, see Figure 8-8.

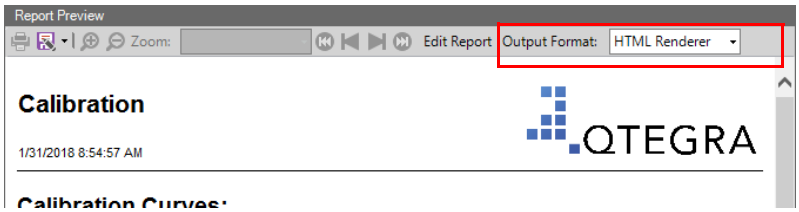


Figure 8-8. Formatting a Report with an HTML renderer

The Report is rendered and the HTML page is displayed.

3. Click the **Save As** button.
   The **Browse For Folder** dialog is opened to select the folder where you want to save the HtmlReport folder with the *index.html* file and all images used.

4. Open the HtmlReport folder and double-click the *index.html* file to view the Report in your browser.

Saving as PDF File

The populated Report can be saved as a standard PDF file by clicking the **Save As** icon from the main reporting toolbar, see Figure 8-9.

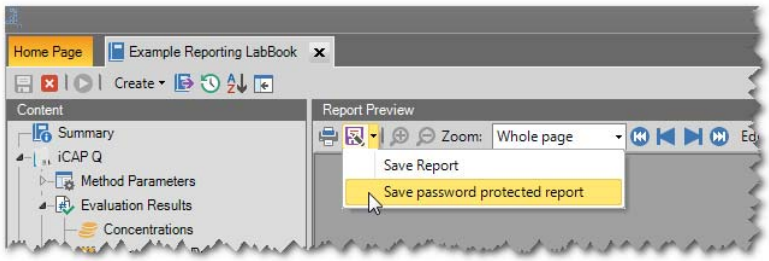


Figure 8-9. Saving a Report as PDF file

❖ **To save a Report**

1. Open the **Reports** view as shown in "To open the Reports view" on page 8-2

2. From the **Report Preview** toolbar, click **Save As** to save the currently displayed Report as a PDF file.

   The Save document dialog is displayed to select the path and to type the file name.

   Tip Saving will always create one Report that is currently selected. You may select each particular Report listed in the Reports section of the Content pane to the left and then click **Save As** to save this Report.

Alternatively, the Report can be saved as a password-protected PDF file.

❖ **To save a password protected Report**

1. Open the **Reports** view as shown in "To open the Reports view" on page 8-2

2. From the **Report Preview** toolbar, expand the **Save As** button to display the menu items. Select **Save password protected Report**, see Figure 8-10.

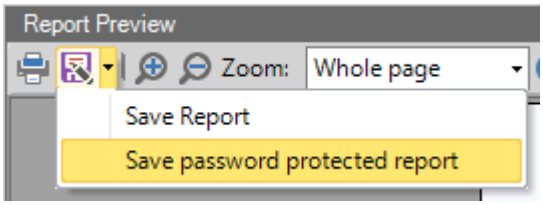


Figure 8-10. Saving a Report as password-protected PDF file

3. The **PDF Password** dialog is displayed to type and confirm the password.

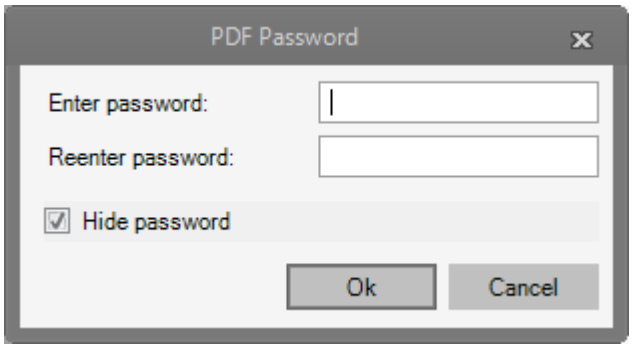


Figure 8-11. PDF Password dialog

4. Select **Hide password** to display an asterisk for every character you are typing into the password fields. This option toggles the display, this means, remove your selection to display the password as it was entered.

5. Type your password and then in the second field, reenter this password.
The **OK** button becomes available when both entries are identical.

The Save document dialog is displayed to select the path and to type the file name.

Tip Saving will always create one Report that is currently selected. You may select each particular Report listed in the Reports section of the Content pane to the left and then click **Save password protected Report** to save this Report.

6. When you open this PDF file from your Windows Explorer, a dialog is displayed to type the password before opening this file.

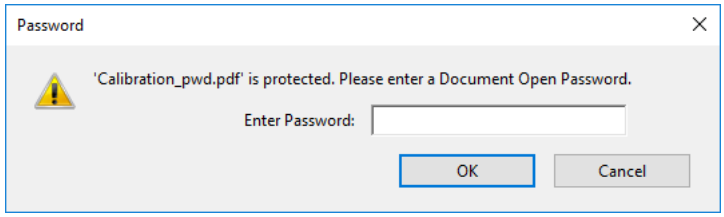


Figure 8-12. Document Open Password dialog

7. Type the correct password to display the Report in your PDF viewer.

Saving as RTF File

The populated Report can also be saved as a file in rich text format (RTF) using the same **Save As** dialog. Instead of the default PDF format, the RTF format must be selected from the drop-down menu of the dialog, see Figure 8-13.

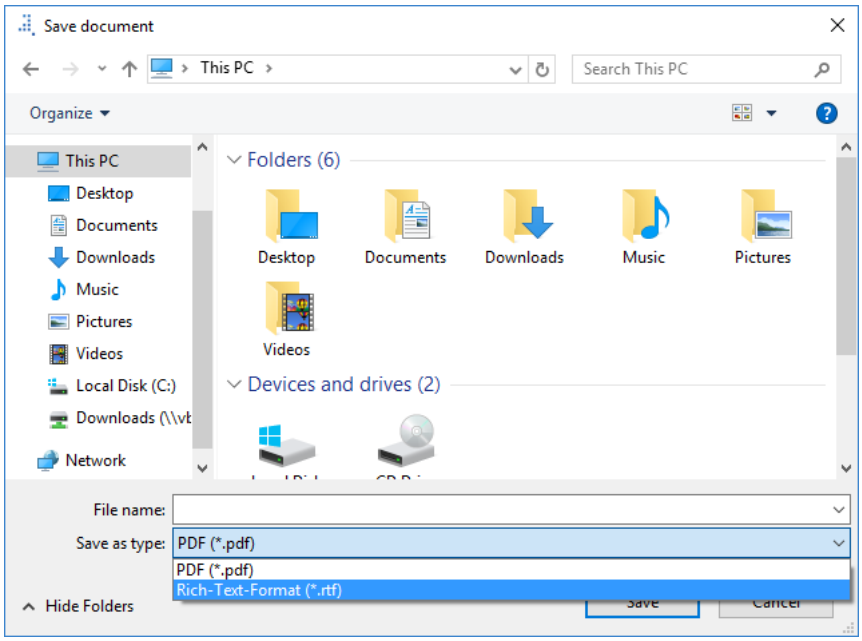


Figure 8-13. Saving a Report as RTF file

Any RTF file so created can, for example, be opened in a text editor, for example, Microsoft™ Word™.

Saving as XML File

The populated Report can be saved as an XML file by selecting *XML Renderer* from the Output Format drop-down menu.

❖ **To save the Report as an XML file**

1. Open the **Reports** view as shown in "To open the Reports view" on page 8-2.
2. From the **Report Preview** toolbar, expand the **Output Format** button to display the menu items. Select **XML Renderer**, see Figure 8-14.

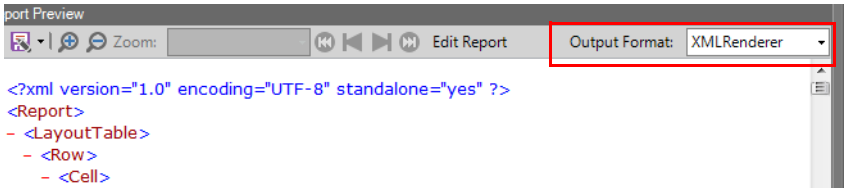


Figure 8-14. Formatting a Report with an XML renderer

The Report is rendered and the XML code is displayed.

3. Click the **Save As** button.
The **Browse For Folder** dialog is opened to select the folder where you want to save the XML file.
4. Finally, use an XSLT template to transform the data.

Automated Report Export

The same export possibilities as described at Printing a Report, Saving as PDF File, Saving as RTF File, and Saving as XML File can be automatically applied for each analysis generated by LabBook-based acquisitions. A combination of hard-copy printouts as well as file exports can be created for either individual analyses or for the entire LabBook of analyses.

The definition of the automatic export of Reports is made per LabBook in the **Content** pane at **Automatic Export > Report Export**, see Figure 8-15.

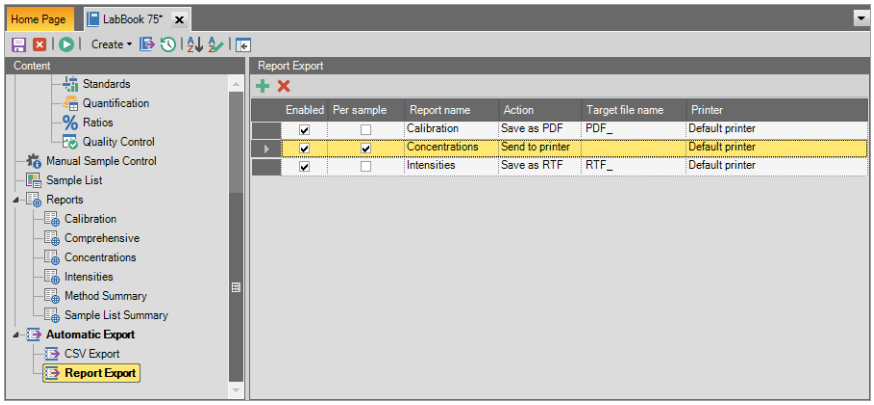


Figure 8-15. Location of automatic export commands within a LabBook

In the example shown in Figure 8-15, the Report “Concentrations” will be produced per analysis as both a PDF file and as a hard-copy (sent to the Windows-defined default printer). A “Comprehensive” Report will be generated as an RTF file. At the end of the LabBook, the “Method Summary” will be exported as an XML file.

The names of any file exported is defined by the **Target File Name** field as shown in Figure 8-15 where any text entered is used as a prefix for the automatically sequentially numbered files generated.

Supplied Reports

Some example Report templates are supplied with Qtegra for your instrument. They address most basic reporting requirements and are listed in Table 8-1.

Table 8-1. Example Report templates supplied with Qtegra ISDS Software

Report Name	Report Content
Basic sample report	Tables for all analytes are displayed with the wavelength, concentration average, and recovery percentage.
Calibration Summary	Calibration lines for all calibrated analytes are displayed along with the equation and correlation coefficient, R^2. Background Equivalent Concentration (BEC) and Detection Limit (LOD) values are also recorded. Following this, the expected and read back concentrations for each standard are listed. Portrait format.
Comprehensive sample report	A single Report containing the most commonly required data. It includes information from the Reports Calibration, Method Summary and Sample List Summary as well as providing the Concentration Average and % RSD precision for every analysis in a LabBook. Portrait format.
	Tip This Report populates tables for analytes depending on their status as Internal Standard or not. It should therefore be edited before use for each LabBook.
Concentrations report	Per run (repeat) concentrations with average and % RSD precision. Landscape format.
Horizontal table report	Concentration average for every analysis in a LabBook. Concentration per line, analytes per column. Portrait format.

Table 8-1. Example Report templates supplied with Qtegra ISDS Software, continued

Report Name	Report Content
Intensities report	Per run (repeat) intensities with average and % RSD precision. Landscape format.
Log-Messages	The Report shows only log entries of the first 5 samples measured. The Log-Message Report lists the entries with Level (UserInfo, Debug), Message string, Category (to indicate the Qtegra module), and the Sub-Category. The list is sorted by Time.
Method Summary	Key analysis method parameters used for data acquisition. Shows the choice of Internal Standard.
Sample List Summary	Index, label, and autosampler position for all analyses in a LabBook-based acquisition. Also shows the Start Time and active user account for each analysis. Portrait format.
Simple sample report	Concentration average, % RSD and Standard Deviation (SD) are shown for every analysis in a LabBook. Portrait format.
Vertical table report	Concentration average for every analysis in a LabBook. Concentration per column, analytes per line. Portrait format.

Using the Qtegra Report Editor

The Qtegra Report Editor is used for creating and editing Report templates. The editor allows creating, loading and saving Report templates, which are used to generate a Report from a LabBook of analyses.

Report templates can be manipulated (created, edited and saved) from an open LabBook. To populate a Report from a given template the LabBook must contain the appropriate data.

This chapter outlines how to work with the Qtegra Report Editor.

Opening a Report Template

❖ **To open a Report template for editing**

1. Open a LabBook.
2. Select the supplied Report template from the list of available Reports (Method Summary, for example).
3. Click the **Edit Report** button (**2** in Figure 8-16).

   The selected Report template is opened up in a new window inside the Qtegra application.

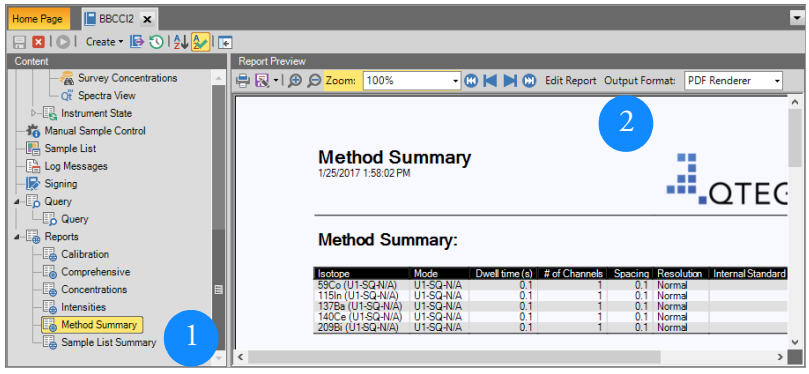


Figure 8-16. Opening a Report template for editing

Structure of the Qtegra Report Editor

The basic structure of the Qtegra Report Editor is shown in Figure 8-17.

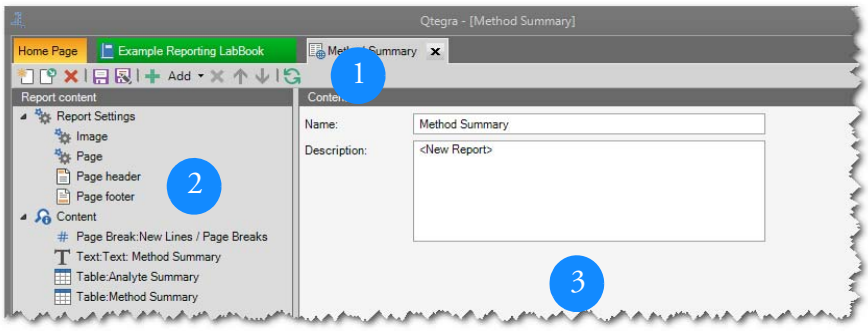


Figure 8-17. Main editor page of Qtegra Report Editor

The Report Editor has the following components:

- The **Toolbar** (**1** in Figure 8-17) that contains the main Report editor-related functions,
- The **Report Content Area** (**2** in Figure 8-17) that shows the structure of the loaded Report template:

  Report Settings: general settings for each page (header, footer, etc.)

  Report Content: the Report objects used in the loaded Report
- The **Report Area** (**3** in Figure 8-17), which displays the details of the selected Content item.

Toolbar

The toolbar provides commands:

- to manipulate Report templates (Load, Save etc.)
- to manipulate content items in Report templates (adding, deleting, moving, etc.).

The possible commands are listed in Table 8-2.

Table 8-2. Commands of toolbar

Function	Description
	Creates a new Report template
	Opens an existing Report template
	Deletes the current Report template
	Saves the current Report template

Table 8-2. Commands of toolbar, continued

Function	Description
	Saves the current Report template under a new name
	Adds a Report content item to the Report template. See "Report Content Items" on page 8-33.
	Deletes the selected content item(s)
	Moves the selected content item(s) up the Report
	Moves the selected content item(s) down the Report
	Applies the Report template to the loaded LabBook

❖ **To create a Report template**

1. From the **Completed LabBooks** list, click to open the LabBook you wish to view.
   The completed LabBook is opened in a new tab.
2. On the toolbar of the LabBook, click Create to open the drop-down menu.
3. Select **New Report**, see Figure 8-18.

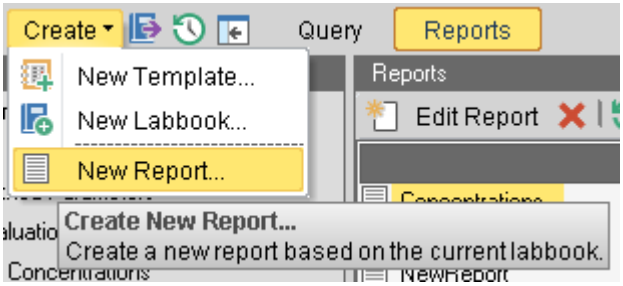


Figure 8-18. Completed LabBook selecting New Report

The Report Editor for the new Report opens in a new tab, see Figure 8-19.

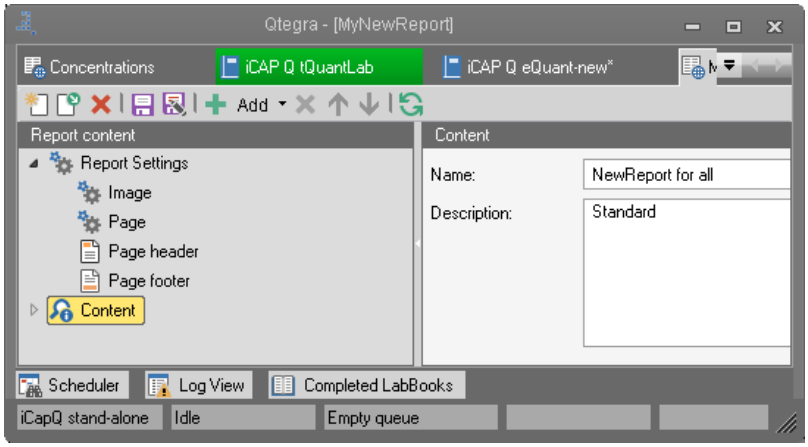
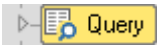


Figure 8-19. Title of Report

Tip You can also open new Reports by clicking **New Report** on the Reports Editor's toolbar.

4. In the **Content** pane, type a **Name** and optionally a **Description** for the Report.
   The **Name** entered is displayed as Report title in the generated Report.

❖ **To delete a Report template**

1. From the **Completed LabBooks** list, click to open the LabBook you wish to view.
   The completed LabBook is opened in a new tab.
2. Click 

in the content pane of your LabBook.
3. On the toolbar of the LabBook, click 

to open the **Reports** view.

4. Select the Report template you wish to delete and click **Delete**, see Figure 8-20.

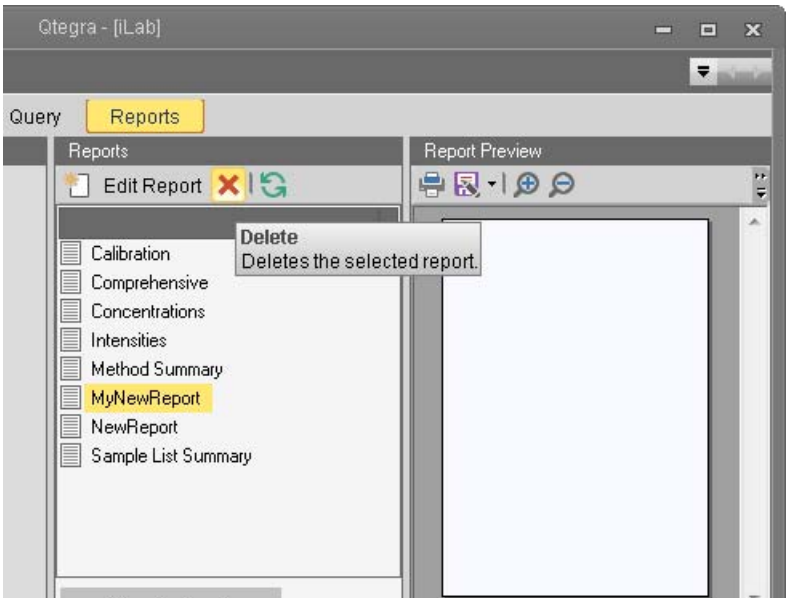


Figure 8-20. Reports page of completed LabBook, deleting Report

The Report template is deleted from the list to the left.

❖ **To save a Report template under a new name**

1. Click **Save** to save the Report template.
The **Save Report** dialog opens, see Figure 8-21.

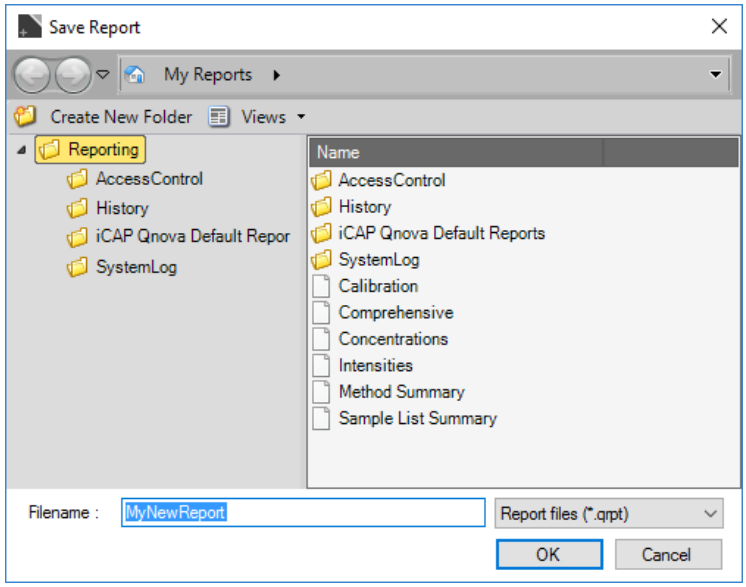


Figure 8-21. LabBook Query Save Report dialog

2. Type a **Filename** and click **OK**.
The file name entered is immediately displayed in the tab of the Report and will be shown in the Reports view in the list on the left.

Tip The shortcut menu of **Reporting** on the left offers commands to create a new folder or to import files. The shortcut menu of a **folder** on the left offers commands to cut, copy, delete, and rename folders.

❖ To generate a Report

1. From the **Completed LabBooks** list, click to open the LabBook you wish to view.
The completed LabBook is opened in a new tab.
2. Click Query in the content pane of your LabBook.
3. On the toolbar of the LabBook, click Reports to open the **Reports** view.
4. Select a Report from the list on the left and click **Execute**.
You can also click Execute Report below the list.
5. The Report is generated as defined in the Report template selected and displayed in the **Report Preview** on the right, see Figure 8-22.

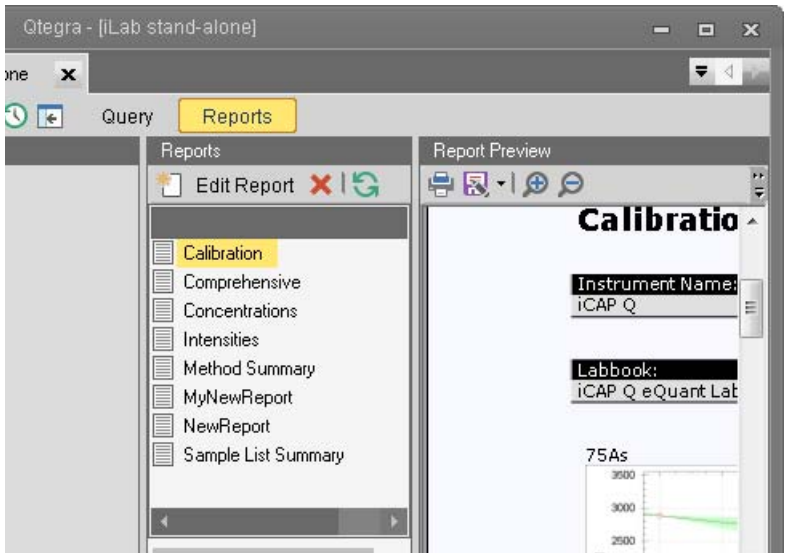


Figure 8-22. Reports page of completed LabBook showing executed Report

6. **Print** the Report.

-or-

Save the Report as desired.

Report Content Area

The Report Content Area shows the content of the Report definition in a tree structure. The main nodes listed in Table 8-3 are available.

Table 8-3. Report Content Area

Node	Description
Report Settings	Contains items, which define the layout of the Report. These items can not be deleted. See "Report Settings Items" on page 8-25.
Content	Contains items, which define the content of the Report that is displayed. See "Report Content Items" on page 8-33.

Report Area

The Report Area allows for the definition of content-specific features.

Editing a Report Template

The supplied Report templates meet the most common reporting requirements. They can be edited as required to generate new templates.

❖ **To edit a Report template**

1. Open a LabBook.
2. From the list of available Reports, select the Report template.
3. Once the Report is displayed with data from the open LabBook, click the **Edit Report** button, see Figure 8-16.

A Report template consists of two sections as shown in Figure 8-23:

- Report Settings
- Content

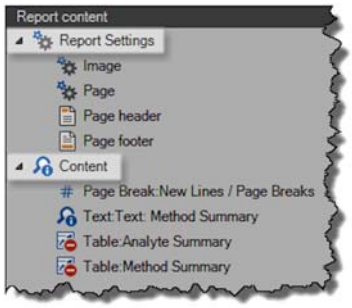


Figure 8-23. Report template consisting of Report Settings and Content

Report Settings are general settings for the Report template that define the look and feel of the Report (page header, footer, etc.). An explanation of each setting is described at "Report Settings Items" on page 8-25.

Content are individual components that add functionality to a Report. An explanation of each content item is described at "Report Content Items" on page 8-33.

In the **Report Content** window, located on the left-hand side of an open Report template, select a particular item. The content-specific properties for the selected item are displayed in the Report Area on the right-hand side for editing, see Figure 8-24. This process is the same for both Settings and Content items.

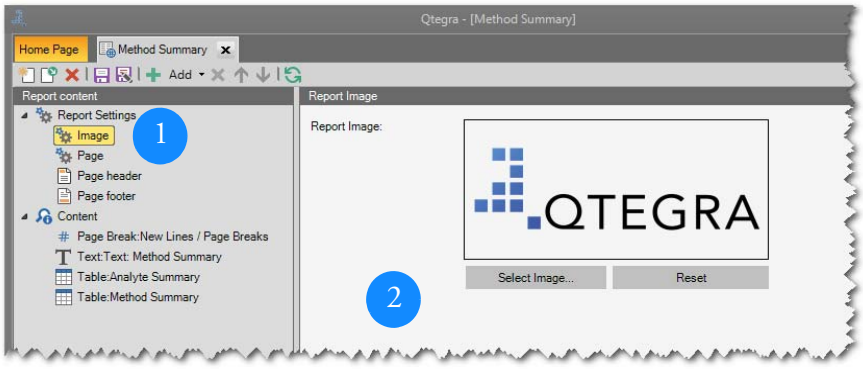


Figure 8-24. Selecting a Report content item for editing

Adding New Content to a Report Template

❖ **To add new content to a Report template**

1. On the Report template toolbar, click the **Add** button. See Figure 8-25.

2. From the drop-down menu showing the available content items, select the content type (*Data* or *Graph*, for example), see Figure 8-25.

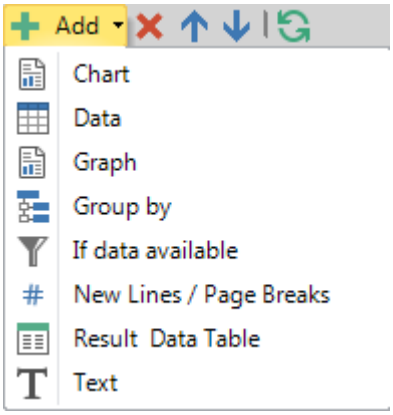


Figure 8-25. Available content types for a Report template

Table 8-4 lists the available content types for a Report template. An explanation of each content item is provided at "Report Content Items" on page 8-33.

Table 8-4. Available content types for a Report template

Content type	Description
Chart	Chart data from a LabBook. See "Chart" on page 8-34.
Data	Numerical data (not results) from a LabBook presented in a table. See "Data" on page 8-40.
Graph	Graphical data from a LabBook. See "Graph" on page 8-44.
Group By	Allows ordering of content by grouping based on an aspect of the LabBook. See "Group By" on page 8-45.
If data available	Items below this item are only displayed if the result of this item contains values.
New Lines/ Page Breaks	Line or page breaks between other content types to improve layout of the Report. See "New Lines/Page Breaks" on page 8-47.
Result Data Table	Results from a LabBook presented in a table. See "Result Data Table" on page 8-47.
Text	User defined text to describe other content in a Report. See "Text" on page 8-51.

Re-Ordering Content

❖ **To change the order of content items in the Report template**

1. Select the content item.
2. On the toolbar, click the ↑ / ↓ buttons.

Report Settings cannot be re-ordered as their positions in the Report template are fixed.

Temporarily Removing Content

The visibility of each content item in a Report is controlled by the **Use in Report** check box. This command is useful during Report creation and editing as content items can be temporarily removed from the display by toggling this field. Content is not permanently deleted from the Report template when using this feature, see Figure 8-26.

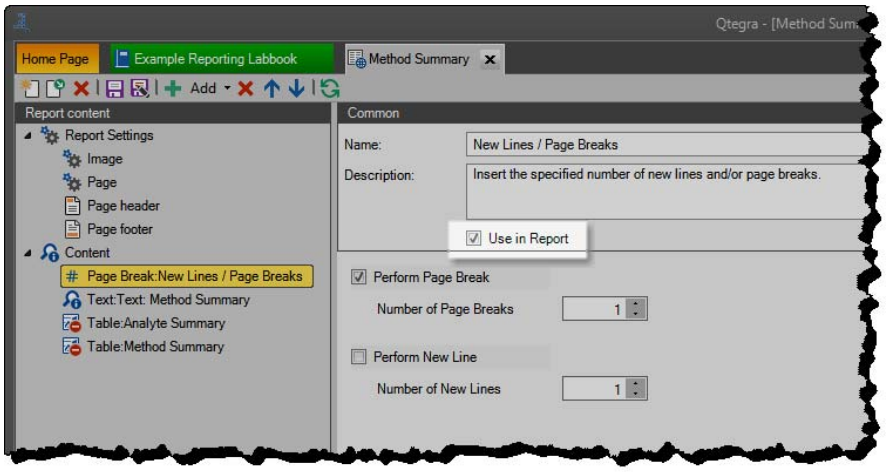


Figure 8-26. Toggling display of content items in Report template

Permanently Removing Content

❖ **To permanently remove content items in a Report template**

1. In the **Report Content** window, select the content items to be permanently removed.
2. On the toolbar, click the **Delete Content** button.

Previewing a Report

Once the Report template is defined, it can be applied to the open LabBook by clicking the **Execute Report** button on the toolbar, see Figure 8-27.

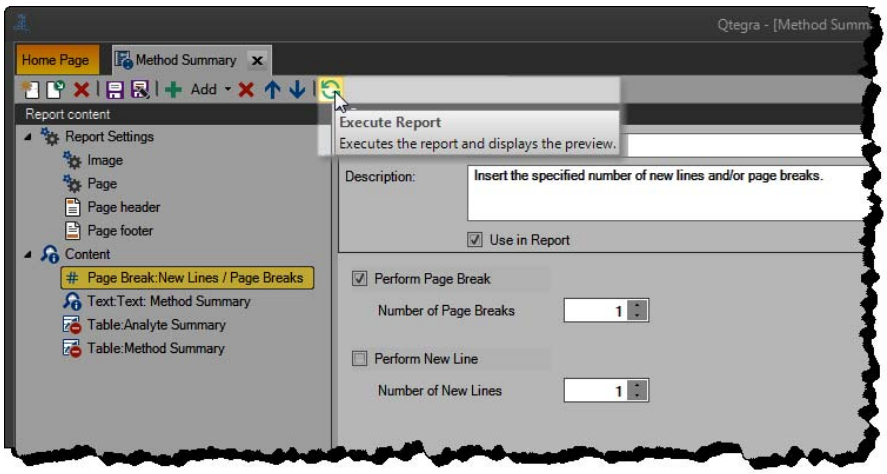


Figure 8-27. Applying a Report template to an open LabBook

Data from the selected LabBook is then used to populate the Report template, and the Report is displayed.

Saving a Report Template

❖ **To save a Report template**

1. Ensure that the edited Report template meets the reporting requirements.
2. Perform one of the two following alternatives:

   a. To save the Report template over a previously defined version, click **Save** on the toolbar.

   b. To create a new Report template, click **Save As** on the toolbar.

Report Settings Items

You create Report presets or templates easiest from the **Reports** view of a completed LabBook in Qtegra.

Generally, you can structure your Report to your needs, add headings, tables and graphs to specify the presentation of the result data.

A typical structure for a Report template is shown in Figure 8-28.

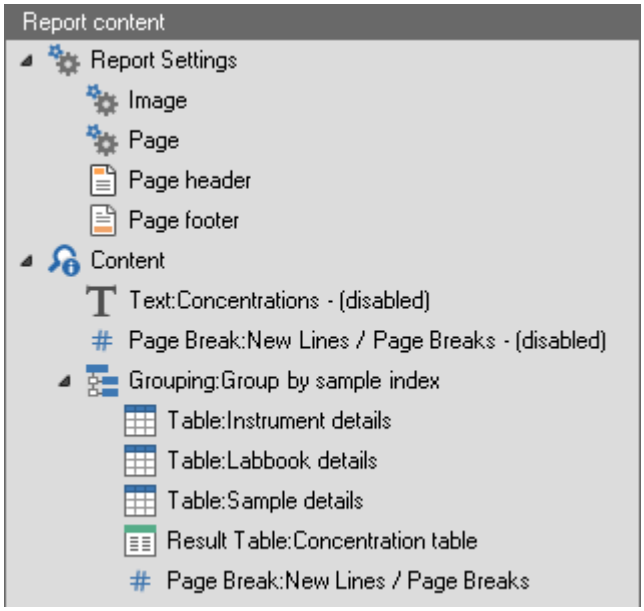


Figure 8-28. Example of the Report Content structure

Image

A user-selectable image can be included at the top right of the Report header. A wide range of image formats is supported. Images are automatically resized for display in the header area. The position of the chosen image cannot be adjusted, see Figure 8-29.

Figure 8-29. Image selection for use in a Report

Two commands are available. They are listed in Table 8-5.

Table 8-5. Commands for image selection

Command	Description
Select Image...	Shows a dialog to select the image file to be used in the Report.
Reset	Resets the image to the default Qtegra image.

This feature can be used, for example, to personalize Reports by adding a company logo to the generated Reports.

Page

The settings for the page type of the Report can be defined here, see Figure 8-30.

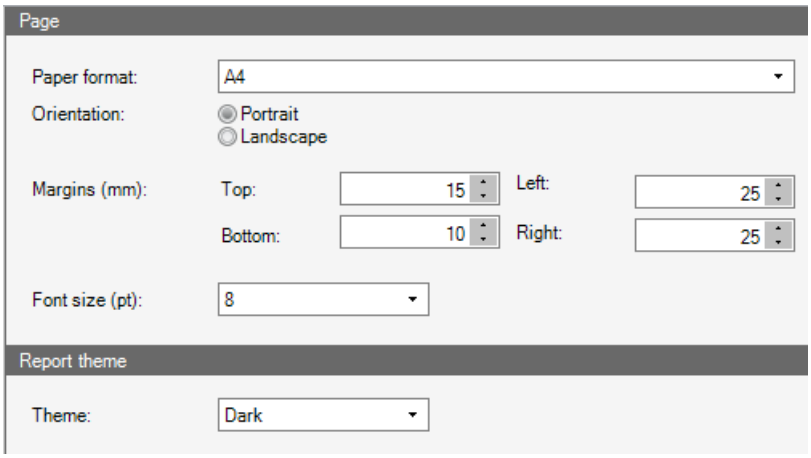


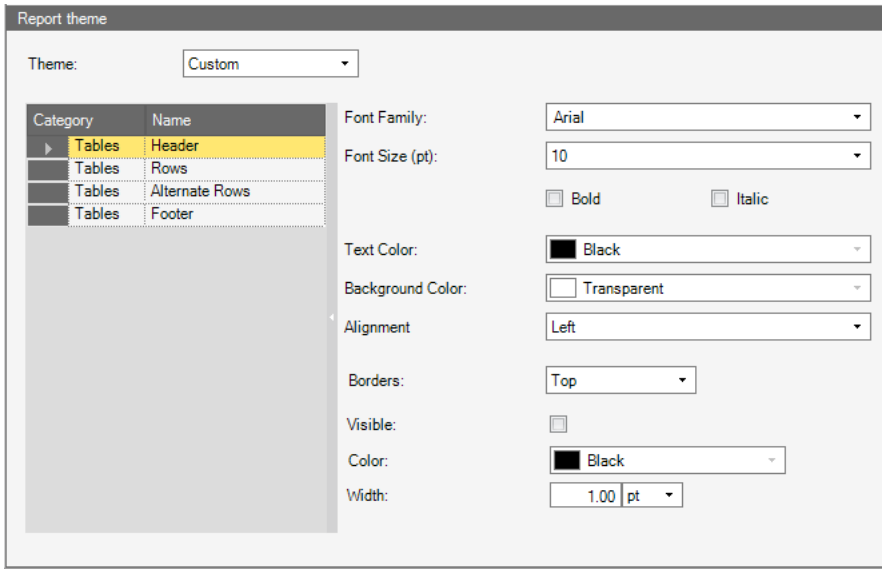
Figure 8-30. Formatting a page of a Report

The commands listed in Table 8-6 are available.

Table 8-6. Commands for page formatting

Command	Description
Paper format	Specify the paper size when saved as or printed.
Orientation	Specify the orientation of the paper.
Margins Top	Top margin, in mm.
Margins Bottom	Bottom margin, in mm.
Margins Left	Left margin, in mm.
Margins Right	Right margin, in mm.
Font Size	Font size for the Report content, in point.
Theme	Select a color theme from the list box. *Dark*, set as default, shows a black background on table headers and alternating gray and white background color on table entries. *Light* shows all tables without background color neither on headers nor on table entries. This would be the recommended theme to be used in Reports that are frequently printed in order to reduce ink usage. Select *Custom* to specify your own color set:

Table 8-6. Commands for page formatting, continued

Command	Description
	The Report theme area is then expanded and provides Font and Color selection boxes to specify all parts of tables. To check your settings, click the **Execute Report** button on the toolbar. For details, see "Previewing a Report" on page 8-25.

Page Header

The settings of the page header of the Report can be defined here, see Figure 8-31.

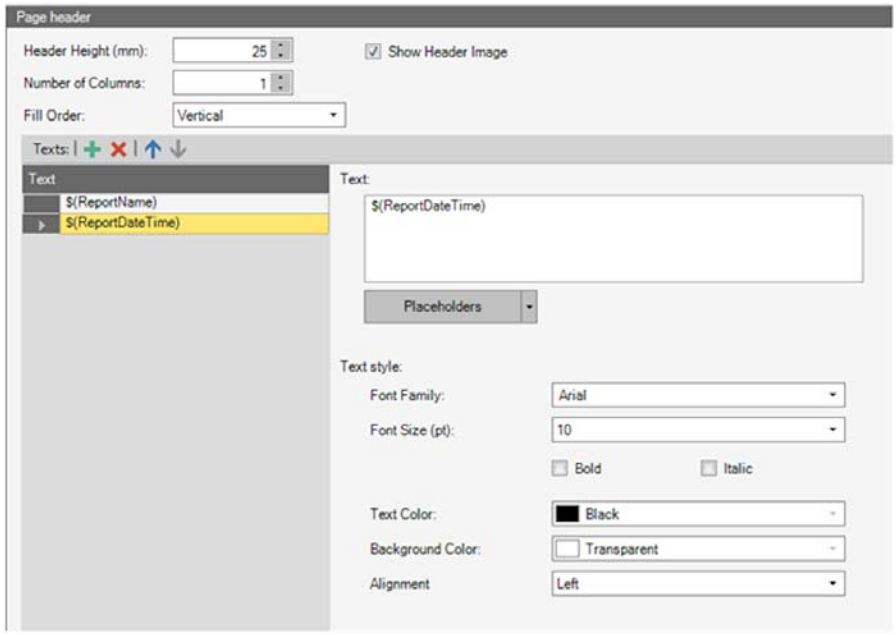


Figure 8-31. Defining page header of Report

The commands listed in Table 8-7 are available.

Table 8-7. Commands to define page header

Command	Description
Header Height	Specify the height of the header, in mm.
Number of Columns	Number of columns for the defined text item(s) displayed in the header.
Fill Order	Define the order in which text items populate the previously defined number of columns.
Show Header Image	If selected, the defined image is displayed in the right corner of the header. See "Image" on page 8-26.
Texts	List of text items that are displayed in the header. See "Header and Footer Text Items" on page 8-31.

Page Footer

The settings of the page footer of the Report can be defined here, see Figure 8-32.

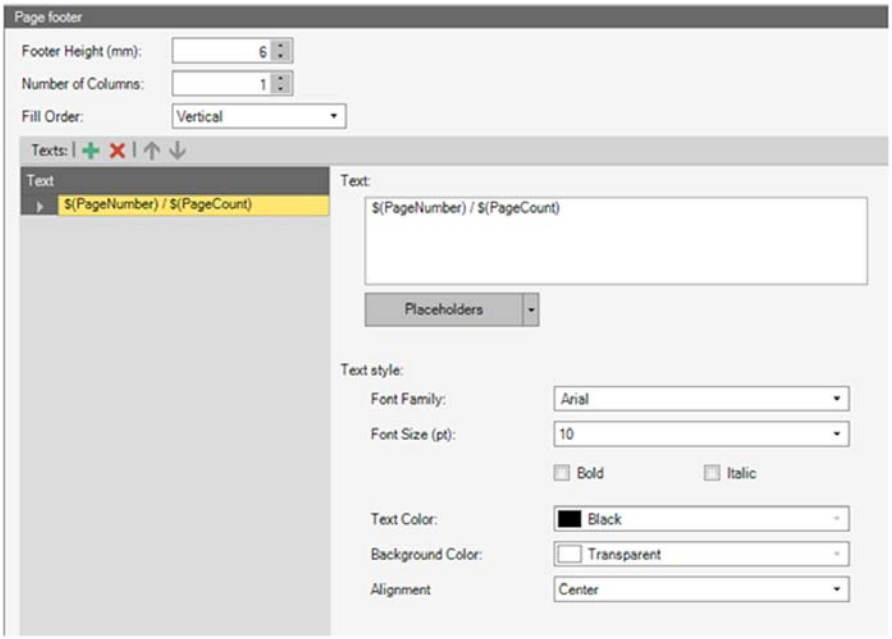


Figure 8-32. Defining page footer of Report

The commands listed in Table 8-8 are available.

Table 8-8. Commands to define page footer

Command	Description
Footer Height	Specify the height of the footer, in mm.
Fill Order	Define the order in which text items populate the previously defined number of columns.
Texts	List of text items that are displayed in the footer. See "Header and Footer Text Items" on page 8-31.

Header and Footer Text Items

Text items are used to define the content of the header and the footer of a Report. The items are arranged in a table-based layout. The table is filled as specified in the **Fill Order** and in **Number of Columns** fields. See Table 8-9 and Table 8-10 as two examples.

Table 8-9. Header and footer text items - Example 1

Example	Result	
Number of columns: 2 Fill Order: Vertical	Text 1	Text 3
Texts: Text 1, Text 2, Text 3	Text 2	

Table 8-10. Header and footer text items - Example 2

Example	Result	
Number of columns: 2 Fill Order: Horizontal	Text 1	Text 2
Texts: Text 1, Text 2, Text 3	Text 3	

Placeholders

Text items can contain placeholders to include Report specific information. The placeholders listed in Table 8-11 are available.

Table 8-11. Placeholders in text items

Placeholder	Description
Report date and time	Creation date and time of the Report.
Report date	Creation date of the Report.
Report time	Creation time of the Report.
Current user	The user name of the currently logged in Windows account.
Page number	The current page number of the Report.
Page count	Total number of pages.
Report name	The name of the Report as specified in the Content section of the Report. See "Content" on page 8-33.
Report file name	The file name of the Report.
Acquired by user	The user name of the currently logged in Windows account when the LabBook was added to the acquisition queue.
Instrument serial number	The serial number of the instrument used for acquisition of the LabBook.

Header and Footer Editor

The header and footer editor is shown in Figure 8-33.

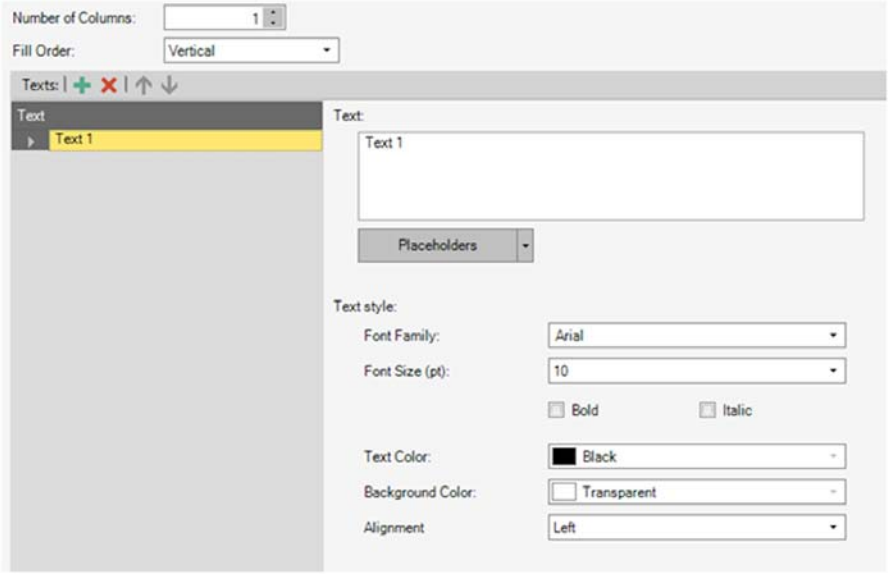


Figure 8-33. Header and footer editor

The commands listed in Table 8-12 are available.

Table 8-12. Commands for header and footer editor

Command	Description
Number of columns	Number of columns for the defined text item(s) displayed in the header or footer.
Fill Order	Order in which text items populate the previously defined number of columns.
Texts	The list of text items that are displayed in the header or footer.
+	Adds a text item.
✕	Removes the selected text item(s).
↑	Move the selected text item(s) up.
↓	Move the selected text item(s) down.

For each text item, the properties listed in Table 8-13 are available.

Table 8-13. Properties for text items

Placeholder	Description
Text	The text to be displayed in the Report.
Placeholders	The list of available placeholders. See "Placeholders" on page 8-31.
Font Family	The font used for the text.

Table 8-13. Properties for text items, continued

Placeholder	Description
Font Size	The font size in point.
Bold	If checked, the text is rendered in bold style.
Italic	If checked, the text is rendered in italic style.
Text Color	The color in which the text is rendered.
Background Color	The background color applied to the text.
Alignment	The text alignment (Left, Center, Right).

Report Content Items

Content

The **Content** item is used to define additional Report information, see Figure 8-34.

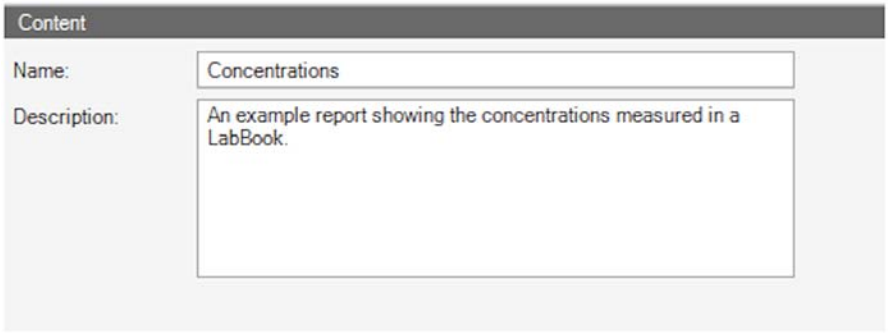


Figure 8-34. Content settings

The fields listed in Table 8-14 are available.

Table 8-14. Fields of content settings

Field	Description
Name	The name of the Report, which is used in the **Report Name** placeholder.
Description	An optional description for the selected Report.

Chart

The Chart item is used to display values as a chart. This tool is used to generate a Performance Report or any type of mass or intensity diagram. The data input sheet offers several setting parameters, see Figure 8-35.

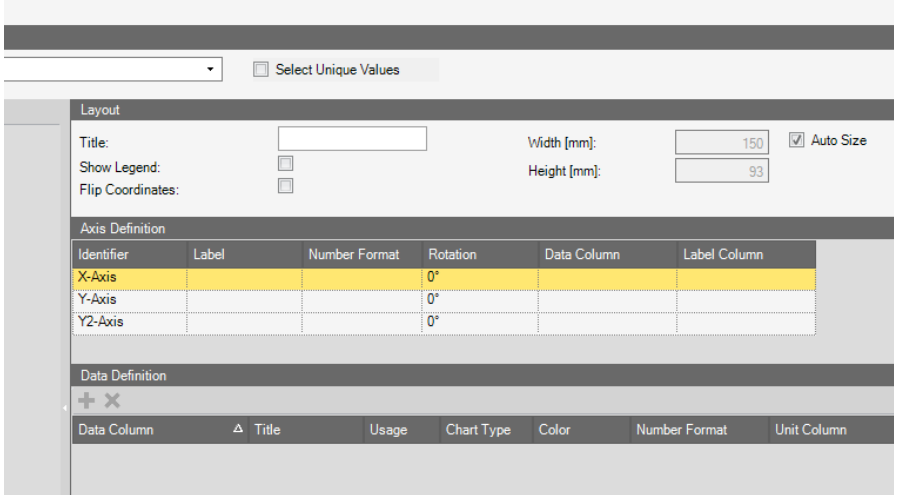


Figure 8-35. Chart settings

The fields listed in Table 8-15 are available.

Table 8-15. Chart settings fields (Sheet 1 of 5)

Field	Description
Name	The name that is displayed in the Report content area for this item. By default, the name is *Chart*.
Description	An optional description.
Use in Report	If selected, this item is rendered when the Report is created.
Source	The data source of any column. Your selection will show the appropriate columns. Select one of the following sources: *Additional acquisition parameters, Analytes, Instrument Information, Interference Correction, LabBook Summary, Measurement Modes, QC MXS Table, Ratios, Results, Sample List, Standard Details, Standards, Survey Scan Settings*.
Select Unique Values	If selected, duplicates are not listed in the table.
Layout area	The Layout area provides some optional parameters. Type or tick the option only if you want the parameter to be visible in each chart.

Table 8-15. Chart settings fields (Sheet 2 of 5)

Field	Description	
	Title	Type a title, for example, “Results” that is shown on top of the chart. 
	Show Legend	Tick this box to display a legend in the top left corner of each chart that explains your color selection from the Data Column area. 
	Flip Coordinates	Tick this box to swap the X- and Y-Axis.
	Width [mm]	When auto size is not selected, type the width of your chart into the edit box. Use this option to show the chart in another size than Qtegra proposes.
	Height [mm]	When auto size is not selected, type the height of your chart into the edit box. Use this option to show the chart in another size than Qtegra proposes.
	Auto Size	Set by default. If selected, the chart is sized as big as possible to fit into the paper format.
Columns	List of available columns specific to the selected Source. Click the item to select and press **<Ctrl>** or **<Shift>** for multiple selection. -or- Press the mouse button and drag over the items to select a range. Selected Columns fields may be added to the Data Definition section, the Sorting tab and the Conditions tab on the lower area.	

Table 8-15. Chart settings fields (Sheet 3 of 5)

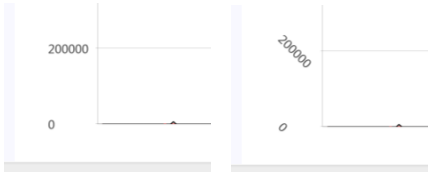
Field	Description	
Axis Definition	Section that provides parameters to define the axis display.	
	Label	Double-click the field and type a label that is shown on the axes. Each axis gets its own label.
	Number Format	See Table 8-19 for details on formatting the numeric output.
	Rotation	Select a rotation angle, for example, *45°*, from the drop-down list to show clockwise rotated labels. Supported range is 0 to 90°. 
	Data Column	From the drop-down list for the X-Axis, select the data column. The drop-down list contains all columns according to the selected source. If nothing is selected, single “steps” are shown.
	Label Column	From the drop-down list for the X-Axis, select the label column. The drop-down list contains all columns according to the selected source.
Data Definition	List of columns that are used for the ordinate (Y-Axis) in the chart. Define chart display parameters for each data column item.	
	Title	Double-click into this cell and type a title if you want to change the default that is copied from the data column.
	Usage	As all the data value appear in the ordinate, select the main Y-Axis or second Y2-Axis.

Table 8-15. Chart settings fields (Sheet 4 of 5)

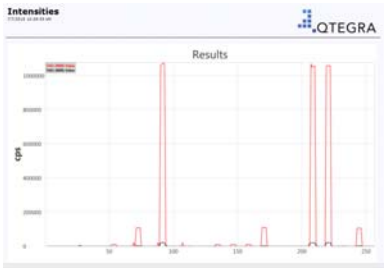
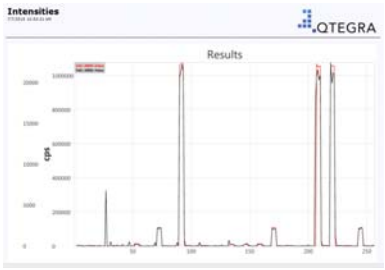
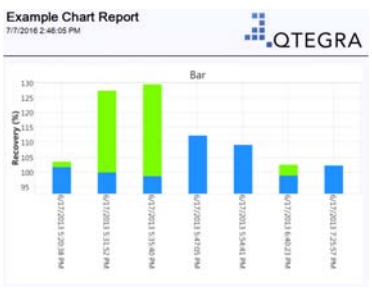
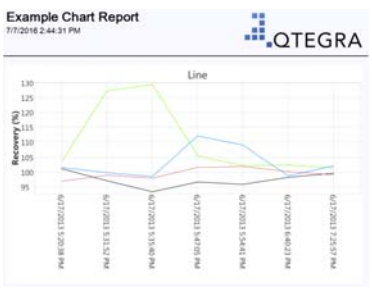
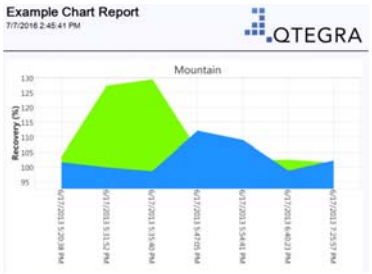
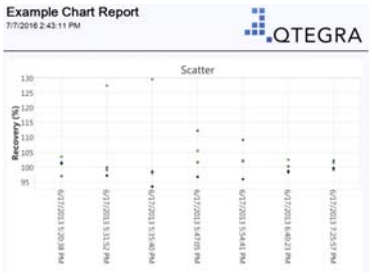
Field	Description
	
	The values for the Y2-Axis are auto-scaled and let the curves use the full height of the chart.
	Chart Type
	Qtegra provides *Bar, Line, Mountain, Scatter*, and *Stern* diagrams as chart type. Select the type for each data column.
	
	
	Color
	Qtegra provides a huge number of colors for the selected chart type. From the drop-down list, select the color for each data column.
	Number Format
	From the drop-down list, select an item that represents the data column. The number format is set in the Axis Definition area.
	Unit Column
	From the drop-down list, select an item that represents the data column.
Sorting	Allows the returned data to be sorted. See "Sorting" on page 8-53.

Table 8-15. Chart settings fields (Sheet 5 of 5)

Field	Description
Conditions	Filters the data. See "Conditions" on page 8-54.
Bookmark Tab	See "Bookmarks" on page 8-52.

Example chart to visualize QC Recoveries

The settings shown in Figure 8-36 are used to compile a scatter chart of the QC recovery.

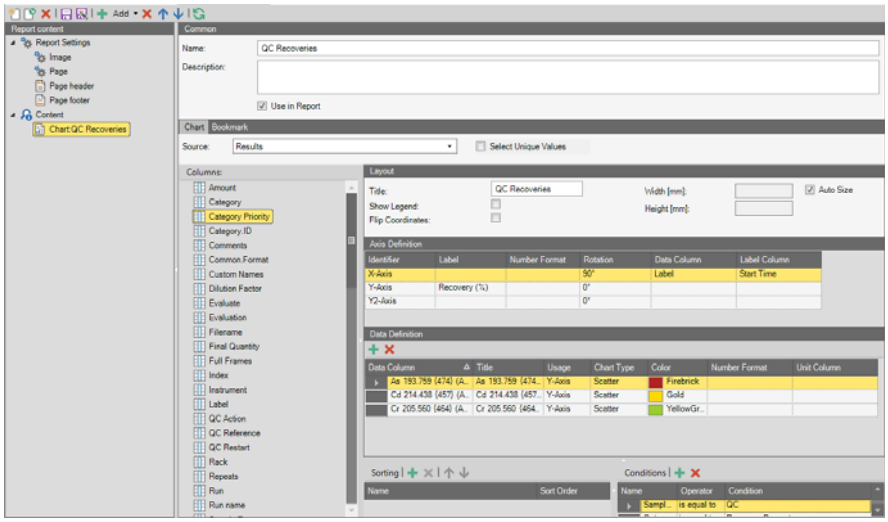


Figure 8-36. Configuration of QC Recovery example chart

In the Axis Definition table, select *Label* as **Data Column** and *Start Time* as **Label Column** for the X-Axis and **rotate** the items by *90°*. Type *Recovery (%)* as **Label** for the Y-Axis.

From the Columns list, select the analytes and add the Source Results to the Data Definition table. In the Data Definition table, select *Scatter* as **Chart type** for all analytes.

In the Conditions table, add *Category* from the **Columns** list and define *Recovery Percentage* as **Condition** with the *is equal to* **Operator**.

Click the **Execute Report** icon on the toolbar (see "Previewing a Report" on page 8-25) to compile a Report that looks as shown in Figure 8-37.

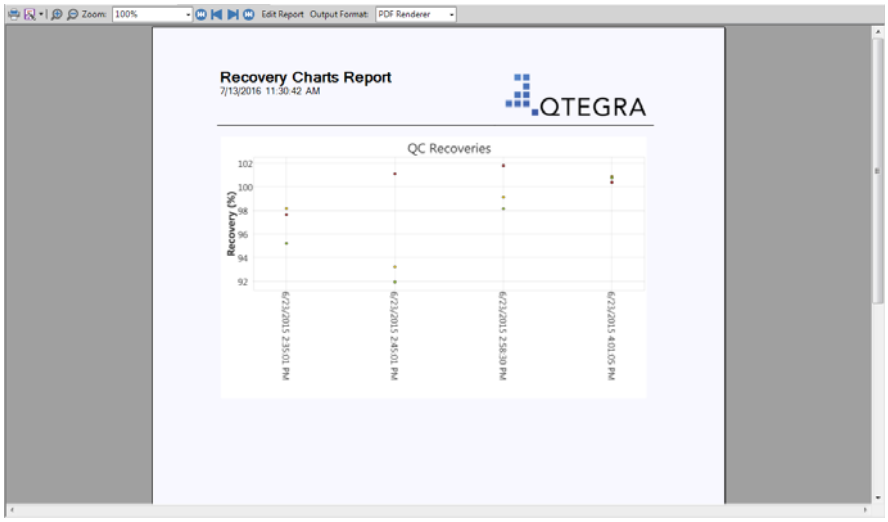


Figure 8-37. Compiled Report of QC Recovery example chart

This example shows that all QC recoveries are in the range of 92 to 102%.

Example chart to visualize Internal Standard Recoveries

The settings shown in Figure 8-38 are used to compile a scatter chart of the Internal Standard recovery.

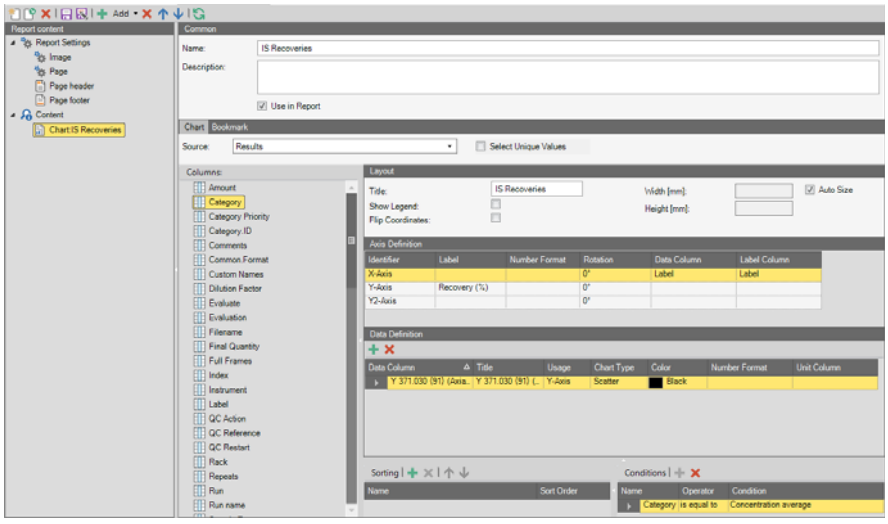


Figure 8-38. Configuration of IS Recovery example chart

Configure the Layout, Axis Definition, Data Definition, and Conditions as described above.

Click the **Execute Report** icon on the toolbar (see "Previewing a Report" on page 8-25) to compile a Report that looks as shown in Figure 8-39.

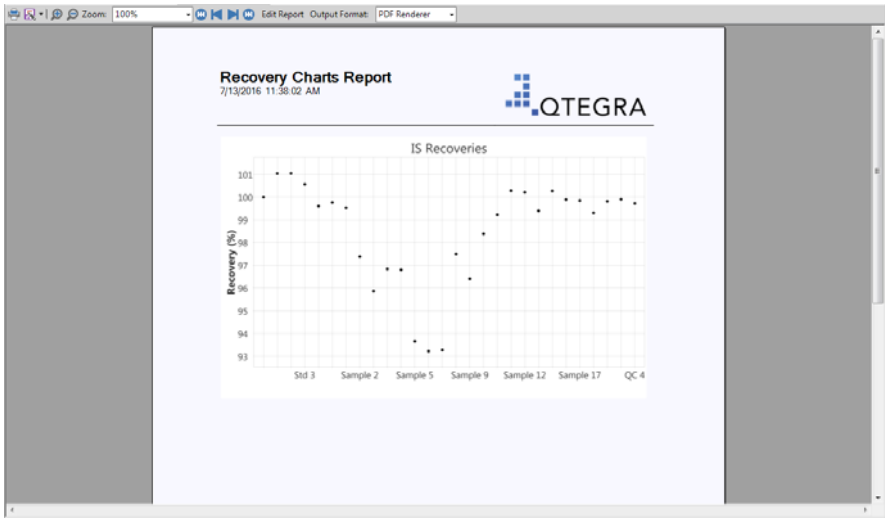


Figure 8-39. Compiled Report of IS Recovery example chart

This example shows the IS recovery for a complete dataset with values in the range of 93 to 101%.

Data

The **Data** item is used for values in a table-based layout, see Figure 8-40.

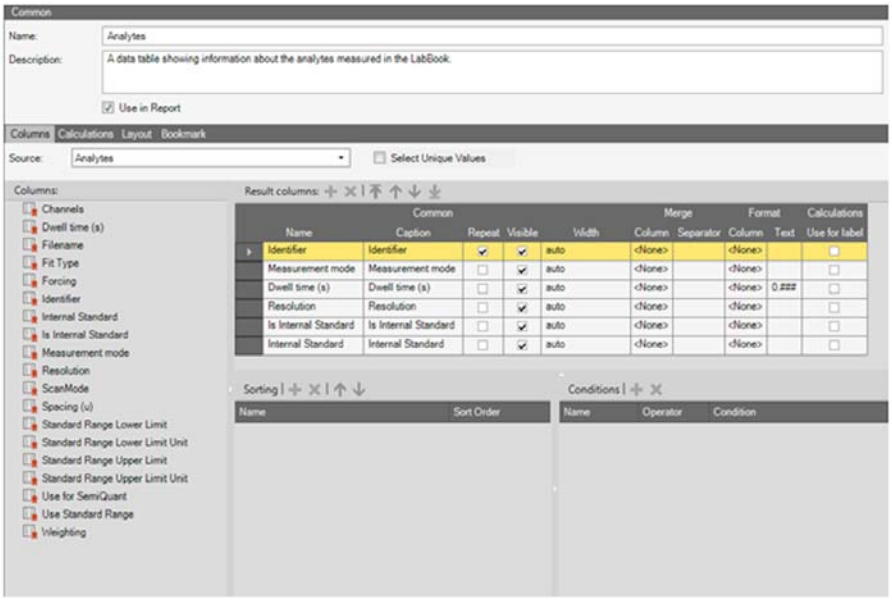


Figure 8-40. Data settings

The fields listed in Table 8-16 are available.

Table 8-16. Data settings fields

Field	Description
Name	The name that is displayed in the Report content area for this item.
Description	An optional description.
Use in Report	If selected, this item is rendered when the Report is created.
Columns Tab	
Source	The data source of any column.
Select Unique Values	If selected, duplicates are not listed in the table.
Columns	List of available columns specific to the selected Source.
Result columns	List of columns that are displayed in the Report.
Sorting	Allows the returned data to be sorted. See "Sorting" on page 8-53.
Conditions	Filters the data. See "Conditions" on page 8-54.
Calculations Tab	See "Calculations" on page 8-56.
Layout Tab	See "Layout" on page 8-57.
Bookmark Tab	See "Bookmarks" on page 8-52.

Result Columns

Result Columns displays the columns that have been selected from the chosen Source. Columns from multiple sources cannot be combined.

For each column the options listed in Table 8-17 can be specified.

Table 8-17. Options for result columns

Option	Description
Common	
Name	The column title as defined in Qtegra.
Caption	User-definable text to represent the Qtegra-defined column title. In this way, data can be displayed under column titles specific to individual requirements.
Repeat	If selected, the column caption is repeated on a new line when the table is too wide for a single line.

Table 8-17. Options for result columns, continued

Option	Description
Visible	If selected, the column is visible in the table.
Width	Column width By selecting **Auto**, the column width is calculated based on the longest entry for the column in the whole table. Otherwise, column width is entered in points.
Merge	
Column	If specified, the content of the current column is merged with the content of the column defined here and displayed as one single column.
Separator	Text used to separate merged columns.
Format	
Column	Reserved for future software versions.
Calculations	
Use for Label	The selected column(s) are displayed in the label text of any calculations defined in the **Calculations** tab.
Text	Defines the formatting of any text returned for a defined column. The text formatting possibilities depend on the column type. See Table 8-18 to Table 8-21.

Table 8-18 shows the standard numeric format strings.

Table 8-18. Numeric format strings

Notation	Summary	Example
C or c	Adds the currency symbol $ in front of the value and rounds the value with two decimals.	$ 123.45
E or e	Exponential notation.	-1.052033E+003
F or f	Integral and decimal digits with optional negative sign.	-1234.57
G or g	The most compact of either fixed-point or scientific notation.	-1.234567890E-25 or -123.456
N or n	Integral and decimal digits, group separators, and a decimal.	1,234.57

Table 8-18. Numeric format strings, continued

Notation	Summary	Example
P or p	Shows the value as percentage value with two decimals. Note: The original unit remains and will therefore appear next to the % symbol.	12,345.67 % ppb
R or r	Displays the value as a real number with 17 digits and a decimal separator.	123.45678901234567
. or #	Rounds the value up or down to an integer value without any group separator.	123

Custom numeric format strings are summarized in Table 8-19.

Table 8-19. Custom numeric format strings

Notation	Before	After
000.00	1.2	001.20
###.##	1.2	1.2
##,#.##	123456789.123	123,456,789.12
#0.0e+0	987654	98.8e4
#,#.##' °K’	12345.678	12,345.68 °K

Standard date and time format strings are summarized in Table 8-20.

Table 8-20. Standard date and time format strings

Notation	Summary	Example for 6/15/2009 1:45:30 PM
d	Short date pattern	6/15/2009
D	Long date pattern	Monday, June 15, 2009
f	Full date/time pattern (short time)	Monday, June 15, 2009 1:45 PM
F	Full date/time pattern (long time)	Monday, June 15, 2009 1:45:30 PM
g	General date/time pattern (short time)	6/15/2009 1:45 PM
G	General date/time pattern (long time)	6/15/2009 1:45:30 PM

Custom date and time format strings are summarized in Table 8-21.

Table 8-21. Custom date and time format strings

Notation	Summary	Example
yyyy-MM-dd HH:mm:ss	6/15/2009 1:45:30 PM	2009-06-15 13:45:30

Graph

The **Graph** item is used to display calibration graphs in the Report, see Figure 8-41.

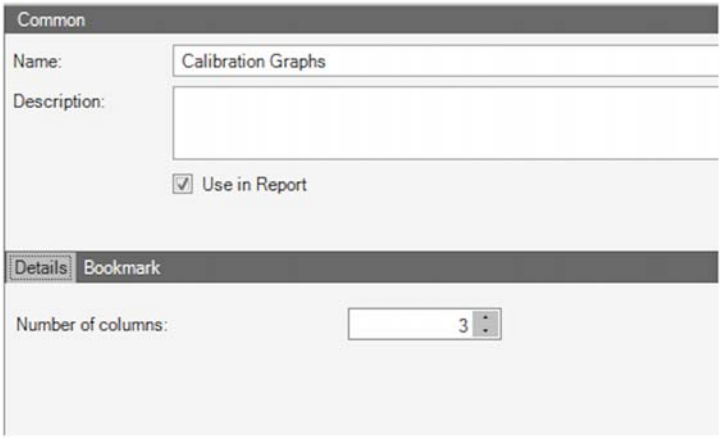


Figure 8-41. Graph content type commands

The fields listed in Table 8-22 are available.

Table 8-22. Graph content type fields

Field	Description
Name	The name that is displayed in the Report content area of this item.
Description	An optional description.
Use in Report	If selected, this item is rendered when the Report is created.
Details Tab	
Number of columns	The number of graphs displayed across the page.
Bookmark Tab	See "Bookmarks" on page 8-52.

You define how many graphs are shown in one row.
The x-axis of each graph represents concentration, the y-axis intensity. Below the graph you will find the formula of the function f(x) and the values for R^2, BEC and LOD.

Group By

The **Group By** item is used to group data based upon criteria defined by another data source. This allows the combination of (multiple) content types per analysis to allow the display, for example, of analysis-specific groups of data, see Figure 8-42.

Figure 8-42. Options for a Group By content item

The fields listed in Table 8-23 are available.

Table 8-23. Fields of Group By content type

Field	Description
Name	The name that is displayed in the Report content area of this item.
Description	An optional description.
Use in Report	If selected this item is rendered when the Report is created.
Details Tab	
Source	The data source used to group data by.
Columns	List of available columns specific to the selected source.
Result columns	List of column(s) used to define the Group By source. Supported columns for grouping are LabBook Summary: Filename, Sample List: Index and Results: Index.
Sorting	Allows the returned data to be sorted. See "Sorting" on page 8-53.
Conditions	Filters the data. See "Conditions" on page 8-54.

Tip This module is for structuring only and must be followed by a Data module, a Graph module or a Result Data Table module to show values.

In the example shown in Figure 8-42 from the supplied Report Calibration, a grouping content item has been added to the Report calibration (**1**). The data source **Results - Index** (**2**) is used to define the content that will be grouped together but **only** when **Sample Type = STD** (**3**).

In this example, for each item that meets the defined grouping criteria (an analysis that has a result **and** has been defined as a STD), a series of content items are displayed, see Figure 8-43.

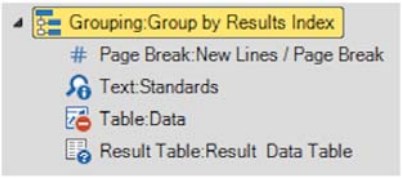


Figure 8-43. Content items defined for analyses that meet the Grouping: Group by Results Index criteria

Each of the grouped content items have their specific definitions as usual. The Report used in this example, **Calibration**, is supplied with Qtegra ISDS Software.

New Lines/Page Breaks

The **New Lines/Page Breaks** item is used to add empty lines and/or page breaks, see Figure 8-44.

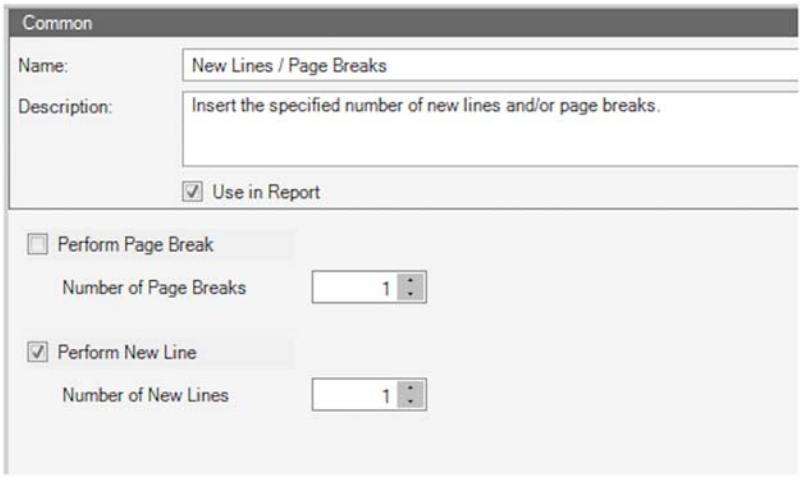


Figure 8-44. New Line/Page Break content type commands

The fields listed in Table 8-24 are available.

Table 8-24. Fields of New Line/Page Break content type

Field	Description
Name	The name that is displayed in the Report content area of this item.
Description	An optional description.
Use in Report	If selected this item is rendered when the Report is created.
Perform Page Break	If selected, page breaks are inserted.
Number of Page Breaks	The number of page breaks inserted.
Perform New Line	If selected, empty lines are added to the Report.
Number of New Lines	The number of empty lines that are added to the Report.

Result Data Table

The **Result Data Table** item is used to display calculated results from a LabBook. The following features are automatically applied to a Result Data Table item:

- Columns that contain no values are hidden.
- The corresponding unit identifier is automatically attached to each analyte column.
- The **Category** column (from the Source **Sample List**) can be used to the displayed name of the text in the **Rows** tab.
- Data listed underneath the **Category** column is sorted automatically using a non user-definable order.
- If selecting **Analytes**, two options are available:

  a. To add all defined analytes to the Report, select the **Analytes** column.

  b. Specific analytes can be added to the Report by selecting them individually from the drop down list under the **Analytes** column.

- The width of all non-repeated columns is identical.
- All analyte results are automatically formatted. The format column is ignored.

The options for the Result Data Table content type are shown in Figure 8-45.

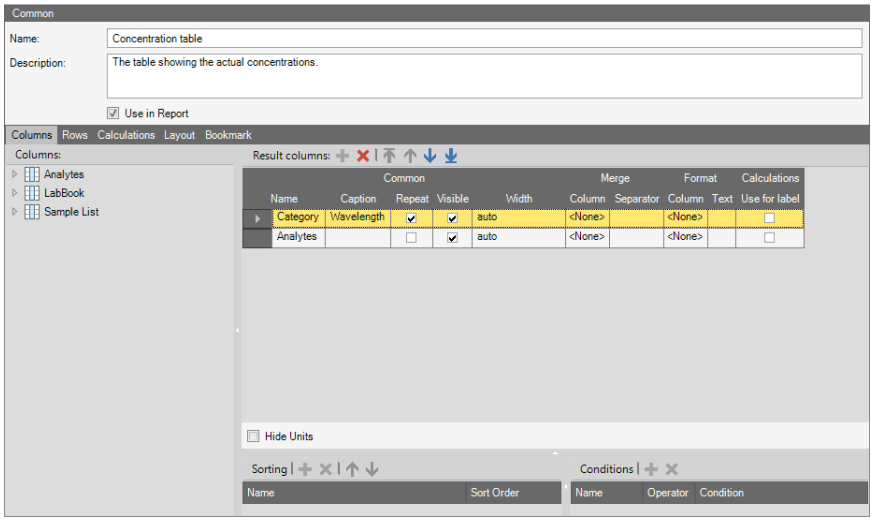


Figure 8-45. Options for Result Data Table content type

The fields listed in Table 8-25 are available.

Table 8-25. Result Data Table content type fields

Field	Description
Common Section	
Name	The name that is displayed in the Report content area of this item.

Table 8-25. Result Data Table content type fields, continued

Field	Description
Description	An optional description.
Use in Report	If selected this item is rendered when the Report is created.
Columns Tab	
Columns	List of available columns. They are grouped together under descriptive headings. Click the triangle next to each header to expand the group.
Result columns	List of columns that are displayed in the Report. See "Result Columns" on page 8-50.
Hide Units	If selected, the unit text for a column is displayed in the header, but **only** if all entries in the column have the same unit type. If different units are used, this button has no effect.
Sorting	Allows the returned data to be sorted. See "Sorting" on page 8-53.
Conditions	Filters the data. See "Conditions" on page 8-54.
Rows Tab	See "Rows" on page 8-50.
Calculations Tab	See "Calculations" on page 8-56.
Layout Tab	See "Layout" on page 8-57.
Bookmark Tab	See "Bookmarks" on page 8-52.

Special Columns

Some of the possible columns have special properties as summarized in Table 8-26.

Table 8-26. Special functions of certain columns

Function	Description
Sample List: Category	This column must be added to allow the name of the lines as selected at the Rows tab to be included. In the example Report **Concentrations** (as shown in Figure 8-45), this column is renamed (using the **Caption** function) to *Wavelength* to allow for easier identification.
Analytes Analyte Ratios Analytes (Survey)	Analytes, Analyte Ratios, and Analytes (Survey) are used as the row or column header in the final results grid.

Result Columns

Result columns displays the columns that have been selected from the chosen source. Columns from multiple column sources can be combined.

Rows

The **Rows** tab is used to select the numerical results displayed in the result table. If no rows are selected, the table displayed in the final Report is empty.

❖ **To add or remove results to or from the table**

Select them from either the **Available** or **Selected** list using the buttons at the bottom of the Rows tab as shown in Figure 8-46.
-or-
Double-click the item.

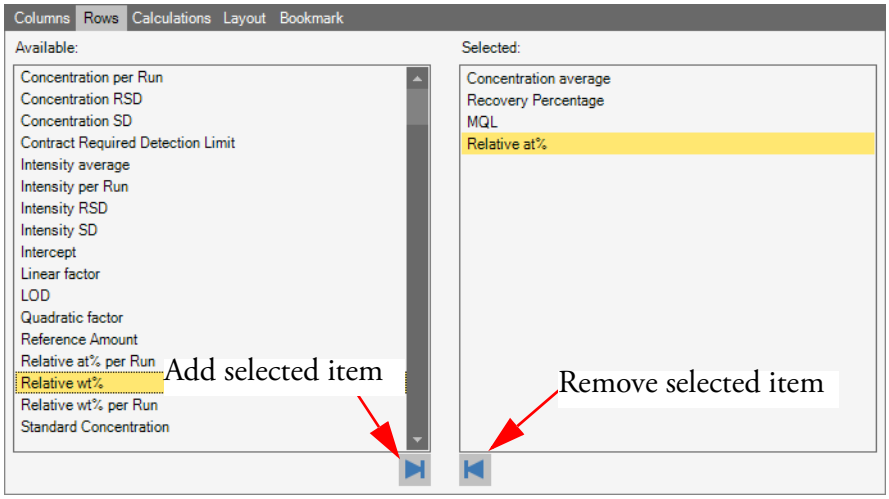


Figure 8-46. Adding or removing data types to or from Result Data Tables

Text

The **Text** item is used to add custom text to the Report, see Figure 8-47.

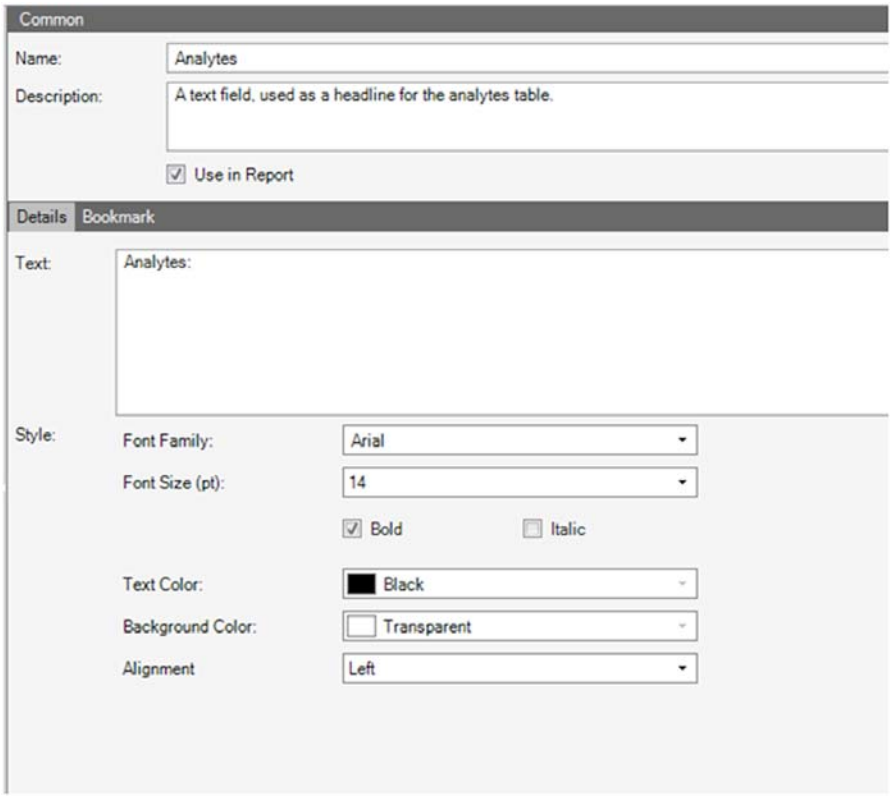


Figure 8-47. Text content type commands

The fields listed in Table 8-27 are available.

Table 8-27. Fields of Text content type

Field	Description
Name	The name that is displayed in the Report content area of this item.
Description	An optional description.
Use in Report	If selected this item is rendered when the Report is created.
Text	The text displayed in the Report.
Style	
Font Family	The font used for the text.
Font Size	The font size in point.
Bold	If checked, the text is rendered in bold style.
Italic	If checked, the text is rendered in italic style.
Text Color	The color in which the text is rendered.

Table 8-27. Fields of Text content type, continued

Field	Description
Background Color	The background color applied to the text.
Alignment	The alignment of the text (*Left, Center, Right*).

Common Items

Bookmarks

Bookmarks are used to generate a table of contents when the Report is saved as a PDF file. If available, a **Placeholders** drop-down menu contains a list of fields, which can be used to define content displayed as bookmark text.

Bookmarks can be created for any Report content item - even those nested inside a **Group By** content item, see Figure 8-48.

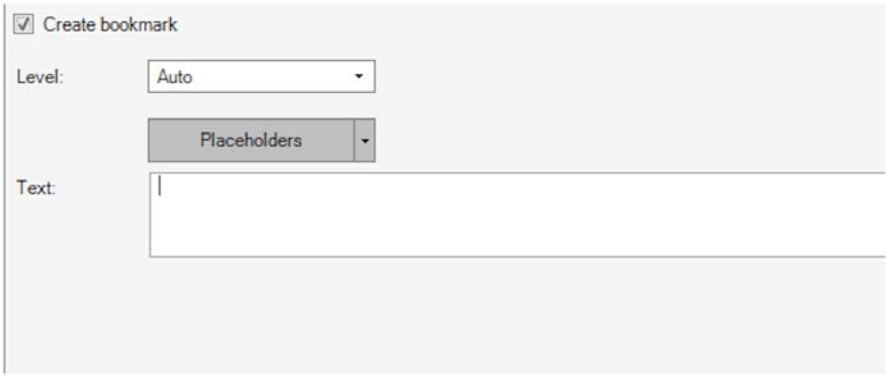


Figure 8-48. Options for bookmark items

The fields listed in Table 8-28 are available.

Table 8-28. Fields of Bookmark content type

Field	Description
Create Bookmark	If selected, a bookmark is created.
Level	Select **Auto** to automatically determine the level of the bookmark in the final PDF file. Otherwise, specify the level that should be used in the table of contents.
Placeholders	Contains the list of placeholders that are currently available. For a Data item and a Result Data Table item, this is the list of result columns selected.
Text	The text that is displayed for the bookmark. Placeholder-specific text will be entered here automatically.

Sorting

The **Sorting** function allows data to be sorted in a user defined order and is used by the following Report content items:

- Data
- Group By
- Result Data Table

❖ **To select a column for sorting displayed data**

1. Select the required column from the list of available columns.
2. On the **Sorting list toolbar**, click **Add**, see Figure 8-49.

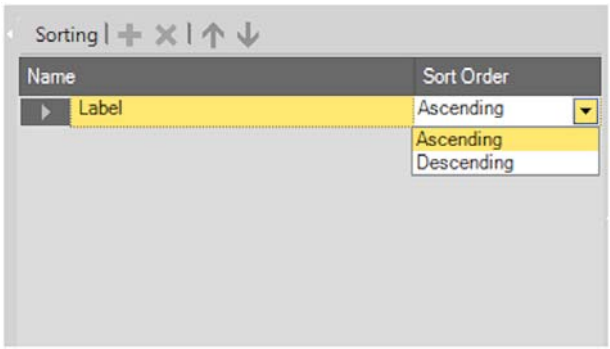


Figure 8-49. Options for sorting commands

The Sorting list toolbar contains the commands summarized in Table 8-29.

Table 8-29. Commands of Sorting list toolbar

Command	Description
+	Adds the selected columns to the sorting list.
✕	Deletes the selected sorting item(s).
↑	Moves the selected sorting item(s) up the list.
↓	Moves the selected sorting item(s) down the list.

The fields listed in Table 8-30 are available.

Table 8-30. Sorting content type fields

Field	Description
Name	The name of the selected column to be used to sort data.
Sort Order	Specify ascending or descending sort order.

Conditions

The **Conditions** function allows data to be filtered by user defined criteria and is used by the following Report content items:

- Data
- Group By
- Result Data Table

Multiple conditions from different columns can be defined by using different operators (see Table 8-32).

❖ **To use a column as a condition to display data**

1. Select the required column from the list of available columns.
2. On the **Conditions list toolbar**, click **Add**.

Figure 8-50 shows the operators for Conditions commands.

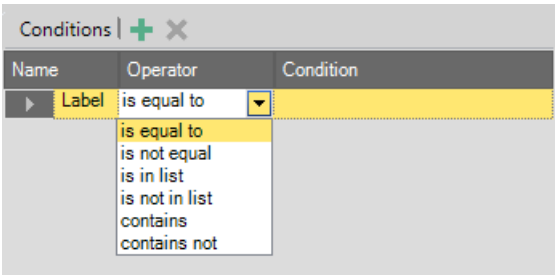


Figure 8-50. Options for Conditions commands

The **Conditions** toolbar contains the commands summarized in Table 8-31.

Table 8-31. Commands of Conditions toolbar

Command	Description
+	Adds the selected columns to the conditions list.
✕	Deletes the selected condition item(s).

The fields listed in Table 8-32 are available.

Table 8-32. Fields of Conditions content type

Field	Description	
Name	The name of the column used for sorting. For example, select *Category* to provide a collection of Conditions (*Concentration average, Intensity average, Recovery Percentage*).	
Operator	The operator used to filter the data depends on the selected column, i.e., not all operators shown below are valid for all columns.	
	Is equal to	Specifies a single value that is used to filter the data in the selected column. Select this value from the Condition drop-down list.
	Is not equal	Specifies a single value that is excluded from the data in the selected column. Select this value from the Condition drop-down list.
	Is in list	Specifies one or more values that are used to filter the data in the selected column. Tick the required values from the Condition drop-down list.
	Is not in list	Specifies a single value that is excluded from the data in the selected column. Tick the rejected values from the Condition drop-down list.
	Contains	Use the wildcard * to filter the data in the selected column. Type the required value in the Condition field. Example: `*myname*` selects all values that contain “myname”.
	Contains not	Specifies a value that does not contain the string entered in the Condition field. Example: `STD` excludes all values that contain “STD”.
	Greater than	Specifies a value that is greater than the value entered in the Condition field.
	Less than	Specifies a value that is less than the value entered in the Condition field.
Condition	The conditions depend on the selected column and operator used.	

Calculations

Calculations are used to apply basic mathematical functions to selected data. Calculations are only available for:

- Data item
- Result Data Table item

Calculations can only be applied to the columns already defined in the result column list. Depending on the selected columns not all calculation types are available.

The options for Calculations are shown in Figure 8-51.

Figure 8-51. Options for Calculations

The **Calculations** toolbar contains the commands summarized in Table 8-33.

Table 8-33. Commands of Calculations toolbar

Command	Description
+	Adds a new calculation item to the calculation list.
✕	Deletes the selected calculation item(s).
↑	Moves the selected calculation item(s) up the list.
↓	Moves the selected calculation item(s) down the list.

The fields listed in Table 8-34 are available.

Table 8-34. Fields of Calculations content type

Field	Description
Calculation	Specifies the calculation type. See "Calculations" on page 8-56.
Group Column	If empty, the calculation is applied to all values of the selected columns once. If a column is selected, the calculation is applied every time the value of the column changes.
Label	The text displayed in the table for the calculation.
Unit	The text for the unit displayed for the calculation.

Table 8-34. Fields of Calculations content type, continued

Field	Description
Format	The format used when displaying the calculation result. See "Result Columns" on page 8-41.
Available Columns	The columns listed are those specified in the Result Columns tab.

The calculation types available are listed in Table 8-35.

Table 8-35. Available calculation types

Calculation type	Description
Entry Count	Number of entries
Minimum	Calculates the minimum
Maximum	Calculates the maximum
Sum	Calculates the sum
Value Replacement	Allows re-ordering of rows in Reports
Average	Calculates the average
Standard Deviation	Calculates the standard deviation
RSD	Calculates the relative standard deviation (% RSD)

Layout

The **Layout** tab is used to define the display of table-related Report Content Items such as Data and Result Data Table.

The Layout options are shown in Figure 8-52.

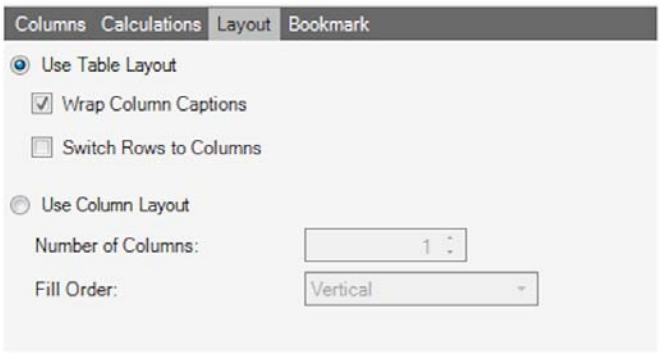


Figure 8-52. Layout options

The check boxes or fields listed in Table 8-36 are available.

Table 8-36. Check boxes or fields at Layout tab

Check box or field	Description
Wrap Column Captions	If checked, the text in the table header is wrapped to save space.
Switch Rows to Columns	If checked, the contents of the defined rows are displayed in columns. This is similar to the Transpose function in Microsoft Excel.
Number of Columns	The number of columns used to display data.
Fill Order	The fill order used to display data.

Table 8-37 shows two examples of using Number of Columns and Fill Order.

Table 8-37. Two examples for using Number of Columns and Fill Order

Example 1	Result	
Number of Columns: 1 Fill Order: Vertical	Label Col 1	Col 1
	Label Col 2	Col 2
	Label Col 3	Col 3

Example 2	Result			
Number of Columns: 2 Fill Order: Vertical	Label Col 1	Col 1	Label Col 3	Col 3
	Label Col 2	Col 2		

Use Column Layout works fine for small data volumes such as showing Index and Sample Type above grouped tables. **Use Table Layout** is suitable for all tables sizes.

Modifying the Performance Report

As an example for changing an originally supplied Report the Performance Report shall be prepared to show “Per-run” data.

❖ **To add Run Data to the Performance Report**

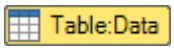
1. From the **Qtegra - [Home Page]**, open Qtegra > File Manager > Reports > Performance Report to see all available Performance Reports.

   Tip Replace the sub-folder and Report to change another Report accordingly.

2. Double-click the Report you wish to modify.
   The Report opens in a Qtegra tab.

3. On the toolbar, click **Edit Report** to open a new tab with the Report editor.

4. Expand the **Add** button and select *Data*.

   The 

   is appended to the Report content and the main area shows the edit boxes.

5. From the **Source** listbox in the Columns tab, select *Sensitivity Run Data*.

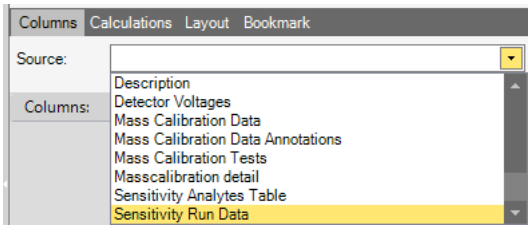


Figure 8-53. Source listbox

   All analytes used in the Performance Report are shown.

6. Select the desired analyte (or press **<Ctrl>** and click to select multiple analytes) and click **Add** on the Result columns toolbar.

   The analytes are listed and may be modified for display as shown above.

7. On the Report Editor toolbar, click **Execute Report** to create the new Report.

8. To change further properties, click **Edit Report** again and change your items accordingly.

Support for Spectra

Spectra information from Survey Scans and Main Runs from eQuant analyses can be added to Reports.

The following examples show how to set up different spectra Reports.

❖ **To add Spectra into a Report**

1. From the Reports toolbar, select **Add > Chart**.

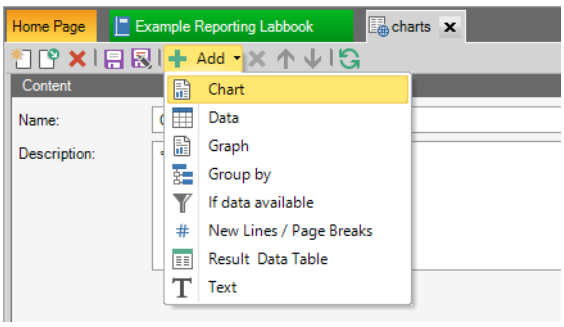


Figure 8-54. Chart item in Add menu

2. From the **Source** selection box, select **Survey and Main Run Intensities**.

3. In the **Axis Definition** section, define the **Labels** to be displayed for the X- and Y-Axis. These should normally be *Mass* for X and *Intensity* for Y.

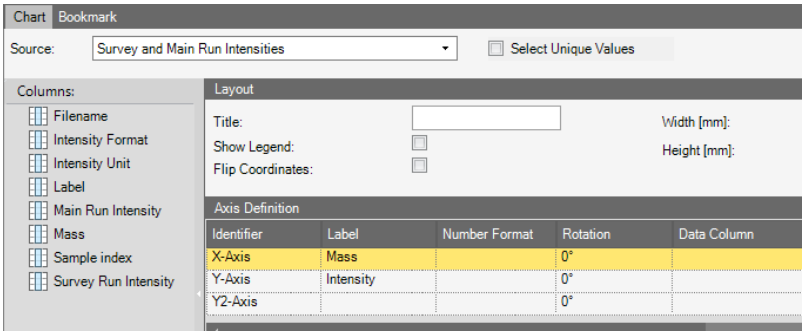


Figure 8-55. Defining the X- and Y-Axes for a 'Spectra Main Runs' Report

4. In the Axis Definition section, select the **Data Column** to be used for display on the X-Axis (normally *Mass*).
With this defined, you can set the **Min** and **Max** mass values to allow a specific mass range to be used.
-or-
Select **AutoMin** and **AutoMax** to display the entire mass range.

5. In the **Data Definition** section, select the **Data Column** to be displayed. This should be either *Main Run Intensity* or *Survey Run Intensity* and should be displayed on either the Y- or Y2-Axis. You

can select from a range of **Chart Types** (*Bar, Scatter* or *Stem*) and the chart **Color** as required.

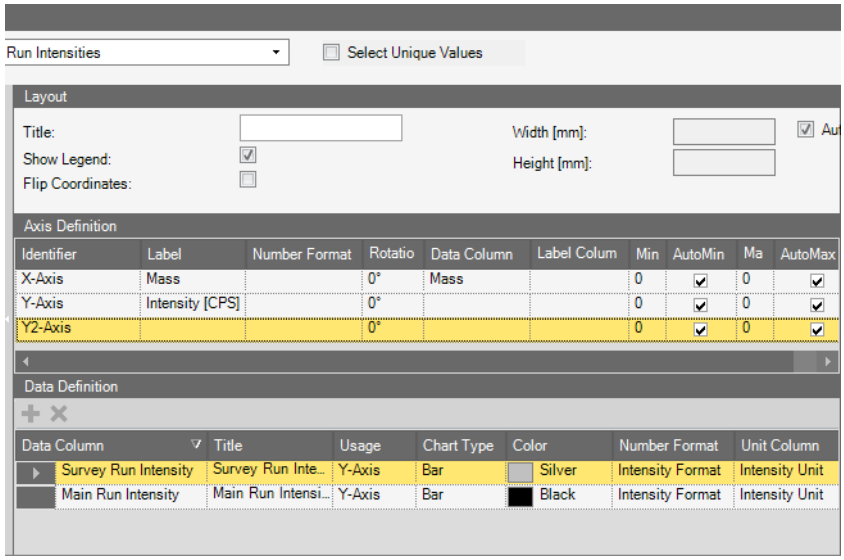


Figure 8-56. Example definition of a 'Spectra Main Runs' Report Template

6. The examples in Figure 8-56 and Figure 8-57 show the definition and resulting display from the supplied 'Spectra Main Runs' Report Template.

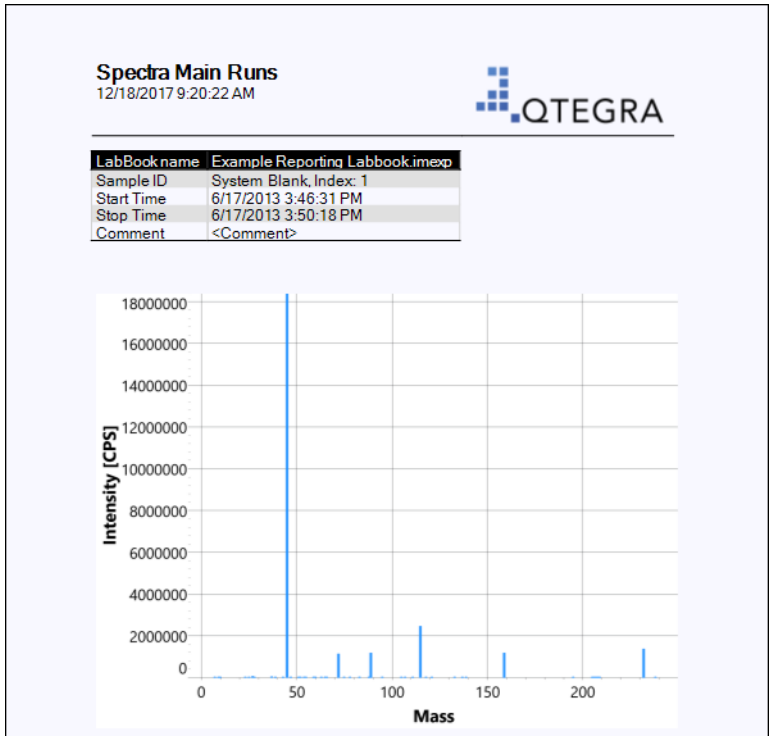


Figure 8-57. Resulting output from an example 'Spectra Main Runs' Report

The chart shows the mass spectrum over the whole mass range.

❖ **To display Recoveries for Internal Standards as charts**

1. From the Reports toolbar, select **Add > Chart**.
2. From the **Source** selection box, select **Analysis Result Table**.
3. In the **Axis Definition** section, define the **Labels** to be displayed for the X- and Y-Axis. For example, use *Sample Index* for X and *IS Recovery (%)* for Y.

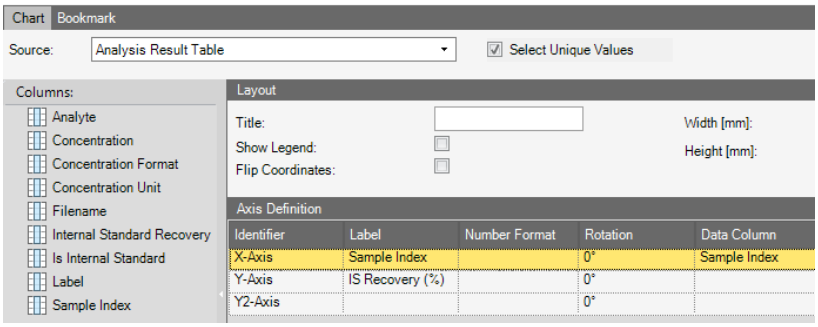


Figure 8-58. Defining the X- and Y-Axes for an IS Recovery Report

4. In the Axis Definition section, select the **Data Column** to be used for display on the X-Axis. This should be *Sample Index* and you can use this value again for the **Label Column**. For the X-Axis (*Sample Index*), select **AutoMin** and **AutoMax** to display recoveries from all analyses in the LabBook. For the Y-Axis (*IS Recovery (%)*), set the **Min** and **Max** recovery values (expressed as a percentage) to allow a specific range of recoveries to be displayed (for example, as defined by a SOP).
   -or-
   Select **AutoMin** and **AutoMax** to display the entire range of recoveries measured.

5. In the **Data Definition** section, select the *Internal Standard Recovery* **Data Column**. You can select from a range of **Chart Types** (*Bar, Scatter* or *Stem*) and the chart **Color** as required.

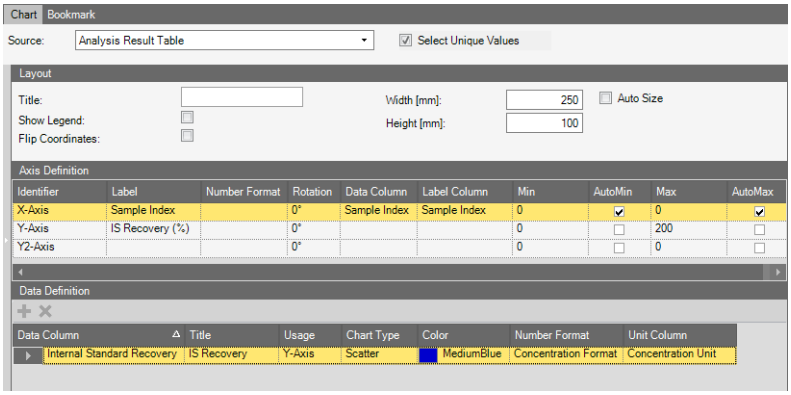


Figure 8-59. Example definition of an IS Recovery Report Template

Tip You can add a **Condition** to, for example, select recoveries for specific Internal Standards to be displayed.

Tip It is not currently possible to display the response from individual Internal Standards, or to label the responses in the chart.

6. The examples in Figure 8-59 and Figure 8-60 show the definition and resulting display from the supplied 'IS_Recoveries' Report Template.

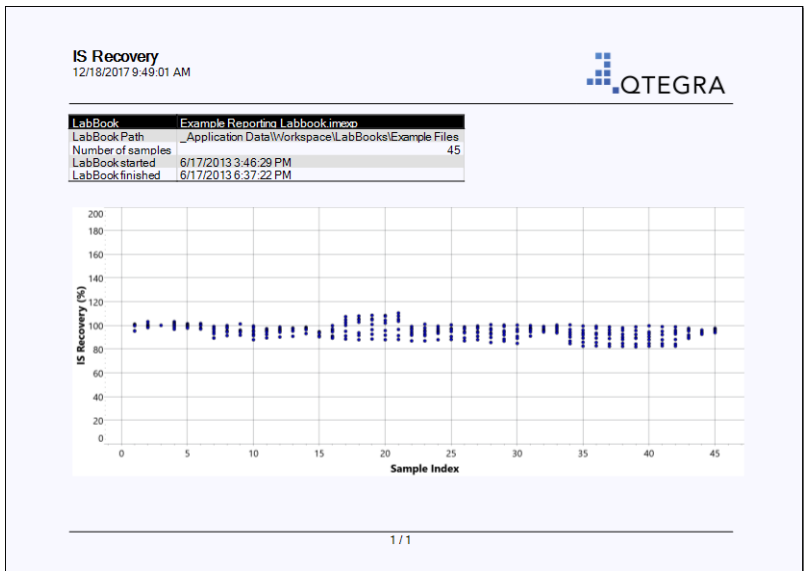


Figure 8-60. Example for an Internal Standard Recovery chart

The chart shows the Internal Standard recoveries from the entire LabBook.

❖ **To display Recoveries for Quality Control values as charts**

1. From the Reports toolbar, select **Add > Chart**.
2. From the **Source** selection box, select **Quality Control Values**.
3. In the **Axis Definition** section, define the **Labels** to be displayed for the X- and Y-Axis. For example, use *Sample Index* for X and *QC Recovery (%)* for Y.

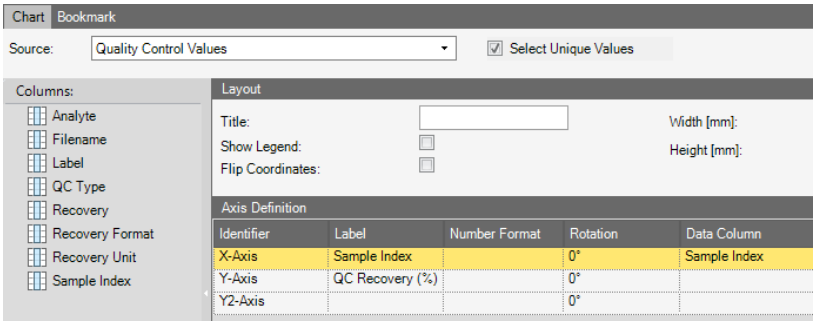


Figure 8-61. Defining the X- and Y-Axes for a Quality Control Recovery Report

4. In the Axis Definition section, select the **Data Column** to be used for display on the X-Axis. This should be *Sample Index* and you can use this value again for the **Label Column**. For the X-Axis (*Sample Index*), select **AutoMin** and **AutoMax** to display recoveries from all analyses in the LabBook. For the Y-Axis (*QC Recovery (%)*), set the **Min** and **Max** recovery values (expressed as a percentage) to allow a specific range of recoveries to be displayed (for example, as defined by a SOP).
   -or-
   Select **AutoMin** and **AutoMax** to display the entire range of recoveries measured.

5. In the **Data Definition** section, select the *Recovery* **Data Column**. You can select from a range of **Chart Types** (*Bar, Scatter* or *Stem*) and the chart **Color** as required.

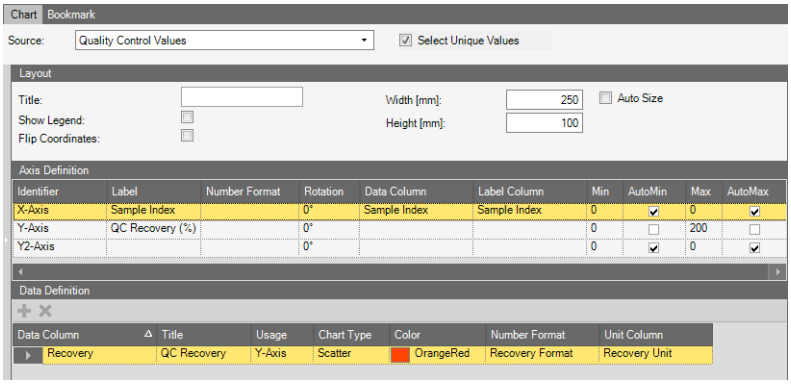


Figure 8-62. Example definition of a Quality Control Recovery Report Template

Tip You can add a **Condition** to, for example, select recoveries for specific analytes or specific QC types to be displayed.

6. The examples in Figure 8-62 and Figure 8-63 show the definition and resulting display from the supplied 'QC_Recoveries' Report Template.

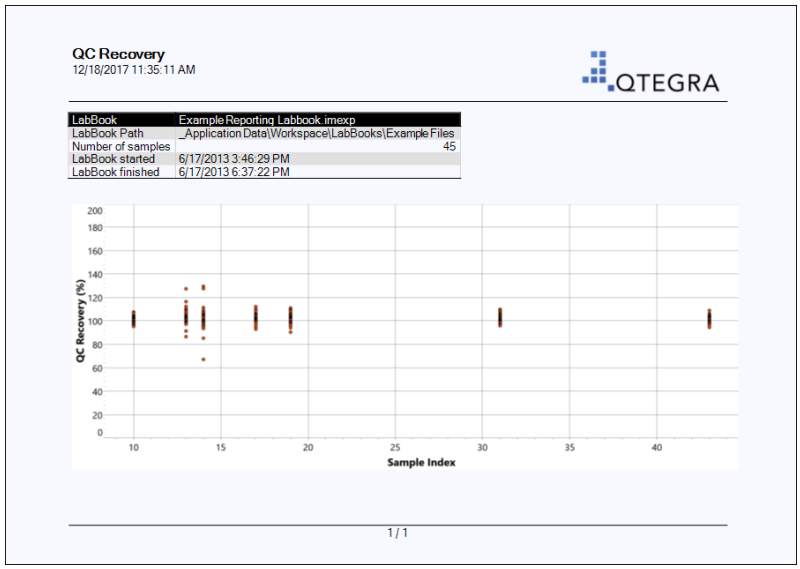


Figure 8-63. Example for a Quality Control Recovery chart

The chart shows the Quality Control recoveries from the entire LabBook.

Qtegra Report Preview

This chapter describes how to work with the Qtegra Report Preview.

The Report Preview is used to display the generated Report based on a selected Report template. The Report Preview window for the supplied Concentrations Report template is shown in Figure 8-64.

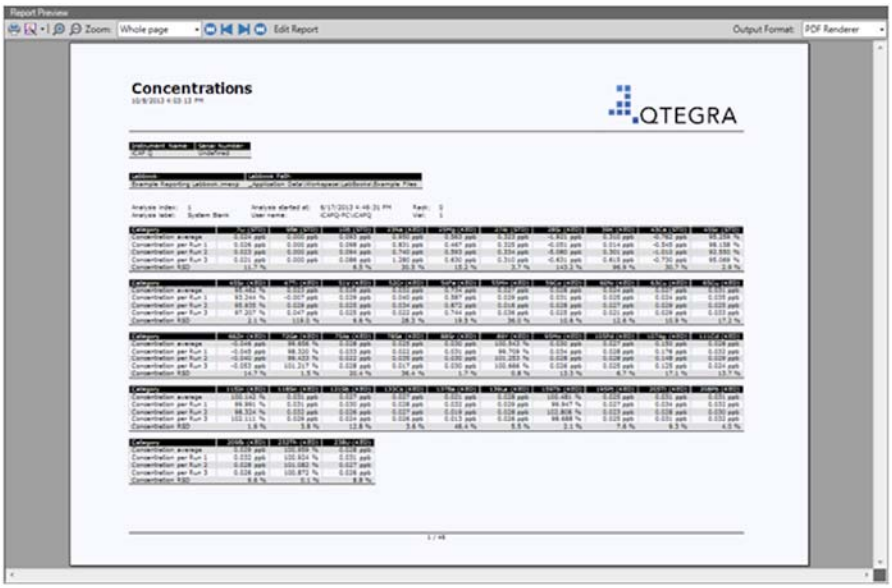


Figure 8-64. Report Preview window for Concentration Report template

The Report Preview has the components:

- Report Preview toolbar
- Preview Area

Report Preview Toolbar

The Report Preview toolbar provides functions to:

- Print and export the Report
- Zoom and navigate through the pages in the Report

The commands of the Report Preview toolbar are listed in Table 8-38.

Table 8-38. Commands of Report Preview toolbar

Command	Description
	Prints the current Report.
	Saves the Report in PDF or RTF format. Saves the XML file in XML format.
	Zooms in the display.

Table 8-38. Commands of Report Preview toolbar, continued

Command	Description
	Zooms out the display.
Zoom	Select one of the listed zoom levels.
	Go to first page.
	Go to previous page.
	Go to next page.
	Go to last page.

Preview Area

In the preview area, one page of the current Report is displayed at the currently selected zoom level. You can navigate through the Report with the page command buttons or by rotating the mouse wheel.

9

Method Parameters

The Method Parameters within a LabBook are dependent on the evaluation method assigned to the LabBook (see "Evaluation Methods" on page 9-2). For every application an appropriate LabBook can be created.

Contents

Evaluation Methods

Qtegra ISDS Software offers a range of **Evaluation** methods (see Figure 9-1) to be selected when creating a LabBook to accommodate any type of analysis required.

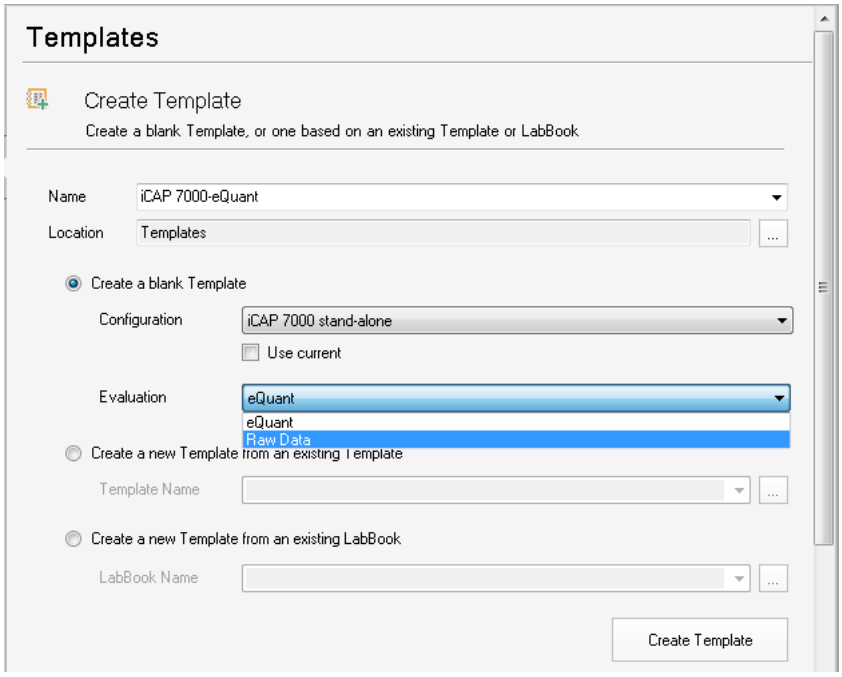


Figure 9-1. Evaluation types drop-down menu

Tip Any values entered that are not within the given range are marked with an ❗.

The main applications for the evaluations are summarized in Table 9-1.

Table 9-1. Evaluation methods

Evaluation	Description
eQuant	Uses external element concentrations to quantify element concentrations in an unknown sample. For the analysis of unknown samples with matching standards, calibration graphs can be acquired and used for the fully quantitative analysis of unknown samples.
Raw Data	Displays the acquired raw intensities, which are then used by the different evaluations.

Method Parameters Settings

In the Method Parameters section, you define all measurement settings for your analytes. The availability of each parameter is controlled by the type of evaluation defined for the Template.

All Method Parameters and the evaluation method for which they are available are listed in Table 9-2.

Table 9-2. Method Parameters of Qtegra

Method Parameter	Evaluation
Analytes	eQuant, Raw Data
Measure Modes	eQuant, Raw Data
Acquisition parameters	eQuant, Raw Data
Monitor Analytes / Intelligent Uptake and Rinse	eQuant, Raw Data
Inter-Element Correction	eQuant, Raw Data
Standards	eQuant
Quantification	eQuant
Ratios	eQuant
Quality Control	eQuant (after activating “Use QC” in the Quantification view)

Analytes

For all Template types, the analytes to be acquired during the measurement are selected in the Method Parameters view **Analytes**.

Analytes can be selected from the periodic table display in the **Elements** page, see Figure 9-2.

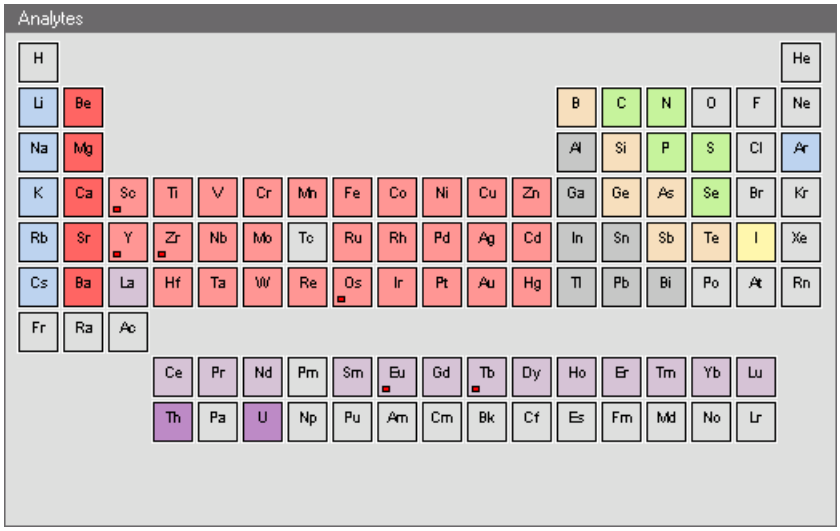


Figure 9-2. Analytes

See "Color Scheme of the Periodic Table" on page 14-62 for details on the periodic table.

Default element properties defined in the database are automatically selected for wavelength, relative intensity, state, and possible interferences of the selected element . These element properties can be redefined by the Administrator in "Acquisition Parameters" on page 9-14.

In the **Analyte Library**, see Figure 9-3, lines can be selected from a tabulated list where the availability for analysis or choice to use as default can be defined. Lines can also be deleted or new lines can be added.

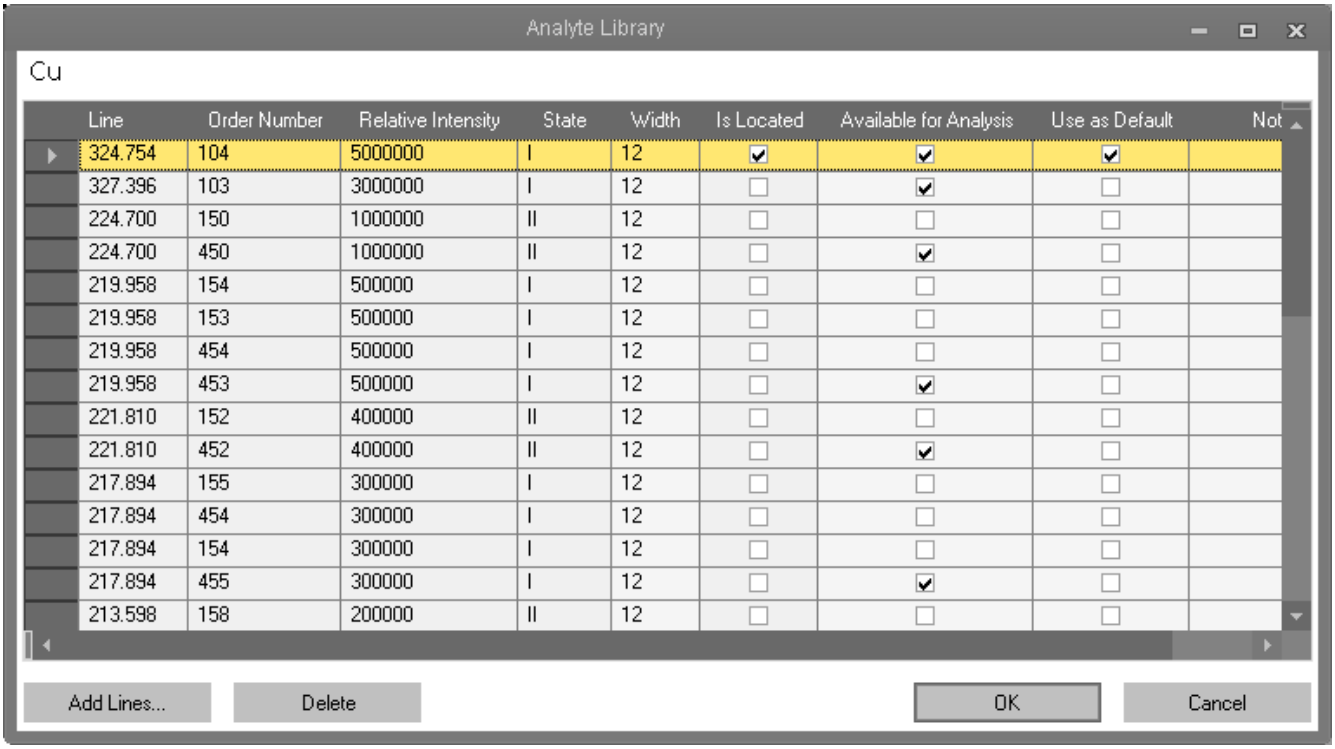


Figure 9-3. Analyte Library

For some elements, several analytical wavelengths are displayed in descending order of relative intensity. Usually, one of the wavelengths is more sensitive, and performs better (improved precision and detection limits) than the others for particular applications.

❖ **To open the Analytes view of a LabBook**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook.
2. Expand Method Parameters and click **Analytes** to open the **Analytes** view of the LabBook.

❖ **To select lines for analytes intensity**

1. Open the **Analytes** view of the Template.
2. Right-click an element in the periodic table.

The details of the element are displayed with symbol, wavelength, relative intensity, state and known interferences as stored in the element database, see Figure 9-4.

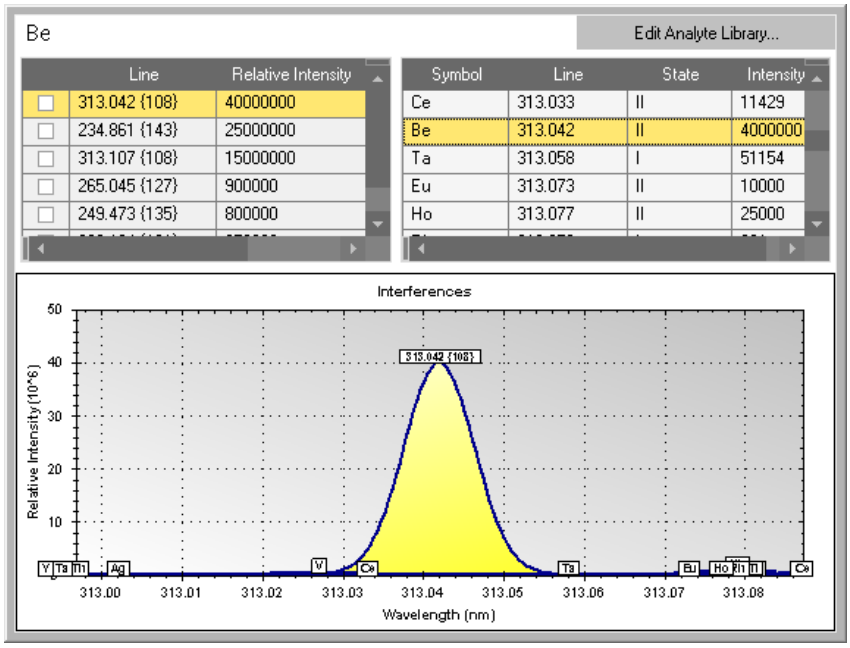


Figure 9-4. Details and interferences of an element

The wavelength of the analyte is displayed in the yellow graph.

3. Select a check box for a **Line** on the left to show the interferences of the selected line for the analyte, see Figure 9-5.

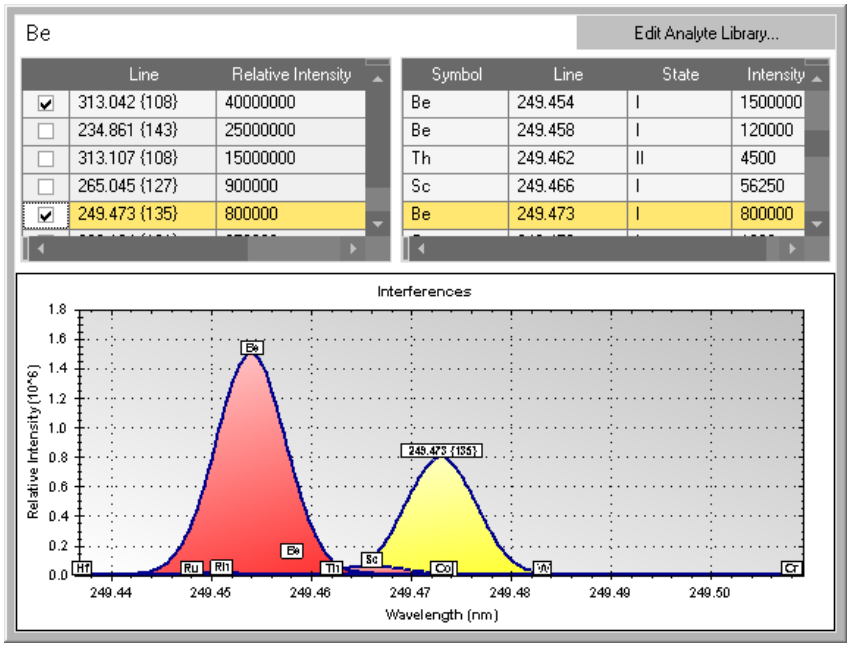


Figure 9-5. Selected interferences of an element

The wavelength of the interference is displayed in the red graph.

4. Click Edit Analyte Library... .
The **Analyte Library** for this element is displayed, see Figure 9-6.

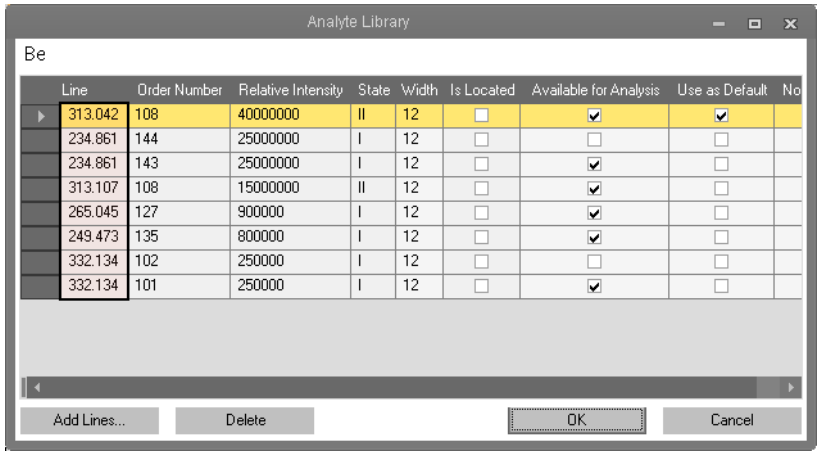


Figure 9-6. Editing Analyte Library

5. Select the **Available for Analysis** and **Use as Default** check boxes as appropriate.

6. Click **OK**.
The changes are applied to the data base.

❖ **To add a line to the analyte library**

1. Open the **Analytes** view of the Template.

2. Right-click an element in the periodic table.

The details of the element are displayed with symbol, wavelength, relative intensity, state and known interferences as stored in the element database, see Figure 9-7.

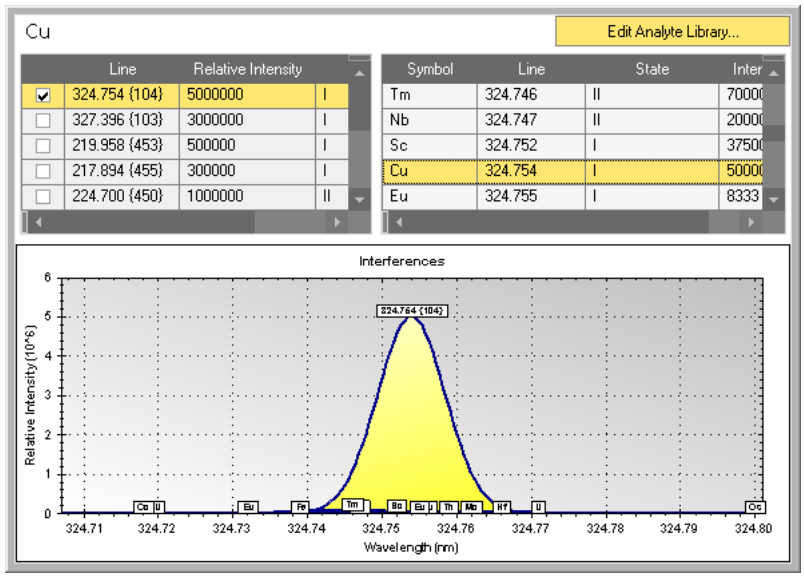


Figure 9-7. Details of an element

3. Click Edit Analyte Library... .

The **Analyte Library** for this element is displayed, see Figure 9-8.

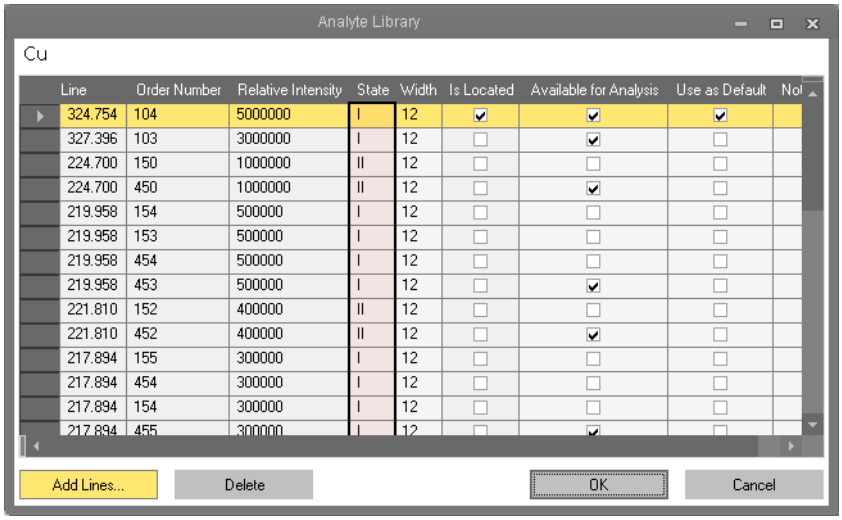


Figure 9-8. Editing Analyte Library

4. Click Add Lines... .
Here you can also delete a line.

The **Extend Analyte Library** dialog for this element is displayed, see Figure 9-9.

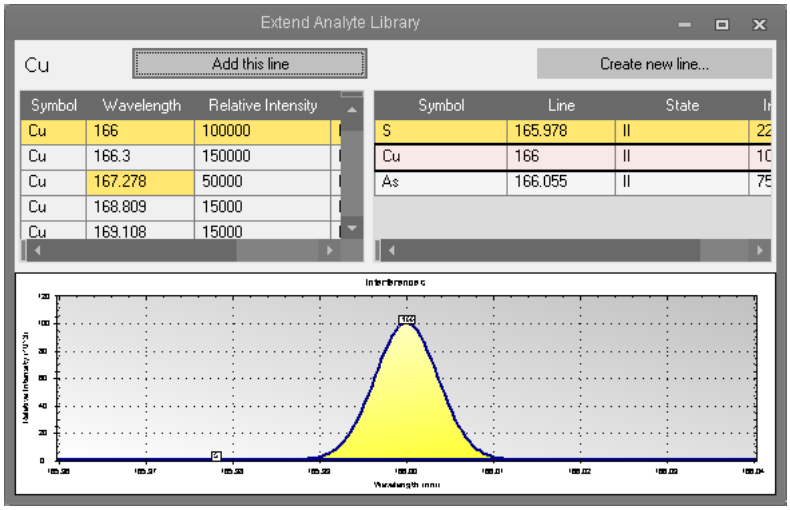


Figure 9-9. Extend Analyte Library

5. Select a line from the table to be added.

6. Click Add this line .
The **Analyte Library** dialog opens.

❖ **To create a new line in the analyte library**

1. Open the **Analytes** view of the Template.

2. Right-click an element in the periodic table.

   The details of the element are displayed (see Figure 9-10) with symbol, wavelength, relative intensity, state and known interferences as stored in the element database.

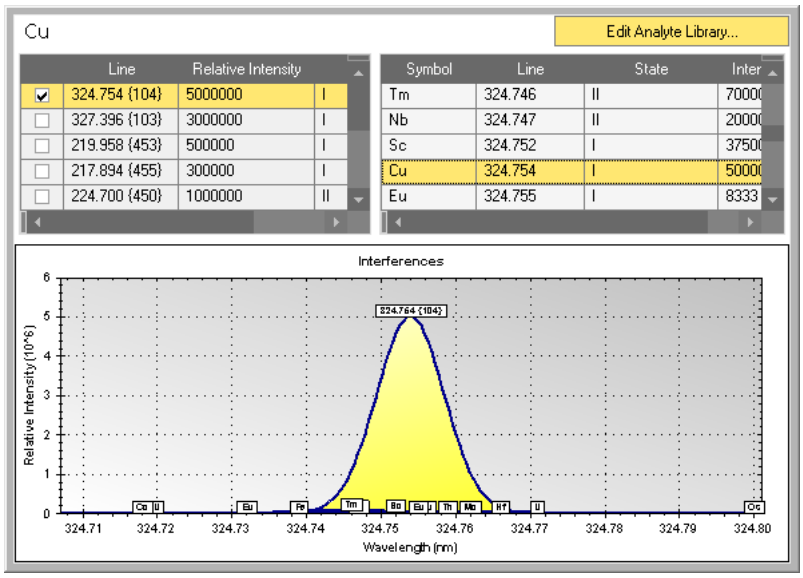


Figure 9-10. Details of an element

3. Click Edit Analyte Library... .

   The **Analyte Library** for this element is displayed, see Figure 9-11.

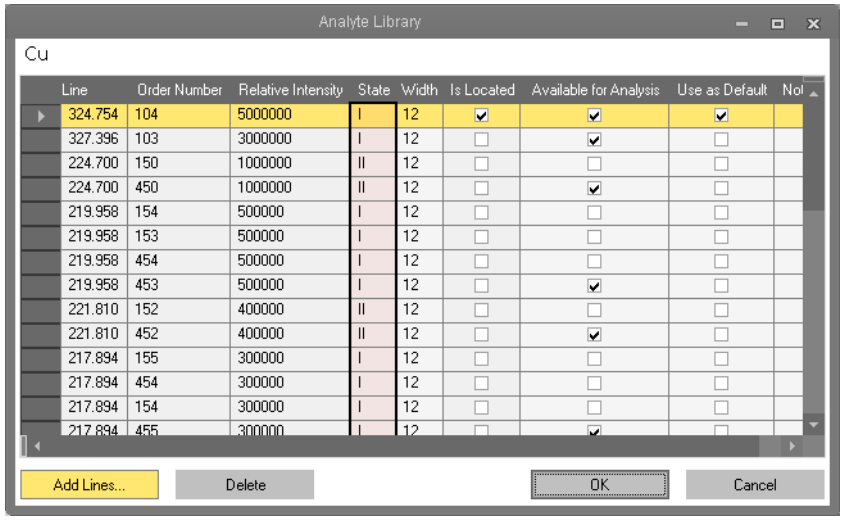


Figure 9-11. Editing the Analyte Library

4. Click Add Lines... .

The **Extend Analyte Library** dialog for this element is displayed, see Figure 9-12.

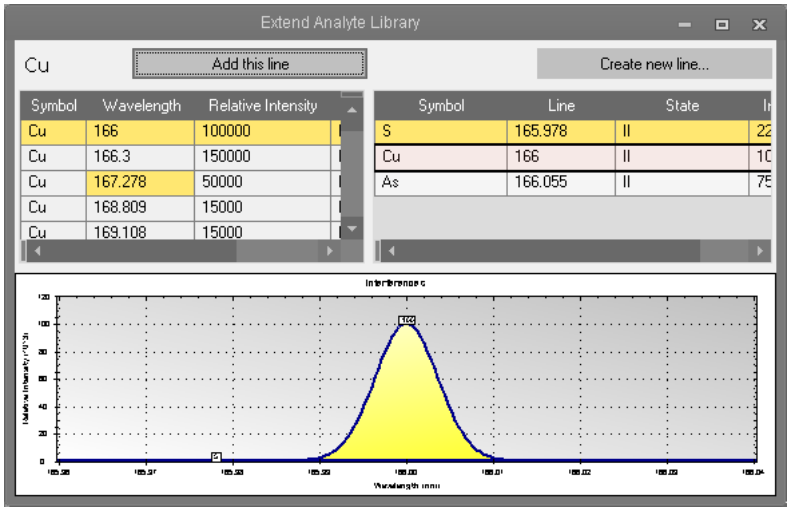


Figure 9-12. Extend Analyte Library

5. Click Create new line....

The **Create a Line** dialog opens, see Figure 9-13.

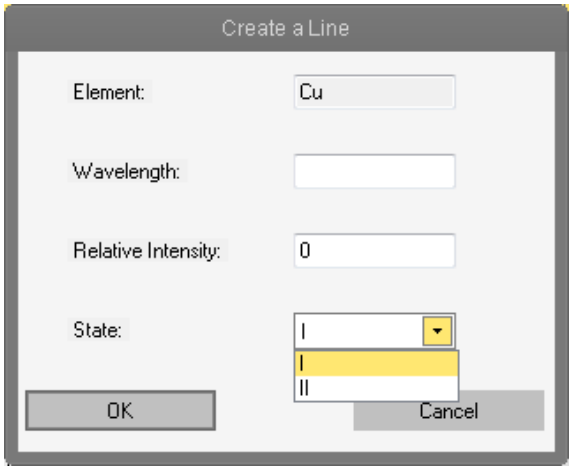


Figure 9-13. Create a Line dialog

6. Enter **Wavelength** and **Relative Intensity**.
7. Select a **State** from the drop-down list.
8. Click **OK**.
   The **Analyte Library** dialog opens.
9. Click **OK**.
10. Click **Save** to save the changes.

❖ **To delete a line from the analyte library**

1. Open the **Analytes** view of the Template.

2. Right-click an element in the periodic table and click Edit Analyte Library... .

   The **Analyte Library** for this element is displayed, see Figure 9-14.

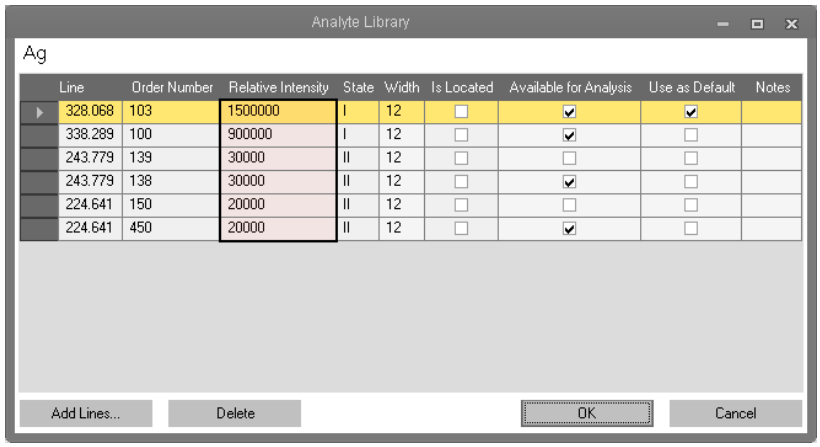


Figure 9-14. Analyte Library example

3. Select the line you wish to delete and click Delete , see Figure 9-15.

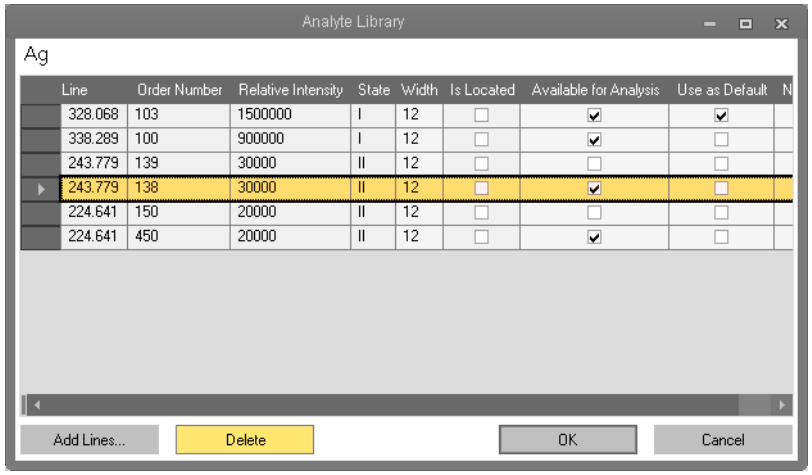


Figure 9-15. Deleting a line from the Analyte Library

   The line is deleted from the Analyte Library for this element in the global database.

4. Click **OK** to close the **Analyte Library** dialog.

5. Click **Save** to save the changes to the global database.

Measure Modes

In the Method Parameter view **Measure Modes** of Qtegra, the analysis conditions such as radial/axial view, exposure time, RF (radio frequency) power and nebulizer gas flow either in the **UV** range or in the **Visible** range, and the flows for the coolant gas, auxiliary gas and additional gas, are defined.

These conditions can be saved as different **Modes** of analysis that can then be chosen in the Acquisition Parameters section for each of the selected analytes, see Figure 9-16.

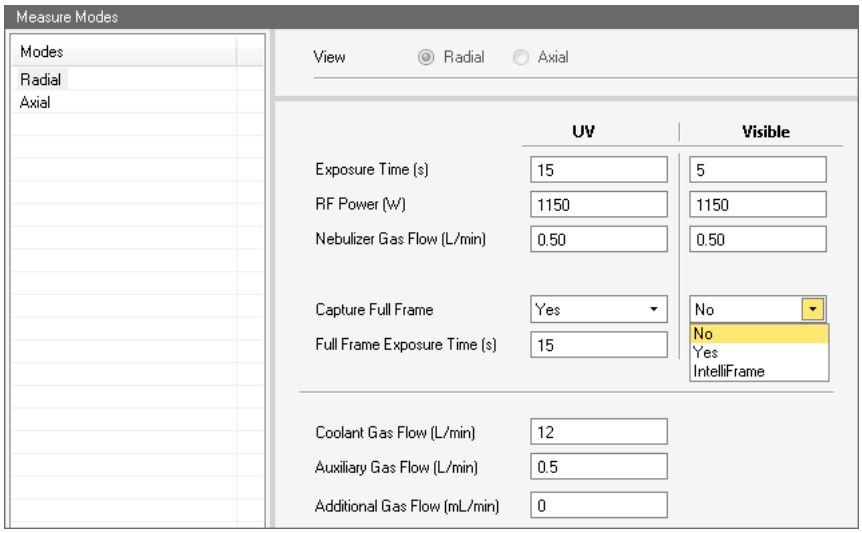


Figure 9-16. Measure Modes

The parameters of the **Measure Modes** view are explained in Table 9-3.

Table 9-3. Measure Modes parameters

Parameter	Description
Exposure Time (s)	The longest period in seconds that the signal will be collected prior to processing. Depending on instrument configuration and analytical wavelengths selected in the method, up to four separate maximum integration periods may be required. **UV** range: *1* to *120* and **Visible** range: *1* to *120*. For typical applications, a reasonable starting point is *15* seconds for the low wavelength range, and *5* seconds for the high wavelength range. **Tip** **UV/Visible** range selection is useful for optimizing the method as you can set the high wavelengths, for example, alkali metals, to have a lower RF power and higher nebulizer flow, and leave the optimal parameters for the lower wavelengths (UV) in the same method.
RF Power (W)	The RF power value can be adjusted from *750* to *1350* W (or to *1600* W, depending on the model).

Table 9-3. Measure Modes parameters, continued

Parameter	Description
	Tip All Duo instruments are software restricted to *1350* W RF as the highest value. The radial iCAP 7400 instrument is restricted to *1600* W RF as its highest value. The iCAP 7200 instrument uses a single fixed RF value of *1150* W.
Nebulizer Gas Flow (L/min)	The nebulizer gas flow value can be adjusted from *0* to *1.5* L/min.
	Tip This option is only displayed for iCAP 7400 and 7600 instruments.
Capture Full Frame	A Full Frame image includes all lines that are emitted by the sample within the selected wavelength range. Two Full Frame images are required to fully describe the sample. **Yes** activates full frame acquisition and **Full Frame Exposure Time** can be entered. **No** deactivates **Full Frame Exposure Time** and full frame acquisition is not performed. With **IntelliFrame** the system collects a series of images at various times (0.03 s, 0.3 s, 3.0 s, 10 s and 30 s) and then determines the appropriate period of time to collect intensity data for each line, to avoid saturation. **Full Frame Exposure Time** is deactivated.
Full Frame Exposure Time (s)	Exposure time of full frame acquisition. Activated when **Captured Full Frame** is set to *Yes*.
Coolant Gas Flow (L/min)	The coolant gas flow is fixed at *12* L/min for all iCAP 7200 and 7400 instruments, and is only adjustable for iCAP 7600 instruments from *10* to *20* L/min.
Auxiliary Gas Flow (L/min)	The auxiliary gas flow can be adjusted from *0* to *2* L/min (iCAP 7600 instrument), or *0* to *1.5* L/min (iCAP 7200 and 7400).
Additional Gas Flow (L/min)	This option only appears where an additional gas Mass Flow Controller is fitted. It is an accessory that is exclusive to the iCAP 7600 instrument and can be used, for example, to remove Carbon from organics applications. The additional gas flow can be adjusted from *0* to *200* mL/min.

Measure Modes parameters are defined in order to optimize the analysis by the radial and/or axial configurations.

In the radial configuration, the plasma is viewed from the side. The radial plasma view offers less sensitivity than the axial view, however, it is preferable for analyzing difficult samples such as organics or very high dissolved solid matrices, as the plasma viewing position can be optimized to reduce background emissions.

In the axial configuration, the plasma is viewed end-on (along the length of the plasma). The axially viewed plasma configuration offers greater sensitivity. It is used for applications requiring the lowest detection

limits, than radial configuration, but has higher susceptibility to matrix interferences, as the entire plasma is viewed, increasing the quantity of light observed from both analyte and background emissions.

❖ **To open the Measure Modes view**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook.
2. Expand Method Parameters and click **Measure Modes** to open the **Measure Modes** view.

❖ **To define Measure Modes for the analysis**

1. Open the **Method Parameters > Measure Modes** view.
2. Select the **Radial** or **Axial View**.
3. Define the **Exposure Time (s)**, **RF Power (W)** and **Neb Gas Flow (L/min)** for **UV Range** and in **VIS Range**.
4. Enter the flows in L/min for **Coolant**, **Auxiliary** and **Additional Gas Flow**.

Acquisition Parameters

For all LabBook types, the list of analytes selected for the LabBook is displayed in the **Acquisition Parameters** view of the Qtegra tool. Acquisition details such as analysis mode, pump details and laser triggering settings as well as measure modes, left and right background, start and stop time, and intensity factor can be defined.

The **Acquisition Parameters** view is shown in Figure 9-17.

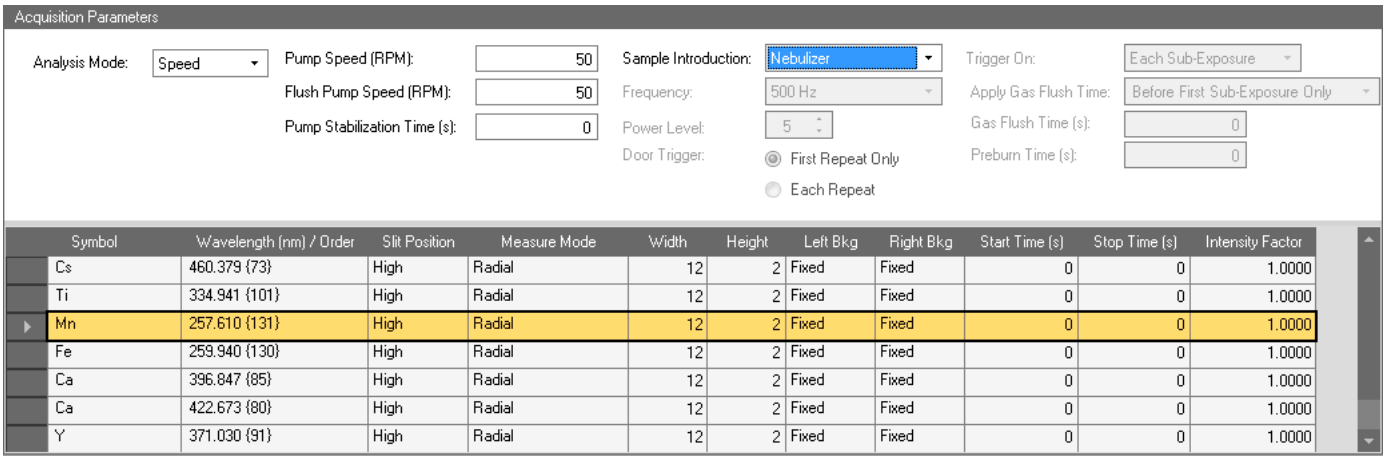


Figure 9-17. Acquisition Parameters view

The **Analysis Mode** parameters are explained in Table 9-4.

Table 9-4. Analysis Mode parameters

Parameter	Description
Analysis Mode	**Normal** mode is the traditional analysis mode which is per replicate. **Speed** mode is a unique mode of analysis which analyzes all radial/high wavelength elements for all replicates, then all axial/low wavelength elements for all replicates. Speed mode of analysis saves time as it removes the need for settle times when switching from one plasma view to the other. **Sprint** mode operates in a similar manner to Speed. This mode removes any overhead time associated with the pre-exposure ensuring minimum sample analysis time. The mode is ideally suited for trend analysis and where sample numbers are high. **Tip** These options are only available for iCAP 7600 instruments. The iCAP 7200 instrument uses only the *Normal* mode and the iCAP 7400 instrument uses the *Normal* and the *Speed* modes for analysis.
Pump Speed (RPM)	Speed of pump in revolution per minute (RPM). Pump rate for analysis. The range is *0* to *125* rpm.
Flush Pump Speed (RPM)	Speed of flush pump in revolution per minute (RPM). Pump Speed for uptake. The range is *0* to *125* rpm. Setting this value higher than the Pump Speed will enable faster sample throughput.

Table 9-4. Analysis Mode parameters, continued

Parameter	Description
Pump Stabilization Time (s)	Pump stabilization time in seconds. This is the time taken to change from the Flush Pump Speed to the Pump Speed. The range is *0* to *1000* seconds. If different values are set for the Flush Pump Speed and the Pump Speed, then it is recommended to use at least a 5-second stabilization delay as this allows the pump to slow down incrementally and avoids wearing the pump tubing out unnecessarily quickly.
Sample Introduction	**Nebulizer** uses the nebulizer settings. With **SSEA**, the values for **Frequency, Power Level, Gas Flush Time (s)**, and **Preburn Time (s)** can be entered, and the **Door Trigger** can be set to **First Repeat Only** or **Each Repeat**. For **Laser**, you can trigger the laser for each sub-exposure or each sample. If **Trigger On** is set to **Each Sample, Apply Gas Flush Time** is set to **Before Each Sample**. If **Trigger On** is set to **Each Sub-Exposure, Apply Gas Flush Time** can be selected from the drop-down list as **Before Each Sub-Exposure** or **Before First Sub-Exposure Only**. The **Gas Flush Time (s)** can be defined for each.

The **Acquisition Parameters** are explained in Table 9-5.

Table 9-5. Acquisition parameters

Column	Description
Symbol	Symbol for the element.
Wavelength (nm)/Order	Wavelength for the element as defined in the Analyte Library.
Slit Position	Displays the position of the slit. It is automatically set (*High* or *Low*) according to the wavelength chosen for the element.
Measure Mode	Measure Mode for the element. The drop-down list shows all Measure Modes defined for this Template (LabBook). The plasma may be viewed axially for applications requiring the lowest detection limits or radially to minimize matrix effects.

Table 9-5. Acquisition parameters, continued

Column	Description
Width	The width of the subarray for each wavelength/element can be defined individually. Default value is *13*.
Height	Default values are *5* for UV and *2* for Visible.
Left Bkg	Left background correction. **None** Turns off the background correction for that side. **Fixed** is the default option. Allows you to define where the background should be placed. **Auto** Allows the software to choose the lowest background point in the subarray. The Qtegra ISDS Software will only select background correction points which are plus or minus one pixel of the positions that the user set.
Right Bkg	Right background correction. **None** Turns off the background correction for that side. **Fixed** is the default option. Allows you to define where the background should be placed. **Auto** Allows the software to choose the lowest background point in the subarray. The Qtegra ISDS Software will only select background correction points which are plus or minus one pixel of the positions that the user set.
Start Time (s)	Displays the start time of the measurement in seconds.
Stop Time (s)	Displays the stop time of the measurement in seconds.
Intensity Factor	Multiplies the signal counts by the entered value to achieve a scale expansion. The default is *1* or no scale expansion. The valid range for the intensity factor is *0.0001* to *1000*.
	For this method parameter, the toolbar of the Template (LabBook) additionally offers the **AutoPeak** function. During Auto Peak Adjust, the peak locations for the method lines associated with each high standards will be finely adjusted. The usual way to perform this routine is by aspirating the highest concentration calibration standard for the method. The CID (Charge Injection Device) will then fine tune the position of each method line onto the chip. This will then be used as the default position for this line until the next auto peak adjustment takes place. If the iCAP 7000 Plus Series ICP-OES has been switched off (by the main power supply) for a longer period of time, an auto peak adjustment should be carried out to optimize the peak location on the CID camera. A standard that contains all of the lines of interest is used and the system automatically makes the appropriate fine adjustment.

If the AutoPeak routine is unsuccessful, there are two general scenarios to this. Either the solution is too weak for the line analyzed, or too strong. Simply aspirate a more suitable solution.

Tip If an argon humidifier is configured with the sample introduction, you may need to allow a delay after failures before re-initializing the AutoPeak routine.

Another additional function on the toolbar is **Time Study**. Time Study performs a basic transient signal analysis and is a helpful tool during method development. For example, it can be used to determine the correct uptake and wash time for the analysis.

❖ **To open the Acquisition Parameters view**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook or Template.

2. Expand Method Parameters and click **Acquisition parameters** to open the **Acquisition Parameters** view.

❖ **To duplicate analyte rows**

1. Open the **Method Parameters > Acquisition Parameters** view.
2. Click the gray field in front of the row or rows to select the analytes you wish to duplicate.
   This way, analytes in one sample can be defined to be measured with different settings.
3. Right-click the selected rows.
   A shortcut menu opens, see Figure 9-18.

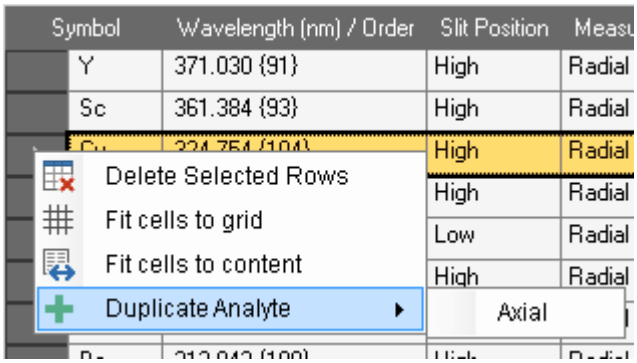


Figure 9-18. Duplicate rows of Acquisition Parameters

4. Select **Duplicate Analyte > Axial** (or **Radial** as offered) from the shortcut menu.
   The selected line is duplicated.

Tip To delete a row, select the row, then press **<Delete>** and confirm the message dialog.

❖ **To define the Acquisition parameters**

1. Open the **Method Parameters > Acquisition Parameters** view. The **Symbol** column lists all analytes selected for this LabBook.

   The **Wavelength (nm) /Order** for each analyte is shown as defined in "Analytes" on page 9-3.

   The **Slit Position** is automatically set.

2. Select a **Measure Mode** from the drop-down menu.
3. Define the **Width** and **Height** of the subarray for the wavelength.
4. For each analyte, select the background identification mode in **Left Bkg** and **Right Bkg** from the drop-down list.
5. Enter **Start Time** and **Stop Time** where applicable and define the **Intensity Factor**.
6. Select the **Analysis Mode** from the drop-down list.
7. Define the **Pump Speed**, **Flash Pump Speed** and **Pump Stabilization Time**.
8. Select the **Sample Introduction** system and define the corresponding parameters (see Table 9-4).
9. Click **Save** in the toolbar to save the changes to your LabBook.

❖ **To adjust AutoPeak**

1. Open the **Method Parameters > Acquisition Parameters** view.
2. On the toolbar, click **AutoPeak**.
   The **Select analytes** dialog opens, see Figure 9-19.

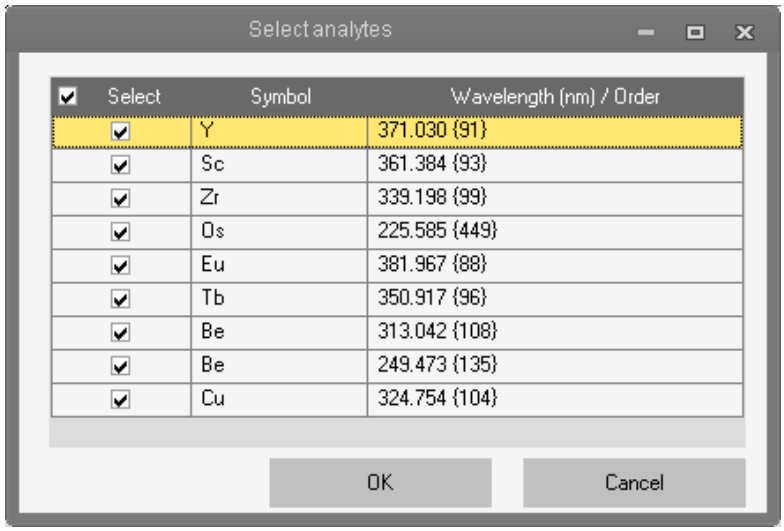


Figure 9-19. Select AutoPeak analytes

3. Select the analytes you wish to perform AutoPeak for.
4. Click **OK**.
   The **Waiting for user response** dialog opens, see Figure 9-20.

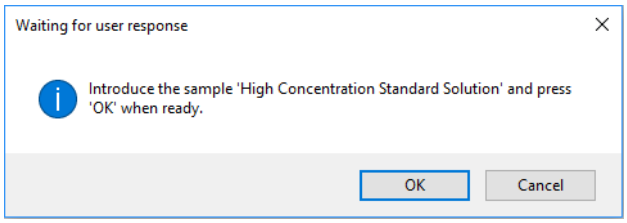


Figure 9-20. AutoPeak user response dialog

5. Start aspirating the high concentration standard solution for some seconds.
6. Click **OK**.
7. Aspirate until the test is finished.
   The progress and result of the test is shown in the message bar at the bottom of Qtegra 

.

❖ **To start Time Study wizard**

1. Open the **Method Parameters > Acquisition Parameters** view.
2. On the toolbar, click **Time Study**.
   The **Time Study Wizard** opens, see Figure 9-21.

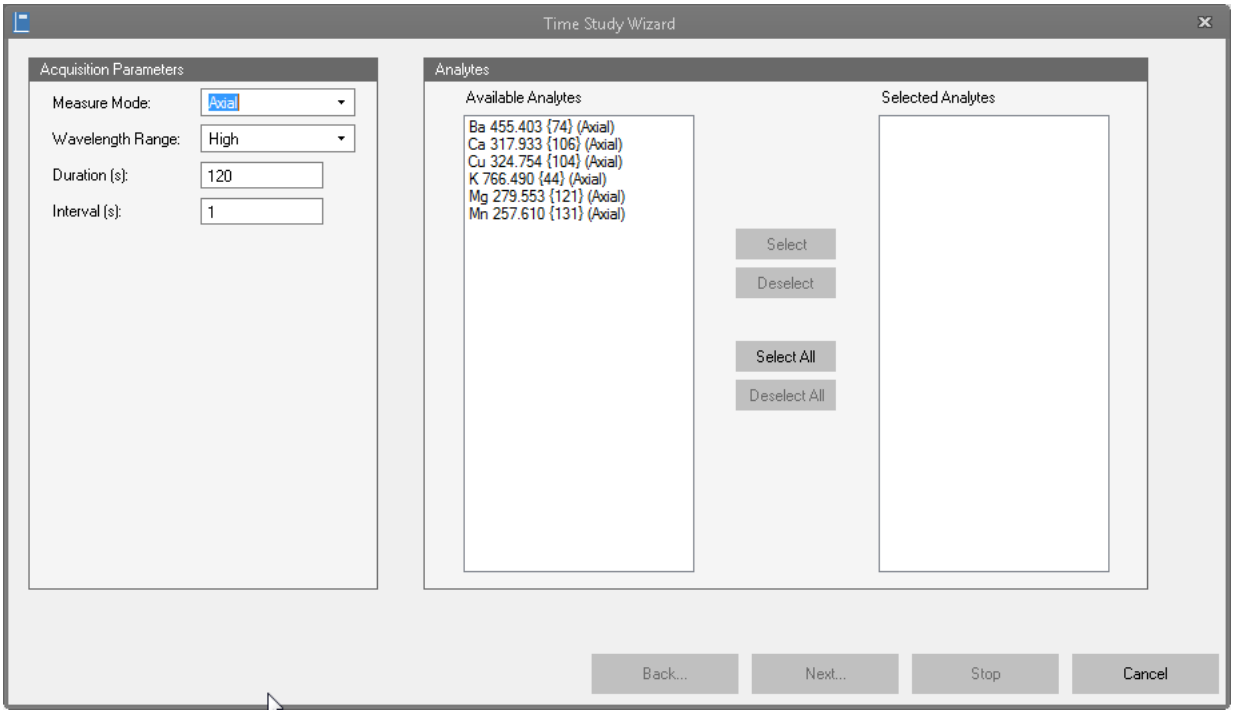


Figure 9-21. Time Study Wizard

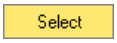
The **Time Study Wizard** includes settings for **Acquisition Parameters** on the left and settings for **Analytes** on the right.

3. Select **Radial** or **Axial** from the drop-down list for **Measure Mode** on the left.

4. Select **High** or **Low** from the drop-down list for **Wavelength Range**.

5. Enter a value for **Duration (s)**.

6. Enter a value for **Interval (s)**.



7. In the **Available Analytes** list, select the elements to be analyzed and click **Select**.
The elements are moved to the **Selected Analytes** list.

Tip Press **<Ctrl>** to select multiple analytes.

8. Click **Next**.
The **Time Study Wizard** changes to shows a graphical display with a progress bar during exposure, see Figure 9-22.

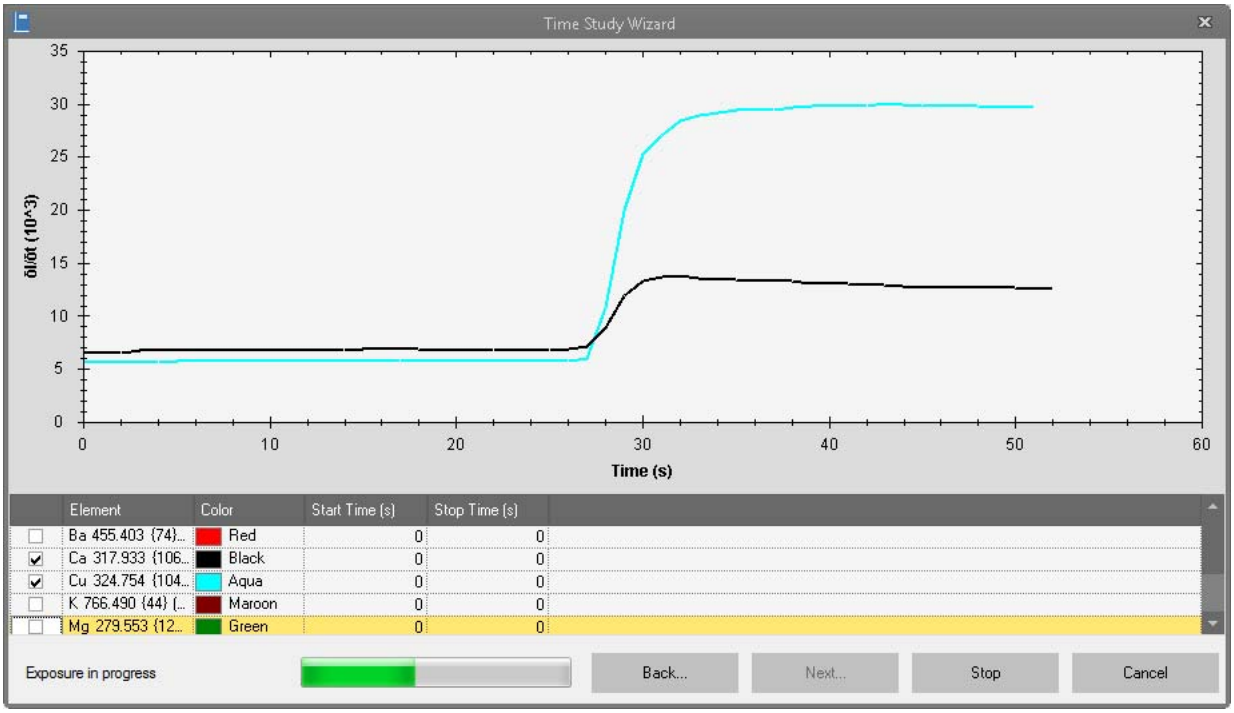


Figure 9-22. Time Study Wizard with graphical display and progress bar of exposure

After exposure you can view the results, see Figure 9-23.

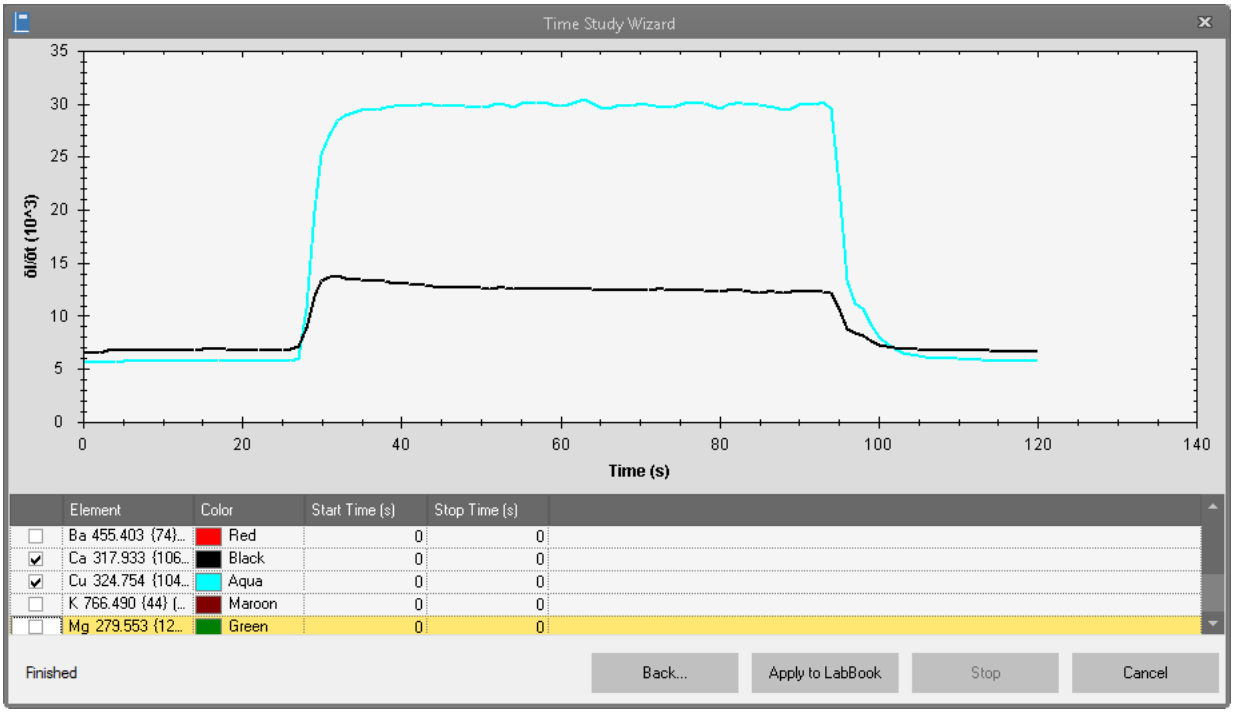


Figure 9-23. Time Study Wizard exposure finished

9. Right-click the graph to open a shortcut menu, see Figure 9-24.

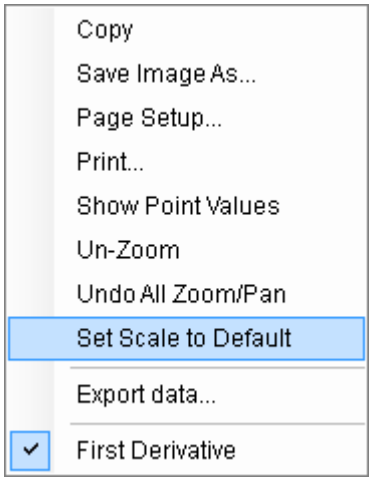


Figure 9-24. Time Study Wizard shortcut menu

The items of the shortcut menu allow you to change the zoom and page setup, copy, print or save the image, show point values or export the data. You can also click and drag to zoom into the graph.

10. Click **Finished** to close the Time Study Wizard.

Intelligent Uptake and Rinse

For all LabBook types, the **Intelligent Uptake and Rinse** view of Qtegra is available.

In the **Intelligent Uptake and Rinse** view, the minimum and maximum delays are defined in the upper part of the view. Parameters for each analyte are set in the table in the lower part, see Figure 9-25.

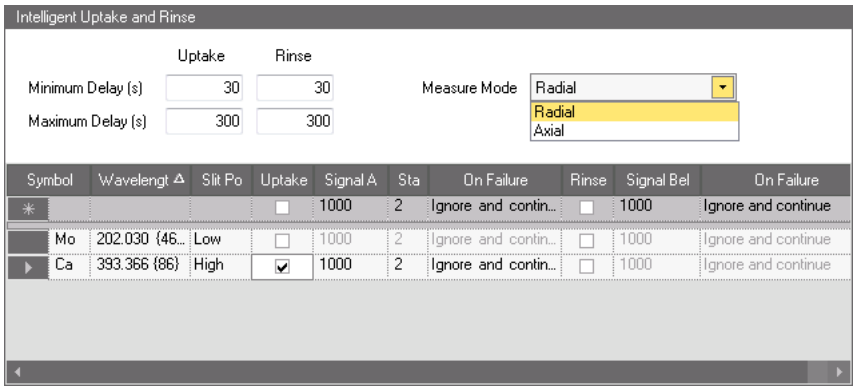


Figure 9-25. Intelligent Uptake and Rinse

The **Intelligent Uptake and Rinse** section can be used to trigger the data acquisition of the instrument to decrease the overall measurement time and increase reproducibility. The **Uptake** starts when the signal for the specified value for the analyte or analytes is stable. If this value falls below the specified value after the measurement has been completed, the **Wash** (Rinse) procedure starts.

❖ **To open the Intelligent Uptake and Rinse view of a LabBook**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook as described in "Opening a Template" on page 4-37.
2. Expand the Method Parameters and click **Intelligent Uptake and Rinse** to open the **Intelligent Uptake and Rinse** view.

❖ **To define the Intelligent Uptake and Rinse settings**

1. Open the **Intelligent Uptake and Rinse** view.
2. Enter the **Uptake** and **Rinse** values for **Minimum Delay (s)** and **Maximum Delay (s)**.
   The default values *30* and *300* are the recommended ones when using standard tubes.
3. Select a **Measure Mode** *Radial* or *Axial* from the drop-down list.
4. In the table, click in the first cell in the **Symbol** column, and enter an element abbreviation.
   The corresponding (default) **Wavelength** is displayed as soon as you select another cell.

5. Press **<Enter>**.
   The new line is added to the table.

6. Select **Uptake** to activate **Signal Above**, **Stability** and **On Failure** for this line and element.
   Define the values and select the action to be performed when failing from the drop-down list.

7. Select **Rinse** to activate **Signal Below** and **On Failure** for this line and element.
   Define the value and select the action to be performed when failing from the drop-down list.

8. Define the settings for each sample line in the table.

Inter-Element Correction

In the **Inter-Element Correction** view in Qtegra, corrections for direct spectral interferences can be defined.

❖ **To open the Inter-Element Correction view**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook as described in "Opening a LabBook" on page 4-23.

2. Expand Method Parameters and click **Inter-Element Correction** to open the **Inter-Element Correction** view.

❖ **To define inter-element corrections**

1. Open the **Inter-Element Correction** view.

2. Select **Enable** for the element you wish to define the correction for, see Figure 9-26.

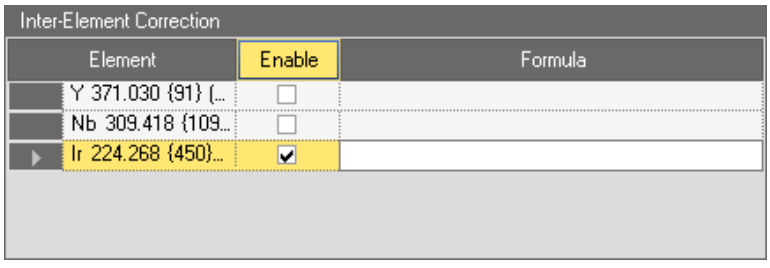


Figure 9-26. Select element for correction

3. In the **Formula** column, double-click the cell next to the selected element.
   A second table opens on the right, see Figure 9-27.

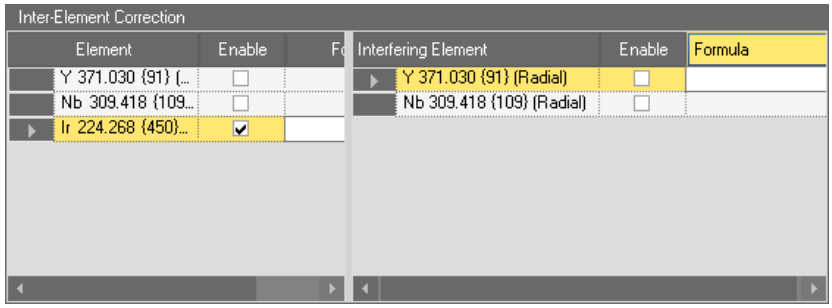


Figure 9-27. Enter formula for correction

4. Select **Enable** for the interfering element and enter the formula for the correction. Use a capital "X" to represent the interfering element. Use mathematical symbols, like * (multiply with), / (divide by), + (plus), or - (minus) for operational commands. Stop typing the formula with **<Enter>**. The correction formula is then shown in the left table.

5. Repeat step 4 for each element you wish to define a correction for.

Tip Inter-Element Corrections can also be defined in a measured LabBook, see "Intensities" on page 10-46.

Standards

For all LabBook types, the **Standards** view in the Qtegra tool allows you to define standards based on the selected evaluation.

Standards are materials containing a known concentration of an analyte. They provide a reference to determine unknown concentrations or to calibrate analytical instruments.

The accuracy of an analytical measurement is how close a result comes to the true value. Determining the accuracy of a measurement usually requires calibration of the analytical method with a known standard. This is often done with standards of several concentrations to make a calibration or working curve.

This section defines all information about the solutions used to calibrate the instrument. For aQuant and eQuant, additionally calibration types can be defined in the Quantification view.

Once a standard is created, the elements of the standard can be selected in the periodic table, see Figure 9-28.

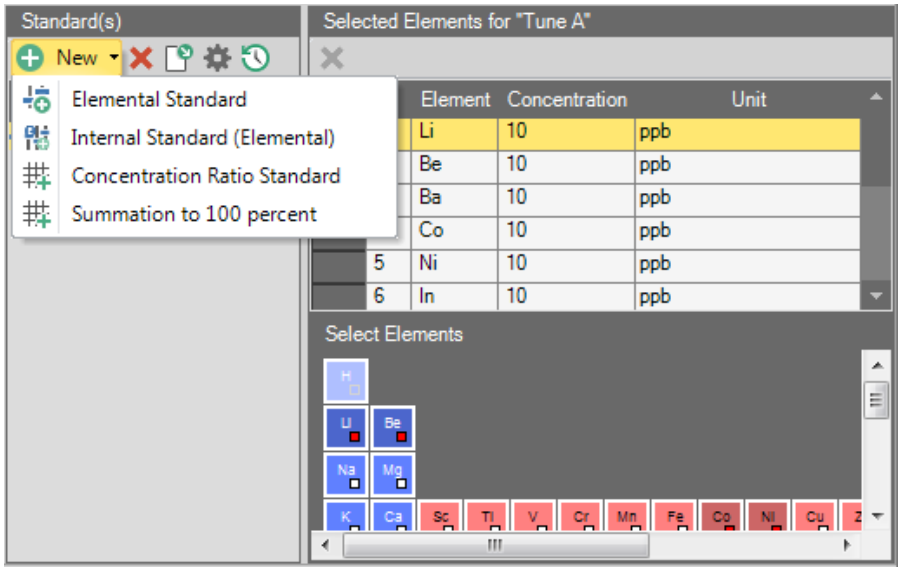


Figure 9-28. Standards view

The columns of the table above the periodic table define the properties of the elements, see Table 9-6.

Table 9-6. Specification of standard elements

Column	Description
No	Automatically assigned number in ascending order.
Element	Displays the symbol for the chemical element contained in this standard file.

Table 9-6. Specification of standard elements, continued

Column	Description
Concentration	Displays the concentration for the element in the standard file. By default, the concentration is set to *10*. This default can be changed and stored, see Table 9-7. Recommendation for quantification standards is to prepare standards at concentrations that cover the concentration range expected in the samples. Recommendation for Internal Standards is to use an internal standard analyte, which is not present in any of the samples. Then add it in equal concentration to all samples and standards or by spiking manually into all samples. The analytical lines referenced to an Internal Standard report a corrected concentration value based on the ratio of analyte to Internal Standard intensities.
Unit	Displays the concentration unit for the element in the standard file. By default, the unit is set to *ppm*. This default can be changed and stored, see Table 9-7.

The commands of the **Standards** view of a LabBook are summarized in Table 9-7.

Table 9-7. Commands of the Standards view

Command	Description
	To create a new list of standards or of Internal Standards (for eQuant), see "Creating New Standards" on page 9-30.
	To delete the selected standards list. In the list of Standard(s), select the standards you want to delete. Click this button, or right-click and select **Delete** from the shortcut menu to delete the selected standards. Confirm the message dialog.

Table 9-7. Commands of the Standards view, continued

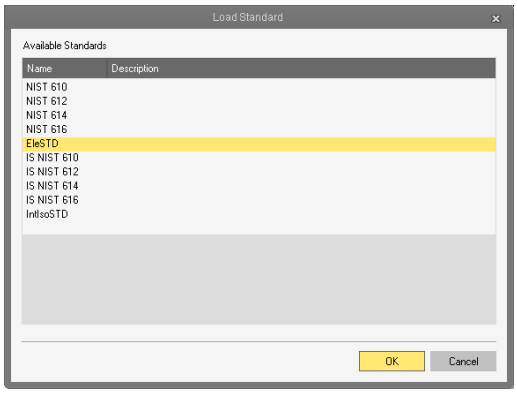
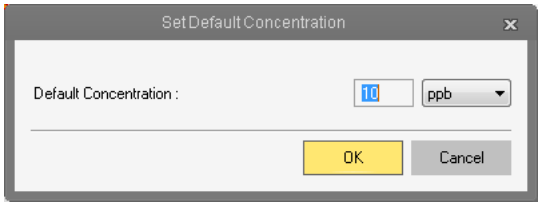
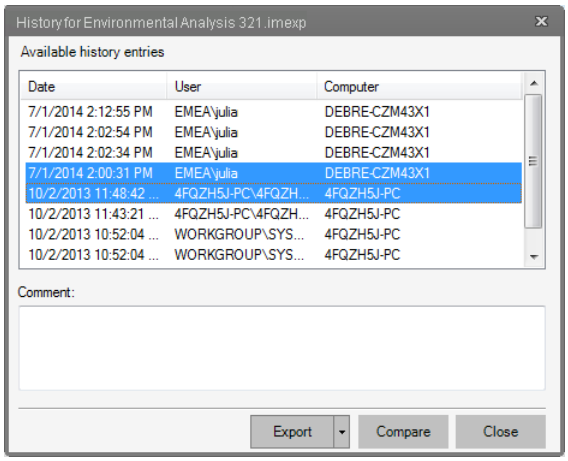
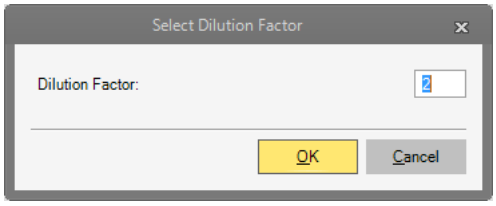
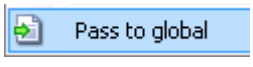
Command	Description
	To load standards from the global standards database. The **Load Standard** dialog opens:  Select a standard from the list and click **OK** -or- Double-click to load the standards into the **Standards** view.
	To edit the default concentration and unit. The **Set Default Concentration** dialog opens:  In this example, the Default Concentration of the analytes in the solutions is set to *10 ppb* and will therefore be used for every new analyte added to the table.

Table 9-7. Commands of the Standards view, continued

Command	Description
	To view, compare and export the history of a LabBook. The **History** dialog for this LabBook opens.  To compare the history entries, press **<Ctrl>** or **<Shift>** and select the range of history entries you wish to compare.

The shortcut menu of the Standard(s) list provides two further commands, shown in Table 9-8:

Table 9-8. Shortcut menu commands of the Standards view

Command	Description
	To **copy** the selected standards list. The **Select Dilution Factor** dialog opens:  Type the dilution factor the copy shall use. Click **OK** to create a standards list getting the name of the source including the suffix "_Copy". The concentration of all elements is automatically recalculated on the dilution factor you entered.
	To save the selected standards list to the global database. In the list of Standard(s), select the standards you want to pass to the global database. Right-click and select **Pass to global** from the shortcut menu to save the selected standards to the global database.

The accuracy of an analytical measurement is how close a result comes to the true value. Determining the accuracy of a measurement usually requires calibration of the analytical method with a known standard. Internal Standards are materials containing a known set of analytes. Internal Standards are used to correct for instrumental drifts in sensitivity and sample specific signal suppression or enhancement. Internal standardization can help compensate for sample viscosity effects and plasma loading to improve the accuracy and precision of analytical results in Inductively Coupled Plasma - Optical Emission Spectrometry (ICP-OES).

Quantification standards are materials containing a known concentration of an analyte. They provide a reference to determine unknown concentrations or to calibrate analytical instruments.

The quantification standard defined here can be selected and used in the "Sample Definition for a Template" on page 5-5. When defining the calibration standards in that section, dilution factors can be applied to the standard.

Internal Standards used for quantification are also created here. Their definition as Internal Standards is done in the **Quantification** view, see "Quantification" on page 9-33.

❖ **To open the Standards view**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook.
2.  Expand Method Parameters and click **Standards** to open the Standards view.

Creating New Standards

Standards created in the **Standards** view of a LabBook or Template in the Qtegra tool are created for the current LabBook but can be saved to the global database.

Tip Global database standards are created in the Configurator applet, see "Standards" on page 3-31.

❖ **To create a new standard**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook.
2. Open the **Method Parameters > Standards** view.
3.  Before entering the elements of the standards, you may define the default concentration. On the toolbar, click **Set default concentration** to open a dialog, where you can select the mainly used concentration and unit, for example, *ppb* or *µg/L*.

4. Expand 

to select the standards type (*Elemental Standard, Internal Standard, Concentration Ratio Standard, Summation to 100 percent*) from the drop-down menu.

5. In the **Add New Standard** dialog, type the **Standard Name** and optionally a **Standard Description**.
For Elemental Standards and Isotope Dilution Standards, tick **Create standard using analyte list** if you want to use the standards as defined.

6. Select the analytes. The way of selection depends on the selected standard.

    a. **Elemental standards** with a known concentration of an analyte provide a reference to determine unknown concentrations or to calibrate analytical instruments. For Elemental Standards, click the elements in the periodic table to add or remove analytes.

        i. Define the properties of the analyte as required.

    b. **Internal Standards (elemental)** are used to monitor any drift in signal sensitivity with time during a set of analyses. Corrections are made by comparing the sensitivity for the Internal Standards in each run of a sample with the sensitivity of the internal standard at a reference point at the start of the experiment. The results of this comparison are then used to correct all of the other analytes in the sample on a per-run basis. It is recommended to use at least one Internal Standard in any multi-element determination.

        i. Add the analyte to the table by clicking the element in the periodic table.

        ii. Define the properties of the analytes as required.

    c. For the **Concentration Ratio Standard** you define a base element. The base element is the main element in the mixture (for example, alloys). This element depends on the analysis to be made.

        i. Add the analyte to the table by clicking the element in the periodic table.
        The default line of the element is added to the table. Concentration ans Unit are added according to the default concentration.

        ii. To remove the analyte, click the respective element in the periodic table again.

        iii. In the table, right-click the element you wish to define as base element.
        A shortcut menu opens.

In this section, the exclamation mark ❗ indicates that the base element has not been selected yet.

iv. Select **Set as base element** from the shortcut menu.
The exclamation mark ❗ disappears.

v. Enter the **Concentration** for each element.

vi. Enter the **Residual Concentration [%]**, see Figure 9-29.

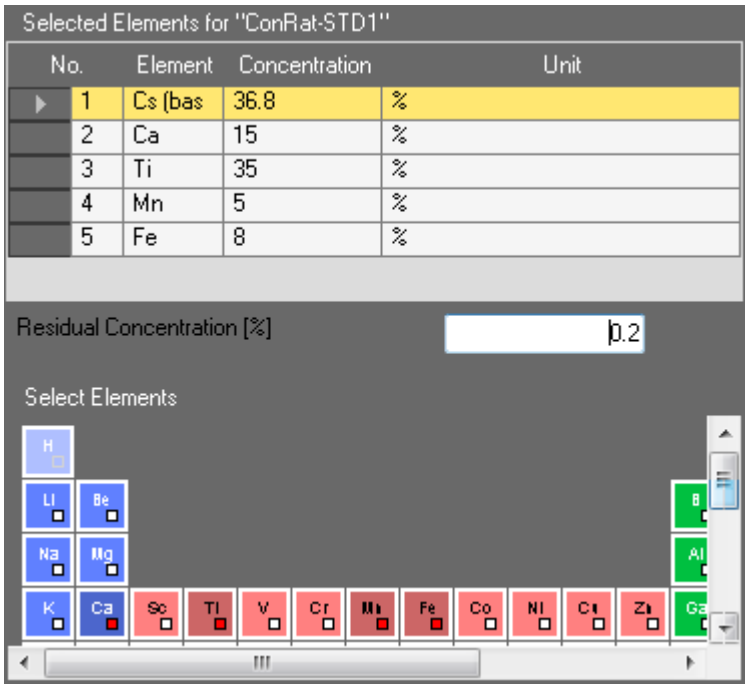


Figure 9-29. Enter Residual Concentration

The Residual Concentration represents the concentrations of residual elements in the sample (for example, impurities). A limit (percentage) needs to be defined.

vii. Define the properties of the analytes as required.

d. **Summation to 100%** is a special case where no base concentration is stated. The element list is populated with all elements. A provision is made for a small residual. When you specify this mode, the residual is initially 100% and reduces as you enter the concentrations of elements. As in the case of Concentration Ratios, the final value of the residual should be well below 1%. The standard concentrations for all elements including the residual will add up to 100%.

i. Add the analyte to the table by clicking the element in the periodic table.
The default line of the element is added to the table.

ii. Enter the Concentration for each analyte.
The Residual Concentration is automatically subtracted from the initial value of 100%.

iii. To remove the analyte, click the respective element in the periodic table again.

iv. Define the properties of the analytes as required.

Loading Standards

As an Administrator, you can generate standards by use of the Configurator tool, see "Standards" on page 3-31. As a User, you may load these standards into your Template or LabBook.

❖ **To load standards**

1. Open the **Method Parameters > Standards** view of the LabBook.
2. To import a list of standards into your LabBook.
   a. On the toolbar, click **Open** to get a list of all preset standards.
   b. Double-click the standard you wish to load into your LabBook. The associated elements and their concentration in the standard solution are displayed on the right-hand pane.

Editing an Existing Standard File

Existing standards can be edited and saved to your Template or LabBook.

❖ **To edit an existing standard file**

1. Open the **Method Parameters > Standards** view.
2. In the **Standards** list, select the standard to be edited.
3. If required, change the default concentration.
4. Click the elements in the periodic table to add or remove analytes.

Quantification

The **Quantification** view in Qtegra allows you to set the calibration and quantification strategy for each analyte.

All analytes selected in the Analytes view are shown in the **Quantification** view, see Figure 9-30.

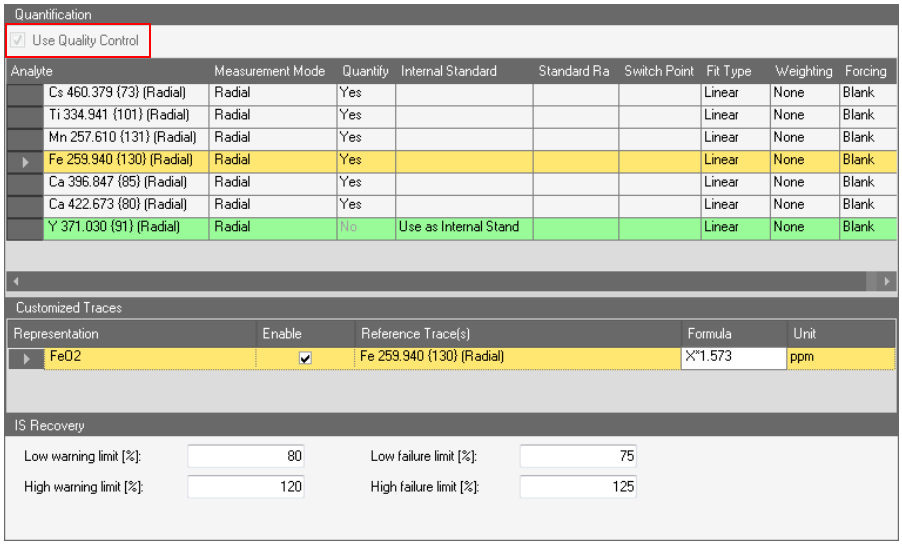


Figure 9-30. Quantification view with Use Quality Control check box

For eQuant Templates only, the **Use Quality Control** check box (see Figure 9-30) is available to enable the Quality Control Method Parameter of Qtegra ISDS Software, see "Quality Control" on page 10-5.

For trace analyses such as oxide analysis, traces can be added or customized in the **Customized Traces** table. This feature allows converting an element concentration into a molecule concentration, see page 9-38.

Calculation Traces can be added to allow calculation of average, maximum, minimum, standard deviation, and sum, see page 9-39.

Multi-Calibration trace is a tool that will enable switching from a sensitive wavelength to a less sensitive wavelength depending on the measured concentration.

For eQuant evaluations only, if an Internal Standard is used, warning limits and failure limits of its recovery can be entered (as percent values) into the fields of the **IS Recovery** section at the bottom of the page. In the results view, after measurement, results outside these warning limits are indicated with yellow, and if they are outside the failure limits, the values will be shown in red. This Internal Standard Test can also be found on the Quality Control page, see "Internal Standard Test" on page 10-24.

The parameters that can be defined for the Quantification table are summarized in Table 9-9.

Table 9-9. Parameters of Quantification table

Column	Description
Analyte	Displays analytes selected in the analytes view (see "Analytes" on page 9-3). The analytes are listed in ascending order according to atomic mass.
Measurement Mode	Shows the Measurement Mode defined for this analyte.
Quantify	Defines whether this analyte is to be quantified or not. **Yes** is automatically selected for all elements in the analyte list of the acquisition parameters.
	No is displayed for analytes that have been selected as internal standards in the **Internal Standard** column. They are removed from the list of Quantified wavelengths. **No** is also displayed for any analyte that has been selected from the Molecule section, for example, doubly charged ions, oxides, background ions. See "Analytes" on page 9-3.
Internal Standard	Once Internal Standards are defined they are added to the drop-down list of the cells in the Internal Standard column. The operator may define any Internal Standard wavelength desired. If **Use as Internal Standard** is selected, this line is shown with a green background.
Standard Range	To control the calibration range. Values outside this range are excluded from calibration.
Switch Point	**Switch Point** is used in conjunction with the Multi-Calibration Trace as it will indicate the concentration from which the next wavelength for a set element will be used. For example, if you have line1, line2 and line3 for element A, switch points can be defined as X1 for line1 and X2 for line2 with X1 < X2. Then, concentrations displayed for A will be measured from line1 and will switch to line2 if the concentration measured using line1 is > X1, same for line2 and X2. For line3, the switch point can be left "open" and any results will be reported or X3 can be entered, which will act as a limit over which results should not be reported. This feature enhances linearity of the calibration for an element and can be used in conjunction with the **Standard Range** to define the best calibration range for each wavelength.

Table 9-9. Parameters of Quantification table, continued

Column	Description
Fit Type	By default the calibration fit is set to **Linear**. All concentration calibrations should be linear with the signal response in the instrument. Nearly cancels out the weighting of higher amounts, which means a nearly equal weighting for low and high concentrations.
	In the rare case that a non-linear calibration is acquired, you can define a **2nd Order** calibration fit. Leads to a disproportionate weighting of smaller amounts.
Weighting	By default set to **None**, where higher weighting of higher amounts or signal values results. With the default setting, calibration points of higher concentrations have a stronger influence on calibration than calibration points of lower concentrations. As a result, the slope line of the calibration curve is influenced more strongly by the calibration points of the higher concentrations. This makes sense, as the determined area values of lower concentrations often show a stronger scattering, which can lead to a distortion of the result.
	If **Absolute SD** is selected, Absolute Standard Deviation is used. The standard deviation calibration variable is the square root of the Variance calibration variable. The Absolute SD estimates the standard deviation based on a random sample. The standard deviation is a measure for the deviation from the average value (the mean).
	If **Relative SD** is selected, Relative Standard Deviation (RSD) is used. The RSD is the standard deviation in relation to the size of the measured values (average); that is, the standard deviation is normalized. In contrast to absolute standard deviations, relative standard deviations can be compared (for values around 1000 a standard deviation of 1 is minor, for values around 10, this is a major deviation).
	If **1/Concentration** is selected, Blanks are ignored (as their concentration is 0) and *Forcing* is set to Blank. Each measured point is weighted by its concentration. This setting is used to increase the influence of smaller values.
	If **1/Concentration^2** is selected, Blanks are ignored (as their concentration is 0) and *Forcing* is set to Blank. Each measured point is weighted by its squared concentration. This setting is used to extra increase the influence of smaller values.

Table 9-9. Parameters of Quantification table, continued

Column	Description
Forcing	**No** forcing for the calibration.
	If **Zero** is selected, the calibration curve is forced through zero.
	If **Blank** (not for aQuant evaluation) is selected, the forcing of the calibration is set to run through the blank. Default setting is Blank.
	If **Zero Standard** is selected, the calibration curve is forced through the concentration of the Zero Standard. Here, forcing through *Blank* or forcing through *Zero* cannot be used as the Zero Standard concentration is different from zero.

❖ **To open the Quantification view**

1. Expand Method Parameters and click **Quantification** to open the **Quantification** view of the LabBook.

❖ **To activate Quality Control (QC) for eQuant evaluations**

1. Open the **Method Parameters > Quantification** view of the LabBook.
2. Select **Use Quality Control** above the table, see Figure 9-31.

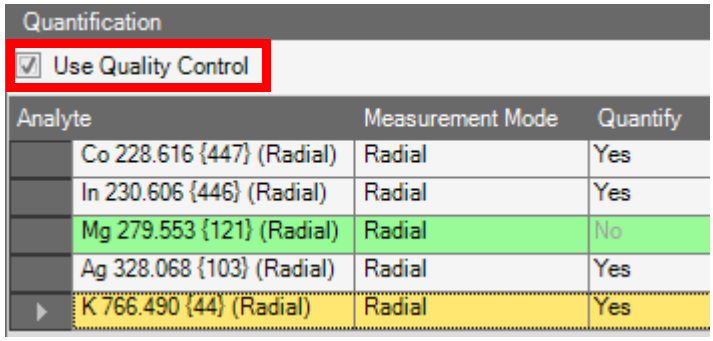


Figure 9-31. Activating Quality Control in Quantification view

The new Method Parameter **Quality Control** is displayed immediately.

❖ **To set the quantification parameters**

1. Open the **Method Parameters > Quantification** view of the LabBook.
2. Click  in the cell of the **Internal Standard** column to open the drop-down list.

   a. Select *Use as Internal Standard* to define this analyte to be used as Internal Standard.
   If you set the value to **No** in the **Quantify** column, this wavelength will not be quantified.

b. In the lines of the other analytes (with *Yes* in the Quantify column), select the defined **Internal Standard** from the drop-down list.

3. Define the **IS Recovery settings** at the bottom of the page.
4. Define the values and units for **Standard Range**, if applicable.
5. Define the value and unit for **Switch Point**, if applicable.
6. Click in the cell of the **Fit Type** column to open the drop-down list and select an entry to distinguish between *Linear* and *2nd Order*.
7. Click in the cell of the **Weighting** column to select *Absolute SD, Relative SD, 1/Concentration,* or *1/Concentration*^{2}. See Table 9-9 for details on the weighting options.
8. Click in the cell of the **Forcing** column to open the drop-down list.

   a. Select *Zero* to define that calibration is forced through zero for this analyte.

   b. If you select *Blank*, the calibration is set to run through the blank for this analyte.

   c. If you select *Zero Standard*, the calibration curve is forced through the concentration of the Zero Standard.

   d. If you select *No*, no forcing for the calibration is performed.

9. Repeat for all analytes or use the fill-down option to apply a setting to more than one analyte.

Adding Traces

Traces are used to add additional information to the quantification. Traces can be added from the shortcut menu of selected analytes on the Quantification view.

❖ **To add Customized Traces to the Quantification**

1. Open the **Method Parameters > Quantification** view of the LabBook.
2. Right-click the desired analyte in the table you wish to customize the trace for, see .
3. From the shortcut menu, select **Add customized trace** or **Add customized multi-calibration trace**.

A new table **Customized Traces** is added to the Quantification view below the Analyte table, see Figure 9-32.

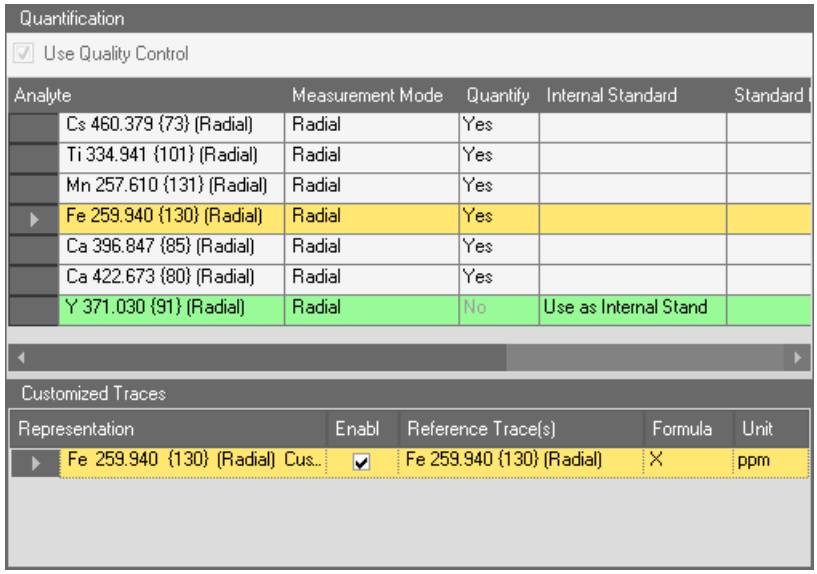


Figure 9-32. Customized Traces table

4. If you selected **Add customize multi-calibration trace**, define the **Switch Point** for the trace, and select **Reference Trace(s)** from the drop-down list.

5. Define **Representation**, select the **Enable** check box to activate the line, type a **Formula**, for example, a product like *X*1.5*, and select a **Unit** from the drop-down list, see Figure 9-33.

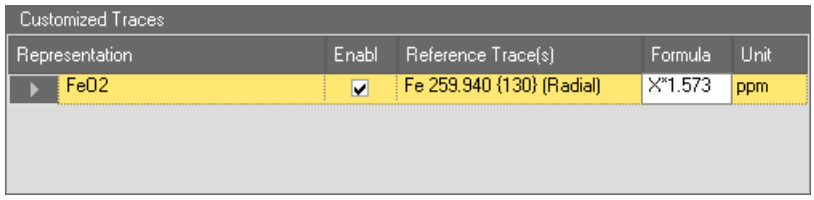


Figure 9-33. Customized trace formula entered

6. To delete a line from this Customized Traces table, select the line and press **<Del>**.

❖ **To add Calculation Traces to the Quantification**

1. Open the **Method Parameters > Quantification** view

2. Right-click multiple selected analytes you wish to calculate the traces for.

3. On the shortcut menu, expand **Add calculation trace** and select the operator you wish to use, see Figure 9-34.

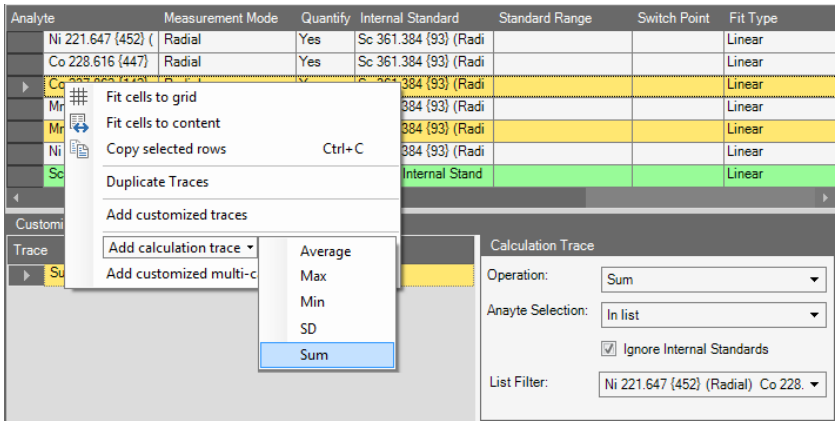


Figure 9-34. Calculation traces from shortcut menu of a LabBook

4. Below the table with the analytes, the Customized Traces table and Calculation Trace view are shown. The trace is shown with the name of the operator but the name can be changed.

Tip As Qtegra does not allow to use the same trace name in multiple lines, a further selection of the operator already used causes an error. In this case, double-click the existing trace name and change the name.

In the Calculation Trace, the **Operation** listbox shows your selection from the shortcut menu. Here, you can change to another operator if desired. This change does not affect the trace name.

Beside *All* the **Analyte Selection** listbox provides *Contains, In list, Not contains, Not in list* for fast and easy selection of all desired analytes.
Tick **Ignore Internal Standards** to exclude Internal Standards from the analyte selection.
The **List Filter** box is filled from your selection of analytes, which can be modified afterward.

5. After your LabBook is measured you can view the customized traces in the Evaluation Results > Concentrations list and also add the traces to a Report.

Ratios

The **Ratios** view of all LabBook types in the Qtegra tool allows you to define analyte ratios for the measurement.

The Ratios table shows the ratio of Analyte 1 and Analyte 2, see Figure 9-35.

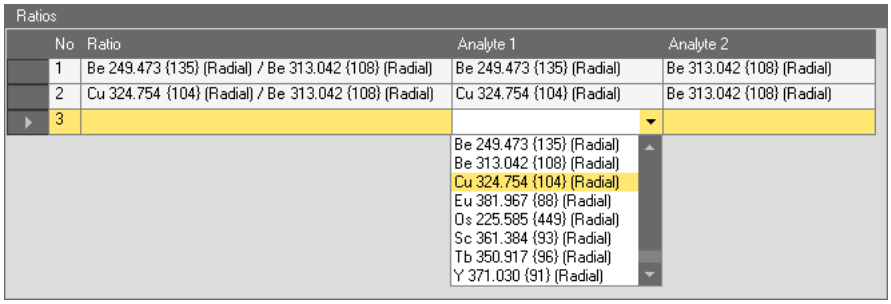


Figure 9-35. Ratios

The parameters that can be defined for the Ratios view are summarized in Table 9-10.

Table 9-10. Columns of Ratios table

Column	Description
No	Automatically assigned number in ascending order.
Ratio	Displays the ratio of **Analyte 1** and **Analyte 2** columns.
Analyte 1	First analyte to be selected for Ratio (numerator). All analytes selected for this LabBook in the Analytes view are displayed in the drop-down list.
Analyte 2	Second analyte to be selected for Ratio (denominator). All analytes selected for this LabBook in the Analytes view are displayed in the drop-down list.

❖ **To open the Ratios view**

1. From the **Qtegra - [Home Page]** navigation pane, open a LabBook.
2. Expand Method Parameters and click **Ratios** to open the Ratios view of the LabBook.

❖ **To define analyte ratios**

1. Open the **Method Parameters > Ratios** view of the LabBook.
2. Expand the cell of the column 1 to display the list of available analytes.
3. Select an analyte for column 1.
   The analyte selected in this column 1 is the numerator in the Ratio column.

4. Expand the cell of the column 2 to display the list of available analytes.

5. Select an analyte for column 2.
The analyte selected in column 2 is the denominator in the Ratio column.

   The ratio of both analytes is displayed in the Ratio column.

6. Click **Save** to save your LabBook.

❖ **To delete rows**

1. Open the **Method Parameters > Ratios** view.

2. Right-click the cell in front of a row.
A shortcut menu opens, see Figure 9-36.

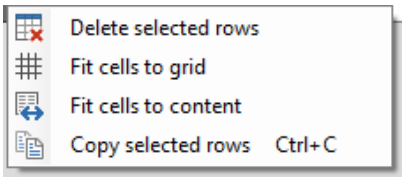


Figure 9-36. Ratio table shortcut menu

3. Select **Delete selected rows**.
A dialog opens.

4. Click **Yes** to delete the selected row.

Quality Control (eQuant only)

For eQuant evaluations only, the **Quality Control** view in the Qtegra tool allows a full quality control (QC) methodology. QC samples interspersed at strategic points in a batch of samples are used to gauge how well the instrument and the analytical method are performing. For details, see "Quality Control" on page 10-5.

Defining Detection Limits (eQuant only)

The Detection Limits are used by some of the QC types to determine whether the sample has passed or failed or even whether the test should be performed in the first place. For details, see "Defining Detection Limits for eQuant LabBooks" on page 10-25.

Defining QC Settings in Sample Definition (eQuant only)

The QC settings are specified for each sample in the Sample Definition section of the eQuant LabBook in the Qtegra tool. The Sample List of the LabBook is generated from the definition given in the Sample Definition section. For details, see "Defining QC Settings in Sample Definition of eQuant Templates" on page 10-30.

10

Analysis with eQuant Evaluation

The evaluation method eQuant is typically employed for routine analyses of liquid samples. It uses external element concentrations to quantify concentrations of elements in an unknown sample. Calibration graphs can be acquired and used for the fully quantitative analysis of unknown samples. A different evaluation strategy can be chosen for each analyte and also for each wavelength of an analyte.

Employment of the iCAP 7000 Plus Series ICP-OES instrument with an autosampler allows for high throughput of samples in the daily work of a laboratory.

Contents

Tip Be sure a Configuration has been created for your system setup, see "Experiment Configurator" on page 3-15.

Setting Up the Template

In the Qtegra tool, all settings for your measurement are entered in the Template. For analysis with eQuant evaluation this includes defining the elements in your calibration solution as well as the analytes of your samples.

Tip For a detailed description of all parameters in a Template, see "Method Parameters Settings" on page 9-3.

❖ **To define Template settings**

1. Create a Template with the Configuration for your system with iCAP 7000 Plus Series ICP-OES, the eQuant evaluation, and, for example, an autosampler.

2. Open the **Method Parameters > Analytes** view of the Template. See "Analytes" on page 9-3 for a general explanation.

3. In the periodic table, select the analytes of your calibration solution and your samples.
   First, the calibration curve of known samples must be acquired for later comparison of the intensities of analytes with this calibration curve.

4. Open the **Measure Modes** view of the Template.

5. Define the parameters for the **Radial** and **Axial View**, as appropriate.
   See "Measure Modes" on page 9-12 for details.

6. Open the **Method Parameters > Acquisition Parameters** view of the template.
   See "Acquisition Parameters" on page 9-14 for a general explanation.

7. For each analyte, select the background identification mode in **Left Bkg** and **Right Bkg** from the drop-down list, enter the **Start** and **Stop Time**, and enter the **Intensity Factor**.

8. Open the **Method Parameters > Intelligent Uptake and Rinse** view of the Template.

9. Set the delays and parameters for the analytes.
   For details, see "Intelligent Uptake and Rinse" on page 9-23.

10. Open the **Method Parameters > Inter-Element Correction** view of the Template.

11. Define the corrections for direct spectral interferences.
    For details, see "Inter-Element Correction" on page 9-24.

12. Open the **Method Parameters > Standards** view of the Template.

13. Click **New** to define a **Standard** as described in "Creating New Standards" on page 9-30.

14. Click **New** to define an **Internal Standard** as described in "Creating New Standards" on page 9-30.

    For definition of an Internal Standard, choose an element that is not present in your sample, but that is as near as possible to the mass of the analyte you wish to quantify. This element should then be added with the same concentration to each sample and standard. The elements of the InternalStandard should not react with the analytes or generate additional spectral interferences on the masses of the analytes. Obviously, also no interferences of the analytes should lie on the spectra of the elements in the Internal Standard.

15. Open the **Method Parameters > Quantification** view of the Template.

16. Type and select the values as described in "Quantification" on page 9-33.
    Fit Type in most cases is *Linear*.
    For analytes selected to be used as Internal Standard the setting for **Quantify** is automatically set to *No*.

17. Select the **Use Quality Control** check box if you wish to use this feature.
    The additional Method Parameter **Quality Control** is shown immediately.

    Tip For details on the Quality Control tests, see "Quality Control (eQuant only)" on page 9-42.

18. Open the **Method Parameters > Ratios** view of the Template.

19. Select the **Analyte 1** and **Analyte 2** from the drop-down lists.
    The Ratios page provides the option to set several user defined ratios, which are displayed after the measurement of the LabBook. For details, see "Ratios" on page 9-40.

    Tip For details on all parameters, see "Method Parameters Settings" on page 9-3.

❖ To define Sample Definition

1. Open a Template with the Configuration for your system with iCAP 7000 Plus Series ICP-OES, the eQuant evaluation, and, for example, an autosampler.

2. Define **Initial Actions, Continuing Actions** and **End Actions** as appropriate.
   To define Initial Actions and End Actions rows is typically appropriate for a high amount of analyses with a routine method.

3. In the **Continuing Actions** section, define **Label** for each row.

4. Enter a value for **Repeats**.
   The value **3** is typically appropriate.

5. For **Sample Type**, select *STD* for the calibration solution from the drop-down list, *UNKNOWN* for the samples, and *BLK* or *AVERAGE BLK* for blanks.

   When analyzing samples with complex matrices using the standard addition mode, the ZERO STD should be selected as the calibration blank. A series of spikes (Spike 1, Spike 2, etc.) of that same sample are used to construct a calibration curve. The curve is then interpolated to determine the concentration of the original unknown sample and subsequent other samples can be determined against this calibration.

6. Select the previously created **Internal Standard** from the drop-down list.

7. In the columns for rack and vials, set the positions of the samples in the autosampler.
   The titles of these columns vary with the autosamplers.

   Tip For details, see "Sample Definition for a Template" on page 5-5.

Quality Control

The **Quality Control** view of Qtegra allows a full quality control (QC) methodology. QC samples interspersed at strategic points in a batch of samples can be used to monitor a range of aspects of the analytical run being performed.

The Quality Control view, see Figure 10-1, allows you to set quality control tests for the measurement.

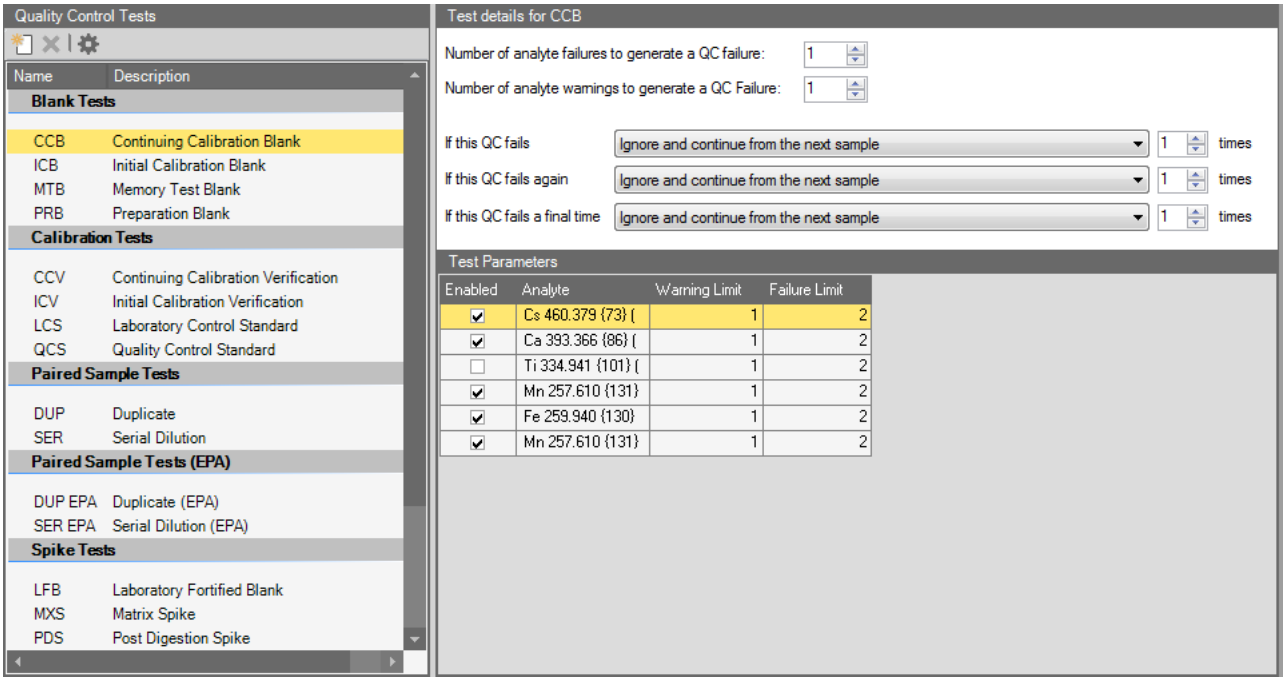


Figure 10-1. Quality Control page of Qtegra

Tip The Quality Control settings are displayed under Method Parameter only when the **Use Quality Control** check box has been selected in the parameter "Quantification" on page 9-33.

Quality Control tests can only be defined before a LabBook is placed on the Scheduler. A limited series of Quality Control parameters can be changed post analysis. Please see "Post Analysis Modification of QC Parameters" on page 10-33.

❖ To open the Quality Control view

1. Expand Method Parameters and open the **Quality Control** (QC) view.

Tip The Quality Control view is only available after Use Quality Control has been ticked in the Quantification view.

Quality Control Failure Rules

Failure rules for QC tests are defined in the Method Parameter Quality Control in Qtegra, see Figure 10-2.

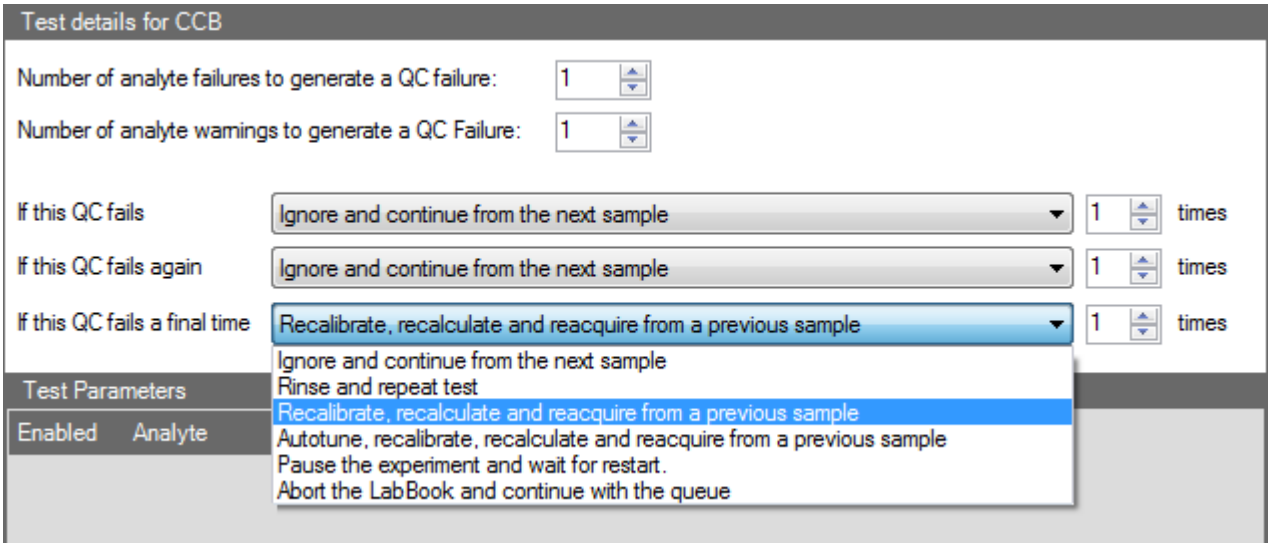


Figure 10-2. Quality control failure rules in the Test details area for each QC test

In the first part of **Test details**, the number of failures can be defined, see Table 10-1.

Table 10-1. Settings for number of failures

Parameter	Description
Number of analyte failures to generate a QC failure	To define how many analytes must fail before the flag message is generated. Click  to change the value. -or- Type the new value directly. **Recommended setting:** 1
Number of analyte warnings to generate a QC failure	The number of successive warnings to generate a QC failure can be set separately. This defines the number of successive warning states for an analyte in a given QC sample type to go through before becoming an absolute failure. Click  to change the value. -or- Type the new value directly. **Recommended setting:** 3

If the QC test fails, a number of options can be defined individually in the second part of **Test details** in the case that:

- The QC fails

- The QC fails again
- The QC fails a final time

The options available are listed and explained in Table 10-2.

Table 10-2. Settings for failure rules

Action	Description
Ignore and continue from the next sample	This action ignores that a QC failure has been registered and continues acquiring the Sample List.
Rinse and repeat test	This action repeats the test after a rinse step has been performed. A failed QC will automatically trigger an identical copy of the QC sample to be inserted into the Sample List after the failed QC. This step will be repeated once.
Recalibrate, recalculate, and reacquire from a previous sample	Upon QC failure, this action will automatically insert a copy of the calibration block and the QC sample immediately after the failed QC sample. A QC pass from the repeated tests will then allow the Sample List to be resumed from a named sample, which is defined in the QC Restart column in the Sample Definition table.
Pause the experiment and wait for restart	Upon QC failure, the LabBook will be paused and waiting to be restarted, giving the user time to manually find and remove the root cause for the failure.
Abort the LabBook and continue with the queue	Upon QC failure, the LabBook will be aborted and the Scheduler will continue with other scheduled LabBooks if there are any.

If a QC test fails, the first action is normally to rinse and repeat the test. If the test fails again, it might be advisable to recalibrate and repeat or to ignore and continue.

Each incident of this test will have exactly the same condition. Once defined, for example, whenever an ICB is defined in the Sample List, the same conditions will be used every time. The parameters can be set separately for each of the tests, for example, CCB can use one set of tests, whereas ICB uses a tighter set.

Quality Control Test Parameters

In the lower right pane of the Quality Control view, Qtegra provides a list, which is populated with all analytes defined in your LabBook. The QC Test Parameters list also shows the Warning and Failure limits.

❖ **To copy a set of limit values to the Test Parameters grid**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
On the left, the available Quality Control Tests are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to define.
   On the right, the corresponding **Test details** and **Test Parameters** are shown.

4. In the **Test Parameters** table, double-click the Warning Limit or Failure Limit cell you wish to change the entry and type the new value.

5. Click anywhere in the table.
   -or-
   Press **<Enter>** to enter the value.

6. Click and drag the mouse pointer from this first entry you wish to copy over all cells of the column to be changed with this value.

7. Right-click your selected range to open the shortcut menu, see Figure 10-3.

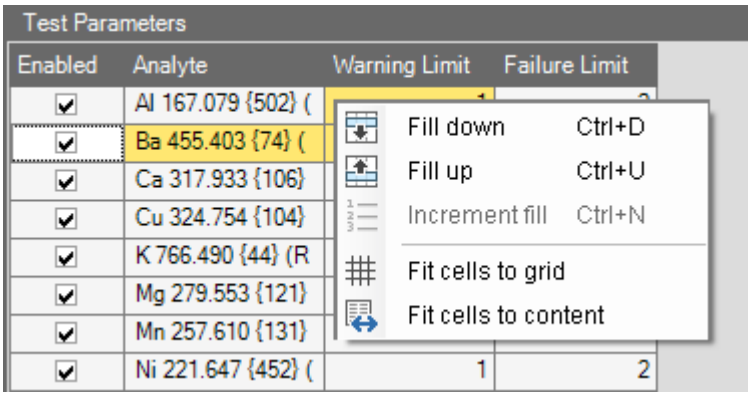


Figure 10-3. Quality Control Test Parameters shortcut menu

8. Select **Fill down** or **Fill up**, as appropriate.
   The entries from the first selected cell are copied down or up to all cells selected.
   -or-
   Press **<Ctrl> + <D>** or **<Ctrl> + <U>** to copy the initial value.

Quality Control Tests

Qtegra is supplied with predefined settings for QC test types. These settings can be edited according to your requirements and saved in the Qtegra Template or LabBook.

❖ **To create a new Quality Control Test**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
   On the left, the available Quality Control Tests are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to duplicate and define.

4. On the toolbar of Quality Control Tests, click **New**.
A dialog box opens, see Figure 10-4.

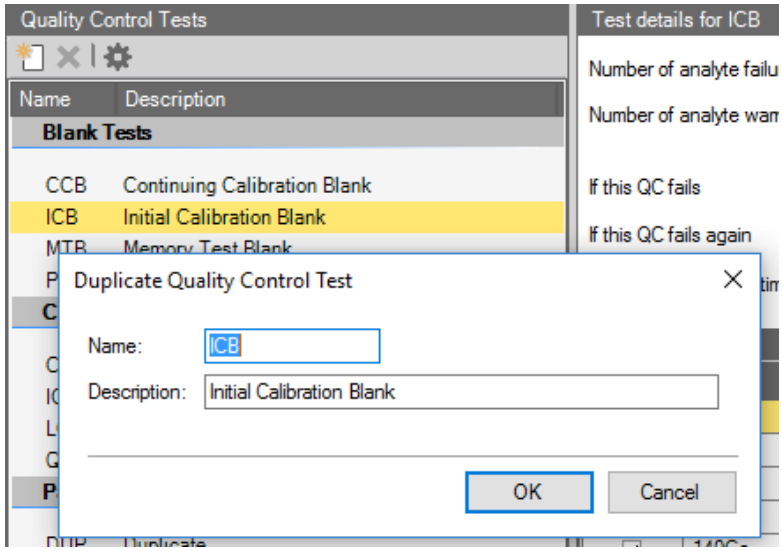


Figure 10-4. Duplicate Quality Control Test window

5. Type a **Name** and **Description** for the new quality control test.

6. Click **OK**.
The new test is added to the list. The Test details and Test Parameters are also copied and may be changed.

❖ **To delete a new Quality Control Test**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
On the left, the available Quality Control Tests are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to delete, see Figure 10-5.

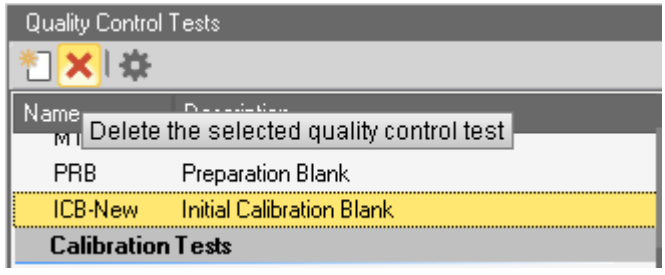


Figure 10-5. Delete non-default Quality Control Test

Tip Predefined Quality Control Tests can not be deleted.

4. Click **Delete**.
   The selected Quality Control Test is immediately deleted from the list.

Blank Verification Tests

Several types of blank verification tests are offered in the Method Parameter Quality Control in Qtegra, see Figure 10-6.

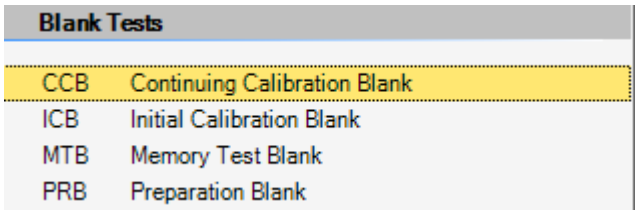


Figure 10-6. QC settings for blank verification

Anywhere in the Sample List, blanks can be analyzed and checked to see if the instrument background for the analyte has drifted either up or down.

The **Blank Test** types limits are based on contract required detection limits (CRDLs). The warning and failure QC limits are based on multiples of the set limits. The analyte will fail if the calculated value is above the failure limit.

The **Blank Tests** available for blank verification are summarized in Table 10-3. The last two columns show typical QC requirements of the US EPA.

Table 10-3. Quality control blank tests

Test type	Description	Purpose	Frequency	Limits
CCB	Continuing Calibration Blank	a continuing periodic check on the signal at blank levels	every 10 samples	< 3 x IDL (Instrumental Detection Limit)
ICB	Initial Calibration Blank	initial check of signal at blank level	after initial calibration	< 3 x IDL
MTB	Memory Test Blank	checks the level of memory (or carry over) of a high concentration sample into the subsequent sample	user definable	user definable
PRB	Preparation Blank	checks the sample preparation methodology for possible contamination	required for each batch of samples	< 3 x IDL

Warning and Failure Limits

The failure and warning limits are multiples of the detection limit, for example, if the detection limit is at *10* ppb, the warning might be at a blank concentration of *1.5* times the detection limit and the failure limit might be at 3 times the detection limit, in this case *15* and *30* ppb respectively.

❖ **To define QC settings for blank tests**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
   On the left, the available **Quality Control Tests** are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to define.
   On the right, the corresponding **Test details** and **Test Parameters** are shown.

4. If desired, change the **Number of analyte failures to generate a QC failure** and change the **Number of analyte warnings to generate a QC failure**. For details, see "Quality Control Failure Rules" on page 10-6.

5. Select the action to take place **If this QC fails**.

6. Select the action to take place **If this QC fails again**.

7. Select the action to take place **If this QC fails a final time**.

8. Clear the **Enabled** check box next to the analyte to skip this analyte, see Figure 10-7.

Test Parameters

Enabled	Analyte	Warning Limit	Failure Limit
☑	Al 167.079 {502} (	1	2
☑	Ba 455.403 {74} (	1	2
☑	Ca 317.933 {106}	1	2
☑	Cu 324.754 {104}	1	2
☑	K 766.490 {44} (R	1	2
☑	Mg 279.553 {121}	1	2
☑	Mn 257.610 {131}	1	2
☑	Ni 221.647 {452} (	1	2

Figure 10-7. Quality Control blank test parameters

By default, all analytes defined in the LabBook are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.
Analytes selected as Internal Standards are not considered for QC tests.

9. Define the **Warning Limit** and **Failure Limit** for each analyte. For details, see "Quality Control Test Parameters" on page 10-7.

Calibration Verification Tests

Several types of calibration verification tests are offered in the Method Parameters, Quality Control view, see Figure 10-8.

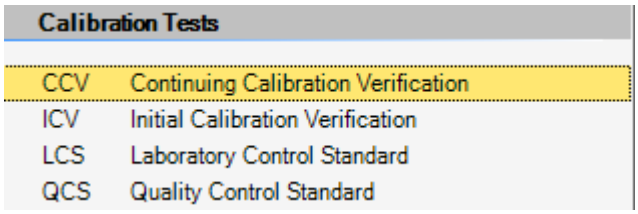


Figure 10-8. Table of QC settings for external calibration verification

Standards of known concentration are dispersed within the samples to check if the concentration calibration is still valid.

Each individual test is associated with a standard in the Sample Definition section and can be defined in the QC section with relative warning or failure limits, and the number of QC failures and warnings of individual analytes to generate a QC failure.

The **Calibration Tests** available for the external calibration verification are summarized in Table 10-4. The last two columns show typical QC requirements of the US EPA.

Table 10-4. Quality Control calibration tests

Test type	Description	Purpose	Frequency	Limits
CCV	Continuing Calibration Verification	a continuing periodic check on accuracy and drift	every 10 samples	90-110%
ICV	Initial Calibration Verification	checks the calibration against a second calibration source	after initial calibration	90-110%
LCS	Laboratory Control Sample	checks the accuracy of the entire analytical process	every 20 samples	80-120% (EPA Method 6010C) 70-130% ISM02.3D
QCS	Quality Control Standard	checks the accuracy of the entire analytical process	once per batch	±10% (EPA Method 200.7)

Warning and Failure Limits

For each analyte the lower and higher warning and failure limits can be set individually. A QC failure and a QC warning are different, the warning limit is always set to tighter specifications than the failure limit. If the QC exceeds the warning limits, a QC warning will be generated and a certain number of consecutive QC warnings for a particular analyte will then lead to a QC failure. If the QC test of the analyte gives results outside the QC failure limits, it will become an instant failure; if results are within the warning limits, the analysis carries on until it reaches the number of successive warnings specified for that QC test type and analyte. The next time it is outside the QC warning limit, it will then become a failure. If the QC value for the warning analyte in that QC test type passes the next test, the counter is reset to zero and the analysis continues. If warning limits are not required, they should be set to the same as the failure limits.

❖ **To define QC settings for calibration tests**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
   On the left, the available **Quality Control Tests** are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to define.
   On the right, the corresponding **Test details** and **Test Parameters** are shown.

4. If desired, change the **Number of analyte failures to generate a QC failure** and change the **Number of analyte warnings to generate a QC failure**. For details, see "Quality Control Failure Rules" on page 10-6.

5. Select the action to take place **If this QC fails**.

6. Select the action to take place **If this QC fails again**.

7. Select the action to take place **If this QC fails a final time**.

8. Clear the **Enabled** check box next to the analyte to skip this analyte, see Figure 10-9.

Test Parameters

Enabled	Analyte	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)
☐	Al 167.079	75	80	120	125
☑	Ba 455.40	75	80	120	125
☑	Ca 317.93	75	80	120	125
☑	Cu 324.75	75	80	120	125
☑	K 766.490	75	80	120	125
☑	Mg 279.55	75	80	120	125
☑	Mn 257.61	75	80	120	125
☑	Ni 221.647	75	80	120	125

Figure 10-9. Quality Control calibration test parameters

By default, all analytes defined in the LabBook are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.
Analytes selected as Internal Standards are not considered for QC tests.

9. Define the **Low Failure Limit (%)**, **Low Warning Limit (%)**, the **High Warning Limit (%),** and **High Failure Limit (%)** for each analyte. For details, see "Quality Control Test Parameters" on page 10-7.

Paired Sample Tests

Several types of paired sample tests are offered in the Method Parameters, Quality Control, see Figure 10-10.

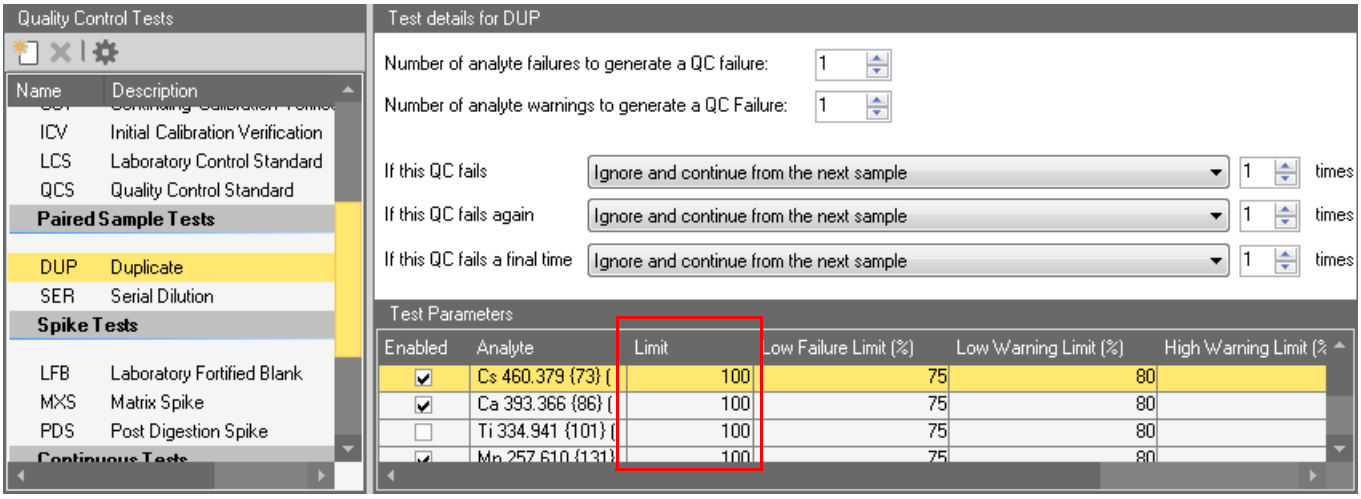


Figure 10-10. Table of QC settings for paired sample

Paired samples are used to assess the method-reproducibility between two defined samples. The QC software will monitor the first defined sample and determine if the second sample is significantly above or below user defined recovery limits.

Whereas the Duplicate Test (DUP) determines the relative percent difference (RPD) between two identical samples, the Serial Dilution Test (SER) determines if the sample matrix affects the data quality by changing the percent recovery after a certain dilution of the sample. To perform an analytically meaningful comparison between the DUP and SER analyses, the concentration in the original sample must have a concentration at least a certain multiple above the detection limit, for example, 200 times higher. This reference detection limit is set via the **Contract Required Detection Limits** dialog (CRDL, see Figure 10-26) that is opened when you click the **Edit the contract required detection limits** button on the toolbar (see Figure 10-11).

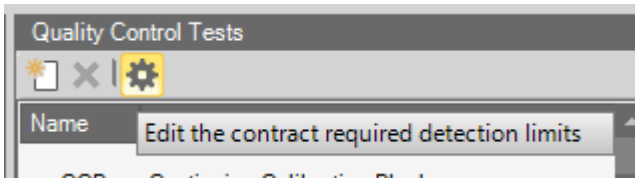


Figure 10-11. Quality Control Tests toolbar with CRDL button

Double-click an entry (see rectangle in Figure 10-10) to change the concentration and select the desired unit from the drop-down menu.

See "Defining Detection Limits for eQuant LabBooks" on page 10-25 for a detailed description. The software will not perform the test if the sample is too close to the detection limit, as it would only lead to excessive failure generation.

$$c_{measured} > Limit \times CRDL$$

The **Paired Sample Tests** available are summarized in Table 10-5. The last two columns show typical QC requirements of the US EPA.

Table 10-5. Quality control paired sample tests

Test type	Description	Purpose	Frequency	Limits
DUP	Duplicate	checks the reproducibility of results by analyzing an unknown sample in duplicate	1 per 20 samples per matrix	±20% RPD
SER	Serial Dilution	checks for matrix effects by assessing the variation of result for an unknown sample before and after dilution	1 per 20 samples per matrix	±20% of the original undiluted result after dilution correction (EPA Method 6010D)

Warning and Failure Limits

The same rules as for other QC tests apply for setting the lower and higher warning and failure limits.

❖ **To define QC settings for paired sample tests**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
On the left, the available **Quality Control Tests** are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to define.
On the right, the corresponding **Test details** and **Test Parameters** are shown.

4. If desired, change the **Number of analyte failures to generate a QC failure** and change the **Number of analyte warnings to generate a QC failure**. For details, see "Quality Control Failure Rules" on page 10-6.

5. Select the action to take place **If this QC fails**.

6. Select the action to take place **If this QC fails again**.

7. Select the action to take place **If this QC fails a final time**.

8. Clear the **Enabled** check box next to the analyte to skip this analyte, see Figure 10-12.

Test Parameters

Enabled	Analyte	Limit	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)
☐	Al 167.079 {502} (	100	75	80	120	125
☑	Ba 455.403 {74} (	100	75	80	120	125
☑	Ca 317.933 {106}	100	75	80	120	125
☑	Cu 324.754 {104}	100	75	80	120	125
☑	K 766.490 {44} (R	100	75	80	120	125
☑	Mg 279.553 {121}	100	75	80	120	125
☑	Mn 257.610 {131}	100	75	80	120	125
☑	Ni 221.647 {452} (	100	75	80	120	125
☑	P 177.495 {490} (	100	75	80	120	125
☑	Zn 213.856 {458}	100	75	80	120	125
☐	Y 371.030 {91} (R	100	75	80	120	125

Figure 10-12. Quality Control Paired Sample Test Parameters

By default, all analytes defined in the LabBook are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.
Analytes selected as Internal Standards are not considered for QC tests.

9. Define the **Limit** for each analyte. The QC test is only performed if the QC concentration is greater than the product of CRDL and specified limit. The default value is *100*, corresponding to the following formula:

$$c_{measured} > Limit \times CRDL$$

where $c_{measured}$ is the concentration of the QC sample, *CRDL* the contract required detection limit, and *Limit* the value from the test parameter table. If the condition is not fulfilled, the QC step for this analyte is skipped and QC passes.

10. Define the **Low Failure Limit (%)**, **Low Warning Limit (%)**, the **High Warning Limit (%),** and **High Failure Limit (%)** for each analyte. For details, see "Quality Control Test Parameters" on page 10-7.

Paired Sample Tests (EPA)

Paired sample tests (EPA) are offered in the Method Parameter Quality Control in Qtegra, see Figure 10-13.

Paired Sample Tests (EPA)	
DUP EPA	Duplicate (EPA)
SER EPA	Serial Dilution (EPA)

Figure 10-13. Table of QC settings for paired sample tests (EPA)

Paired samples are used to assess the method-reproducibility between two defined samples. These EPA tests only check an absolute limit value.

To keep the calculation independent from the (plain) DUP and SER paired sample tests, Qtegra ISDS Software provides paired sample tests following the EPA calculations with a different recovery calculation, see "Paired Sample Tests (EPA conform)" on page 13-6. In the Test Parameters table, only the Limit, Warning Limit, and Failure Limit can be defined, see Figure 10-14.

Test Parameters

Enabled	Analyte	Limit	Warning Limit (%)	Failure Limit (%)
☑	Ba 455.403 {74} (Radi	100	20	25
☑	Ca 393.366 {86} (Radi	100	20	25
☐	Cu 324.754 {104} (Rad	100	20	25
☑	K 766.490 {44} (Radial	100	20	25
☑	Mg 279.553 {121} (Rad	100	20	25
☑	Mn 257.610 {131} (Rad	100	20	25

Figure 10-14. Table of QC settings for paired sample tests (EPA conform)

Define the **Warning Limit (%)** and **Failure Limit (%)** for each analyte. For details, see "Quality Control Test Parameters" on page 10-7.

The **Paired Sample Tests (EPA)** available are summarized in Table 10-6.

Table 10-6. Quality control paired sample tests (EPA)

Test type	Description	Purpose	Frequency	Limits
DUP (EPA)	Duplicate (EPA)	checks the reproducibility of results by analyzing an unknown sample in duplicate	1 per 20 samples per matrix	±20% RPD
SER (EPA)	Serial Dilution (EPA)	checks for matrix effects by assessing the variation of result for an unknown sample before and after dilution	1 per 20 samples per matrix	±20% of the original undiluted result after dilution correction (EPA Method 6010D)

Spike Tests / Spike Tests (ARC)

Several types of spike tests are offered in the Method Parameter Quality Control in Qtegra, see Figure 10-15.

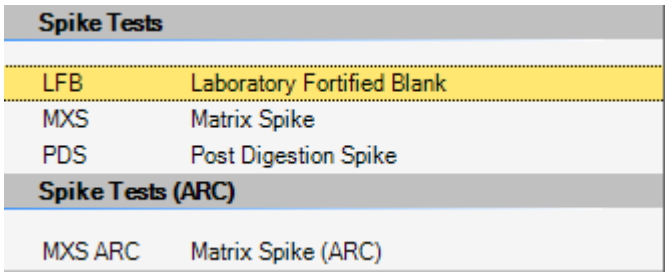


Figure 10-15. Table of QC settings for spike recovery tests

Spike tests are used to determine the recovery of a known addition of analyte to a particular sample. The rightmost two columns in Table 10-7 show typical QC requirements of the US EPA.

Table 10-7. Quality control spike recovery

Test type	Description	Purpose	Frequency	Limits
LFB	Laboratory Fortified Blank	checks the recovery of analytes in a matrix-free sample	every 20 to 30 samples	85-115% (EPA Method 200.8)
MXS	Matrix Spike	checks the recovery of a spike in the sample matrix	every 20 samples	80-120% (EPA Method 6020A) 30-70% ILM05.2D

Table 10-7. Quality control spike recovery

Test type	Description	Purpose	Frequency	Limits
PDS	Post Digestion Spike	checks the recovery of analytes spiked into an unknown sample after preparation (digestion)	1 per 20 samples per matrix	75-125%
MXS ARC	Matrix Spike with Alternative Recovery Calculation	based on an alternative recovery calculation that avoids negative recoveries in cases where spike concentrations are too low compared to unspiked samples		

Warning and Failure Limits

Apply the same rules as for other QC tests for setting the lower and higher warning and failure limits.

❖ **To define QC settings for spike tests**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
On the left, the available **Quality Control Tests** are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to define.
On the right, the corresponding **Test details** and **Test Parameters** are shown.

4. If desired, change the **Number of analyte failures to generate a QC failure** and change the **Number of analyte warnings to generate a QC failure**. For details, see "Quality Control Failure Rules" on page 10-6.

5. Select the action to take place **If this QC fails**.

6. Select the action to take place **If this QC fails again**.

7. Select the action to take place **If this QC fails a final time**.

8. Clear the **Enabled** check box next to the analyte to skip this analyte, see Figure 10-16.

Test Parameters

Enabled	Analyte	Qualifier	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)
☐	Al 167.079 {502} (	100	75	80	120	125
☑	Ba 455.403 {74} (	100	75	80	120	125
☑	Ca 317.933 {106}	100	75	80	120	125
☑	Cu 324.754 {104}	100	75	80	120	125
☑	K 766.490 {44} (R	100	75	80	120	125
☑	Mg 279.553 {121}	100	75	80	120	125
☑	Mn 257.610 {131}	100	75	80	120	125
☑	Ni 221.647 {452} (	100	75	80	120	125
☑	P 177.495 {490} (	100	75	80	120	125
☑	Zn 213.856 {458}	100	75	80	120	125

Figure 10-16. Quality Control spike test parameters

Generally, all analytes defined in the LabBook are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.
Analytes selected as Internal Standards are not considered for QC tests.

9. Define the **Qualifier** for each analyte. The QC test is only performed if the ratio of spike concentration and unspiked concentration is greater than the specified Qualifier. Default value is *100*, corresponding to a spike/unspiked ratio of 1/1, expressed in percent, following the formula:

$$\frac{c_{spike}}{c_{unspiked}} \cdot 100 > Qualifier$$

where c_{spike} is the concentration of the spike, $c_{unspiked}$ the concentration of the unspiked QC sample, and *Qualifier* the value from the test parameter table. If the condition is not fulfilled, the QC step for this analyte is skipped and QC passes.

10. Define the **Low Failure Limit (%)**, **Low Warning Limit (%)**, the **High Warning Limit (%),** and **High Failure Limit (%)** for each analyte. For details, see "Quality Control Test Parameters" on page 10-7.

Continuous Tests

Several types of continuous tests are offered in the Method Parameter Quality Control in Qtegra, see Figure 10-17.

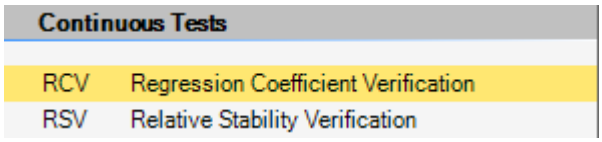


Figure 10-17. Table of QC settings for continuous tests

The continuous test RCV checks the correlation coefficient of the calibration to make sure that only accurate calibration data is used for the quantification of unknown samples.

With the continuous test RSV, the relative stability of the obtained signal can be verified. A certain threshold value can be defined, either related to signal intensity in CPS or concentration, so that sample concentrations not greater than the threshold value are not included in this QC test. This way, QC failures for very low concentrations or intensities can be avoided.

Continuous tests are active for all BLKs, standards and samples to continuously monitor the performance during analysis.

Two different **Continuous Tests** are available. The last two columns in Table 10-8 show typical QC requirements of the US EPA.

Table 10-8. Quality control spike recovery

Test type	Description	Purpose	Frequency	Limits
RCV	Regression Coefficient Verification	checks that the linearity of the calibration is within (above) the specified warning and failure limits	every calibration	0.95 Failure 0.9
RSV	Relative Stability Deviation Verification	checks that the relative signal stability of the main run data is within (below) the specified warning and failure limits	every samples	5% Failure 10%

Warning and Failure Limits

The same rules as for other QC tests apply for setting the lower and higher warning and failure limits.

❖ **To define QC settings for continuous tests**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
On the left, the available **Quality Control Tests** are listed, see Figure 10-1.

3. Select the *Quality Control Test* you wish to define.
On the right, the corresponding **Test details** and **Test Parameters** are shown.

4. If desired, change the **Number of analyte failures to generate a QC failure** and change the **Number of analyte warnings to generate a QC failure**. For details, see "Quality Control Failure Rules" on page 10-6.

5. Select the action to take place **If this QC fails**.

6. Select the action to take place **If this QC fails again**.

7. Select the action to take place **If this QC fails a final time**.

8. Clear the **Enabled** check box next to the analyte to skip this analyte, see Figure 10-18.

Test Parameters

Enabled	Analyte	Warning Limit	Failure Limit
☐	Al 167.079 {502}...	0.95	0.9
☑	Ba 455.403 {74}...	0.95	0.9
☑	Ca 317.933 {106...	0.95	0.9
☑	Cu 324.754 {104...	0.95	0.9
☑	K 766.490 {44} (...	0.95	0.9
☑	Mg 279.553 {12...	0.95	0.9
☑	Mn 257.610 {13...	0.95	0.9
☑	Ni 221.647 {452}...	0.95	0.9
☑	P 177.495 {490}...	0.95	0.9
☑	Zn 213.856 {458...	0.95	0.9

Figure 10-18. Quality Control: continuous test RCV parameters

By default, all analytes defined in the LabBook are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.

9. For the continuous test **RCV**, define the **Warning Limit** and **Failure Limit** for the analytes. For details, see "Quality Control Test Parameters" on page 10-7.

10. For the Continuous Test **RSV**, select the parameters to be verified for each analyte from the drop-down list **Verify**, see Figure 10-19.

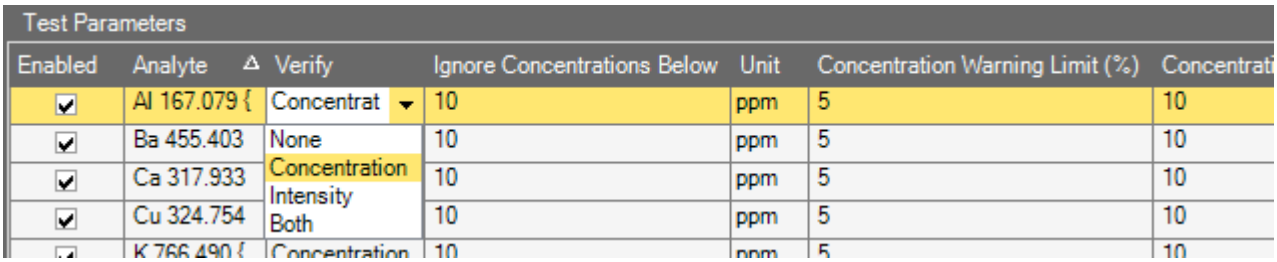


Figure 10-19. Quality Control: continuous test RSV parameters, left part

11. Set the value for **Ignore Concentration Below** and define a **Unit**, if activated.
    Set the **Concentration Warning Limit (%)** and **Concentration Failure Limit (%)**.

12. Set the value for **Ignore Intensities Below**, if activated.
    Set the **Intensity Warning Limit (%)**and **Intensity Failure Limit (%)**, see Figure 10-20.

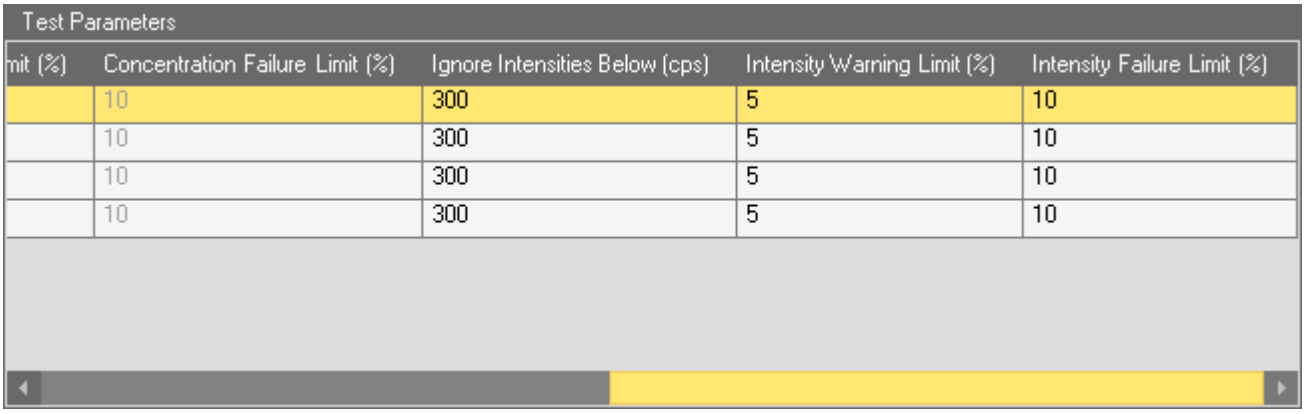


Figure 10-20. Quality Control: continuous test RSV parameters, right part

Internal Standard Test

An Internal Standard test is offered in the Method Parameter Quality Control in Qtegra, see Figure 10-21.

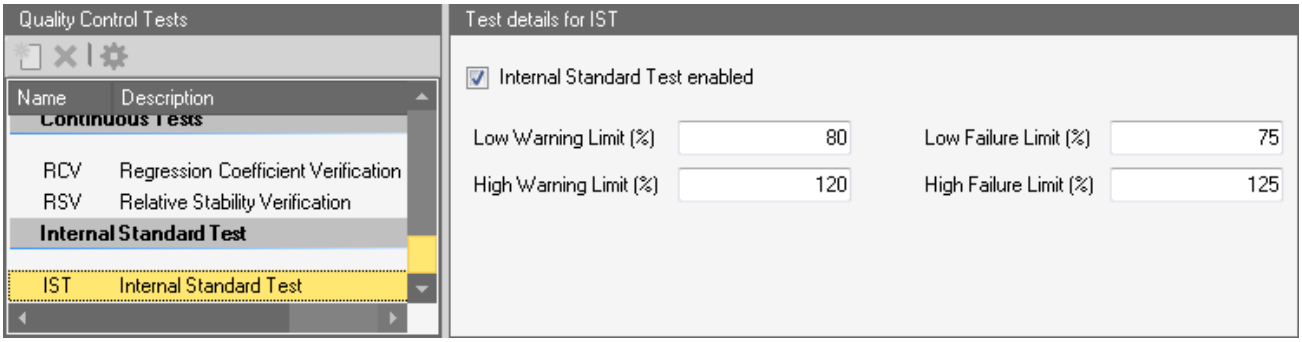


Figure 10-21. Quality Control: test details for IST

Like the continuous test, the Internal Standard test is activated for every entry in the Sample List to evaluate performance and make sure that potentially occurring matrix effects can be corrected for.

If an Internal Standard is used, warning limits and failure limits of its recovery in percent can be entered.

Tip The Internal Standard test can also be found in the Quantification view, in the field of the **IS Recovery** pane at the bottom of the view, see "Quantification" on page 9-33.

❖ **To define QC settings for Internal Standard Tests**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.
   On the left, the available Quality Control Tests are listed, see Figure 10-1.
3. Select the *Quality Control Test* you wish to define, for example.
   On the right, the corresponding **Test details** are shown, see Figure 10-21.
4. Tick **Internal Standard Test enabled** to activate this feature.
5. Define the **Low Warning Limit (%)** and **High Warning Limit (%)** for the analytes.
6. Define the **Low Failure Limit (%)** and **High Failure Limit (%)** for the analytes.

Defining Detection Limits for eQuant LabBooks

The Detection Limits are used by some of the QC types to determine whether the sample has passed or failed or even whether the test should be performed in the first place.

The Quality Control view of the eQuant LabBook in Qtegra allows the definition of contract-required detection limits for the measurement, see Figure 10-22.

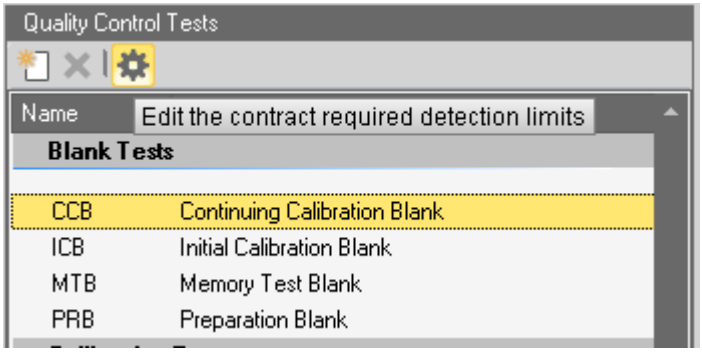


Figure 10-22. Opening contract-required detection limits

The contract required detection limits are defined by the laboratory operator and can be either experimentally derived from data previously acquired or set as values that are prescribed by regulators such as the US EPA. They are used as part of the Blank Verification QC tests and also as a pre-test validation for the Paired Sample Tests.

The detection limits are edited in the dialog **Contract Required Detection Limits**. It is also possible to import or export detection limits. The elements of the dialog are summarized in Table 10-9.

Table 10-9. Detection limits

Column	Description
Symbol	Displays the analytes selected for the Template (LabBook).
Concentration	Defines the detection limit for this analyte.
Unit	This column defines the unit of the detection limit. By default, the unit is *ppm*. Several units are offered to be selected from the drop-down list. The units can be different for each analyte. The detection limits are used later in certain QC tests.
Import	Import Contract Required Detection Limits. See "To import an existing analyte list" on page 10-27.
Export	Export Contract Required Detection Limits. See "To export the currently loaded analyte list" on page 10-29.

Tip Any analytes (cells) that are not required for the LOD checks can be left blank.

❖ **To enter detection limits for the defined analytes**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.

3. On the toolbar, click **Edit the contract required detection limits**. A dialog opens, see Figure 10-23.

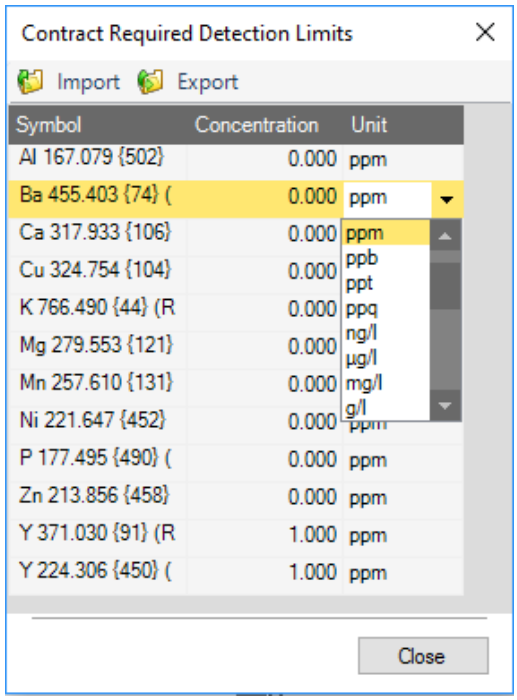
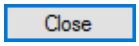


Figure 10-23. Contract Required Detection Limits dialog

4. Click the **Concentration** cell next to an analyte and type a value for the detection limit.
5. Expand the **Unit** cell to select a unit from the drop-down list. The default unit is *ppm*.
6. Repeat until all detection limits are set.



7. Click **Close**.

❖ **To import an existing analyte list**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.

3. On the toolbar, click **Edit the contract required detection limits**. A dialog opens, see Figure 10-24.

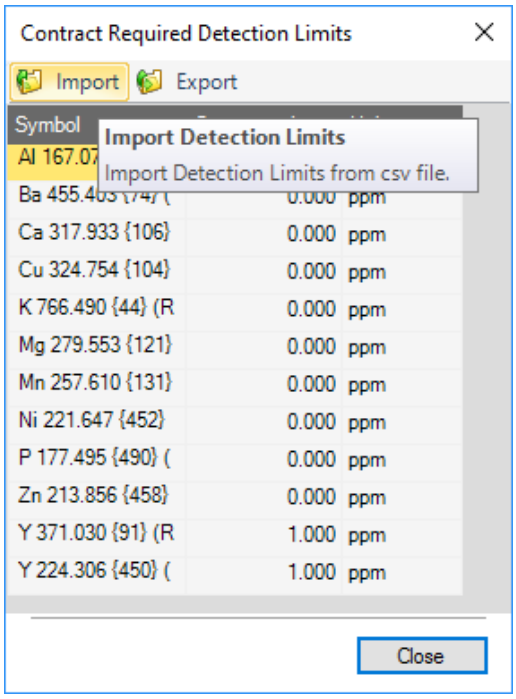


Figure 10-24. Contract Required Detection Limits import

4. Click **Import** to open the **Import detection limits** dialog.
5. Select the directory of your CSV file.
6. Select the CSV file you wish to import, see Figure 10-25.

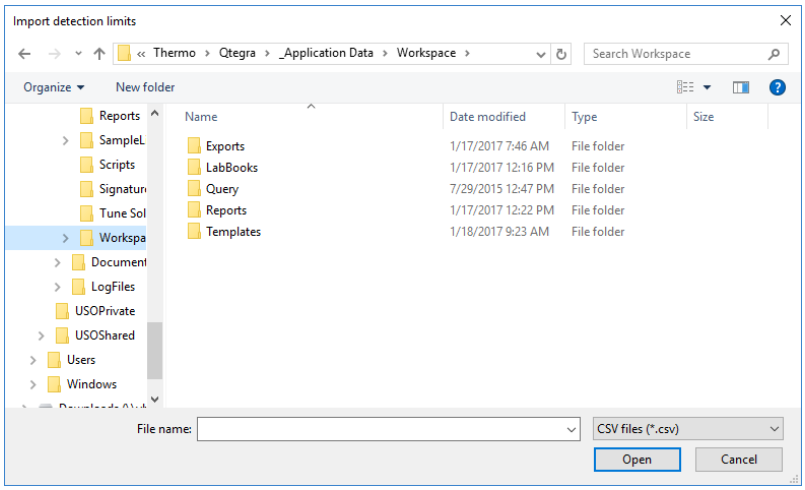
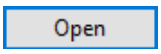
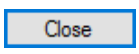


Figure 10-25. Import detection limits dialog



7. Click **Open** to load the file.
The CSV file is imported into the table to be edited as required.



8. Click **Close** to close the **Contract Required Detection Limits** dialog.

❖ **To export the currently loaded analyte list**

1. Open a LabBook with the eQuant evaluation and activated **Quality Control**.

2. Open the **Method Parameters > Quality Control** view.

3. Click **Settings**.
A dialog opens, see Figure 10-26.

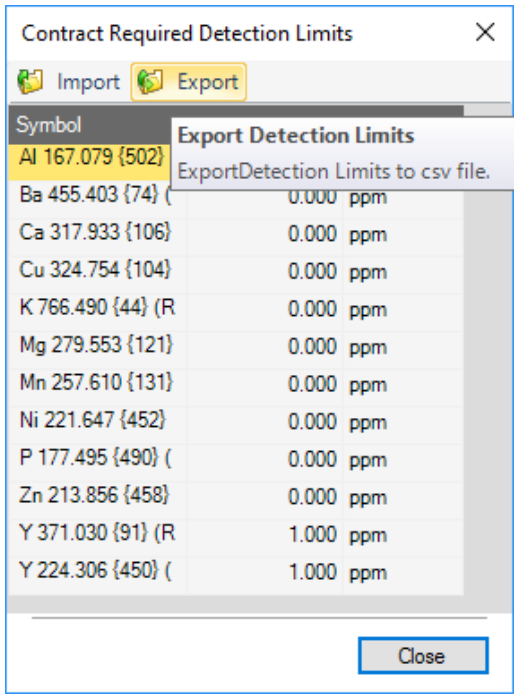


Figure 10-26. Contract Required Detection Limits export

4. Click **Export** to open the **Export detection limits** dialog, see Figure 10-27.

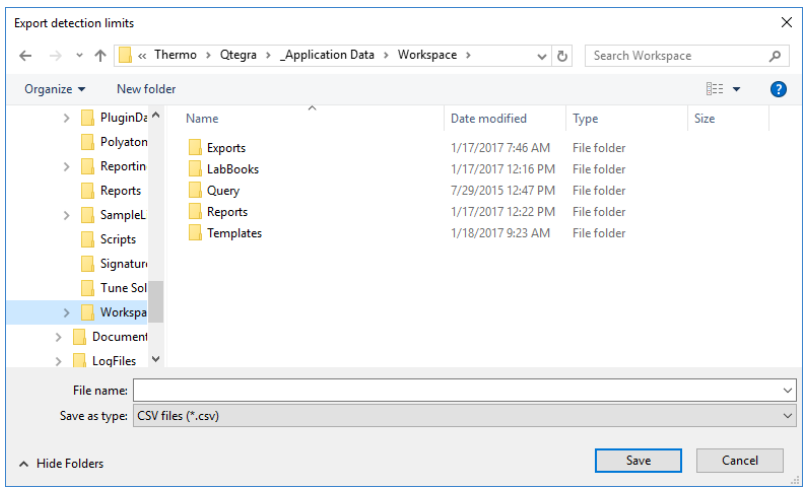
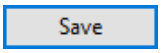


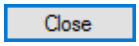
Figure 10-27. Export detection limits dialog

5. Select the directory of your CSV file.

6. Type a name for the CSV file you wish to export.



7. Click **Save** to save the file.
The CSV file is exported.



8. Click **Close** to close the **Contract Required Detection Limits** dialog.

Defining QC Settings in Sample Definition of eQuant Templates

The QC settings are specified for each sample in the Sample Definition section of the eQuant Template in Qtegra. The Sample List of the LabBook is generated from the definition given in the Sample Definition section.

QC samples can be defined as **Initial Actions**, for example, ICB or ICV, as **Continuing Actions** with the appropriate value for Interval, or in special cases as **End Actions**.

Tip For details on Quality Control, see "Quality Control" on page 10-5.

❖ **To define QC settings in Sample Definition**

1. Open a Template with the eQuant evaluation and activated **Use Quality Control**, see "Quantification" on page 9-33.
2. Define your Quality Control Test, see "Quality Control" on page 10-5.
3. Click 

Sample Definition to open the Sample Definition view of the Template.
4. Add as many **Initial**, **Continuing** and **End Actions** rows as you need for your experiment.

   Tip Initial and End Actions rows will only be done once at the beginning and respectively the end of the experiment. A single row in the Continuing Actions block will be repeated according to the Intervals specified. The Continuing Actions rows block will be repeated as required depending on the number of samples entered when creating a LabBook from this Templates, see "Creating LabBooks" on page 4-24.
5. Type a **Label** for each row and define the columns to your needs.

   Tip For details on the columns, see "Sample Definition for a Template" on page 5-5.
6. Type a **Label** and select **QC** for the column **Sample Type** for your QC rows.

7. For your **Initial Actions** QC row, select a QC test type, for example, ICB or ICV from the drop-down list to specify the **QC Action**.

8. Select a **Standard** where required by the QC test, see Figure 10-28.

Initial Actions

Label		M	Sample T	Internal Standard	Standard		QC	QC Rest		Rack	Vial
BLK	0	3	BLK	Internal Standard		1	None			1	1
Calibration 0.5 J	0	3	STD	Internal Standard	0.5 J	1	None			1	2
Calibration J	0	3	STD	Internal Standard	J	1	None			1	3
Calibration 2J	0	3	STD	Internal Standard	2 J	1	None			1	4
Rinse	0	3	UNKNOWN	Internal Standard		1	None			1	5
ICB	0	3	QC	Internal Standard		1	ICB	Next sample		1	6
ICV	0	3	QC	Internal Standard	J	1	ICV	Next sample		1	7
Rinse	0	3	UNKNOWN	Internal Standard		1	None			1	5

Figure 10-28. QC action ICV defined as Initial Actions row

9. Select an action from the drop-down list for the column **QC Restart** for your Initial Actions QC row.
This action takes effect if the QC test failed.

10. For **Continuing Actions** rows, type a **Label** and select **QC** for the column **Sample Type** for your QC test rows.
The color of the row changes to light red to indicate a QC sample type.

11. Select a **Standard** where required by the QC test, and select an action from the **QC Restart** and **QC Action** drop-down lists, see Figure 10-29.

Continuing Actions

Interval		K	Label	S	M	Sample T	Internal Stan	Standard		QC Action	QC Restart	QC Reference	Rack	Vial
1			BLK	0	3	UNKNOWN	Internal Standard		1	None		BLK	Standard	1
1			PRB	0	3	QC	Internal Standard		1	PRB	After previous QC		Standard	1
1			Sample 1	1	3	UNKNOWN	Internal Standard		1	None		Sample 1	Standard	1
1			DUP	0	3	QC	Internal Standard		1	DUP	After previous QC	Sample 1	Standard	1
1			SER	0	3	QC	Internal Standard		100	SER	After previous QC	Sample 1	Standard	1
1			LFB	0	3	QC	Internal Standard	J	1	LFB	After previous QC	BLK	Standard	1
1			MXS	1	3	QC	Internal Standard	2 J	1	MXS	After previous QC	Sample 1	Standard	1
1			PDS	0	3	QC	Internal Standard	J	1	PDS	After previous QC	Sample 1	Standard	1
1			MTB	0	3	QC	Internal Standard		1	MTB	After previous QC		Standard	1
1			Rinse	0	3	UNKNOWN	Internal Standard		1	None			Standard	1
10			LCS	0	3	QC	Internal Standard	LCS STD	1	LCS	After previous QC		Standard	1
10			QCS	0	3	QC	Internal Standard	QCS STD	1	QCS	After previous QC		Standard	1

Figure 10-29. QC test types example definitions in Sample Definition

In our example, all QC samples are shown once correctly defined for purely demonstrative reasons. Usually, you choose only one or two QC types in your experiment.

For some QC test types, for example **MXS**, you may refer to this QC test row with a <*unique ID*>. The <*unique ID*> can be freely defined. This exact same <*unique ID*> needs to be entered for **QC Reference** in the sample row from which you wish to refer.

12. Type a <*unique ID*>, in this example, *BLK* and *Sample 1*, in the **QC Reference** column of the appropriate UNKNOWN sample rows.

13. Repeat this <*unique ID*> in the appropriate QC test row.
In this example, *BLK* is repeated in the **QC Reference** column for the **QC Action** column **LFB**, and *Sample 1* is repeated in the **QC Reference** column for the **QC Action** column **DUP**, **SER**, **MXS**, and **PDS**.

14. Define **End Actions** rows, as appropriate, see Figure 10-30.

End Actions

Label	Surv	M	Sample Type	Internal Standard	St	D	QC Action	Q	]Q	Rack	Vial
Rinse	0	3	UNKNOWN	Internal Standard		1	None			Standard	1
Rinse	0	3	UNKNOWN	Internal Standard		1	None			Standard	1
Rinse	0	3	UNKNOWN	Internal Standard		1	None			Standard	1

Figure 10-30. QC Sample Definition End Actions

In this example, the QC Action column entries are defined as *None*.

15. Create a LabBook from this Template as described in "Creating a LabBook for Analysis with eQuant Evaluation" on page 10-35.

❖ **To use averaged unspiked analyses**

For the QC tests Paired Sample, Paired Sample EPA, Spike and Spike ARC, an average calculated from multiple unspiked samples can be used in recovery calculations.

1. Assign multiple unspiked analyses their own individual QC Reference tag.

2. Enter these tags in the QC Reference for the Spike Recovery QC test. The average of the tagged unknown analyses will be used in the Spike Recovery calculation.

	Label	rnal St	Standard	Dilution	QC Action	QC Restart	QC Reference	Special Blank
1	Blk			1	None			
2	Blk			1	None			
3	Blk			1	None			
4	Blk			1	None			
5	Blk			1	None			
6	STD 0.5 ppb		STD 0.5 ppb	1	None			
7	STD 5 ppb		STD 5 ppb	1	None			
8	STD 50 ppb		STD 50 ppb	1	None			
9	Unknown			1	None			
10	Unknown			1	None		Ref1	
11	Unknown			1	None		Ref2	
12	Unknown			1	None		Ref3	
13	Unknown			1	None			
14	QC		STD 5 ppb	1	MXS	QC.Next	Ref1,Ref2,Ref3	
15	Unknown			1	None			

Figure 10-31. Assigning multiple unspiked unknown analyses for use in a MXS recovery QC test

Tip Use a comma as a separator for multiple QC Reference tags.

Post Analysis Modification of QC Parameters

If you want to make changes in the defined QC tests after the LabBook is completed, you must grant the relevant Qtegra user group with the appropriate access rights. For details, see "Granting Access Rights" on page 3-4.

Tip Initially, no Qtegra user group has appropriate access rights to make these changes.

❖ To change QC parameters

1. With the correct access rights, open your LabBook and select the Sample List, see Figure 10-32.

	Label	rnal St	Standard	Dilution	QC Action	QC Restart	QC Reference	Special Blank
1	Blk			1	None			
2	Blk			1	None			
3	Blk			1	None			
4	Blk			1	None			
5	Blk			1	None			
6	STD 0.5 ppb		STD 0.5 ppb	1	None			
7	STD 5 ppb		STD 5 ppb	1	None			
8	STD 50 ppb		STD 50 ppb	1	None			
9	Unknown			1	None			
10	Unknown			1	None			
11	Unknown			1	None			
12	Unknown			1	None			
13	Unknown			1	None			
14	QC		STD 5 ppb	1	CCV	QC.Next		
15	Unknown			1	None			

Figure 10-32. Initial view of a Sample List

Tip Only the QC parameters QC Action and QC Reference can be edited post analysis.

2. For example, when changing the QC Action to a Spike Test (in the example change from *CCV* to *MXS*), the QC Reference must sometimes also be modified.

	Label	rnal St	Standard	Dilution	QC Action	QC Restart	QC Reference	Special Blank
1	Blk			1	None			
2	Blk			1	None			
3	Blk			1	None			
4	Blk			1	None			
5	Blk			1	None			
6	STD 0.5 ppb		STD 0.5 ppb	1	None			
7	STD 5 ppb		STD 5 ppb	1	None			
8	STD 50 ppb		STD 50 ppb	1	None			
9	Unknown			1	None			
10	Unknown			1	None			
11	Unknown			1	None			
12	Unknown			1	None			
13	Unknown			1	None			
14	QC		STD 5 ppb	1	MXS	QC.Next		
15	Unknown			1	None			

Figure 10-33. Changed QC Action with red indicator showing that a QC Reference must be provided before continuing

3. Tag the QC Reference for an Unknown (in rows 9 up to 12, see Figure 10-34) with a unique (string and/or number) identifier.

4. Enter the sample identifier for the QC Reference in the QC sample (row 14, see Figure 10-34).
The red warning symbol disappears when all tags are referenced.

	Label	rnal St	Standard	Dilution	QC Action	QC Restart	QC Reference	Special Blank
1	Blk			1	None			
2	Blk			1	None			
3	Blk			1	None			
4	Blk			1	None			
5	Blk			1	None			
6	STD 0.5 ppb		STD 0.5 ppb	1	None			
7	STD 5 ppb		STD 5 ppb	1	None			
8	STD 50 ppb		STD 50 ppb	1	None			
9	Unknown			1	None			
10	Unknown			1	None		Ref1	
11	Unknown			1	None			
12	Unknown			1	None			
13	Unknown			1	None			
14	QC		STD 5 ppb	1	MXS	QC.Next	Ref1	
15	Unknown			1	None			

Figure 10-34. QC Action with tagged QC Reference

Creating a LabBook for Analysis with eQuant Evaluation

The LabBook should be based on the Template that you created for your eQuant analysis in Qtegra.

❖ **To create the LabBook for your eQuant analysis**

1. From the **Qtegra - [Home Page]** navigation pane, click **LabBooks**. The **LabBooks** view of Qtegra opens.
2. Type a **Name** for the LabBook and select a **Location**, see Figure 10-35.

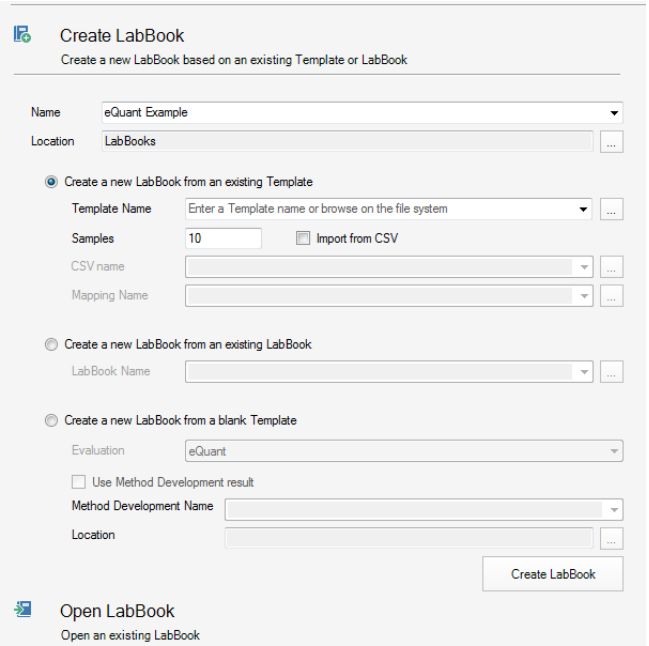


Figure 10-35. Typing the name for an eQuant LabBook

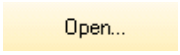
3. Select **Create a new LabBook from a Template**.
4. Select your eQuant **Template Name** from the drop-down list.
5. Type a number for **Samples**.
   To import a Sample List, click **Import from CSV**, and select a **CSV name** and a **Mapping Name** from the drop-down list.
6. Click **Create LabBook** to create the new LabBook.
   A new tab opens for the new LabBook.
7. Check all Method Parameters.
8. Check the Sample List.
9. Make sure that the settings for the autosampler are corresponding to the actual position of vials in the autosampler.

Acquiring Data with an eQuant LabBook

Intensity and concentration data can be reviewed in Qtegra ISDS Software for completed analyses. Spectra View furthermore offers the possibility to look at the emission spectra acquired during the Full Frames runs.

❖ **To run a LabBook**

1. From the **Qtegra - [Home Page]** navigation pane, click **LabBooks**. The **LabBooks** view opens.



2. On the lower part of this view, click **Open**. The **Browse for LabBook** dialog opens.
3. Select the LabBook.
4. Click **OK** to open the LabBook in a new tab.

5. Click **Schedule** to add the LabBook to the Scheduler. If **Automatic** has been selected for **Start Queue** in the **Options** settings of the Scheduler (see "Customizing Scheduler Settings" on page 4-76), the LabBook is started immediately.

During the start of the measurement, the instrument is checked automatically. This check includes a check of the slide valve that may have been set into a closed state. If so, Qtegra indicates *Opening Slide Valve* in the status bar to inform the user about the current state. The slide valve then is opened automatically. Qtegra waits for 5 seconds and repeats the opening procedure if the closed state remains. After a third insufficient trial the LabBook is suspended.

Results and Post Analysis Data Evaluation

For details on viewing results, see "Viewing the Results of a Measurement" on page 6-32.

Depending on the needs of your laboratory, additional, post analysis data evaluation of results may be required.

By inspecting the measured LabBook you may be able to identify potential issues with the measurement and correct or minimize their effect through re-evaluation.

Any changes to the calculated data stored in a LabBook are recorded and can be saved with comments. At no time is the raw, acquisition data in the LabBook modified.

Concentrations

In the Evaluation Results **Concentrations** view of the LabBook in Qtegra, the results of the quantitative analysis are summarized. As with the Sample List, blanks (BLK) are displayed in blue, standards (STD) in yellow, QCs in red and UNKNOWNs in white. The mean, standard deviation (SD) and relative standard deviation (RSD) values as well as the results of each main run are shown when you expand the line. An

entry can be added or removed from the calculation by right-clicking and selecting **Include entry** or **Exclude entry** from the shortcut menu, see Figure 10-36.

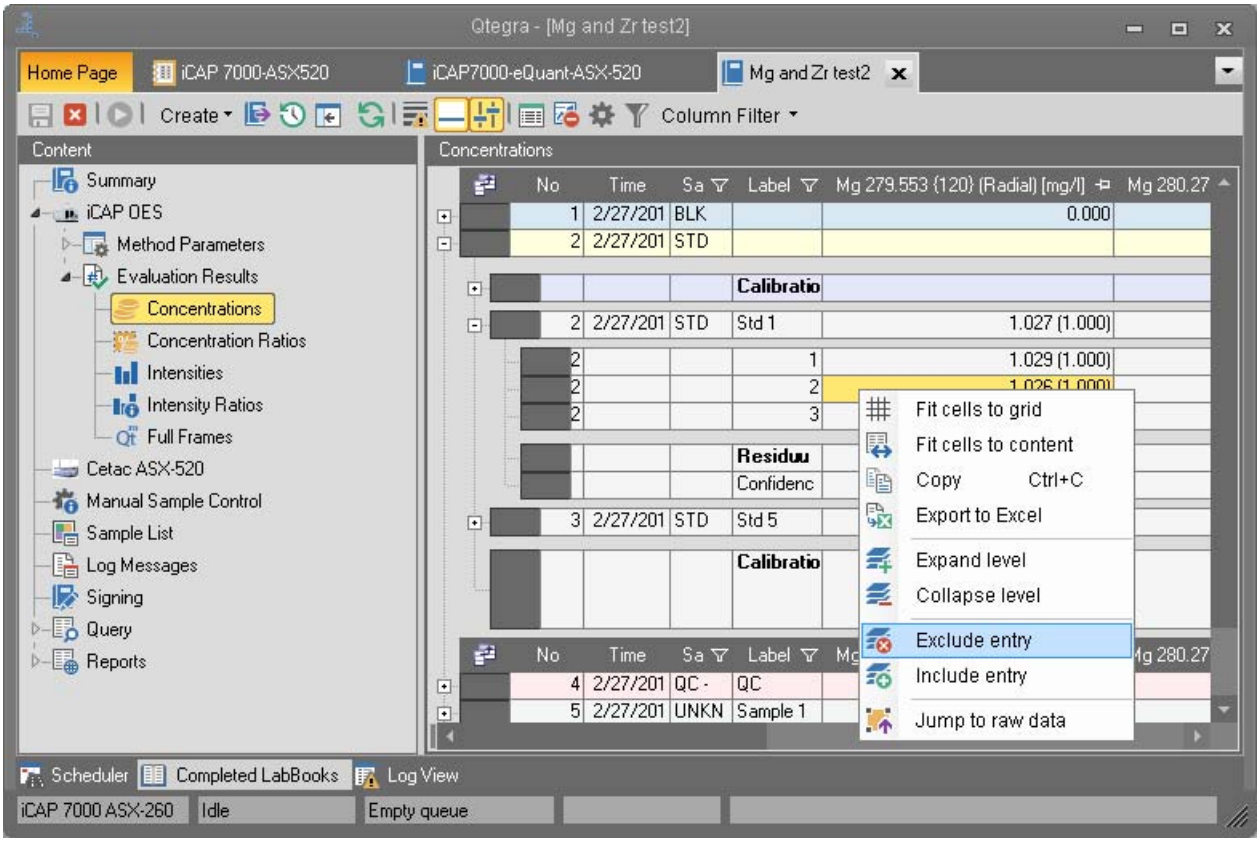


Figure 10-36. Evaluation Results: Concentrations with shortcut menu

Tip When using a very large LabBook, a recalculation, for example, initiated by excluding or including an entry, takes time to display final results. For this busy state, Qtegra displays an additional icon on the toolbar of the Intensities view, the Concentrations view, and the Concentration Ratios view to indicate the calculation running in the background, see Figure 10-37. You can proceed with your next steps, but be aware that the displayed values may change as long as the animated indicator is shown.

Figure 10-37. Busy indicator for background calculation

From the shortcut menu (see Figure 10-36), click **Jump to raw data** for an entry to open the **Intensities** view that shows the corresponding intensity value. This allows you to verify the value.

Values in brackets represent the expected concentration of the standard. The recovery of the internal standard is displayed in percent relative to the first sample acquired. Double-click one of these values to plot the recovery against the sample number.

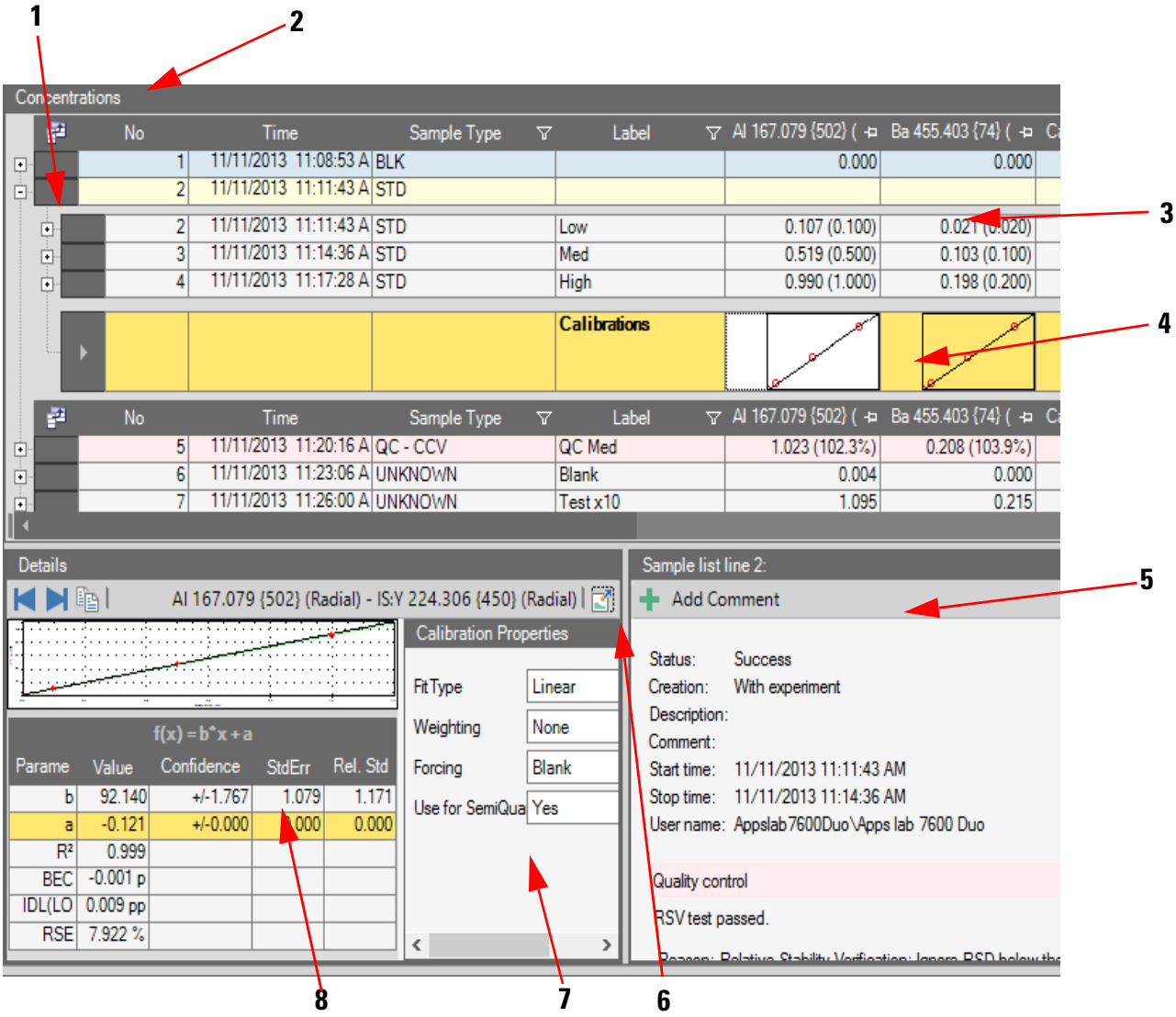
❖ To display details

1. In the Evaluation Results Concentrations list, click the first cell (**1** in Figure 10-38) of the desired line to select one sample.
   The selected sample is indicated by a triangle and highlighted with yellow background.

2. On the toolbar, click **Display Details** (**2** in Figure 10-38),
   -or-
   Double-click a cell with the concentration value,
   -or-
   Click **[+]** in front of the sample line to expand the entry and double-click the thumbnail of the calibration curve.

An enlarged graph of the calibration curve is displayed on the lower left side (**8** in Figure 10-38), including the calculated values for the background equivalent concentration (BEC), the instrumental detection limit (IDL) as well as the most common statistical data to assess the

quality of the fit. The green area in the graph represents the confidence delta at 90% while each point is displayed with its standard deviation, see Figure 10-38.



Labeled Components: 1=Triangle as selection indicator, 2=Details button, 3=selected line, 4=thumbnail of calibration curve, 5=Comment tile, 6=Maximize button, 7=Calibration Properties tile, 8=Details view with parameter table

Figure 10-38. Evaluation Results: Concentrations details

The values are automatically updated when values are included or excluded or the settings in the "Quantification" on page 9-33 view of the Method Parameters are changed.

You can further enlarge the graph by clicking **Maximize** (**6** in Figure 10-38). Right-click the graph to display options to copy or save the graph or to display the data logarithmically.

Click **Restore** to fit the graph back to its initial pane.

Comments for each sample line can be added by clicking **Add Comment** (**5** in Figure 10-38) in the right tile of the **Details** view.

Calibration Properties (**7** in Figure 10-38) may be adjusted locally from this view as well. Any change in calibration properties made to an element here is applied locally to both the calibration and displayed results in the Concentrations view.

The toolbar of the Concentrations view offers a button to perform a **Recalculation**.

Buttons with correction functions allow to switch on/off the mathematical **Interference Correction** and to switch on/off the **Use** of **Internal Standards**. In the Comment tile, the Quality Control results are always shown based on the correction functions (including the **Blank Correction**) enabled. In case you have copied a LabBook from a LabBook where the correction functions of the Method Parameters are not used, the Quality Control nevertheless shows the values with correction functions.

Click **Blank Correction** to switch on/off the blank correction. If no ZERO STD is selected, the blank correction includes the measured intensity of the different wavelengths into the calibration plot with a concentration of *0* (BLK). If one or more samples in the Sample List are indicated as ZERO STD (to perform a standard addition), the correction is done by subtraction of the intensities determined for this sample.
Blank correction can lead into negative concentrations as Qtegra consequently calculates the measured concentration minus BLK concentration, see Figure 10-39.

Sample Type	Label	Ni 345.847 {97} (
UNKNOWN	NKO	0.320
UNKNOWN	NKO	0.296
BLK		0.348
ZERO STD		0.915
UNKNOWN	R0	0.327
	1	0.332
	2	0.321
	Mean:	**0.327**
	RSD [%]:	2.5
	SD:	0.0

	Ni 345.847 {97} (
	0.320
	0.296
	0.348
	0.567
	-0.021
1	-0.016
2	-0.027
	-0.021
	38.3
SD:	0.0

Figure 10-39. Analyte concentration before and after Blank correction

The history of the changes made to the LabBook are displayed by clicking **History** on the toolbar. Options to export the results are shown by clicking **Export** (see Figure 6-3). The button **Create** allows you to set up a new LabBook or Template from the one already measured with its current settings. See also "LabBook Toolbar" on page 6-2.

Internal Standard Correction

The reference value of an Internal Standard (IS) is defined by the average intensity of the Internal Standard analyte in the first blank of the current standard block or by the first standard in case a blank is not present.

Internal Standard correction is applied on a per run basis. That means, the per run intensities of both the analyte and its defined internal standard are ratioed to generate the internal standard corrected intensities which carried through in the calculation process.

You can change an Internal Standard correction for each measured sample after completion of the LabBook.

❖ **To change an Internal Standard correction**

1. Open your finished LabBook.
2. Select **Concentrations** from the Evaluation Results section to display the table of all measured samples.

3. Right-click the concentration cell of an UNKNOWN or QC sample to open the shortcut menu, see Figure 10-40.

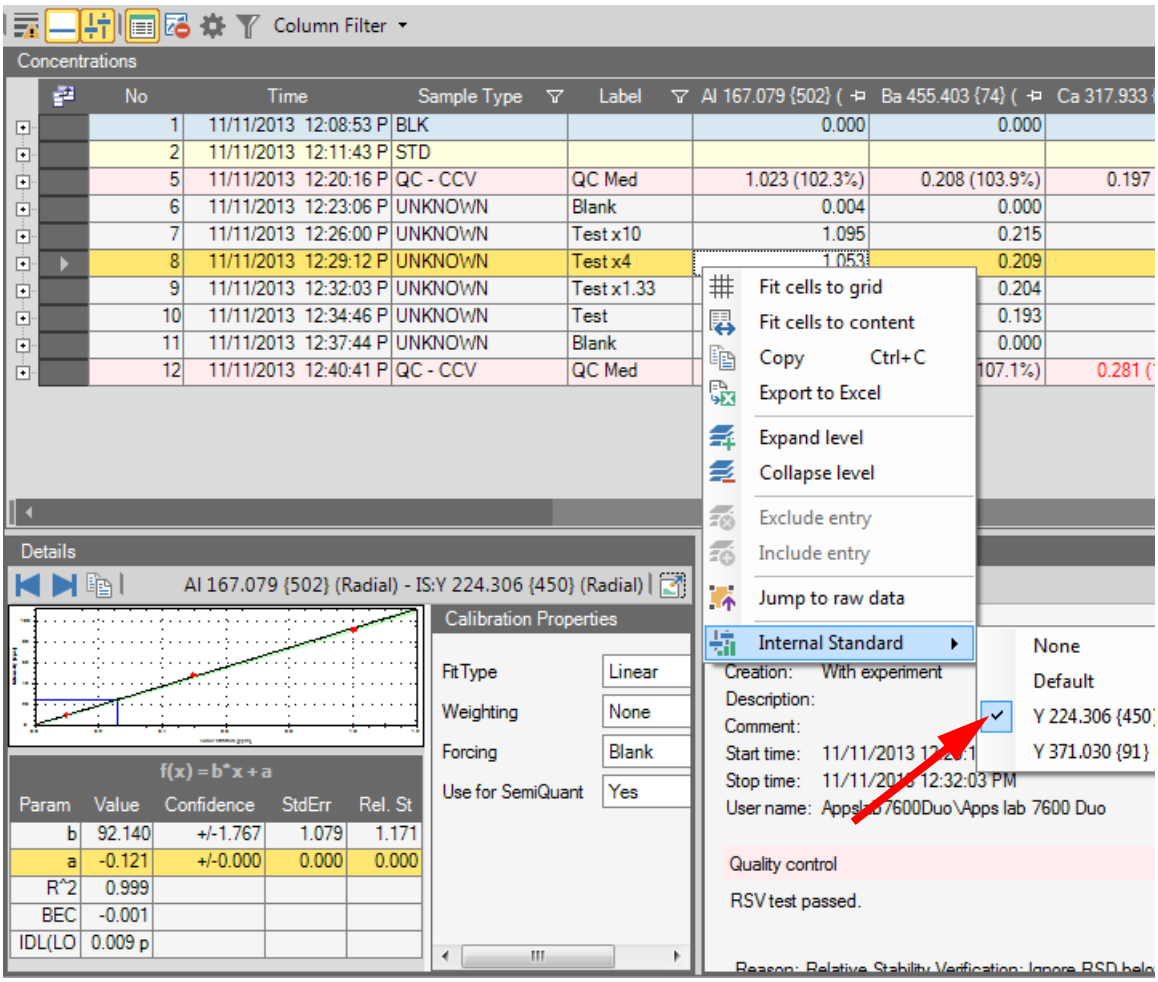


Figure 10-40. Shortcut menu for Internal Standard

4. Open the sub-menus from **Internal Standard** to select the desired Internal Standard for this element.
   The currently selected choice for IS correction is highlighted by a check mark.

5. At the same time you will see the change made in the Details view of the calibration curve for that analysis, see the red arrow on Figure 10-40, where the element and its corresponding IS are shown.

Tip When you select a series of cells either per element (column), per analysis (line), or by freehand selection and select an Internal Standard from the shortcut menu, you are changing the IS for the selected cells only. Right-click selection of the Internal Standard is only possible for the UNKNOWN and QC sample types. If your selection contains the sample types BLK, STD, AVERAGE BLK, ZERO STD, right-click choice of Internal Standard is not available.

Through this right-click selection of Internal Standard you are **not** changing the selected IS in non-selected cells or for the Blanks and Standards in the LabBook.

To change the IS selection used in the calibration (BLKs and STDs) you must update the **Quantification**.

Changes to IS selection in the **Quantification** page overwrite any changes made locally in **Concentrations** and set the IS in all analyses (BLK, STD, UNKNOWN etc).

❖ To reset Internal Standard settings of one analyte

1. To set the Internal Standard of the current selection back to the default, right-click the current selected concentration cell to open the shortcut menu.

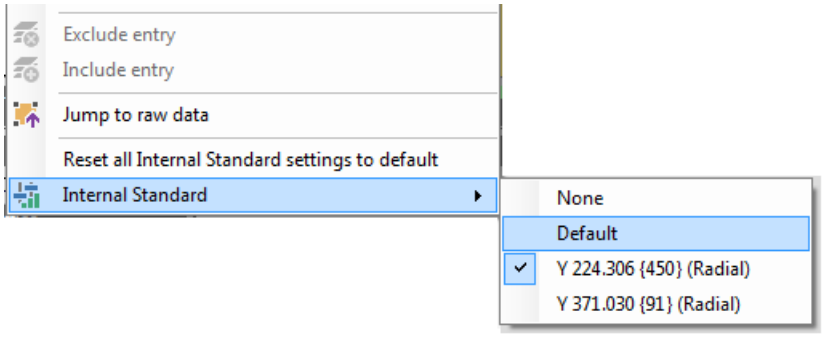


Figure 10-41. Shortcut menu with Internal Standard item

2. Select **Internal Standard** > **Default**.
The Internal Standard changes to the default element, which is defined in the Quantification view.

Tip Resetting the Internal Standard to Default does not affect the Calibration Properties parameters shown in the Details view. This command only sets the Internal Standard back to the default element.

❖ To reset all Internal Standard settings

1. To set the Internal Standard settings for all analytes back to the defaults, right-click anywhere in the **Concentrations** table to open the shortcut menu.

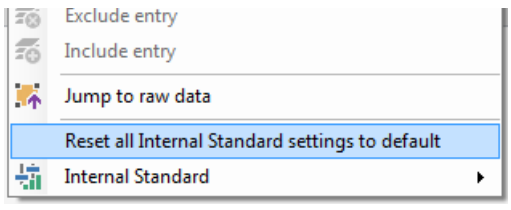


Figure 10-42. Shortcut menu with Reset all Internal Standard item

2. Select **Reset all Internal Standard settings to default**.
   All Internal Standards change to the respective elements, which are defined in the **Quantification** view.

   Tip Resetting all Internal Standard settings to default does not affect the Calibration Properties parameters shown in the Details view. This command only sets all Internal Standards back to the defaults.

Dependencies between the Quantification and the Concentrations View

To understand the effect for the **Concentrations** view on changes on the **Quantification** view, some user actions will be described.

As shown above, changes to the Internal Standard can be performed per analyte. You can also change the Calibration Properties per analyte. These changes remain as set by you and are shown in the Details tile on the **Concentrations** view. Further activities on the **Concentrations** view, for example, changing or resetting Internal Standards, do not affect the Calibration Properties.

Tip When copying a LabBook from a LabBook, the Internal Standards are taken from the default settings defined in the **Quantification** view.

When you change parameters in the **Quantification** view, it will affect the calculation shown on the **Concentrations** view. That means, all changes on the **Quantification** view have an impact on the evaluation results. If, for example, the IS for an analyte has been changed in the **Concentrations** view and the IS for the same analyte is then later set to another item on the **Quantification** view, the selection in the **Quantification** takes priority.

Concentration Ratios

The Evaluation Results **Concentration Ratios** view of the LabBook shows the ratios for each pair of wavelengths entered in the Method Parameters section related to the determined concentrations, see Figure 10-43.

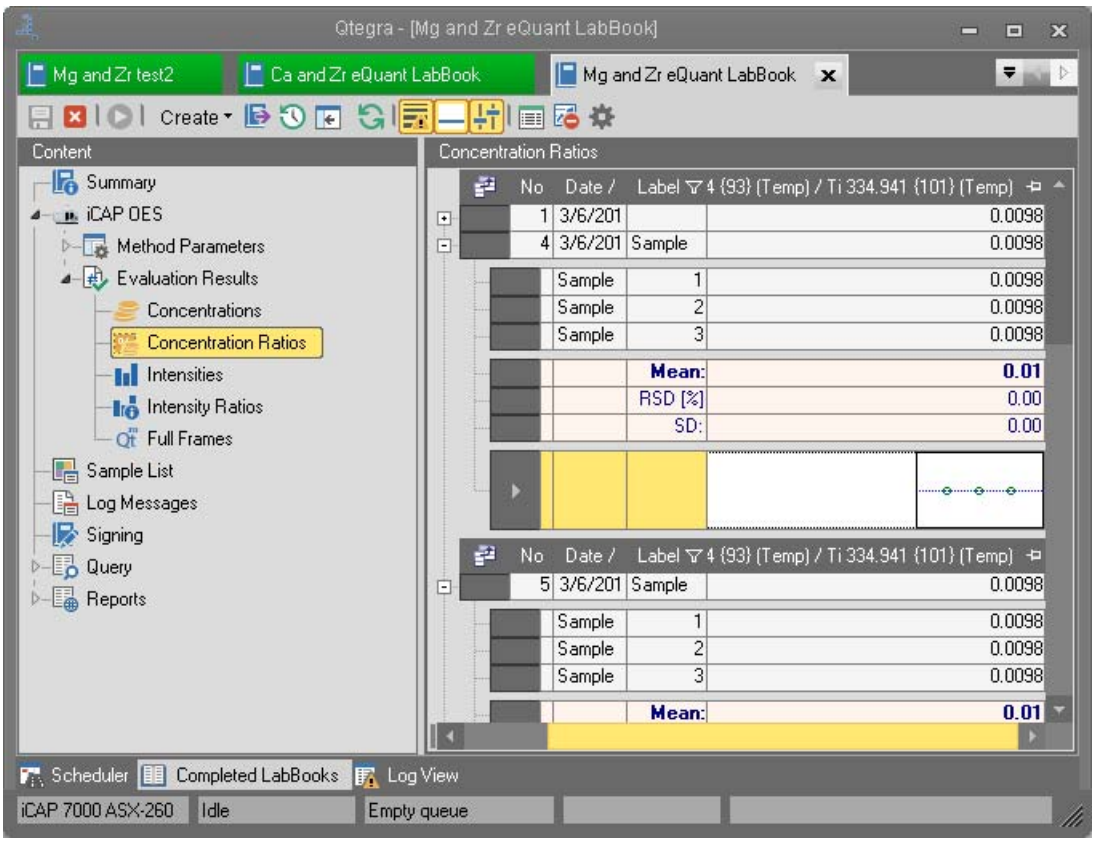


Figure 10-43. Evaluation Results: Concentration Ratios

Intensities

The Evaluation Results **Intensities** view of the LabBook in Qtegra displays the raw intensities. If the entries are shown in bold type, at least one sweep within one main run was measured using the analog mode of the detector. If the entries are displayed in blue instead of black, they

were manually edited, for example, the result of one main run was removed from the calculation of the average after the measurement, see Figure 10-44.

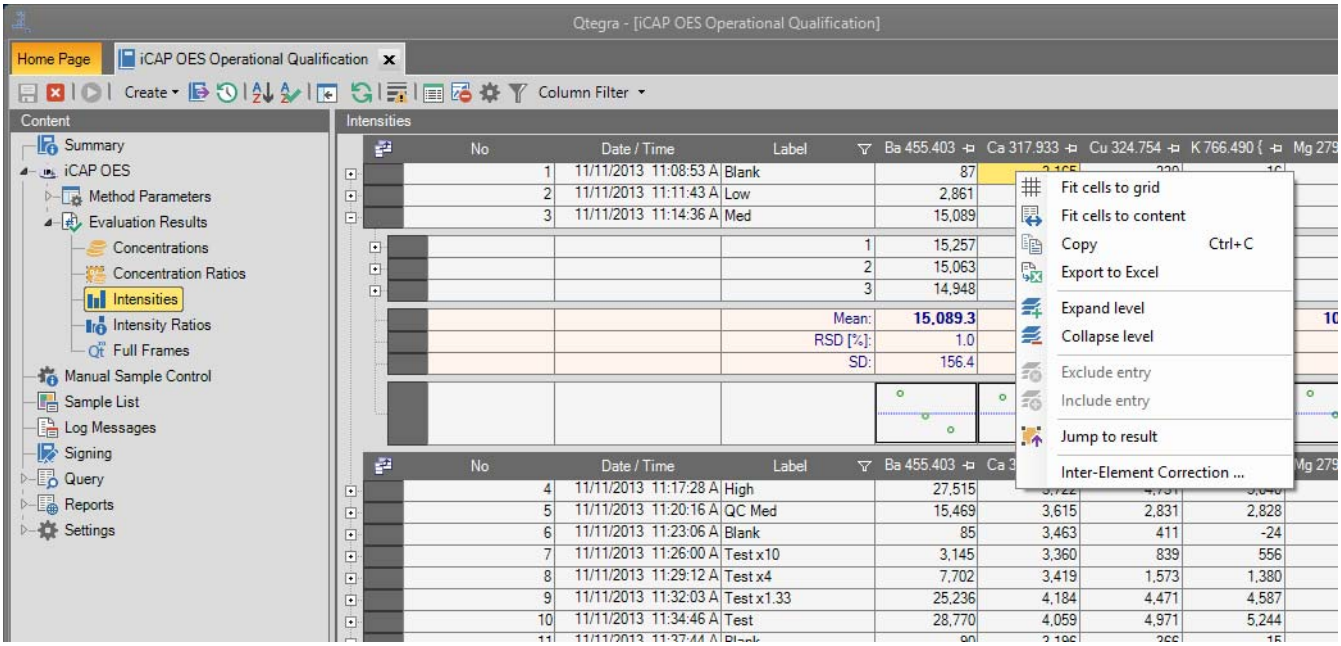


Figure 10-44. Evaluation Results: Intensities with shortcut menu

From the shortcut menu, select **Jump to result** for an entry to open the **Concentrations** view showing the corresponding concentration value. This allows you to verify the value.

Expand a line to display the mean as well as the standard deviation (SD) and relative standard deviation (RSD) values. In the thumbnails, filled circles indicate that the value was measured in the analog mode, red circles represent excluded entries. The blue line in the Details view represents the mean of the different main runs, see Figure 10-45.

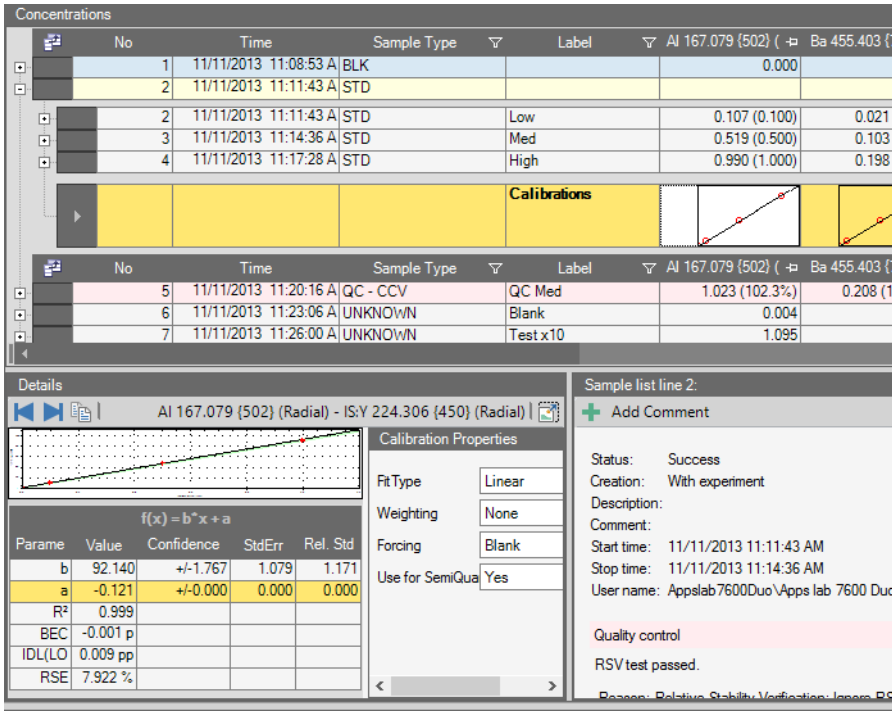


Figure 10-45. Evaluation Results: Concentrations Details

From the Intensities view, right-click the intensity of one of the repeats to open the shortcut menu. When direct spectral overlaps occur, the Inter-Element Correction attempts to correct those (and subsequent contaminated data) by applying a ratioed correction factor to all samples.

Inter-Element interferences occur when elements in the sample emit light at wavelengths so close to that of the analyte that they contribute to the intensity of the light from the analyte. If such conditions exist, the calculation will yield a high concentration for the analyte. Applying Inter-Element Corrections removes the effects of these non-analyte emissions.

❖ To apply inter-element corrections

1. Select **Inter-Element Correction** to open the dialog as shown in Figure 10-46.

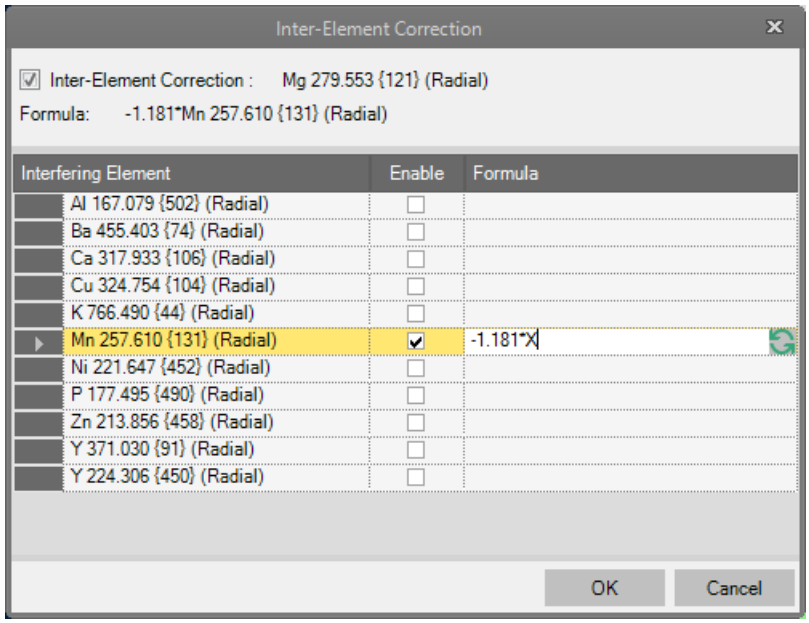


Figure 10-46. Inter-Element Correction dialog

2. Tick the **Enable** check box to activate the correction for the element of the line.

   Click the refresh button of the **Formula** column to show the corresponding correction formula.
   Double-click the formula to change it.

3. Click **OK** to close the dialog and to apply the changes.

The Inter-Element Correction method parameter allows to visualize all the selected corrections and to select/deselect them. Double-click the intended element(s) to change the formulas. This will prompt a second table where this information can be typed.

Double-click the intensity of one of the repeats to open the subarray plot in the bottom (left side) along with a table (right side), see Figure 10-47.

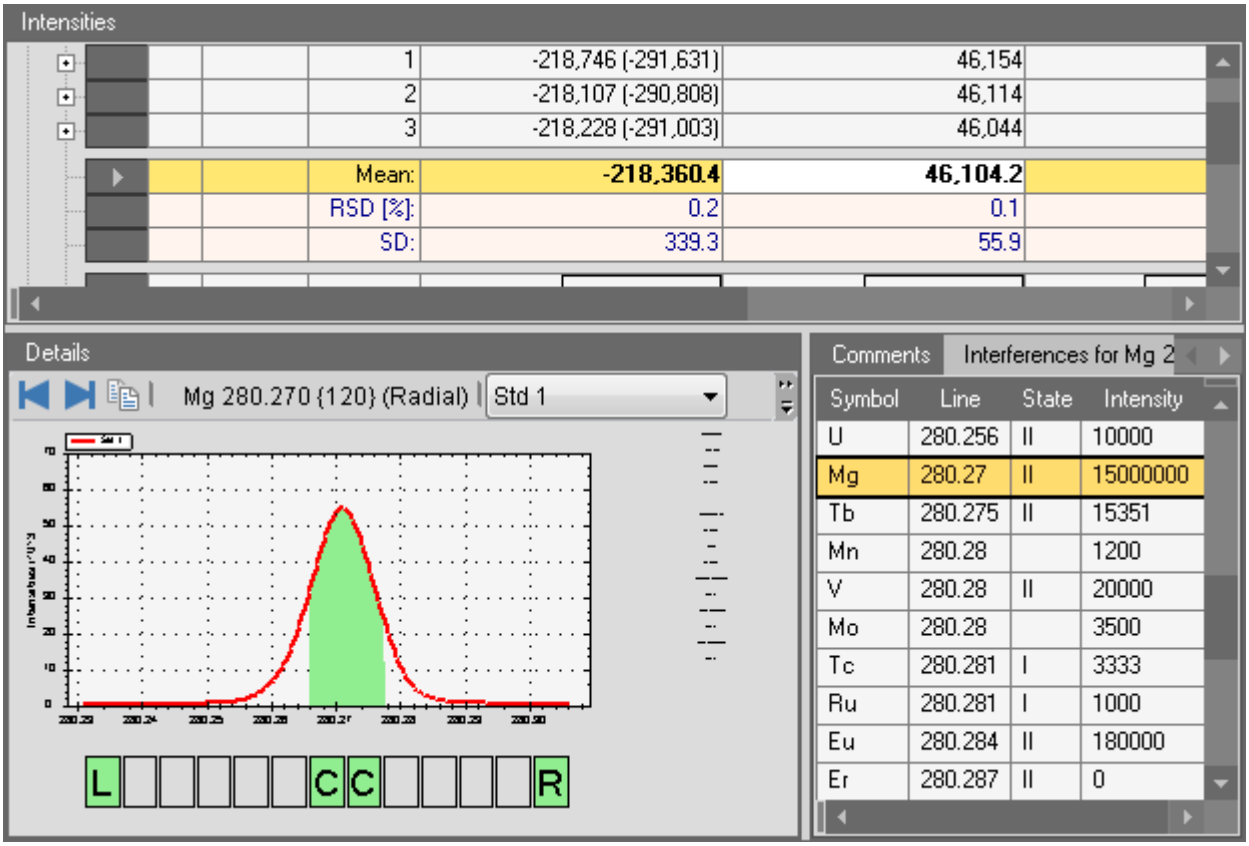


Figure 10-47. Evaluation Results: Intensities subarray plot

The subarray plot represents the region of the CID that has been allocated to that particular element and can be used to determine if a line for a given element is free of interference from lines of other elements. Subarrays are normally examined to check for interferences and ensure that the analytical peak is covered by the central integration area (marked *C* on the subarray plots).

Relevant information related to the analysis is displayed right next to he graph. Wavelength and Intensity change according to the position of the mouse in the graph. Corrected Peak, Peak, Average Background, and Left and Right background change according to the setting in the graph (number of pixels selected).

Right-click the graph to open the shortcut menu, see Figure 10-48.

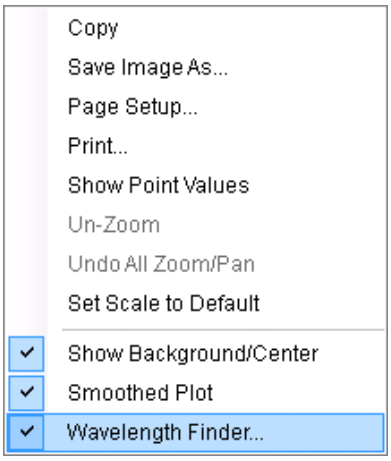


Figure 10-48. shortcut menu of Intensities graph

Without selection, the subarray plot is presented (bar chart). If **Smoothed Plot** is selected, the subarray plot is drawn as a graph, without selection you will see the subarray plot as a bar chart. **Show Background/Center** highlights the central pixel.

The table on the right of the graph is the **Wavelength Finder** and it displays the Symbols with corresponding wavelength (Line), State and Intensity. On the Comments tab, click Add Comment to open the User Comment dialog and to type comments for the selected sample line.

In the toolbar of the **Details** view on the left, **Maximize** enlarges the graph. Click C to change the pre-defined central pixel. Click L and R to change the pre-defined left and right background pixels respectively. Click an empty square to select additional pixels.

Click the analyte column in the Intensities table (right next to **Label**) to overlap the plots of all samples. You can choose the repeat and samples in the drop-down menu, see Figure 10-49.

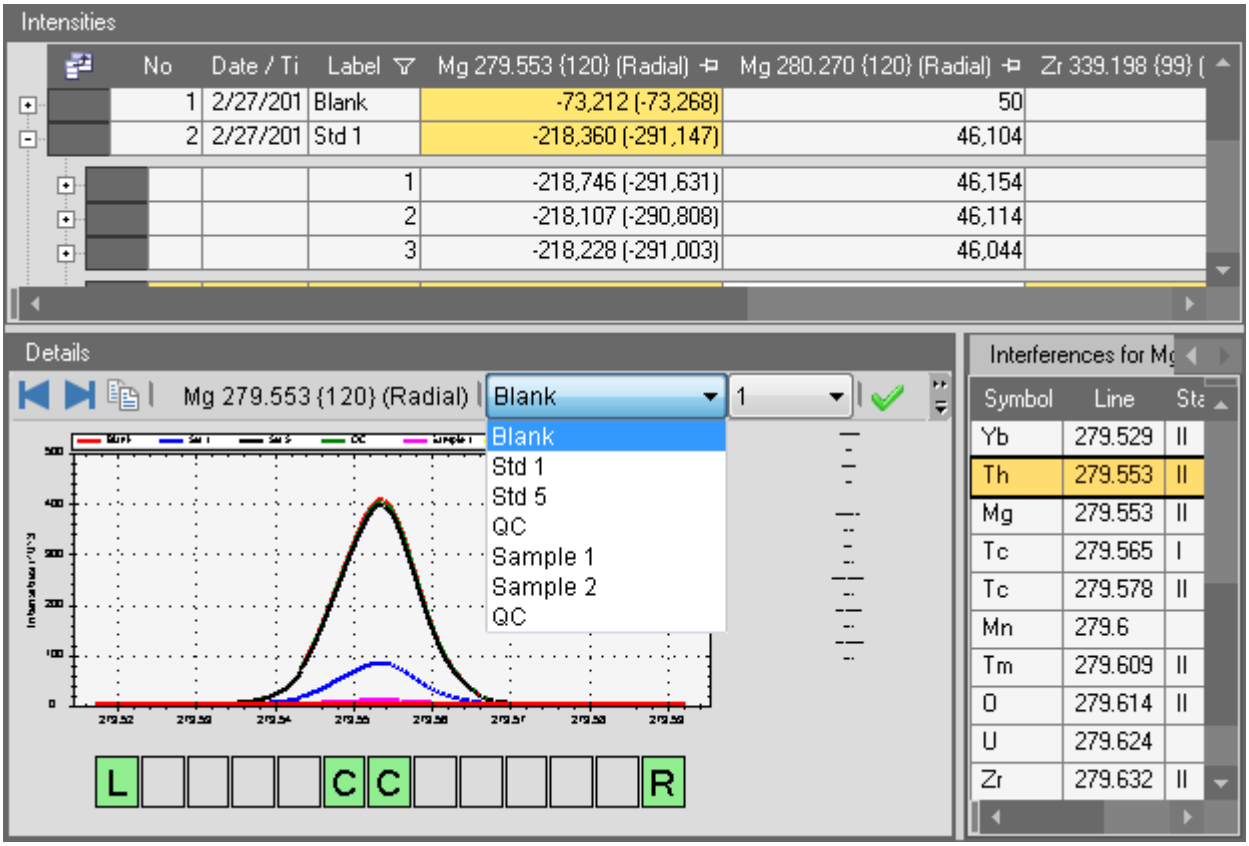


Figure 10-49. Detail subarray plot with drop-down menu

Select the next or previous analyte with the arrows buttons in the toolbar of the **Details** view. Changes are applied with .

Intensity Ratios

The Evaluation Results **Intensity Ratios** view of the LabBook in Qtegra shows the data with reference to the raw intensities. The shortcut menu offers functions to include or exclude single entries, see Figure 10-50.

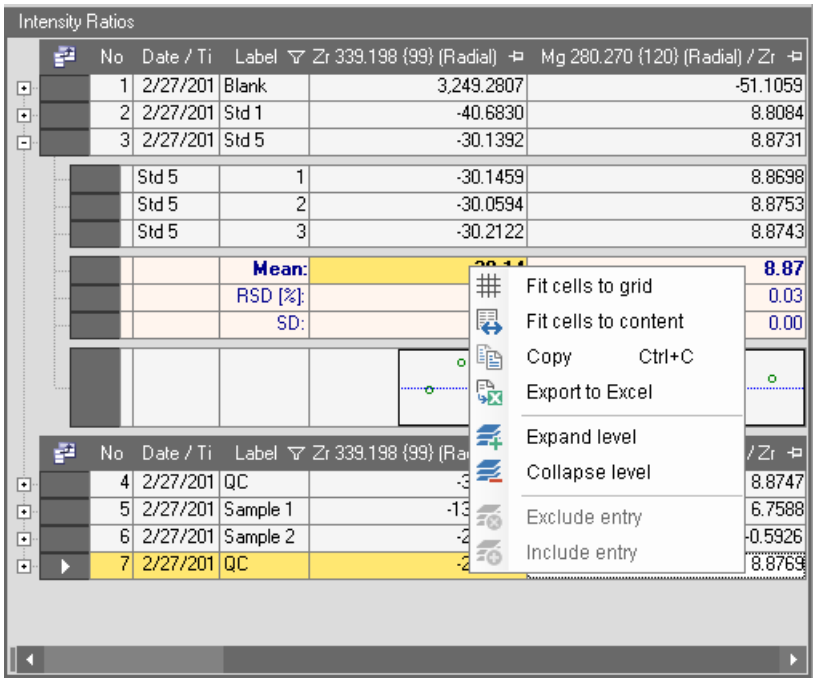


Figure 10-50. Evaluation Results: Intensity Ratios with shortcut menu

Full Frames

With the Evaluation Results **Full Frames** view of the LabBook in Qtegra you can identify all the elements present. Method elements are shown on the right in the **Elements** panel, see Figure 10-51.

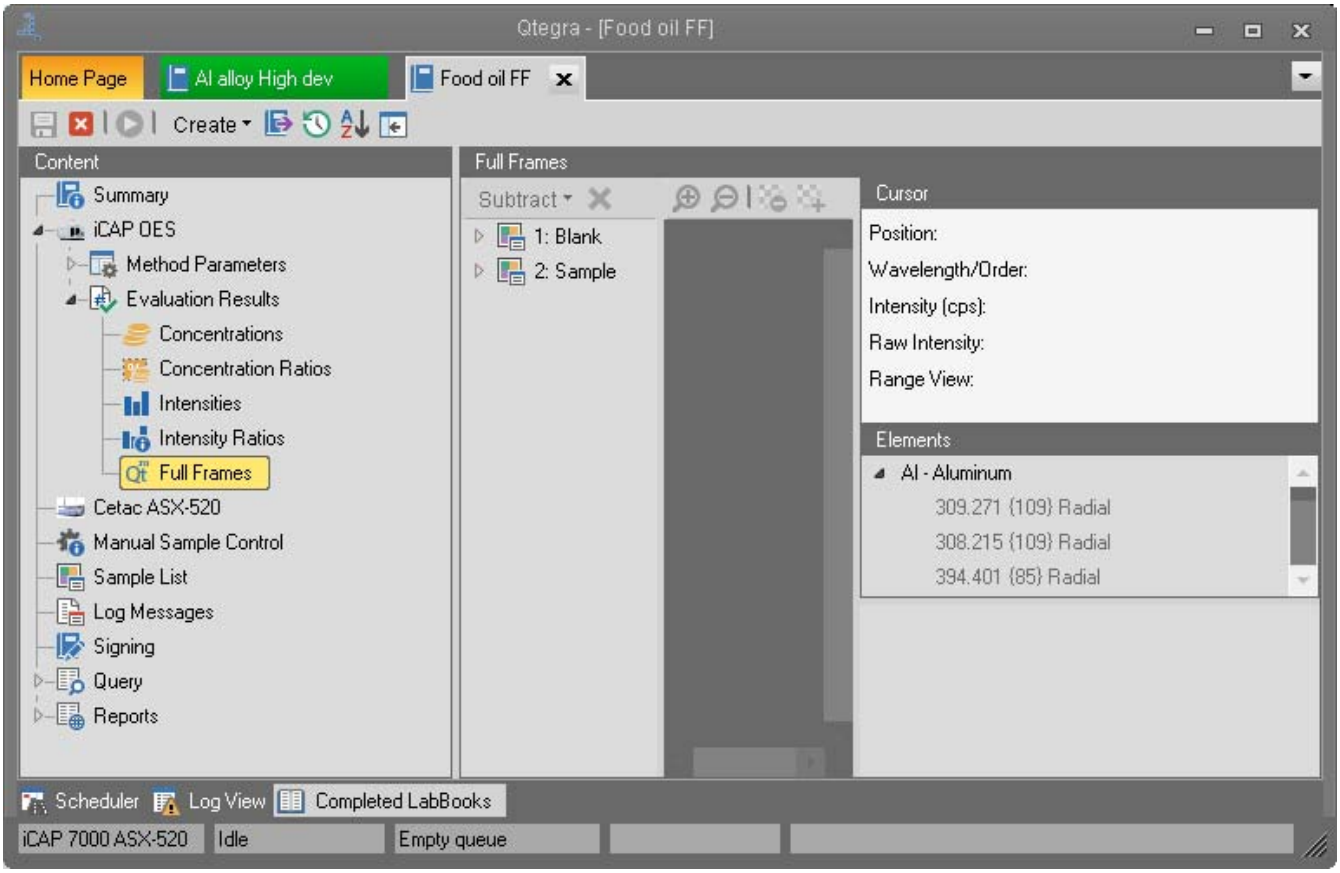


Figure 10-51. Evaluation Results: Full Frames view

The table of **Elements** shows elements and wavelengths that are available.

Click a sample line listed below **Full Frame** to show the graphical representation, see Figure 10-52.

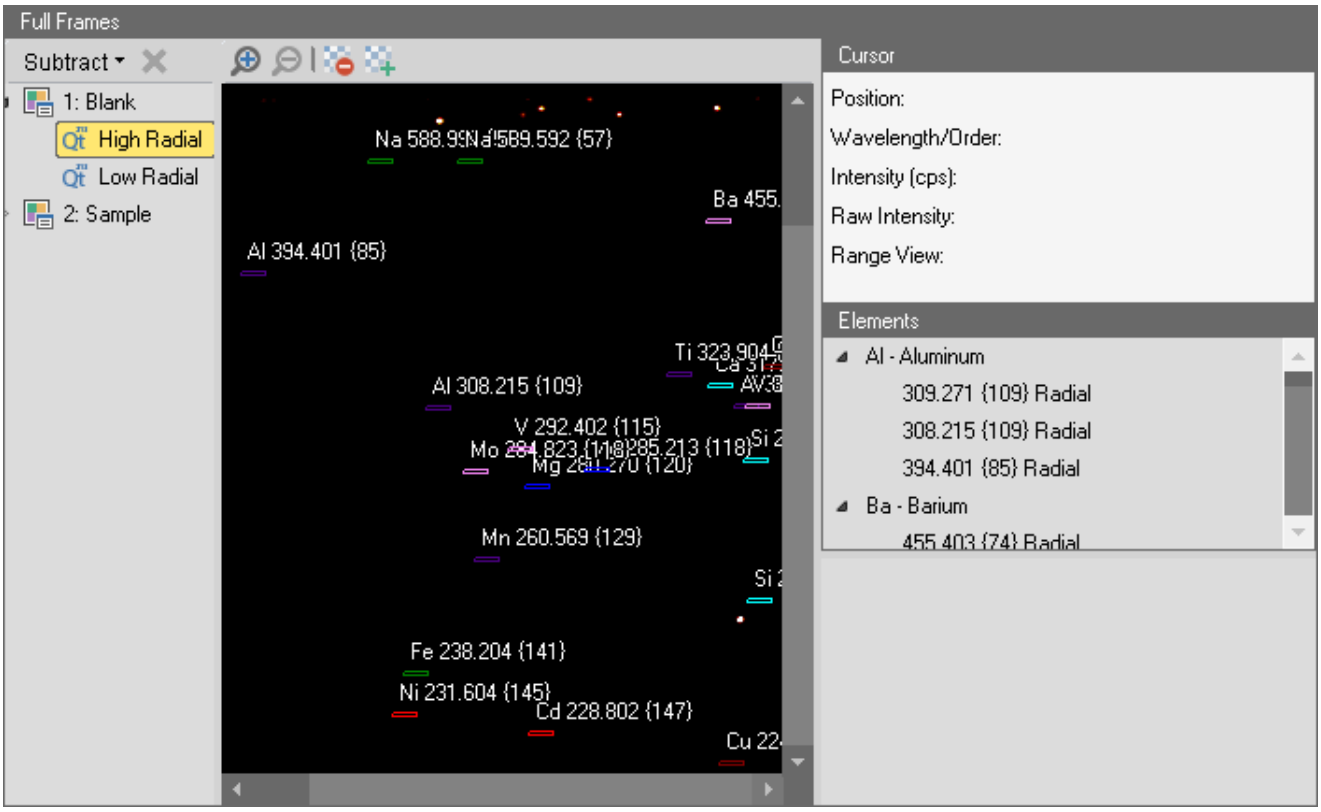


Figure 10-52. Full Frame results with graphical representation

A Full Frame is a graphical depiction of the CID chip. The Full Frame image presents a complete spectrum of all lines that are emitted by the sample.

If additional elements of interest are observed, you can identify them using the wavelength finder function that becomes available on the right side below **Elements** when you click an element in the graphical representation, see Figure 10-53.

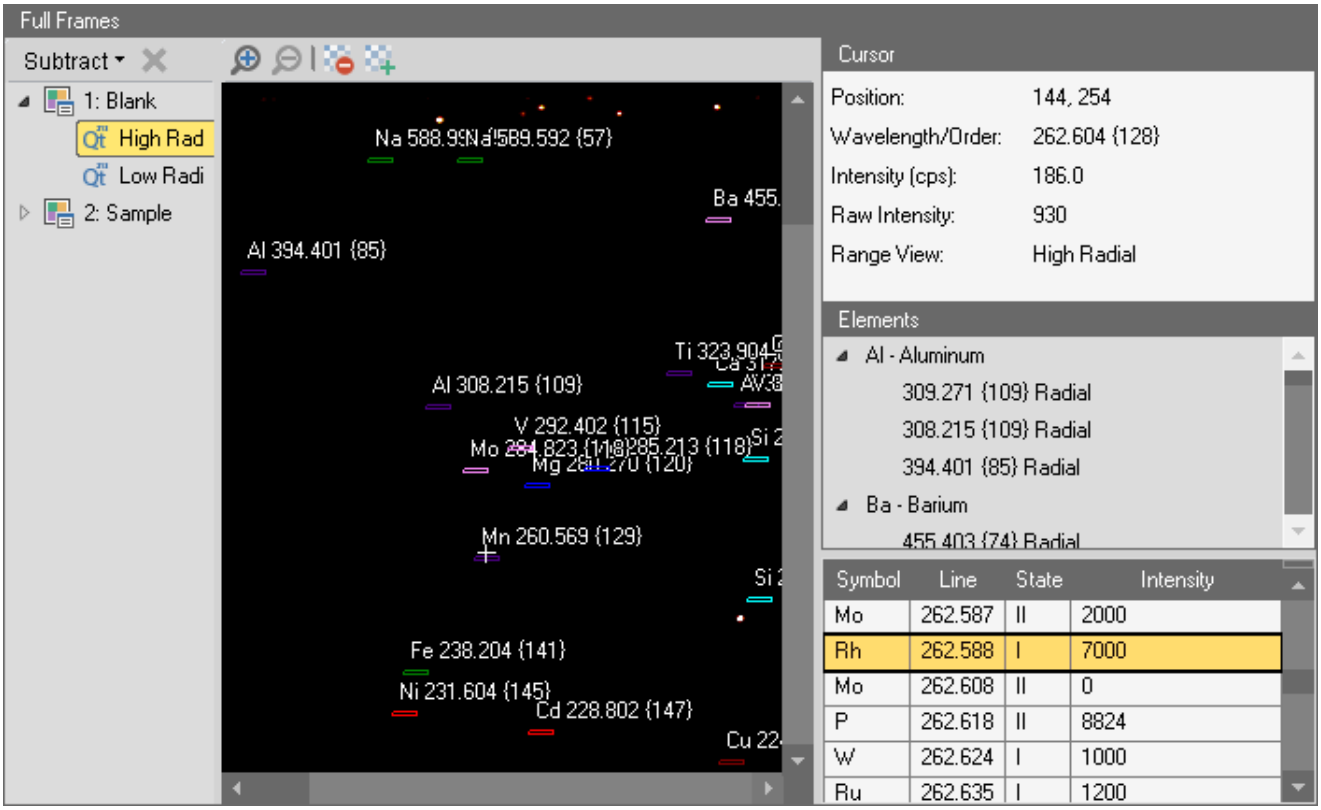


Figure 10-53. Full Frame results showing the wavelength finder

The **Cursor** section on the top right displays the **Position**, **Wavelength/Order**, **Intensity**, and **Raw Intensity** information for the **Range View** selected when you clicked into the full frame image.

You can identify method and non-method elements at the click of a button using the wavelength finder. The zoom function allows you to focus on a particular area of interest. Click to zoom out again.

Right-click a line in **Elements** to zoom into or to remove the selected line, see Figure 10-54.

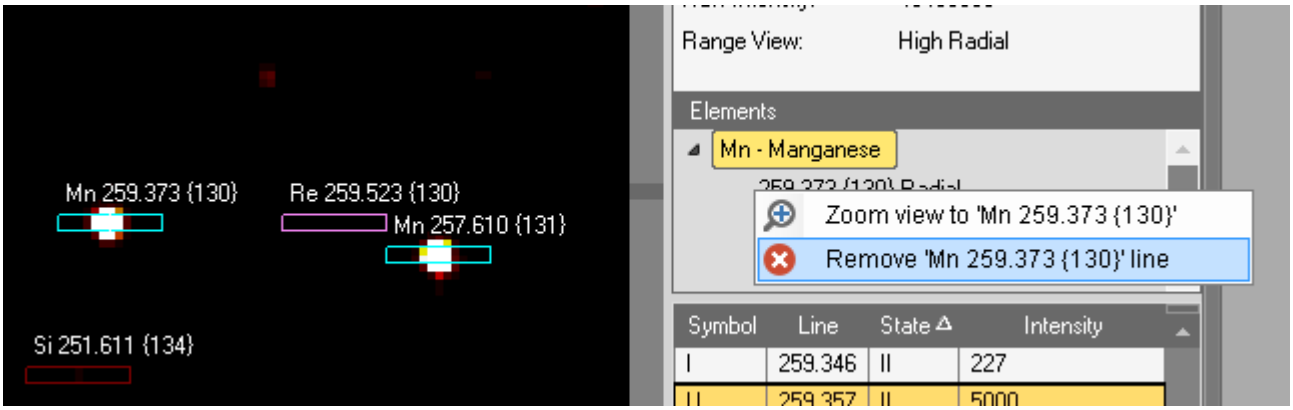


Figure 10-54. Full Frame results showing the Elements shortcut items

From the wavelength list, right-click the element you wish to view, and select **Show <element> line** or the **Show primary <element> lines** from the shortcut menu, see Figure 10-55.

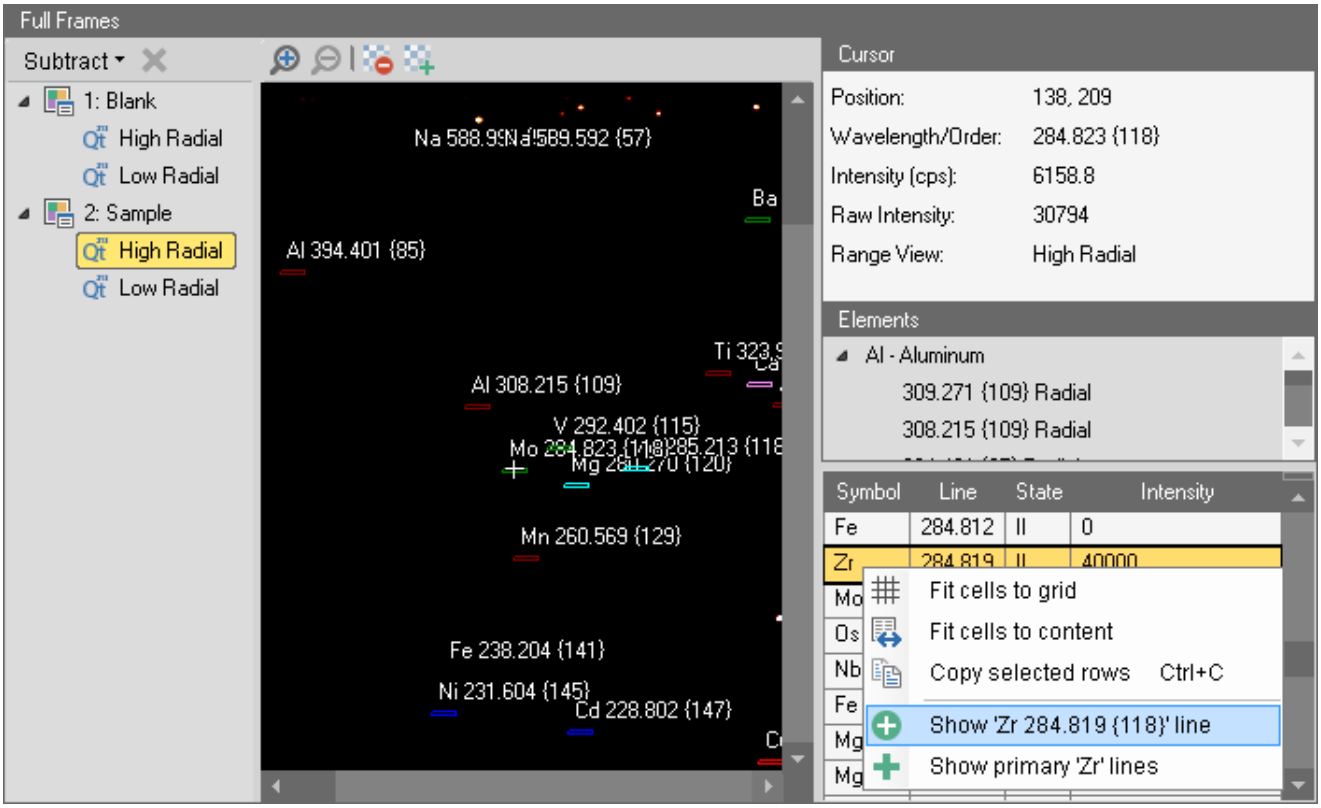


Figure 10-55. Full Frame result view showing the shortcut menu of the wavelength finder

The selected item will be highlighted on the Full Frame display. Right-click the selected element in the wavelength finder to remove it from the display.

Full Frame subtraction allows you to identify contaminants from one batch to the next by subtracting one sample from the other.

Alternatively, a blank sample can be subtracted in order to remove the background, see Figure 10-56.

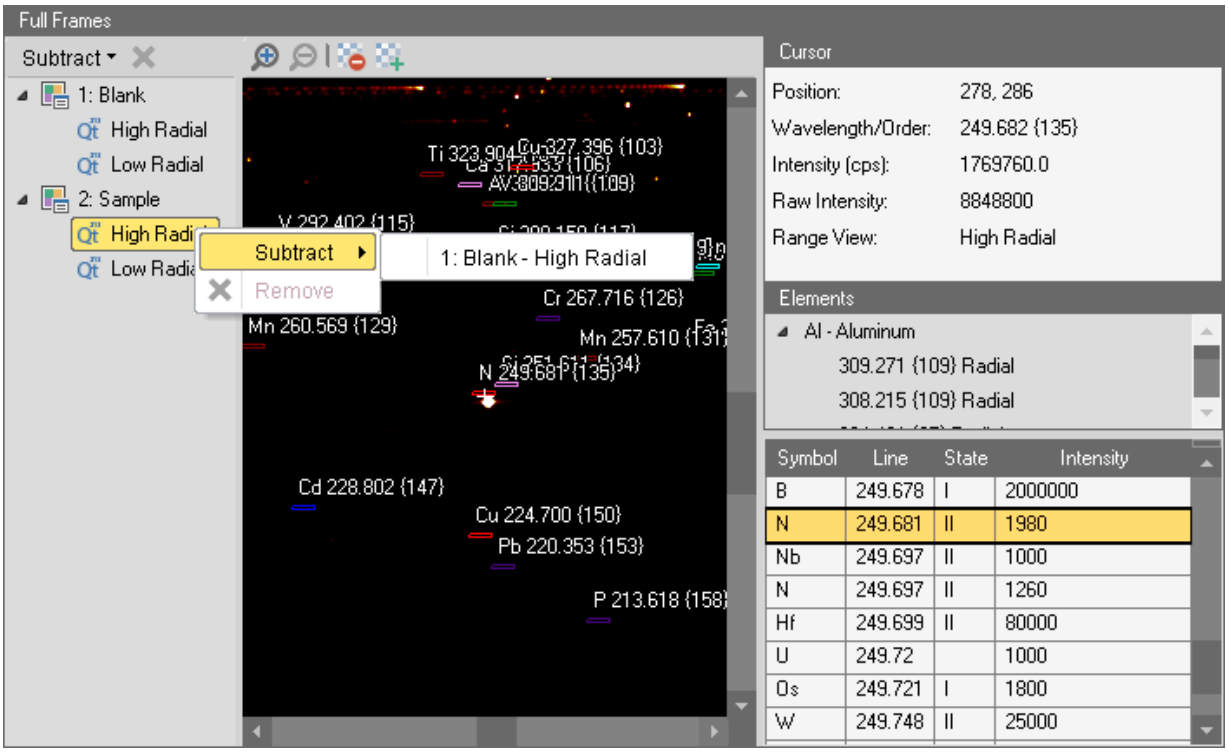


Figure 10-56. Full Frame results view Subtract

When you are working with a Full Frame image, concentrate on the many wavelengths appearing as bright spots in the lower wavelength region of the image.

The top of the image may appear overexposed due to the large amount of background. This background results mainly from argon continuum emission.

The bright spots are elements in your sample. The brightness of the spot is proportional to the concentration of the element, which emits light at that specific wavelength. The brighter the spot, the higher the concentration.

The **Lighten** and **Darken** tools are provided for ease of discrimination between areas of different intensity, so that it is easier to see a line, see Figure 10-57.

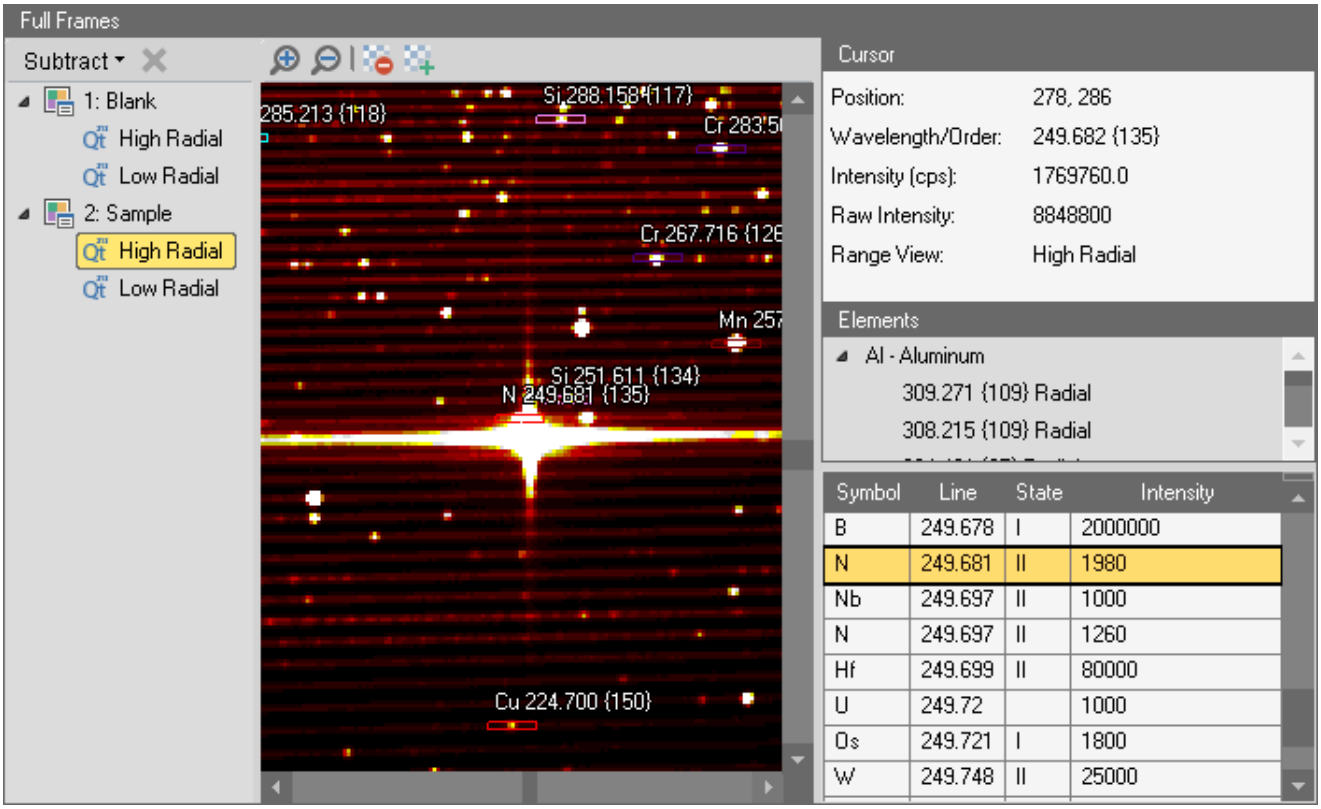


Figure 10-57. Full Frame results view lightened

11

Basic Mathematical Methods

This chapter describes the basic mathematical methods used by Qtegra ISDS Software. It includes information about statistical calculations, linear and polynomial regression as well as Gaussian error estimation for regression analysis.

Contents

Statistical Calculations

Average

For k given values x_1, x_2...x_k the average or mean $\bar{x}$ is defined by

$$\bar{x} = \left(\sum_{i=1}^{k} x_i \right) / k$$

Standard Deviation (SD)

For k given values x_1, x_2...x_k the standard deviation SD is defined by

$$SD = \sqrt{\frac{1}{k-1} \cdot \sum_{i=1}^{k} (x_i - \bar{x})^2}$$

Relative Standard Deviation (RSD)

With $\bar{x} \neq 0$, the relative standard deviation RSD of the k values x_1, x_2...x_k is given by

$$RSD = \frac{SD}{\bar{x}} \cdot 100\%$$

Tip If the software allows values to be excluded then only the included values are used in the calculation.

Relative Standard Error (RSE)

United States EPA SW-846 method 8000D includes the request to use the RSE evaluate in the acceptability of a calibration by evaluating the difference between the measured and true concentrations in a calibration.

With x_i = actual concentration of the calibration level i, x'_i = calculated concentration at level i, n = number of calibration points, and p = number of terms in the fitting equation (linear = 2, quadratic = 3), the relative standard error (RSE, expressed as %) is given by

$$RSE = 100 \times \sqrt{\left(\sum_{i=1}^{n} \left[\frac{x'_i - x_i}{x_i} \right]^2 \right) / (n-p)}$$

Least Squares Fits (LQF)

For given data pairs (x_0,y_0), $(x_1,y_1)...(x_k,y_k)$ and the polynomial function $f(x)=a_bx^b+...a_2x^2+a_1x+a_0$ the solution of a least squares fit is given as the set of parameters a_0, $a_1...a_b$ which minimizes the sum:

$$\sum_{i=0}^{k}[y_i-f(x)]^2 = Min!$$

or in case of weighting (see Table 13-2):

$$\sum_{i=0}^{k}\omega_i[y_i-f(x)]^2 = Min!$$

Linear Least Squares Fit (LLQF)

The curve used for solving the least squares fit problem is given as $f(x)=a_1x+a_0$. This kind of least squares fit is also commonly known as the determination of the linear regression curve. Its parameters a_1, a_0 can be determined by calculating:

$$a_0 = \frac{\left(\sum_{i=0}^{k}y_i\right)\sum_{i=0}^{k}x_i^2-\left(\sum_{i=0}^{k}x_i\right)\sum_{i=0}^{k}x_iy_i}{k\left(\sum_{i=0}^{k}x_i^2\right)-\left(\sum_{i=0}^{k}x_i\right)^2}$$

$$a_1 = \frac{k\left(\sum_{i=0}^{k}y_ix_i\right)-\left(\sum_{i=0}^{k}x_i\right)\sum_{i=0}^{k}y_i}{k\left(\sum_{i=0}^{k}x_i^2\right)-\left(\sum_{i=0}^{k}x_i\right)^2}$$

Weighting can be applied to the formula.

Quadratic Least Squares Fit (QLQF)

The QLQF uses the same basic algorithm with the difference that $f(x)$ is defined as $f(x)=a_2x^2+a_1x+a_0$. Solving the following system of linear equations solves the problem:

$$A\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^{k} 1 & \sum_{i=0}^{k} x_i & \sum_{i=0}^{k} x_i^2 \\ \sum_{i=0}^{k} x_i & \sum_{i=0}^{k} x_i^2 & \sum_{i=0}^{k} x_i^3 \\ \sum_{i=0}^{k} x_i^2 & \sum_{i=0}^{k} x_i^3 & \sum_{i=0}^{k} x_i^4 \end{bmatrix} \cdot \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^{k} y_i \\ \sum_{i=0}^{k} x_i y_i \\ \sum_{i=0}^{k} x_i^2 y_i \end{bmatrix}$$

Weighting can be applied to the formula.

Correlation Coefficient (R)

The Pearson correlation coefficient, R, is a measure of the strength and direction of the linear relationship between two variables that is defined as the covariance of the variables divided by the product of their standard deviations. In Qtegra ISDS Software, the correlation coefficient is calculated as the square root of the coefficient of determination:

$$R = \sqrt{R^2}$$

Coefficient of Determination (R^2)

For n given values $y_1, y_2 \ldots y_n$ the general definition of the coefficient of determination R^2 is given by

$$R^2 = 1 - \frac{ss_{res}}{ss_{tot}} \text{ with } ss_{res} = \sum_{i=1}^{n} [y_i - f_i]^2 \text{ and } ss_{tot} = \sum_{i=1}^{n} [y_i - \bar{y}]^2$$

R^2 can be related to the unexplained variance since the second term compares the unexplained variance (variance of the model's errors) with the total variance.

Tip In linear least squares regression with an estimated intercept term, R^2 equals the square of the Pearson correlation coefficient between the observed and modeled data values of the dependent variable.

Error Estimation and Confidence Intervals

Error Estimation for Linear Regression

Let $y = a_1x + a_0$ be the formula resulting for the linear regression where $(x_i, y_i)_{1...n}$ are the defining data points. The residual e_i (residuum) is defined as

$$e_i = y_i - \bar{y}_i$$

and the sum of squared errors (SSE) is given by

$$SSE = \sum_{i=1}^{n} e_i^2$$

Since errors are obtained after calculating two regression parameters from the data, errors have *n-2* degrees of freedom. Therefore the mean squared errors (MSE) result in

$$s_e^2 = MSE = \frac{SSE}{n-2}$$

Using the MSE, the standard error for the parameters a_1 and a_0 can be written as:

$$s_{a_0} = s_e \sqrt{\left(\frac{1}{n} + \frac{\bar{x}^2}{\left(\sum_{i=1}^{n} x_i - n\bar{x}^2 \right)} \right)}$$

$$s_{a_1} = \frac{s_e}{\sqrt{\left(\sum_{i=1}^{n} x_i - n\bar{x}^2 \right)}}$$

The relative standard error can be obtained by dividing the standard error by the corresponding value of the parameter. The standard error (half of the confidence delta) of the estimated linear function value at x can be calculated by

$$error(x) = \sqrt{(s_{a_0})^2 + (x \cdot s_{a_1})^2} \text{ (Gaussian Error Estimation)}$$

The

$$100 \cdot (1 - \alpha)\%$$

confidence intervals for a_0 and a_1 can be computed using

$$t[1 - \alpha/2, n - 2]$$

— the 1 - $\alpha/2$ quantile of the *t* distribution with *n-2* degrees of freedom. The confidence intervals are

$$[a_1 - ts_{a_1}, a_1 + ts_{a_1}]$$

and

$$[a_0 - ts_{a_0}, a_0 + ts_{a_0}]$$

Tip If a confidence interval includes zero the regression parameter cannot be considered to be different from zero at the $100 \cdot (1 - \alpha)\%$ confidence level. In case of a preset parameter (for example, forcing through a value) there are *n-1* degrees of freedom.

Reporting Calculations

This chapter describes the functionality and available methods supported by the “Calculations” feature given in the Reporting of Qtegra ISDS Software.

Calculations

Tip New Reports are created in the Qtegra tool of Qtegra ISDS Software, refer to the Help or Software Manual of the system.

The Report items **Result Data Table** and **Data** offer the additional “Calculations” feature. Adding additional column calculations via the below shown control adds additional information to the resulting report table, that is adding, for example, an **Average** calculation to one of the available columns adds an extra line at the end of the table showing the mean of the lines summarized before. See Figure 11-1.

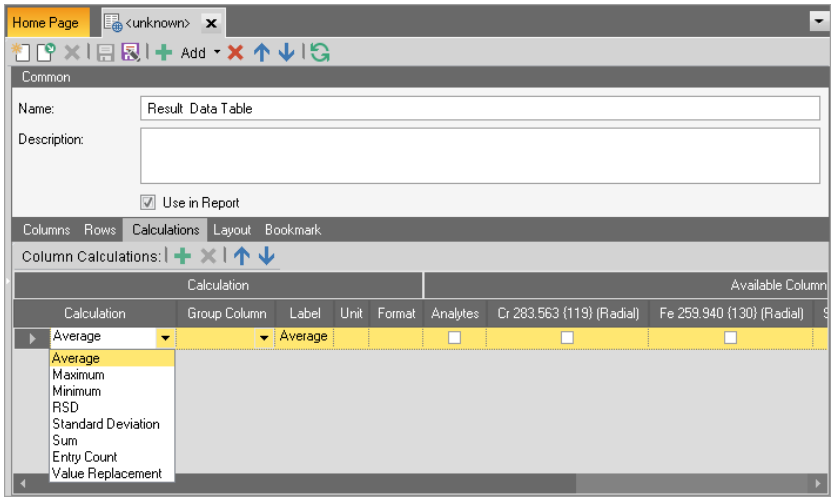
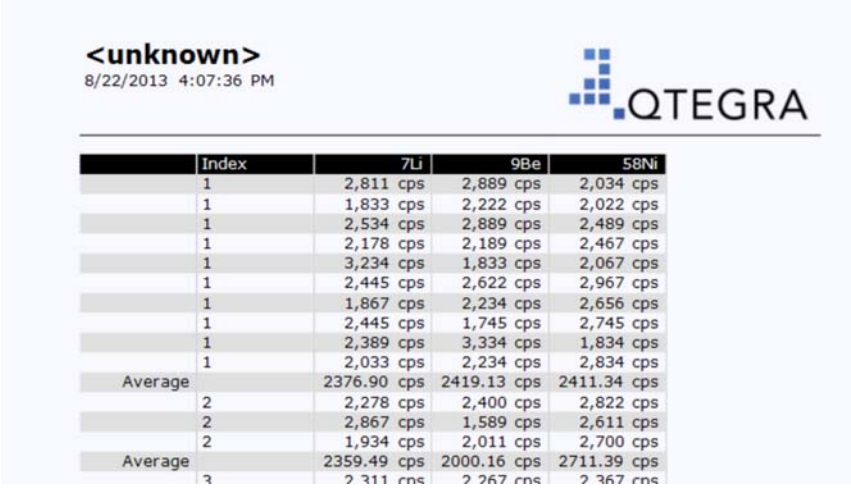


Figure 11-1. Report Calculations

Various calculations are available. The full variety of calculations is only available for numerical columns, whereas **Entry Count** is available for any given column. Multiple calculations can be added to a grid. The natural order given by the defining control also defines the order of addition to the Report page. The **Group Column** feature can be also used to bind a calculation to a certain table column.

Label defines the label value displayed in the final report table. **Unit** and **Format** – a numerical format string, that is 0.000 for displaying three significant digits – are used to format the displayed value.

For example, in case of “Average”, selecting the **Index** column results in executing the averaging for every sample, see Figure 11-2.



	Index	7Li	9Be	58Ni
	1	2,811 cps	2,889 cps	2,034 cps
	1	1,833 cps	2,222 cps	2,022 cps
	1	2,534 cps	2,889 cps	2,489 cps
	1	2,178 cps	2,189 cps	2,467 cps
	1	3,234 cps	1,833 cps	2,067 cps
	1	2,445 cps	2,622 cps	2,967 cps
	1	1,867 cps	2,234 cps	2,656 cps
	1	2,445 cps	1,745 cps	2,745 cps
	1	2,389 cps	3,334 cps	1,834 cps
	1	2,033 cps	2,234 cps	2,834 cps
Average		2376.90 cps	2419.13 cps	2411.34 cps
	2	2,278 cps	2,400 cps	2,822 cps
	2	2,867 cps	1,589 cps	2,611 cps
	2	1,934 cps	2,011 cps	2,700 cps
Average		2359.49 cps	2000.16 cps	2711.39 cps
	3	2,311 cps	2,267 cps	2,367 cps

Figure 11-2. Averaging for every sample

Available Calculation Types

Let k be the number of given values x_1, x_2...x_k from the column using the selected calculation, then the following calculations are done for the list entries of the **Calculation** column, see Table 11-1:

Table 11-1. Calculation types

Calculation Type	Calculation
Average	$\bar{x} = \frac{\sum_{i=1}^{k} x_i}{k}$
Maximum	$Max[x_1, x_2, \ldots, x_k]$
Minimum	$Min[x_1, x_2, \ldots, x_k]$
RSD	$\frac{SD}{\bar{x}} \cdot 100\%$
Standard Deviation	$SD = \sqrt{\frac{1}{k-1}\sum_{i=1}^{k}(x_i - \bar{x})^2}$
Sum	$\sum_{i=1}^{k} x_i$

Table 11-1. Calculation types, continued

Calculation Type	Calculation
Entry Count	k
Value Replacement	Removes Report table lines, meeting defined criteria, and adds the value in the added line.

Value Replacement offers an additional dialog for setting up the replacement criteria. This dialog is identical with the control used for filter conditions, see Figure 11-3.

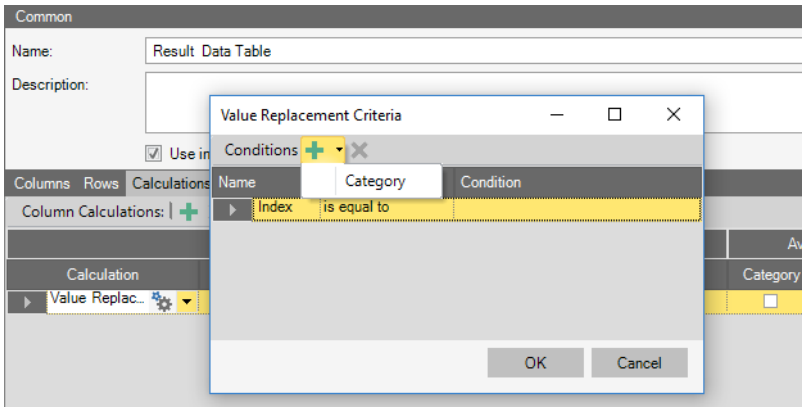


Figure 11-3. Value Replacement Criteria

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Raw Data Processing Algorithms

The Qtegra ISDS Software Data Evaluation is handled by different evaluation modules called Virtual Evaluations (VE). The system currently knows the following common evaluation modules for quantification:

- Raw Data
- eQuant (External Calibration)

This chapter describes the Raw Data structure. The raw data interface, which knows already certain mathematical methods to manipulate the given raw data, is also used by eQuant. Therefore, it is necessary to give a short overview, which data is used as a basis for the evaluation modules.

Contents

Raw Data Handling

The evaluation methods use the structures supported by the Raw Data evaluation method to handle raw data streams. Raw Data itself allows displaying the streams and offers the possibilities to apply an interference correction.

Tip From the programmer's point of view the Data Adapter is the interface offering access to the raw data used by the evaluation methods. Raw data values are based on the number of runs given in the corresponding line of the Sample List.

An exemplary Sample List is shown in Figure 12-1.

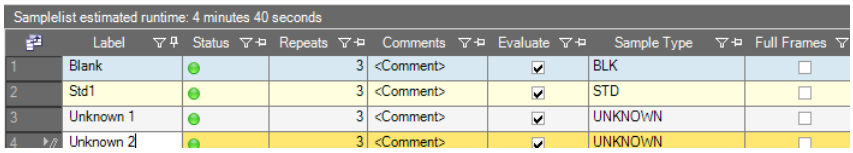

Figure 12-1. Sample list (eQuant with iCAP OES)

Exemplary acquisition parameters are shown in Figure 12-2.

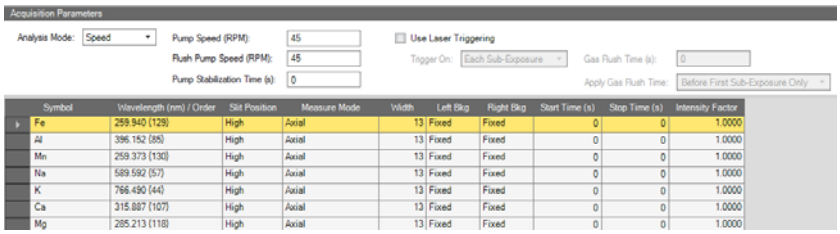

Figure 12-2. Acquisition Parameters (eQuant with iCAP OES)

In Raw Data mode, eQuant offers an interface for external manipulation of the intensity values. This interface is available for each trace on the Intensities View via the Details View. In case of iCAP OES the background correction and the integration area can be defined, see Figure 12-3.

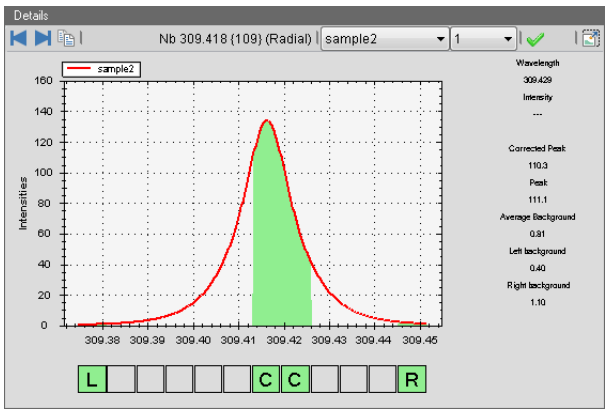

Figure 12-3. Details view (eQuant with iCAP OES)

The measured analyte intensity i_A is defined as the average intensity at the center pixel position's $Average_C$ corrected by the average background intensity $Average_{Bkg}$.

$$i_A = Average_C - Average_{Bkg}$$

The slope of the background curve $Slope_{Bkg}$ is calculated from the difference of the intensities of the left background L_{Bkg} and right background R_{Bkg} divided by the difference of pixel positions of left and right background $Pixel_{LR}$. If multiple pixels are selected, the average pixel position is used.

$$Slope_{Bkg} = \frac{(L_{Bkg} - R_{Bkg})}{Pixel_{LR}} \text{ (per pixel)}$$

with

$$Pixel_{LR} = Pixel_R - Pixel_L$$

The average background intensity $Average_{Bkg}$ is calculated from the intensities of left background L_{Bkg} minus the difference of pixel positions between left background and center position $Pixel_{LC}$ multiplied by the slope of the background curve $Slope_{Bkg}$.

$$Average_{Bkg} = L_{Bkg} - (Pixel_{LC} \times Slope_{Bkg})$$

with

$$Pixel_{LC} = Pixel_C - Pixel_L$$

This way of calculation leads to different average background values if the Center or Left/Right background positions are moved or changed, that means, set or remove the C on the subarray plot.

Interference Correction

The interference correction is the first data correction applied on raw data values.

The nature of the interference correction is always the same. The intensity values of the desired emission lines are interfered by emission lines of other elements (spectral overlap). By measuring these interfering emission lines, a linear correction with k interfering intensities given as values i_1, i_2...i_k and the related correction factors f_1, f_2...f_k can be applied to the measured intensity i with

$$i_{corrected} = i + \sum_{j=1}^{k} f_j \cdot i_j$$

The iCAP OES system offers Inter-Element Correction for the external interference correction, see Figure 12-4:

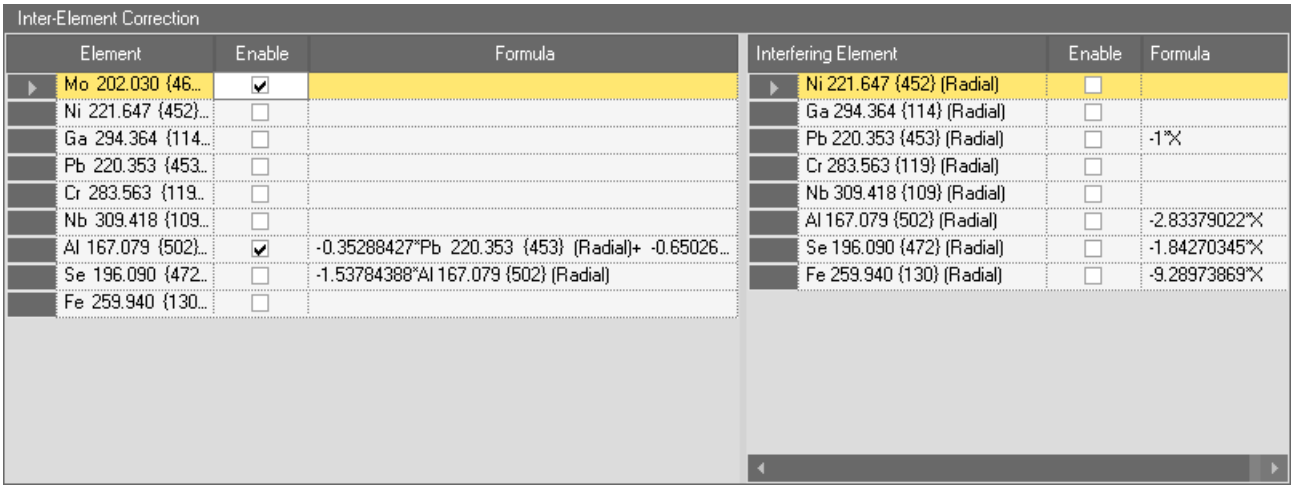

Figure 12-4. Inter-Element Correction with iCAP 7000 Series ICP-OES

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Data Processing Algorithms for eQuant

This chapter describes the evaluation algorithms for the Qtegra ISDS Software used in eQuant evaluation algorithms.

Contents

External Calibration - eQuant

The eQuant VE is the most complex module of the quantification series. It currently offers seven Sample Types to specify measurement blocks using the Sample List. The Standard Editor is used for specifying standards and Internal Standards. The Method Parameters of the VE specify Internal Standards for given emission lines as well as settings for certain calibration properties. The following Sample Types are supported in Table 13-1:

Table 13-1. Sample Types

Sample Types	Chapter/Figure
UNKNOWN	Defines a sample where the contained elements are quantified using the calibration curve from the preceding standard block, or using the Semi-Quant feature if applicable.
STD	The sample line is treated as a standard.
BLK	The last blank value of a blank block is used for blank correction.
AVERAGE BLK	The mean of all average blanks in the current measurement block defines the blank to be used for blank correction.
ZERO STD	Allows working in standard addition mode inside the external calibration module eQuant.

Table 13-1. Sample Types, continued

Sample Types	Chapter/Figure
UPDATE CALIB	Used to correct the current calibration curve.
QC	Defines a sample as quality control sample and applies the selected actions. From the point of evaluation, a QC sample is handled in the same way as an UNKNOWN sample.

Tip For a detailed description of the different available QC modes, refer to the Help or Software Manual of the system.

The sample lines in Figure 13-1 define a valid measurement block consisting of a BLK, four standards, four QC samples and three unknown samples:

Samplelist

	Label	St	Performance Chec	Survey R	User Pre-dilut	Main R	Sample Type	Standard	Dilution Fa	Amount	Final Quantit	QC Action
1	Blank 1		No	2	0	10	BLK		1			None
2	Std 1.0 ppb		No	2	0	3	STD	Tune A	10			None
3	Std 2.5 ppb		No	2	0	3	STD	Tune A	4			None
4	Std 5.0 ppb		No	2	0	3	STD	Tune A	2			None
5	Std 10.0 ppb		No	2	0	3	STD	Tune A	1			None
6	Sample 1		No	2	0	3	QC	Tune A	1			CCV
7	Sample 1		No	2	0	3	QC	Tune A	1			CCV
8	Sample 1		No	2	0	3	QC	Tune A	1			CCV
9	Sample 1		No	2	0	3	QC	Tune A	1			CCV
10	Sample 2		No	2	0	3	UNKNOWN		1			None
11	Sample 3		No	2	0	3	UNKNOWN		1			None
12	Sample 4		No	2	0	3	UNKNOWN		1			None

Figure 13-1. Valid measurement block

A minimal measurement block consists of at least one STD sample line and one UNKNOWN sample line. However, only multiple measurement results assure statistically useful data.

Internal Standardization

Internal Standard emission lines for the Internal Standard correction are defined on the Quantification Page or via the Standard Editor and the Sample List.

Internal Standard Correction

In case Internal Standard correction has been activated and Internal Standard emission lines have been defined, the Internal Standard correction is applied.

The first blank and, in case of the absence of a blank, the first standard defines the reference value for the Internal Standard correction. All other sample lines belonging to this standard block (in means of

quantification) will be corrected against that reference. Every measured intensity i will be corrected with the appropriate Internal Standard correction factor g_{ISC}.

Using the reference sample g_{ISC} is calculated by

$$g_{ISC} = \frac{s_r}{s_t}$$

where s_r and s_t are the reference and target sensitivity of the Internal Standard emission line

$$s_r = \frac{\bar{i}_r}{c_r} \text{ and } s_t = \frac{i_t}{c_s}$$

with $\bar{i}_r$ as the average intensity in the reference sample over all runs, i_t as the target intensity in the corrected sample, and c_r, c_s as the known concentration of the reference and the corrected sample, respectively. The target sensitivity is calculated for every run in every sample differing from the reference.

For every none-standard emission line with an Internal Standard defined, the measured run intensity will be corrected according to

$$i_{corr} = i \cdot g_{ISC}$$

The concentrations c_r and c_s are only applied if Internal Standards with different concentrations are defined. The most common way is to use an equally concentrated spike as an Internal Standard for the whole measurement block. In this case the concentrations c_r and c_s can be ignored.

Tip The quotient s_r / s_t is calculated on a “per run” basis. This means that the averaged quotient for each main run is used to correct the intensities and not the quotient of the averaged values.

Differently concentrated Internal Standards can be defined.

Blanks

A blank analysis represents the baseline above which a signal is detected. Blanks may be measured singularly or in a series of consecutive analyses (a blank block).

In the simplest case, a single analysis is defined as a blank by setting the Sample Type to ‘BLK’ in the Sample List.

In a blank block however, Qtegra can work with blanks in two ways, depending on the choice of Sample Type:

- If all of the blank block analyses are defined as Sample Type 'BLK', the last measured blank analysis is taken as the blank intensity.
- If more than one blank block analysis is defined as Sample Type 'AVERAGE BLK', the average of these analyses is taken as the blank intensity.

$$i_{Blank_{Emission\ line}} = \frac{\sum_{j=1}^{\#\text{blank block lines}} i_{Blank}}{\#\text{blank block lines}}$$

By default, the blank is defined as the zero intensity point in the calibration. For a ZERO STD analysis however, the blank correction is made by subtracting the intensity value of the measured blank from the ZERO STD.

Tip Blank correction is not performed on analytes used as Internal Standards. If a calibration curve is available, this curve will be used to convert the measured intensities into concentrations. The concentration values returned are dependent on the options used for the calibration. For example, only setting 'Forcing = Blank' guarantees a zero concentration.

Limit of Detection (LOD)

The Limit of Detection (LOD) or Instrumental Detection Limit (IDL) of an emission line is defined as a multiple of the standard deviation of blank analysis (SD_{Blank}) associated to a calibration that is converted into a concentration value using the slope of the calibration function (a_1). For eQuant, the following formula specifies the LOD:

$$LOD = \left(\frac{3 \times SD_{Blank}}{a_1}\right)$$

Tip An LOD value can be reported for both types of blank: BLK or AVERAGE BLK.

Tip In the Concentrations Evaluation Results view, LODs are only displayed when a concentration equivalent can be calculated. An LOD value is only calculated for a linear regression calibration. Thus, no LOD value is calculated for a 2nd order calibration.

Method Quantification Limit (MQL)

The Method Quantification Limit (MQL) of an emission line is defined as a multiple of the standard deviation of blank analysis (SD_{Blank}) associated to a calibration that is converted into a concentration value using the slope of the calibration function (a_1). This value is then

corrected by the *Total Dilution Factor* (*TDF*, see "Intelligent Dilution" on page 13-7) applied to the analysis. For eQuant, the following formula specifies the MQL:

$$MQL = \left(\frac{10 \times SD_{Blank}}{a_1}\right) \times TDF$$

Tip The MQL can be sample specific due to different dilution factors used in a LabBook.

Background Equivalent Concentration (BEC)

The Background Equivalent Concentration (*BEC*) for the given emission line is defined based on its current calibration curve *f(x)* with

$$BEC = -f^{-1}(0)$$

the intercept of the calibration curve.

Quality Control (QC)

The QC tests and the recovery calculations are always based on total (measured) concentrations according to the equations mentioned in "Standard Addition within eQuant" on page 13-18. Thus, factors like Dilution, Amount, and Final Quantity are already included.

Currently, Qtegra knows several Quality Control Tests, which are grouped in several sub-categories according to their respective calculation.

Blank Tests

The test value is calculated based on a comparison of the total (measured) concentration (*TMC*) to the user defined Contract Required Detection Limits (*CRDL*). Afterward, the test value is compared to the defined warning and failure limit. Note that the unit of the Contract Required Detection Limits can be different to the ones defined for the standards.

$$Test\ value = \frac{TMC}{CRDL} \cdot 100\%$$

Calibration Tests

The recovery for calibration tests is calculated by comparing the total (measured) concentration (*TMC*) to the theoretical standard concentration (*TSC*).

$$Recovery = \frac{TMC}{TSC} \cdot 100\%$$

Paired Sample Tests

For Paired Sample Tests, the recovery is calculated by comparing the total (measured) concentration (*TMC*) to the concentration of a reference sample (*RSC*).

$$Recovery = \frac{TMC}{RSC} \cdot 100\%$$

Paired Sample Tests (EPA conform)

For EPA conform Paired Sample Tests, the relative percentage difference (*RPD*) is calculated of the total (measured) concentration (*TMC*) and the concentration of a reference sample (*RSC*) using the following formula:

$$RPD = \frac{|TMC - RSC|}{(TMC + RSC)/2} \cdot 100\%$$

Spike Tests

Using a Spike Test, the recovery is calculated by comparing the measured concentration (Total Measured Concentration (*TMC*) of the spiked QC sample minus Unspiked Sample Concentration (*USC*) of a reference sample) with the expected (theoretical) spike concentration (*SC*).

$$Recovery = \frac{TMC - USC}{SC} \cdot 100\%$$

Spike Tests (ARC)

With an Alternative Recovery Calculation (*ARC*), the Spike Test has been modified to avoid negative recoveries in case where spike concentrations are too low compared to unspiked samples. ARC is

calculated as quotient of the total measured concentration of the spiked QC sample (*TMC*) and the sum of unspiked sample concentration (*USC*) and expected (theoretical) spike concentration (*SC*).

$$Recovery = \frac{TMC}{USC + SC} \cdot 100\%$$

Continuous Tests

Using the Regression Coefficient Verification (*RCV*), the Coefficient of Determination R^2 is compared to the entered warning and failure limits. The RCV test is performed at the end of a standard block.

The Relative Stability Verification (*RSV*) is performed for each line. It compares the RSD value of the final calculated concentration and/or the measured intensity against the entered warning and failure limit. Note that the limit of the concentration above which the test is performed can have a different unit than used for the standards.

Internal Standard Tests

The Internal Standard Tests compare the recovery of the Internal Standards against the entered limits.

Intelligent Dilution

For the Intelligent Dilution option Calibration Range, the measured concentration for each analyte (*TMC*) is compared to the entered limit, which is the percentage of the highest calibration point for this analyte (Highest Standard Concentration, *HSC*). The needed dilution is then calculated using the following equation:

$$Dilution\ Factor = \frac{TMC}{HSC \cdot Target\,(\%)}$$

The Total Dilution Factor (abbreviated with *TDF*) is calculated using the following equation:

$$Total\ Dilution\ Factor = Autodilution\ Factor \times Dilution\ Factor$$

Standards

Standards consist of elements with known concentrations, which are the basis of any comparing quantification method. Consecutive standard sample lines are handled as a so-called standard block. Each standard sample line generates one intensity value for each measured emission line. Together with the concentration of the element (known from the standard) this pair of values forms a data point of the calibration curve *f(x)*.

Standard Calibration Properties

The available options for calculating a calibration curve are listed in Table 13-2:

Table 13-2. Options for calibration curve calculation

Option	Description	
Fit Type	Linear	A linear regression curve with $f(x) = a_1x + a_0$ is calculated using the given data points.
	2nd order	A quadratic polynomial fit with $f(x) = a_2x^2 + a_1x + a_0$ will be used.
	Both fit types use the least squares fitting method described in "Least Squares Fits (LQF)" on page 11-3.	
Forcing	None	Value *y* for $x = 0$ is not manipulated.
	Zero	The calibration curve will be forced to fulfill $f(0) = 0$ which is equivalent to set $a_0 = 0$.
	Blank	Defines the calibration curve *f(x)* with $x = 0$ as $f(0) = i^{BLK}_{Emission\ line}$ -or- $f(0) = i^{AVERAGE\ BLK}_{Emission\ line}$ depending on the current blank block mode.

Table 13-2. Options for calibration curve calculation, continued

Option	Description	
Weighting	None	Value will not be weighted.
	Absolute SD	Weight $\omega_k = 1/SD_k^2$ Each point is weighted by the standard deviation SD_k of the analyte over the runs in the sample.
	Relative SD	Weight $\omega_k = 1/(SD_k/\bar{i}_k)^2$ Each point is weighted by the standard deviation SD_k of the analyte over the runs in the sample relative to the mean $\bar{i}_k$.
	1/Concentration	Weight $\omega_k = 1/c_k$ Each point is weighted by the concentration c_k of the analyte. Blanks are ignored as their concentration is 0.
	1/Concentration^2	Weight $\omega_k = 1/c_k^2$ Each point is weighted by the squared concentration c_k^2 of the analyte. Blanks are ignored as their concentration is 0.

Units to be Displayed

The units used to display the calculation results for an analyte depend on the first appearance of that given analyte in a standard. Unit selections are set for the whole experiment.

Quantification of UNKNOWN/QC Samples

Based on the calibration curve *f(x)* the original concentration *c* of the analyte in an UNKNOWN sample is calculated using

$$c = f^{-1}(x)$$

where *x* is the measured intensity. QC samples are handled in the same way as UNKNOWN samples - with the exception that in case where a recovery needs to be used and displayed (for example, CCV) the percentage is calculated based on the before calculated concentration and compared the with defining concentration.

Final Quantity, Amount, and Dilution

If Final Quantity *q*, Amount *a,* and Dilution *d* are specified in the Sample List, the concentration value is corrected by

$$c_{corr} = c \cdot d \cdot \frac{q}{a}$$

Unspecified values are set to *1*. The dilution is differently handled for standards. Dilution, Amount and Final Quantity are applied to the concentration of the stock solution c_{stock} to calculate the expected concentrations c_{exp} for the calibration curve using

$$c_{\exp} = c_{stock} \cdot \frac{1}{d} \cdot \frac{a}{q}$$

Update Calibration

Considering the fact of a drifting instrument without wanting to measure all standards again, it is possible to use a so-called Update Calibration sample line (UPDATE CALIB). This sample is used to calculate a correction value, which will be applied on the preceding calibration block. Therefore, it is necessary that the Update Calibration line uses the same concentration as the correspondent sample line in the standard block (STD).

Tip After any Update Calibration, the calibration function is recalculated. There is no difference in the calculated result in the sample following 6 separate Update Calibrations (according to 6 STDs for example) from using all 6 or just one.

Consider

$$i^{UPDATE\ CALIB}_{Emission\ line}$$

to be the intensity of a measured emission line for a certain concentration, which was also measured inside the preceding standard block sample line with

$$i^{STD}_{Emission\ line}$$

The resulting factor

$$c_{UPDATE\ CALIB} = \frac{i^{UPDATE\ CALIB}_{Emission\ line}}{i^{STD}_{Emission\ line}}$$

is used for scaling any intensity value of the calibration curve for the subsequent sample lines.

The ZERO STD sample type feature offers the same possibilities as described in "Standard Addition within eQuant" on page 13-18 with the chance of combining them with all other available sample types inside the eQuant evaluation.

Tip If a zero standard is used, all blank corrections will be performed by subtracting intensity values.

Quantification Steps

In order to quantify an element, the following methods are applied:

1. Application of Inter-Element Correction if activated and available.
2. Calculation of Internal Standards - a correction will only be applied if activated.
3. If zero standards exist, blank correction is implemented as subtraction blank.
4. Generation of calibration curves based on standards and zero standards.
5. Based on the pre-calculated information the element quantification takes place.

Post-Quantification Calculations

Post-quantification calculations are defined as calculations applied after finishing the element quantification for the current LabBook. The calculation is based on the concentration of the samples, but not on the measured intensities.

Special Blank

The Sample List allows specifying a special blank for each available sample. The sample line defining the use of a special blank will be post-quantification corrected by the subtraction of the average value of the blank concentration (corrected by TDF) from its corresponding

unknown concentration (corrected by TDF). In case of UNKNOWN/QC samples the subtraction takes place using the run values.

Tip The calculation is performed in sequential order. Recursion is not allowed. Each sample line is calculated only once.

If a LabBook looks similar to this example (see Figure 13-2), the concentration of a sample corrected by a special blank is calculated as follows:

$$c_{spBLK} = (c_{sample} \times TDF_{sample}) - (c_{BLK} \times TDF_{BLK})$$

Samplelist estimated runtime: 10 minutes 44 seconds

	Label	Full Frames	Comments	Evaluate	Sample Type	Standard	Special Blank
1	Blank	3	<Comment>	☑	BLK		
2	Standard	3	<Comment>	☑	STD	std high	
3	Sample 1	3	<Comment>	☑	UNKNOWN		
4	Sample 2	3	<Comment>	☑	UNKNOWN		3: Sample 1

Figure 13-2. Example of LabBook with Special Blank correction

Let, for example, the concentration of Sample 1 be 5 ppb and the concentration of Sample 2 be 15 ppb. As Sample 1 is used as special blank for Sample 2 the concentration of Sample 2 is 10 ppb (15-5 ppb).

To understand how a Special Blank correction is calculated by Qtegra and how recursion can occur, read the following examples carefully.

Example 1

Imagine a LabBook with four samples. None of these samples is Special Blank corrected, see Figure 13-3.

Samplelist estimated runtime: 6 hours 59 minutes 12 seconds / 30 minutes 34 seconds remaining

	Label	Rack	Vial	Repeats	Comments	Evaluate	Sample Type	Special Blank
31	Sample 1	3	1	2	<Comment>	☑	UNKNOWN	
32	Sample 2	3	2	2	<Comment>	☑	UNKNOWN	
33	Special Blank	Standard	1	2	<Comment>	☑	UNKNOWN	
34	Sample 3	3	3	2	<Comment>	☑	UNKNOWN	

Concentrations

No	Time	Sample Type	Label	K 766.490 {44} (Radial) [mg/l]
1	11/3/2014 2:40:06 PM	BLK		0
2	11/3/2014 2:42:14 PM	STD		
31	11/4/2014 1:56:49 PM	UNKNOWN	Sample 1	114,290
32	11/4/2014 1:58:50 PM	UNKNOWN	Sample 2	73,273
33	11/5/2014 7:47:38 AM	UNKNOWN	Special Blank	5
34	11/4/2014 2:00:52 PM	UNKNOWN	Sample 3	47,648

Figure 13-3. Sample List and Concentrations view of LabBook without Special Blank correction

The measured concentration of Sample 1 is 114,290 µg/L, of Sample 2 73,273 µg/L, of Sample 3 (Special Blank) 5 µg/L, and Sample 4 47,648 µg/L are not corrected.

Example 2

Imagine a LabBook with four samples. Samples 1, 2, and 4 are **Special Blank corrected** by Sample 3 (concentration of 5 µg/L). In this case, the measured concentration of your samples is decreased by the Special Blank concentration, for example, the measured concentration of Sample 1 is 114,290 µg/L but is shown as 114,285 µg/L (corrected by 114,290 - 5 = 114,285 µg/L), see Figure 13-4.

Samplelist estimated runtime: 6 hours 59 minutes 12 seconds / 30 minutes 34 seconds remaining

	Label	Rack	Vial	Repeats	Comments	Evaluate	Sample Type	Special Blank
31	Sample 1	3	1	2	<Comment>	☑	UNKNOWN	33: Special Blank
32	Sample 2	3	2	2	<Comment>	☑	UNKNOWN	33: Special Blank
33	Special Blank	Standard	1	2	<Comment>	☑	UNKNOWN	
34	Sample 3	3	3	2	<Comment>	☑	UNKNOWN	33: Special Blank

Concentrations

	No	Time	Sample Type	Label	K 766.490 {44} (Radial) [mg/l]
⊞	1	11/3/2014 2:40:06 PM	BLK		0
⊞	2	11/3/2014 2:42:14 PM	STD		
⊞ ▶	31	11/4/2014 1:56:49 PM	UNKNOWN	Sample 1	114,285
⊞	32	11/4/2014 1:58:50 PM	UNKNOWN	Sample 2	73,268
⊞	33	11/5/2014 7:47:38 AM	UNKNOWN	Special Blank	5
⊞	34	11/4/2014 2:00:52 PM	UNKNOWN	Sample 3	47,643

Figure 13-4. Sample List and Concentrations view of LabBook with Special Blank correction

The measured concentration of Sample 2 of 73,273 µg/L is shown as 73,268 µg/L (corrected by 73,273 - 5 = 73,268 µg/L).

Sample 3 is the Special Blank itself and will therefore not be corrected. The measured concentration of 5 µg/L is shown as 5 µg/L.

Finally, the measured concentration of Sample 4 of 47,648 µg/L is shown as 47,643 µg/L (corrected by 47,648 - 5 = 47,643 µg/L).

Example 3 - Pitfall

Imagine a LabBook with four samples. All samples including the Special Blank (Sample 3) are **Special Blank corrected**. In this case, the measured concentration of all your analytes is shown as corrected values, see Figure 13-5.

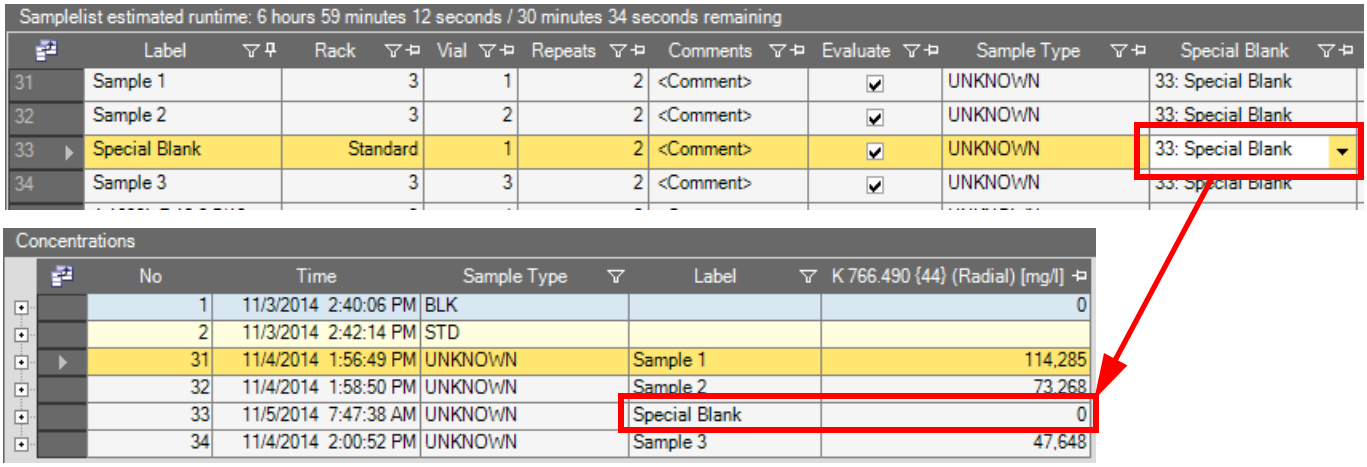


Figure 13-5. Sample List and Concentrations view of LabBook with recurred Special Blank correction

The measured concentration of Sample 1 of 114,290 µg/L is shown as 114,285 µg/L (corrected by 114,290 - 5 = 114,285 µg/L).

The measured concentration of Sample 2 of 73,273 µg/L is shown as 73,268 µg/L (corrected by 73,273 - 5 = 73,268 µg/L).

Tip Sample 3 is the Special Blank itself and will also be corrected. The measured concentration of 5 µg/L is shown as 0 µg/L (5 - 5 = 0 µg/L). From now on, the Special Blank has a concentration of 0 µg/L!

Finally, the measured concentration of Sample 4 of 47,648 µg/L is shown as 47,648 µg/L (corrected by 47,648 - 0 = 47,648 µg/L).

Example 4 - Moving a Special Blank

In the Sample List, let one sample refer to a Special Blank, i.e., the Special Blank column shows an entry with a line indicator. Click the gray field in front of the line and drag the line up or down. Release the mouse button to drop the sample on the desired position.

Tip If the sample line of the Special Blank is moved, then the Special Blank column has to be updated according to the new position of the Special Blank. Therefore, open the drop-down list and click to assign the correct Special Blank with its new line indicator.

Alternative Special Blank

By default the blank concentration (corrected by TDF) is subtracted from the unknown concentration (corrected by TDF) of the sample.

$$c_{spBLK} = (c_{sample} \times TDF_{sample}) - (c_{BLK} \times TDF_{BLK})$$

With Qtegra ISDS version 2.8 SR1, an alternative Special Blank (*AltSpBLK*) calculation has been introduced:

$$c_{AltSpBLK} = ((c_{sample} \times DF_{sample}) - (c_{BLK} \times DF_{BLK})) \times \frac{q}{a}$$

where *DF* is the Dilution Factor, *q* the Final Quantity value and *a* the Amount specified in the Sample List (see "Final Quantity, Amount, and Dilution" on page 13-10).

To use this alternative Special Blank calculation instead of the Special Blank correction, open the Display Settings dialog of your LabBook and set the **Quantification Setting** to *True*, see Figure 13-6.

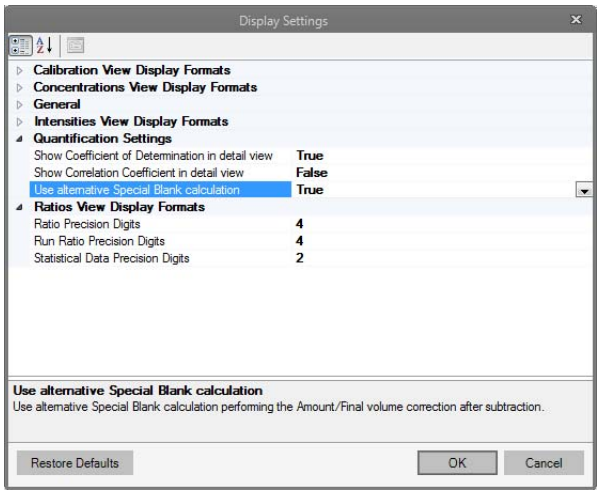


Figure 13-6. Display Settings dialog showing the Quantification Settings

Thus, the setting is only valid for the current LabBook.

Blank Corrected Intensity

The blank corrected intensity per run is calculated from the Internal Standard corrected intensity (per run) subtracted by its zero concentration intensity (intercept, i_{zero}) using

$$i_{BLKcorr} = i_{corr} - i_{zero}$$

The blank corrected intensity average $\bar{i}_{BLKcorr}$ is calculated from the IS corrected intensity average $\bar{i}_{corr}$ subtracted by its zero concentration intensity (intercept, i_{zero}) using

$$\bar{i}_{BLKcorr} = \bar{i}_{corr} - i_{zero}$$

Relative Atom Percent (RelAt%) and Relative Weight Percent (RelWt%)

Relative atom percent (RelAt%) and relative weight percent (RelWt%) are calculated for analytes on the following conditions:

- A multi-calculation trace with "Sum" operator is defined.
- The analyte matches the selection defined for the multi-calculation trace.
- A concentration is available for the analyte.

The relative atom percent (RelAt%) is calculated using

$$RelAt\%_{Analyte} = \frac{\frac{Concentration_{Analyte}}{Mass_{Analyte}}}{\sum_{NthAnalyte=1}^{n} \frac{Concentration_{NthAnalyte}}{Mass_{NthAnalyte}}} \cdot 100$$

The relative weight percent (RelWt%) is calculated using

$$RelWt\%_{Analyte} = \frac{Concentration_{Analyte}}{\sum_{NthAnalyte=1}^{n} Concentration_{NthAnalyte}} \cdot 100$$

with the description shown in Table 13-3.

Table 13-3. Description for RelAt% and RelWt% parameters

Parameter	Description
$RelAt\%_{Analyte}$	Relative atom percent of analyte of interest.
$RelWt\%_{Analyte}$	Relative weight percent of analyte of interest.
$Concentration_{Analyte}$	Concentration of analyte of interest.
$Mass_{Analyte}$	Mass of analyte of interest.

Table 13-3. Description for RelAt% and RelWt% parameters, continued

Parameter	Description
	Tip For isotopical standards, the isotope mass is used for calculation. For elemental standards, the element mass is used for calculation.
n	Amount of analytes matching the selection and having a valid concentration.

Example

If a multi-calculation trace is defined in the quantification view of eQuant (as shown in Figure 13-7), the relative atom percent and relative weight percent are calculated for all but the Internal Standard analytes.

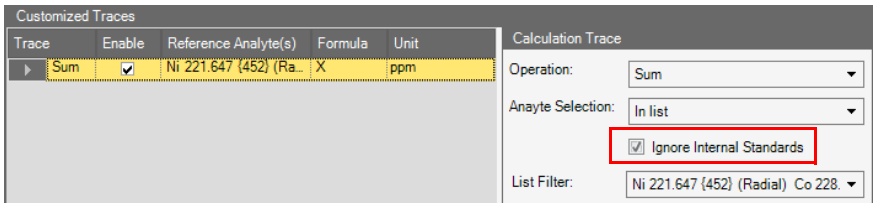


Figure 13-7. Multi-calculation trace sum to ignore IS

Standard Addition within eQuant

With Standard Addition mode, two sample types – ZERO STD defining the sample without a spiked concentration and STD for spiked samples to set up measurement – can be used. A valid zero standard block in the Sample List consists of one ZERO STD measured at the beginning of a sequence of standards. For each ZERO STD and STD block, a 1st order calibration curve is produced for every analyte defined as standard. The curve is constructed from the mean results of given runs using the given concentrations.

The first-order calibration curve is calculated using a linear least squares fit. The available options are listed in Table 13-4:

Table 13-4. Options for calibration curve calculation

Option	Description	
Forcing	No	Value will not be manipulated.
	Zero	The calibration curve will be forced through standard defined as zero spike.

Table 13-4. Options for calibration curve calculation, continued

Option	Description	
Weighting	None	Value will not be weighted.
	Absolute SD	Weight $\omega_k = 1/SD_k^2$ Each point is weighted by the standard deviation SD_k of the analyte over the runs in the sample.
	Relative SD	Weight $\omega_k = 1/(SD_k/\bar{i}_k)^2$ Each point is weighted by the standard deviation SD_k of the analyte over the runs in the sample relative to the mean $\bar{i}_k$.
	1/Concentration	Weight $\omega_k = 1/c_k$ Each point is weighted by the concentration c_k of the analyte. Blanks are ignored as their concentration is 0.
	1/Concentration^2	Weight $\omega_k = 1/c_k^2$ Each point is weighted by the squared concentration c_k^2 of the analyte. Blanks are ignored as their concentration is 0.

Based on the calibration curve, the original concentration c of the analyte in the standard samples is calculated using

$$c = f^{-1}(x)$$

where x is the measured intensity. Having

$$f(x) = a_1 x + a_0$$

the measured concentration of the zero standard is calculated as

$$c_{ZERO\,STD} = \frac{a_0}{a_1}$$

Final Quantity, Amount, and Dilution

If Final Quantity *q*, Amount *a*, and Dilution *d* are specified in the Sample List, the concentration value is corrected by:

$$c_{ZERO\,STDcorr} = c_{ZERO\,STD} \cdot d \cdot \frac{q}{a}$$

Unspecified values are set be *1*.

If Standard Addition in eQuant is used, the derived function *f(x)* can also be utilized for the calculation of concentrations in subsequent UNKNOWN samples. The concentration of the reference standards used to calculate

$$f^{-1}(x)$$

is hereby calculated by:

$$c_{STDcorr} = c_{STD} + c_{ZERO\,STD}$$

Units to be displayed

The units used to display the calculation results for an analyte depend on the first appearance of that given analyte in a standard. Unit selections are set for the complete experiment.

Tip Weighting for the calibration curve is only available if all standard measurements in the current block of the Sample List consist of at least two runs. In all other cases, the option is disabled. Any leading standard samples before the first unspiked sample will be ignored.

14

Settings

This chapter of the *iCAP 7000 Plus Series ICP-OES Software Manual* describes the setting of peripherals that is done prior to the creation of a Template and LabBook.

Contents

Peripherals

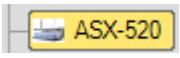
The settings for peripherals such as LC pumps or LC autosamplers can be adjusted in the corresponding view of the Template in Qtegra.

Tip Peripherals are added to the Configuration in the Configurator tool of Qtegra ISDS Software by your Administrator or Thermo Fisher Scientific field service engineer (see "Experiment Configurator" on page 3-15).

Teledyne CETAC ASX-520 / ASX-560 / ASX-1400 Autosampler

The Teledyne CETAC™ Technologies ASX-520 autosampler offers 4 racks and an autotune function. The schematic view and settings described in the following are similar to the Teledyne CETAC Technologies ASX-560, and the Teledyne CETAC Technologies ASX-1400 are therefore valid for these peripherals.

❖ **To adjust the Teledyne CETAC autosampler settings**

1. Open a Template with a Configuration including the Teledyne CETAC ASX-520, Teledyne CETAC ASX-560, or Teledyne CETAC ASX-1400 autosampler.
2. Click 

to open the autosampler view, see Figure 14-1.

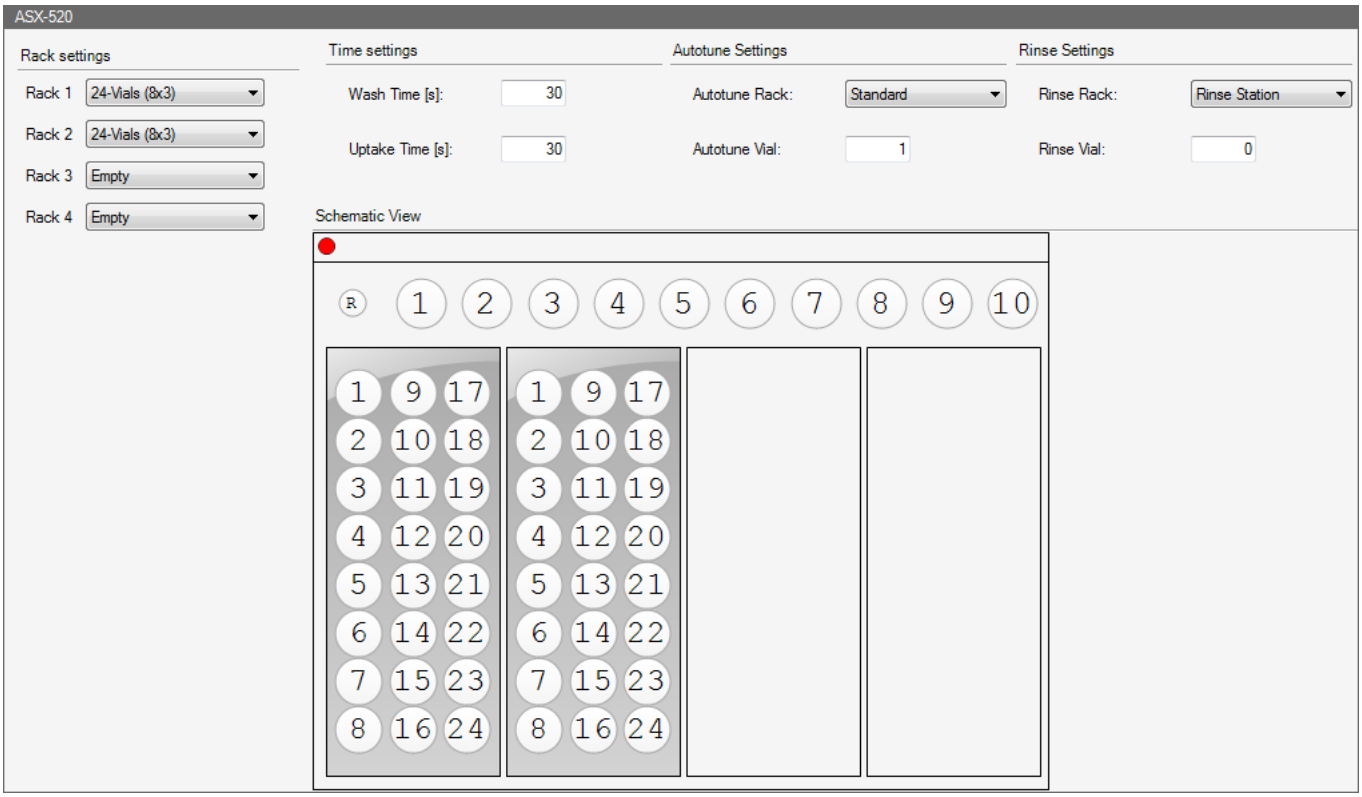


Figure 14-1. Teledyne CETAC ASX-520 settings

3. Select the **Rack settings** from the drop-down menus. On most CETAC autosamplers you can choose between *21-*, *24-*, *40-*, *60-*, and *90-Vials* layout.
   The **Schematic View** shows the selected rack configuration.
4. Under **Time settings**, type the **Wash Time [s]** and the **Uptake Time [s]**.
5. Under **Autotune Settings**, select the **Autotune Rack** from the drop-down menu and type the **Autotune Vial** number.
6. Under **Rinse Settings**, select the **Rinse Rack** from the drop-down menu and type the **Rinse Vial** if the setting is not *Rinse Station*.

Teledyne CETAC ASX-260 / ASX-280 Autosampler

The Teledyne CETAC Technologies ASX-260 autosampler offers 2 racks and an autotune function. The schematic view and settings described in the following are similar to the Teledyne CETAC Technologies ASX-280 and are therefore valid for these peripherals.

❖ **To adjust the Teledyne CETAC autosampler settings**

1. Open a Template with a Configuration including the Teledyne CETAC ASX-260 or ASX-280 autosampler.

2. Click ASX-280 to open the autosampler view, see Figure 14-2.

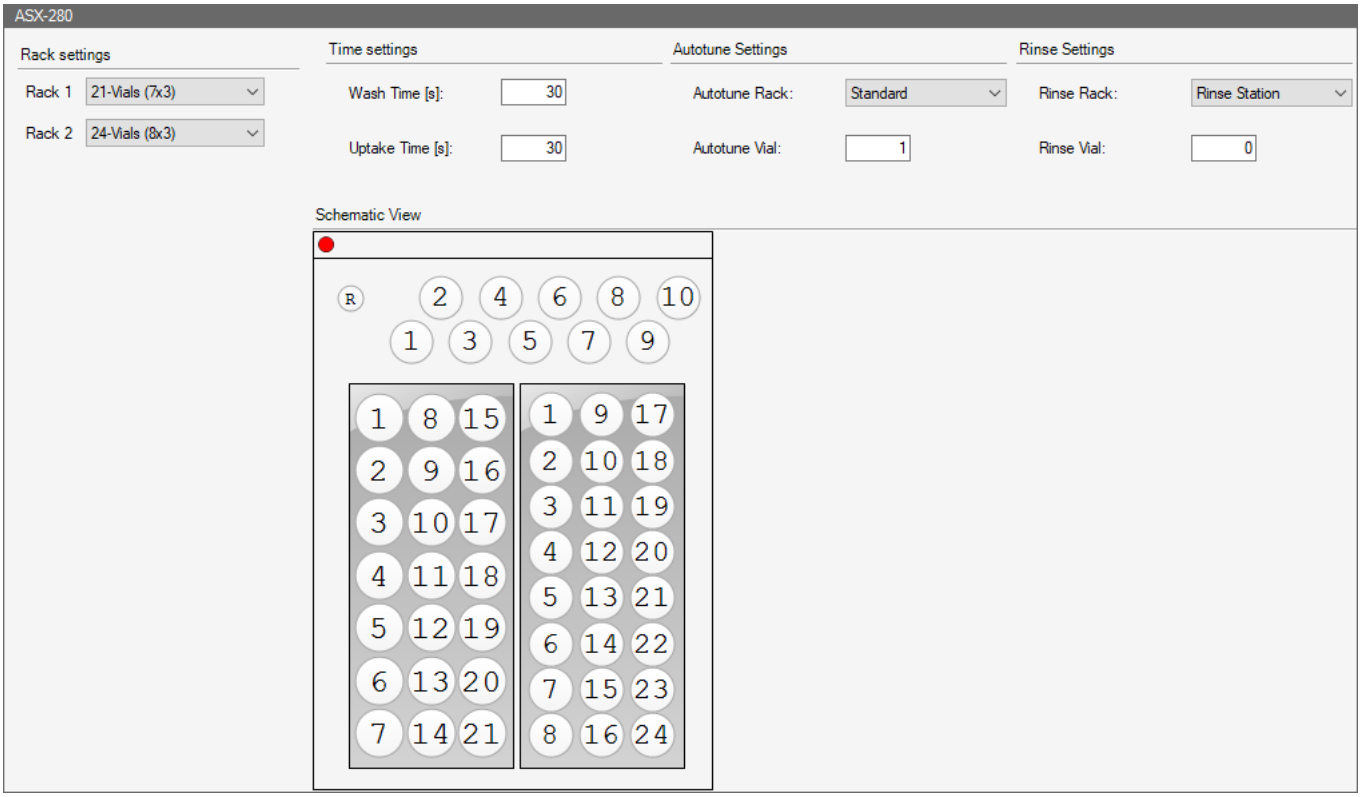


Figure 14-2. Teledyne CETAC ASX-280 settings

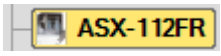
3. Select the **Rack settings** from the drop-down menus. You can choose between *21-*, *24-*, *40-*, *60-* and *90-Vials* layout. The **Schematic View** shows the selected rack configuration.
4. Under **Time settings**, type the **Wash Time [s]** and the **Uptake Time [s]**.
5. Under **Autotune Settings**, select the **Autotune Rack** from the drop-down menu and type the **Autotune Vial** number.
6. Under **Rinse Settings**, select the **Rinse Rack** from the drop-down menu and type the **Rinse Vial** if the setting is not *Rinse Station*.

Teledyne CETAC ASX-100 / ASX-112FR Autosampler

The Teledyne CETAC Technologies ASX-100 autosampler offers 1 rack and an autotune function. The schematic view and settings described in the following are similar to the Teledyne CETAC Technologies ASX-112FR and are therefore valid for these peripherals.

❖ **To adjust the Teledyne CETAC autosampler settings**

1. Open a Template with a Configuration including the Teledyne CETAC ASX-100, or ASX-112FR autosampler.

2. Click 

to open the autosampler view, see Figure 14-3.

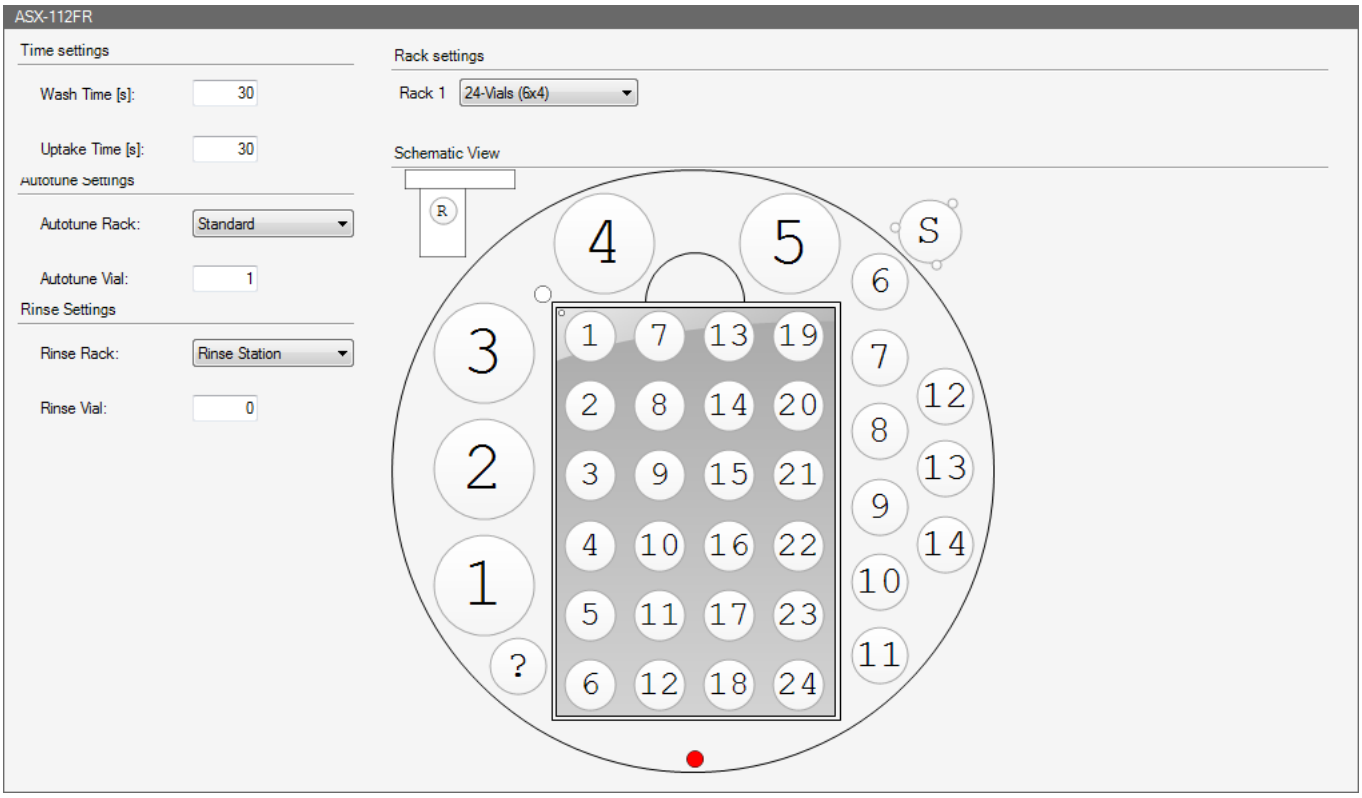


Figure 14-3. Teledyne CETAC ASX-112FR settings

3. Select the **Rack settings** from the drop-down menu. You can choose between *24-, 48-* and *96-Vials* layout.
   The **Schematic View** shows the selected rack configuration.

4. Under **Time settings**, type the **Wash Time [s]** and the **Uptake Time [s]**.

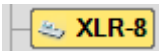
5. Under **Autotune Settings**, select the **Autotune Rack** from the drop-down menu and type the **Autotune Vial** number.

6. Under **Rinse Settings**, select the **Rinse Rack** from the drop-down menu and type the **Rinse Vial** if the setting is not *Rinse Station*.

Teledyne CETAC XLR-8 / XLR-860 Autosampler

The Teledyne CETAC Technologies XLR-8 autosampler offers 8 racks and an autotune function. The schematic view and settings described in the following are similar to the Teledyne CETAC Technologies XLR-860 and are therefore valid for these peripherals.

❖ **To adjust the Teledyne CETAC autosampler settings**

1. Open a Template with a Configuration including the Teledyne CETAC XLR-8 or XLR-860 autosampler.
2. Click 

to open the autosampler view, see Figure 14-4.

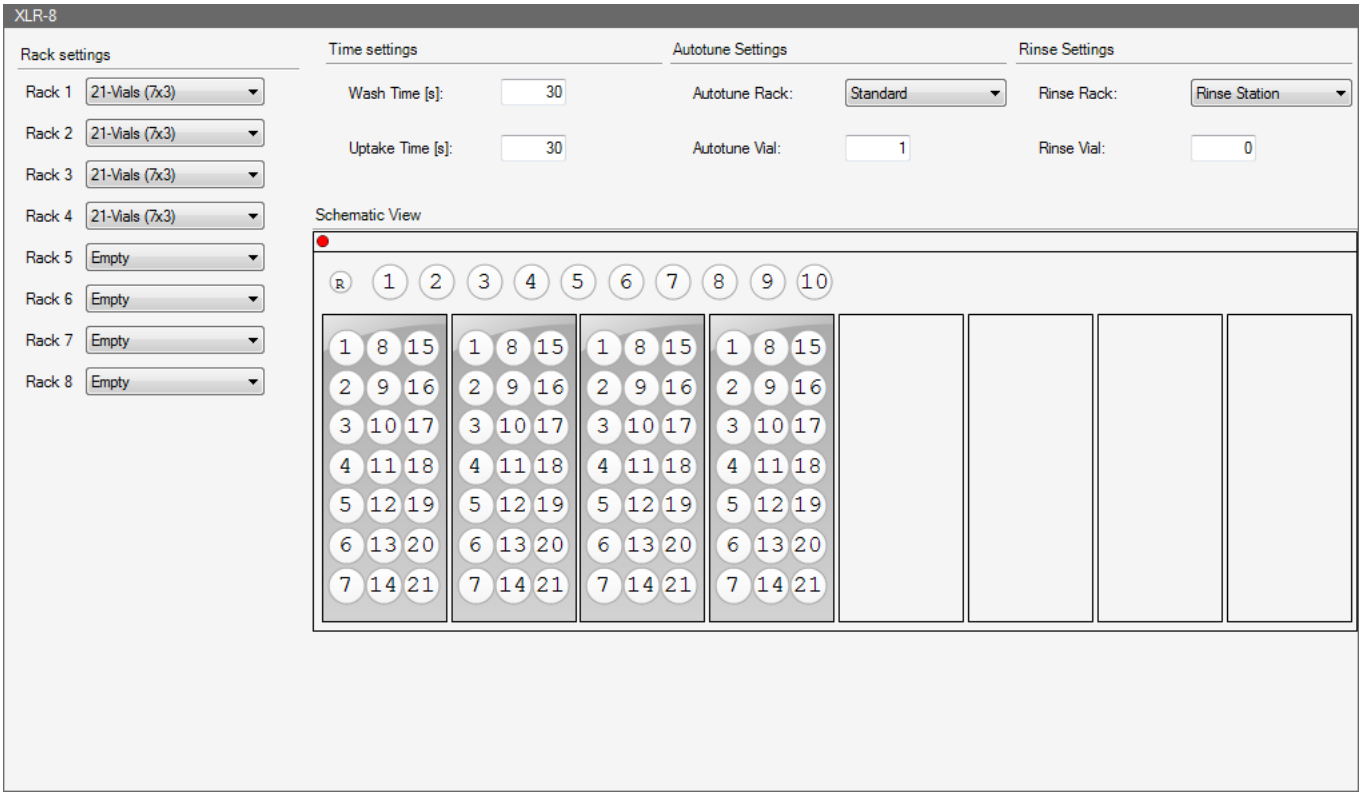


Figure 14-4. Teledyne CETAC XLR-8 settings

3. Select the **Rack settings** from the drop-down menus. You can choose between *21-, 24-, 40-, 60-* and *90-Vials* layout. The **Schematic View** shows the selected rack configuration.
4. Under **Time settings**, type the **Wash Time [s]** and the **Uptake Time [s]**.
5. Under **Autotune Settings**, select the **Autotune Rack** from the drop-down menu and type the **Autotune Vial** number.
6. Under **Rinse Settings**, select the **Rinse Rack** from the drop-down menu and type the **Rinse Vial** if the setting is not *Rinse Station*.

ESI SC-2DX / SC-4Q / SC-8DX Autosampler

Several ESI autosamplers can be connected to your iCAP 7000 Plus Series ICP-OES. The ESI autosamplers including an autodilutor (ESI SC-2DX, ESI SC-4Q, ESI SC-8DX) are configured by the same interface of Qtegra and will therefore be described together.

Tip The settings for Uptake and Wash in the Monitor Analytes view of Qtegra will overwrite these settings for the autosampler.

❖ **To adjust the ESI autosampler settings**

1. Open a Template with a Configuration including the ESI autosampler.
2. In the Content pane, double-click the desired ESI autosampler to expand the entry and to display Method Settings, FAST Methods and Intelligent Dilution.
3. Click 

to open the autosampler view, see Figure 14-5.

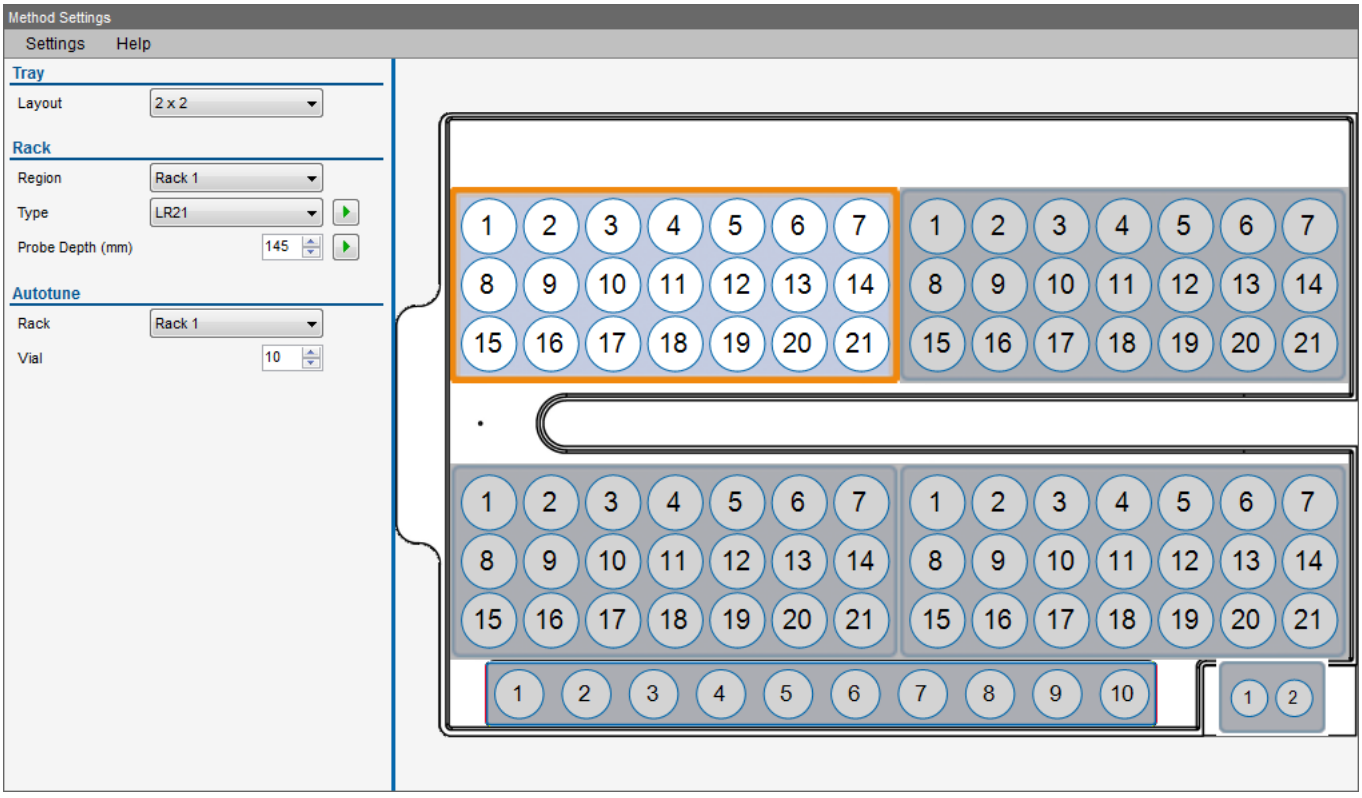


Figure 14-5. ESI SC-4Q settings

Tip The right-hand tile shows a racks layout of your specific ESI autosampler and may vary from the screenshots in this manual.

4. Select **Settings > Racks**.

The ESI SC-4Q autosampler offers 5 racks and a rinse station, see Figure 14-5.
The ESI SC-2DX autosampler offers 3 racks and a rinse station, see Figure 14-6.

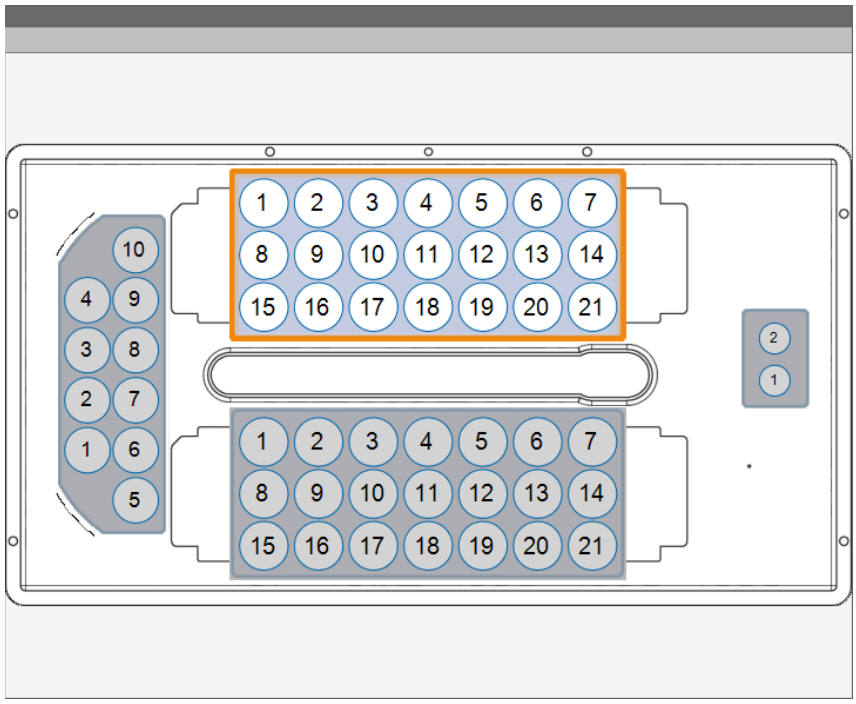


Figure 14-6. ESI SC-2DX settings

The ESI SC-8DX autosampler offers 12 racks and a rinse station, see Figure 14-7.

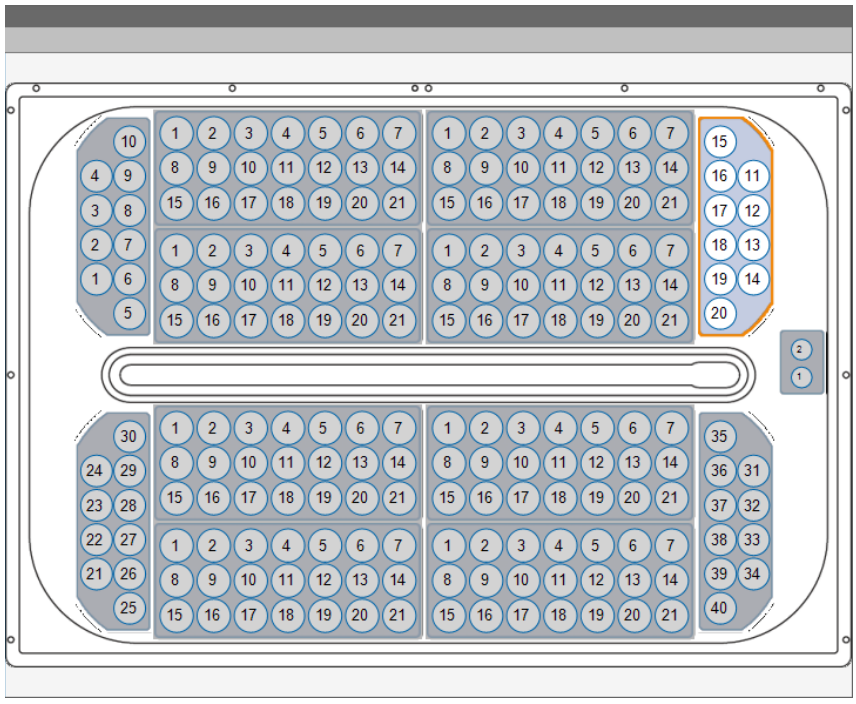


Figure 14-7. ESI SC-8DX settings

5. Select the settings for **Layout** for **Tray**, **Region**, **Type** and **Probe Depth** for **Rack**, and **Rack** and **Vial** for **Autotune**.

6. Select **Settings > Analysis**, see Figure 14-8.

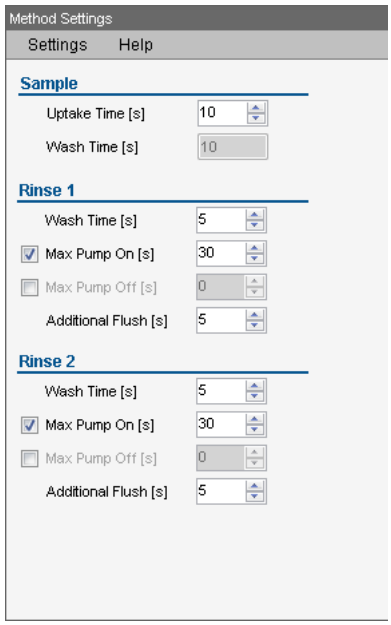


Figure 14-8. ESI autosampler Analysis Settings

7. Under **Sample**, type the **Uptake Time [s].** The **Wash Time [s]** is set to 10 seconds.

8. Under **Rinse 1**, type **Wash Time [s]**, select **Max Pump On [s]** or **Max Pump Off [s]**, and type **Additional Flush [s]**.

9. Under **Rinse 2**, type **Wash Time [s]**, select **Max Pump On [s]** or **Max Pump Off [s]**, and type **Additional Flush [s]**.

10. Select **Settings > Post-Analysis** and then select the action after analysis completed from the drop-down menu, see Figure 14-9.

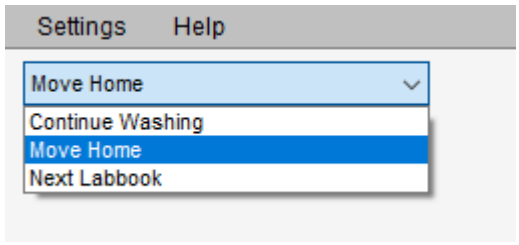


Figure 14-9. Post Analysis drop-down menu

a. With **Continue Washing**, set the **Rinse 1** and **Rinse 2** parameters as shown in Figure 14-8. When selected, after analysis completed the probe moves to the rinse vial and cleans for the specified time.

b. With **Move Home**, type a **Home Shutdown Time** value. When selected, after analysis completed the probe moves to the home position and stops the peristaltic pump.

c. With **Next LabBook**, no additional setting is required. When selected, after analysis completed the next LabBook is started from the Scheduler.

Tip For FAST Methods, see "Autodilution Using the ESI prepFAST II Method" on page 14-24.
See "Using ESI Autosamplers without FAST Method" on page 14-13 for a Configuration without FAST Methods.

11. Click Intelligent Dilution to open the Internal Standard and Calibration setting page, see Figure 14-10.

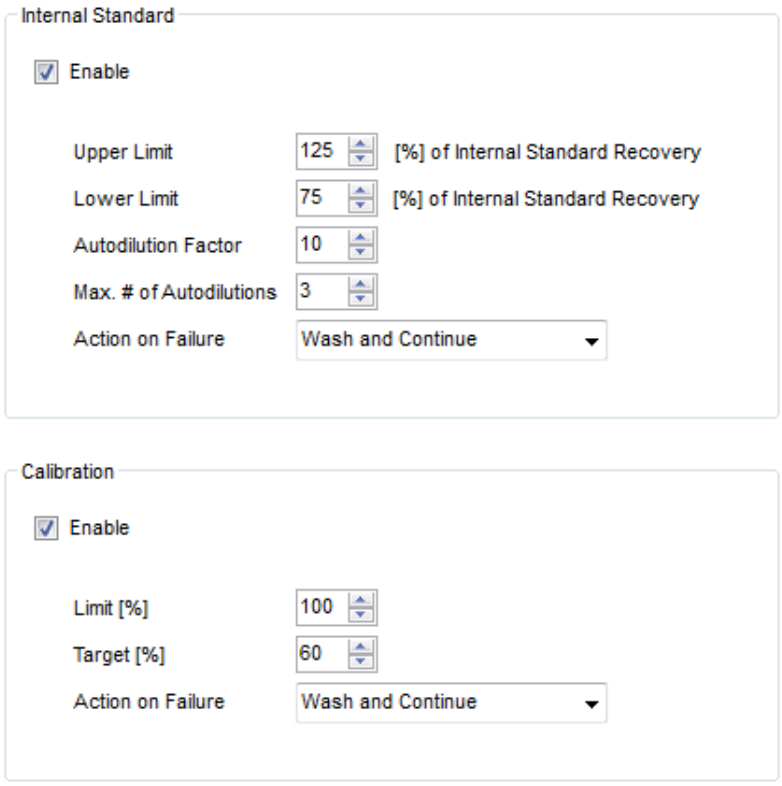


Figure 14-10. ESI Intelligent Dilution settings

12. Set the parameters for **Internal Standard** (see "Calibration Curve created by Autodilution" on page 14-21) and **Calibration** as described in detail, see "Intelligent Dilution Settings" on page 14-16.

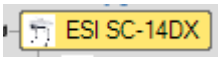
ESI SC-4DX / SC-14DX Autosampler

The ESI SC-14DX autosampler offers 15 racks and a rinse station. The ESI autosamplers ESI SC-4DX and ESI SC-14DX are configured by the same interface of Qtegra and will therefore be described together.

Tip The settings for Uptake and Wash in the Monitor Analytes view of Qtegra will overwrite these settings for the autosampler.

❖ **To adjust the ESI autosampler settings**

1. Open a Template with a Configuration including your ESI autosampler.

2. Select 

to show the autosampler rack layout, see Figure 14-11.

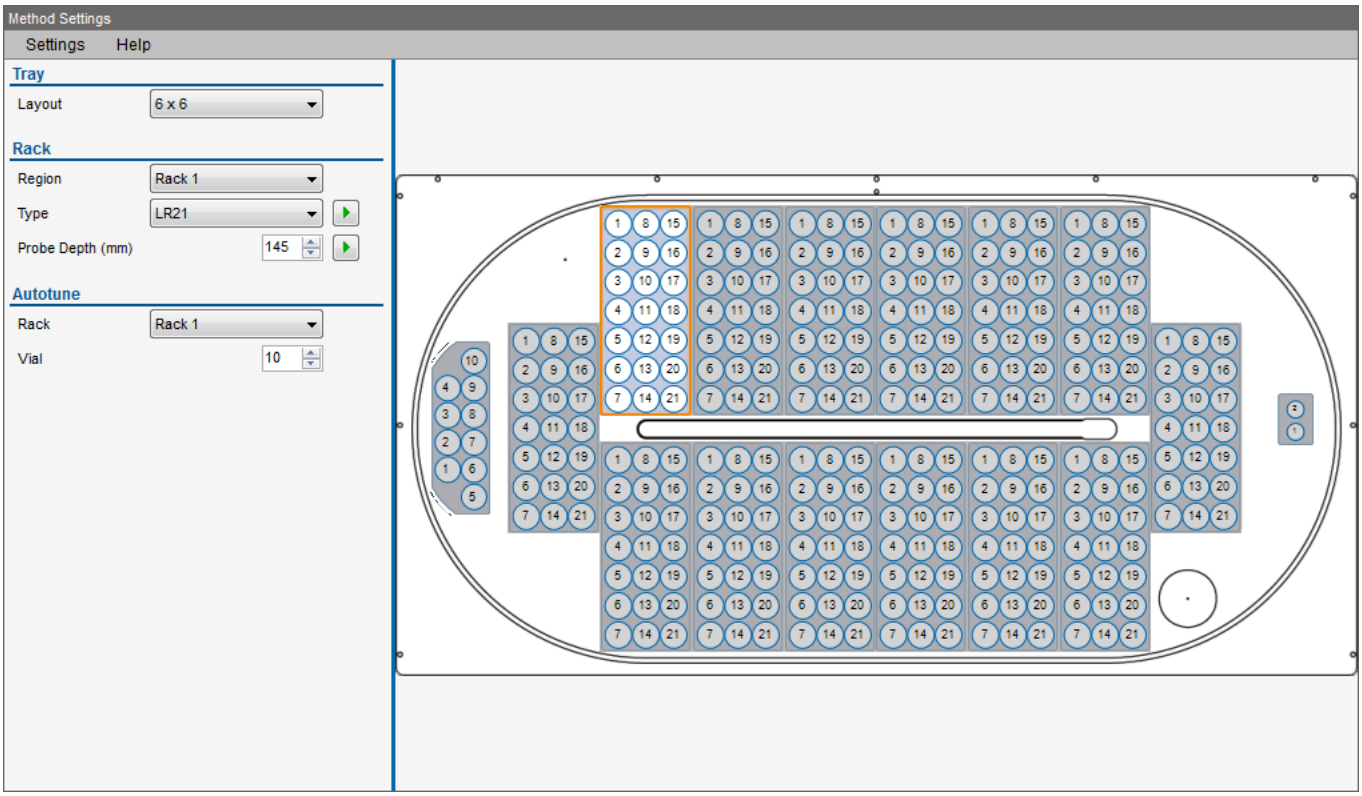


Figure 14-11. ESI SC-14DX settings

3. Select **Settings > Racks**, see Figure 14-12 for the ESI SC-4DX autosampler.

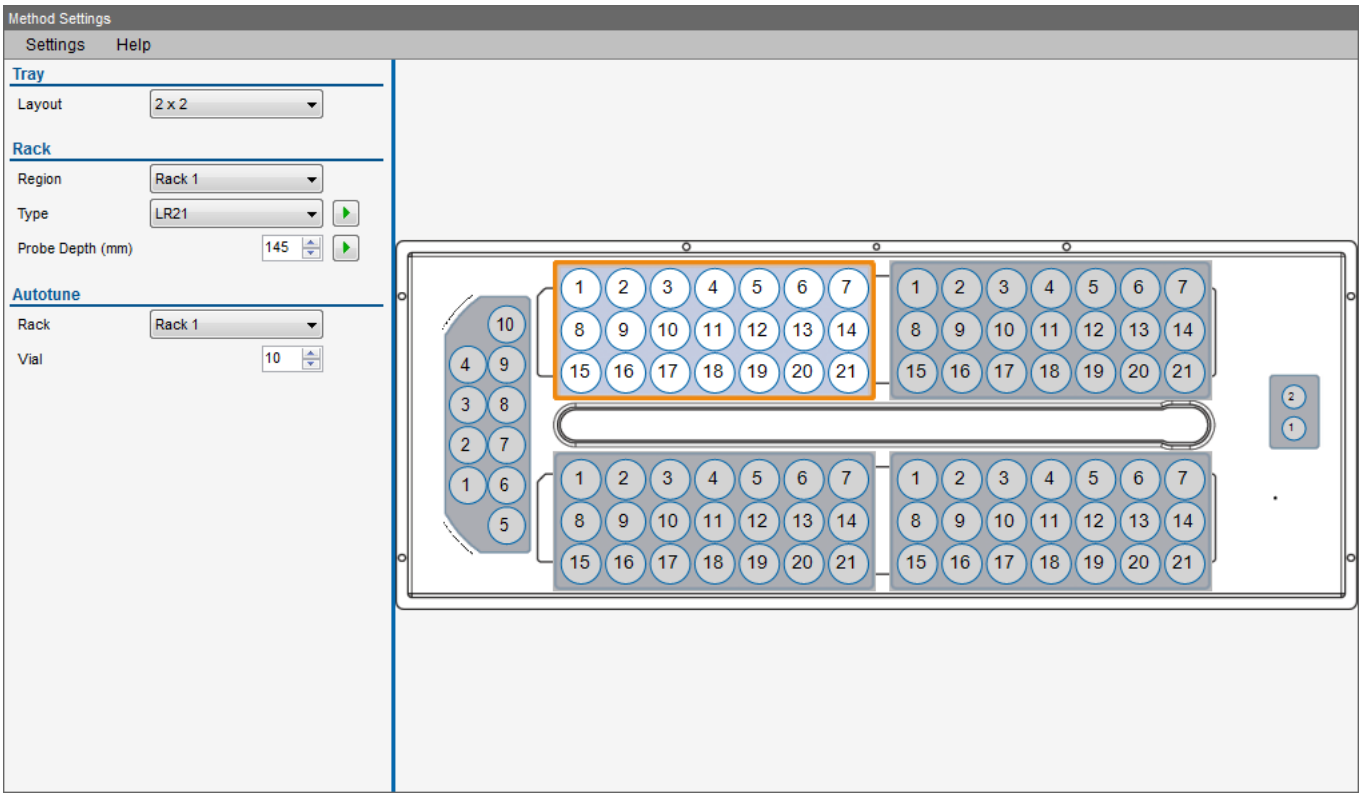


Figure 14-12. ESI SC-4DX settings

4. Select the settings for **Layout** for **Tray**, **Region**, **Type** and **Probe Depth** for **Rack**, and **Rack** and **Vial** for **Autotune**.

5. Select **Settings > Analysis**, see Figure 14-13.

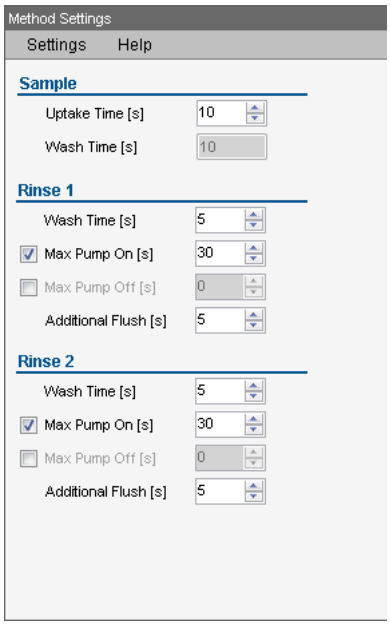


Figure 14-13. ESI autosampler Analysis Settings

6. Under **Sample**, type the **Uptake Time [s].** The **Wash Time [s]** is set to 10 seconds.

7. Under **Rinse 1**, type **Wash Time [s]**, select **Max Pump On [s]** or **Max Pump Off [s]**, and type **Additional Flush [s]**.

8. Under **Rinse 2**, type **Wash Time [s]**, select **Max Pump On [s]** or **Max Pump Off [s]**, and type **Additional Flush [s]**.

9. Select **Settings > Post-Analysis**, and select the action after analysis completed from the drop-down menu, see Figure 14-14.

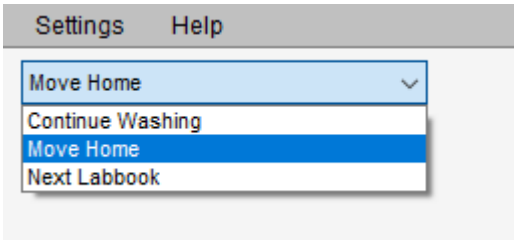


Figure 14-14. Analysis Completed drop-down menu

   a. With **Continue Washing**, set the **Rinse 1** and **Rinse 2** parameters as shown in Figure 14-13. When selected, after analysis completed the probe moves to the rinse vial and cleans for the defined time.

   b. When **Move Home** selected, after analysis completed the probe moves to the home position.
   If a **Home Shutdown Time** is defined, the probe moves to the home position for the set time before the next LabBook from the Scheduler is started.

   c. With **Next LabBook**, no additional setting is required. When selected, after analysis completed the next LabBook is started from the Scheduler without moving the probe to the home position or continuing washing.

10. For 

, see "Autodilution Using the ESI prepFAST II Method" on page 14-24.
See "Using ESI Autosamplers without FAST Method" on page 14-13 for a Configuration without FAST Methods.

Using ESI Autosamplers without FAST Method

This section describes how to set up an ESI autosampler without using the FAST valve.

❖ **To configure the autosampler without using the FAST valve**

1. In the Configurator tool, create the Configuration based on your instrument and peripheral as usual, see "To create a new Configuration" on page 3-16.

   No further Configuration settings are necessary as the defaults can be used.

   If desired check the correct settings as follows.

   a. In the Experiment Configurator applet, right-click the ESI peripheral (for example, ESI SC-4DX) and select **Edit settings** from the shortcut menu, see Figure 3-11.
   The Settings dialog opens, see Figure 14-15.

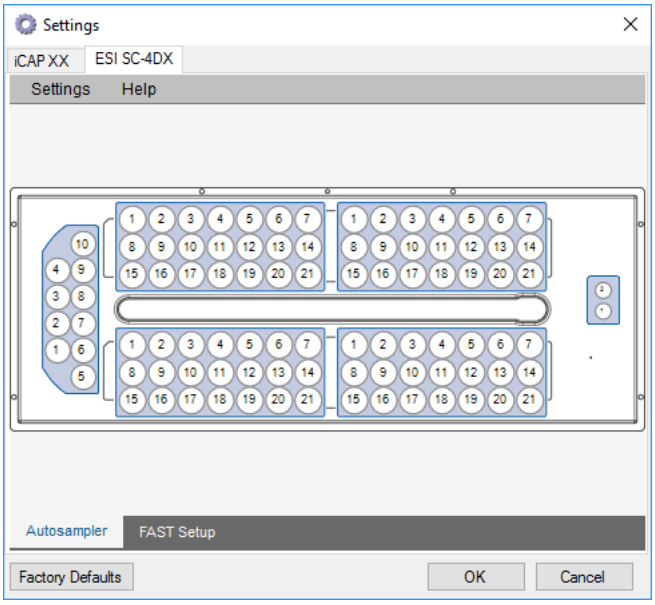


Figure 14-15. Autosampler tab of ESI autosampler

   b. Below the racks layout, select the **FAST Setup** tab.

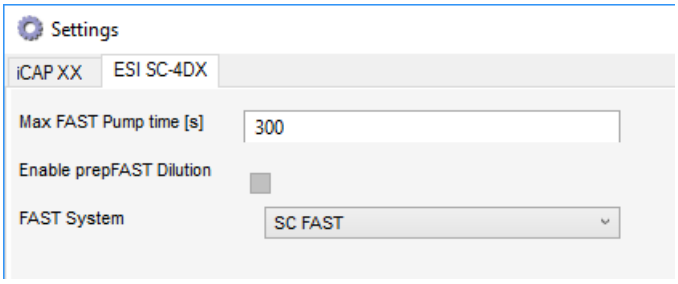


Figure 14-16. FAST Setup tab of ESI autosampler

   c. Leave the **Max FAST Pump time**, **Enable prepFAST Dilution** and **FAST System** drop-down unchanged.

2. Load the Configuration in the Qtegra ISDS Software.

3. On the Dashboard, select the ESI autosampler from the peripheral selector. Define settings for racks, rinse and motors.

4. Select the FAST Method tab, see Figure 14-17.

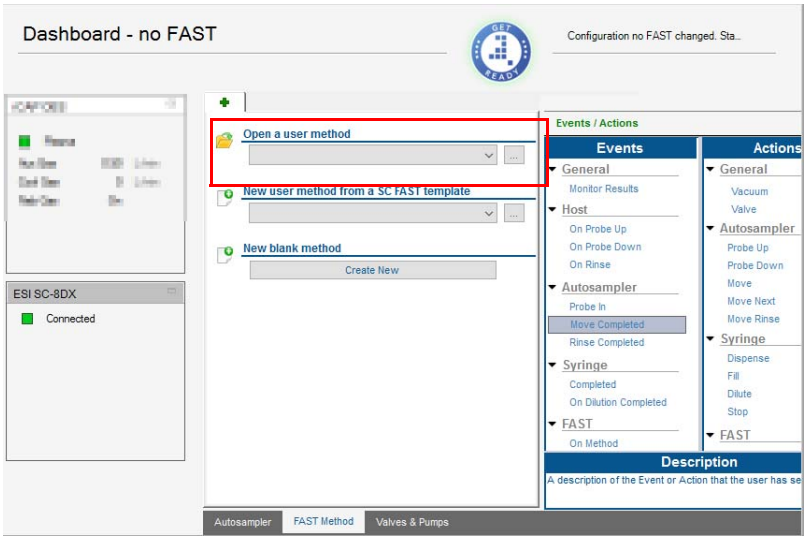


Figure 14-17. FAST Method tab of ESI autosampler on Dashboard

5. Make sure that no FAST Method is selected from the dialog options on this page.

6. You can now create and schedule your LabBook as usual. The autosampler is used with your definition of racks, rinse and motors. No FAST method is used.

7. To ensure the FAST Methods settings in your LabBook, expand the ESI autosampler in the Content pane and select FAST Methods, see Figure 14-18.

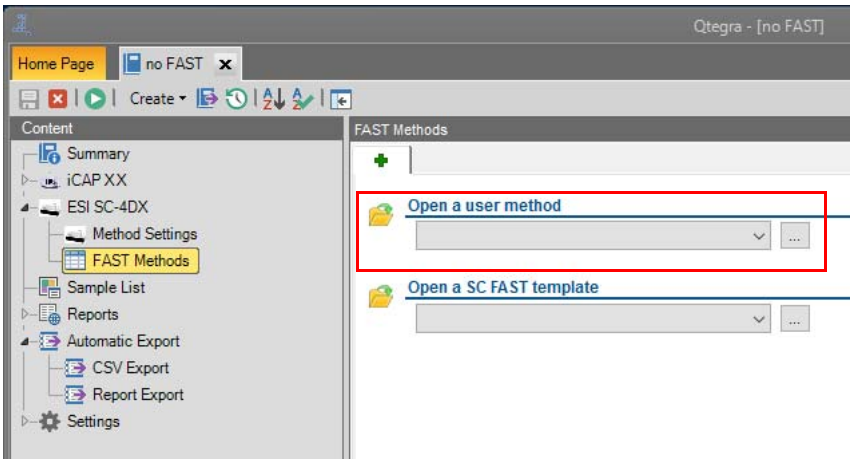


Figure 14-18. FAST Methods of LabBook

8. Make sure that no FAST Method is selected from the dialog options on this page.

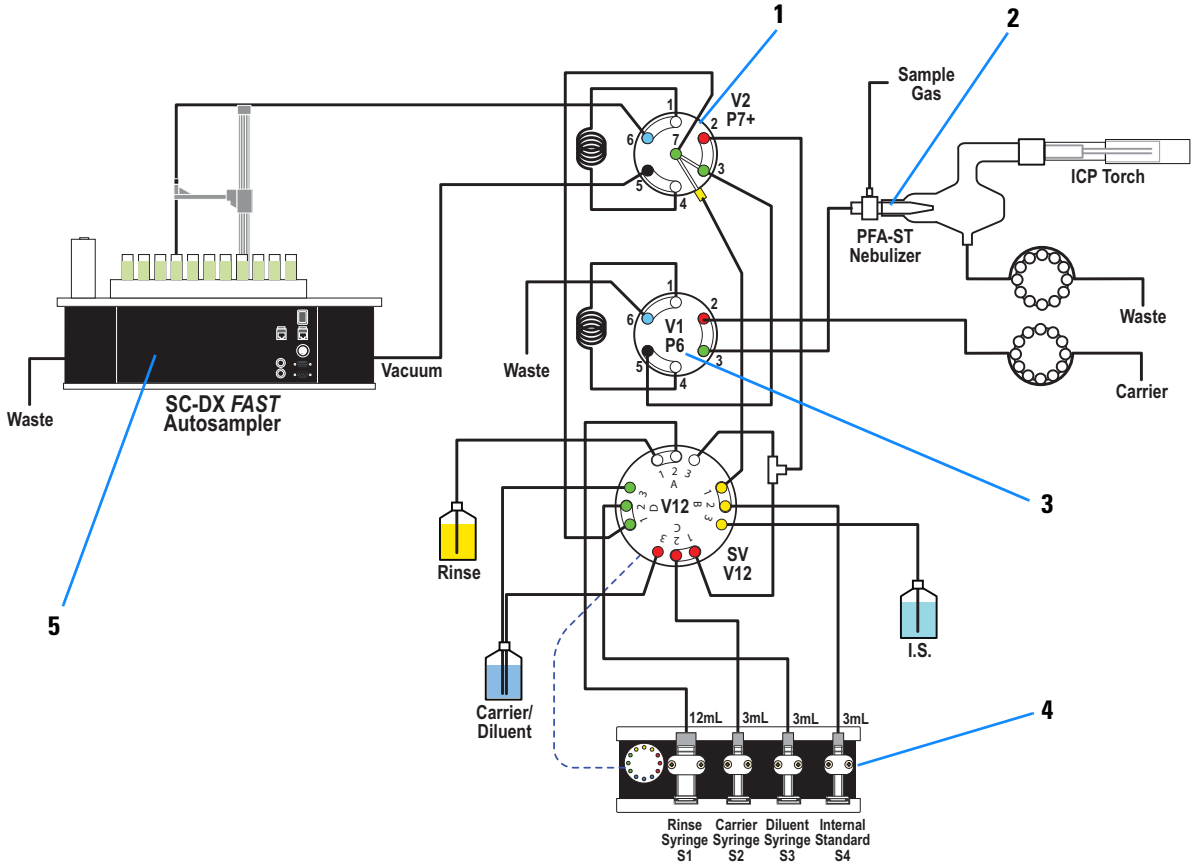
Automatic Dilution Processes

Intelligent Dilution

Intelligent Dilution is an automated iterative process that dilutes samples, which have shown analyte concentrations to be outside the calibration range. It also dilutes samples when one or more of the Internal Standards show an unacceptable recovery due to matrix effects.

Experimental Setup

The setup is shown in Figure 14-19.



Labeled Components: 1=7-port valve (valve 2), 2=PFA nebulizer, 3=6-port valve (valve 1), 4=S400V 4 syringe pump dilution module, 5=Supporting cart

Figure 14-19. The complete prep*FAST* II autodilution system

Intelligent Dilution Settings

When using the prep*FAST* II with the iCAP 7400 ICP-OES, it is possible to automatically dilute samples, which have concentrations that are higher than the calibration range. It also provides the option to

dilute samples, which show matrix effects for the Internal Standard. This is often the case for environmental or industrial samples. The settings, which define the autodilution parameters, are available in the LabBook on the dedicated Intelligent Dilution view, see Figure 14-20.

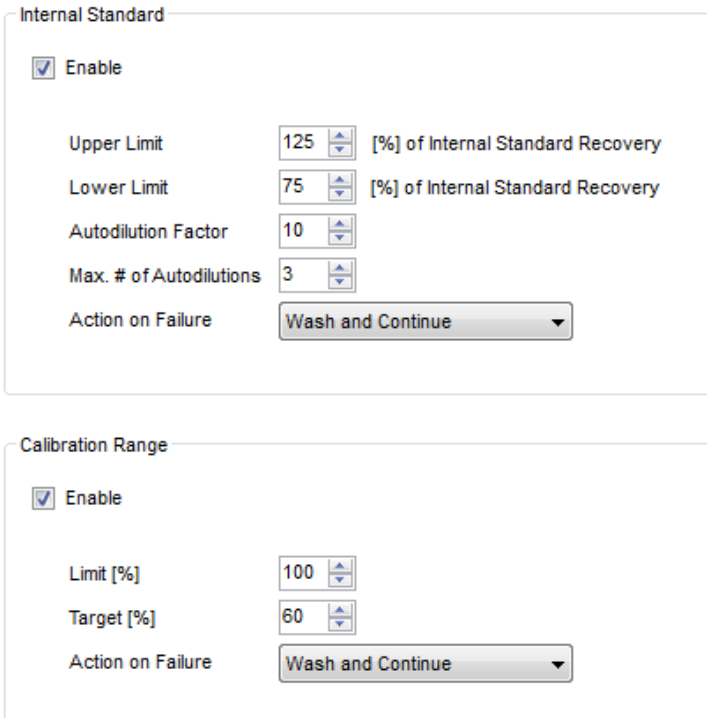


Figure 14-20. Enabling the Autodilution for Internal Standard and Calibration Range

To get a short help, just point to the desired item of this page. A tooltip shows the definition.

For the **Internal Standard** an Upper and a Lower Limit can be defined, between which the recovery of the Internal Standard has to lie. If the recovery rate of any Internal Standard within the LabBook does not meet this criterion, the sample will be diluted according to the set Autodilution Factor, e.g. *10*. If the recovery of at least one Internal Standard is still not within the defined limits, the prep*FAST* II system will try to dilute it further, e.g. by a factor of *20*, until the Maximum Number of Autodilutions has been reached. In this case, the action defined by the Action on Failure drop-down menu will be performed.

For the **Calibration Range** a Limit can be set. If at least one of the investigated analytes shows a concentration above this limit, the sample will be autodiluted. This value is the percentage of the highest calibration standard (STD sample) for any measured analyte. If for example, the highest calibration point is 1 ppm and the limit was set to *120%*, each sample with an analyte concentration above 1.2 ppm will be autodiluted to the Target value. If more than one analyte is out of the calibration range, the highest dilution factor will be applied automatically. This value is again a percentage of the highest calibration

point. With the aforementioned example this would mean that the 1.2 ppm sample is diluted by a factor of 2 to achieve a concentration of 0.6 ppm (60% of the highest calibration point).

❖ **To edit the Internal Standard parameters**

1. Check **Enable** to activate the Internal Standard (IS) section. For details on IS, see "Calibration Curve created by Autodilution" on page 14-21.

2. Type an **Upper Limit** to set the maximum value with regard to the Internal Standard recovery compared to the BLK Internal Standards signal. Usually, the upper limit is set 25% above the maximum value of the Internal Standard recovery, i.e., type a value like *125%*. Values exceeding this limit will then be highlighted in red font in the Concentrations table.

3. Type a **Lower Limit** to set the minimum value with regard to the Internal Standard recovery. Usually, the lower limit is set 25% below the maximum value of the Internal Standard recovery, i.e., type a value like *75%*. Values below this limit will then be highlighted in red font in the Concentrations table.

4. Type an **Autodilution Factor** to dilute your sample solution. With regard to the number of autodilution cycles (see step 5) make sure to type a useful factor. To decrease the concentration slightly, type a small value, for example, 2 or 3. 3 means 2 parts of diluent and 1 part of your sample.

5. Type the **Max. Number of Autodilutions** to define the maximum number of dilution cycles. A typical number of cycles is 3.
The autodilution cycle ends automatically when the IS is in range.

6. From the **Action on Failure** list box, select a procedure that follows the dilution process.
Select **Wash and Continue** to run your experiment as if there is no failure.
-or-
Select **Abort LabBook** to stop the analysis of the current LabBook and run the next LabBook of your Scheduler.
-or-
Select **Abort Scheduler** to stop your experiment.

❖ **To edit the Calibration parameters**

1. Check **Enable** to activate the Calibration section.

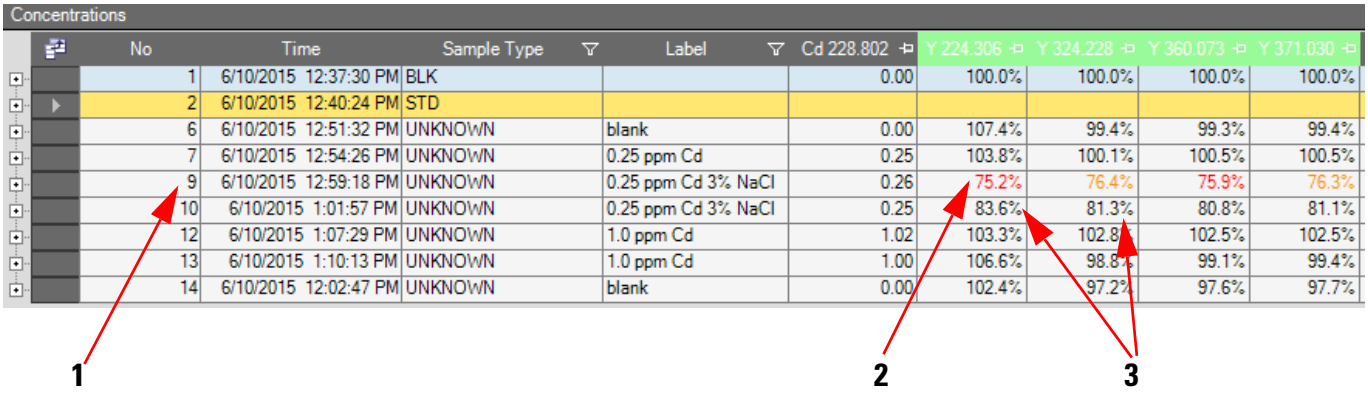
2. Type a **Limit** that defines how much the concentration of the unknown sample can exceed the range. Typically, the limit is set to 100%.

3. Type a **Target** that is used by the autodilutor when your unknown sample exceeds the limit setting. Typically, the target is set to 60% of the maximum concentration.

4. From the list box **Action on Failure**, select a procedure that follows the calibration process.
   Select **Wash and Continue** to run your experiment as if there is no failure.
   -or-
   Select **Abort LabBook** to stop the analysis of the current LabBook and run the next LabBook of your Scheduler.
   -or-
   Select **Abort Scheduler** to stop your experiment.

When the Internal Standard signal recovery is out of range (exceeds upper or lower limit), check these values in the Evaluation Results > Concentrations view. For example, on this LabBook, *sample containing 0.25 ppm Pb in 3% NaCl* in line 9 on the Sample List (**1** in Figure 14-21), the Internal Standard recovery for Y 224.306 shows 75.2% (**2** in Figure 14-21) and for Y 324.228 it shows 76.4%. These values are out of range and the status is indicated with red and orange font in the Results view.

Qtegra adds the new sample automatically (line 10) and runs the sample with the **Autodilution Factor**. The new sample is prepared with *3* fold dilution and the Internal Standard recovery achieved inside the range with Y 224.306 = 83.6% and Y 324.228 = 81.3% (**3** in Figure 14-21).



Labeled Components: 1=line number, 2=out of range values, 3=inside range values after autodilution

Figure 14-21. Example of LabBook missing the limits of Internal Standard recovery

If the autodilution fails, that means if the Internal Standard recovery remains out of range, then the autodilution process will dilute the IS as often as specified in the **Max. Number of Autodilutions** or until the IS concentration remains inside the calibration limits.

From the **Action on Failure** listbox, for this LabBook, *Wash and Continue* is selected.

For example on this LabBook, line 12 (**1** in Figure 14-21) shows *1 ppm Cd* out of range of the **Limit** setting due to the maximum calibration concentration of 0.5 ppm.

The calibration curve is shown in Figure 14-22.

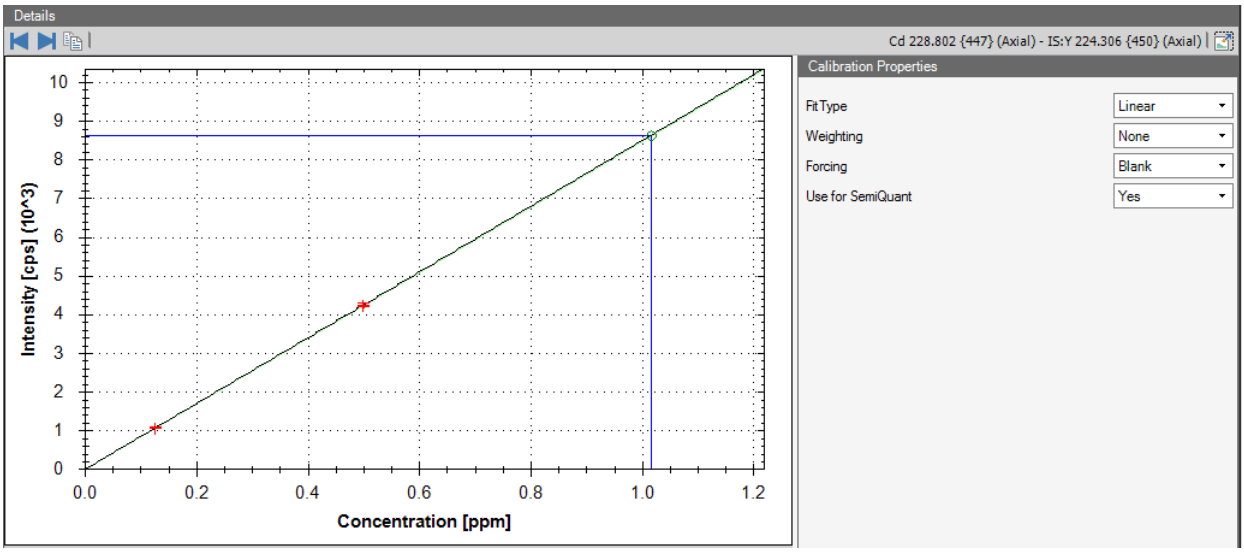


Figure 14-22. Calibration curve of line 12 of LabBook

The autodilutor therefore automatically starts the dilution process. In the **Evaluation Results** view, double-click the entry of line 12 to display the **Details** and **Comment** pane.

In the example LabBook, the **Target** is set to 60%. The autodilution process adds the sample *1.0 ppm Cd* to line 13 and runs with the Total Dilution Factor *3.814* (see Figure 14-27), calculated via f(x) = b × x + a, see Figure 14-23.

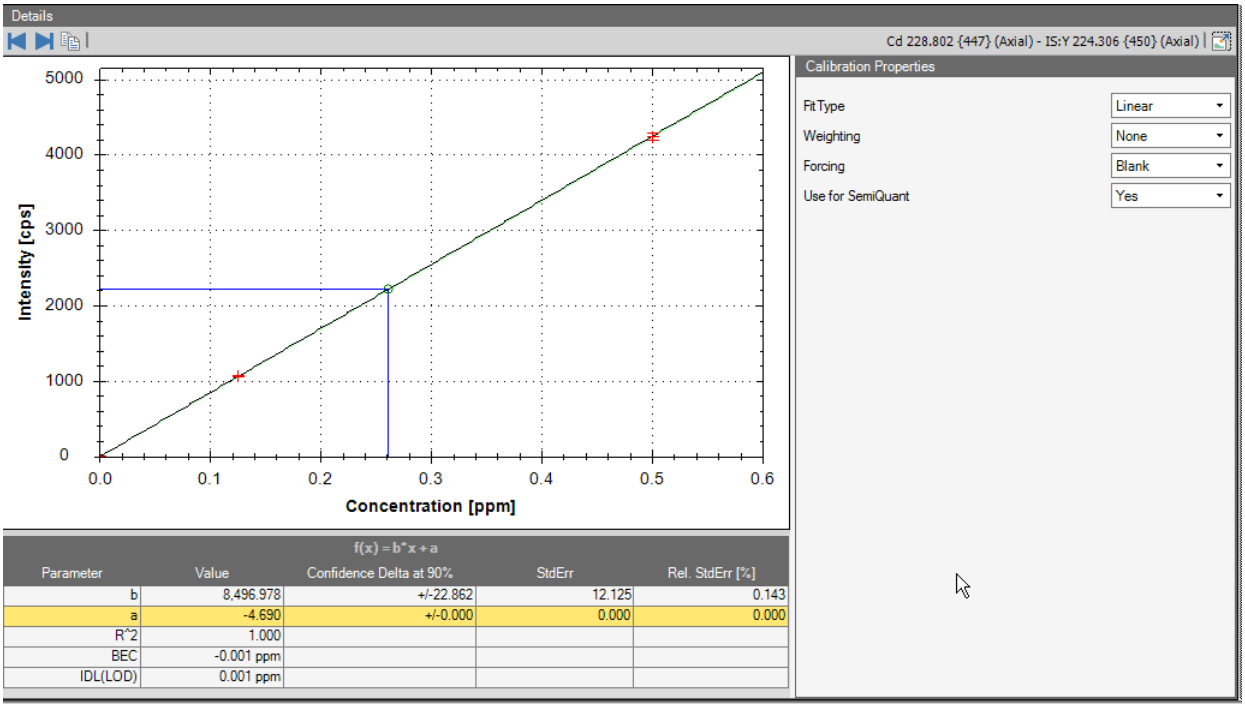


Figure 14-23. Calibration curve and details view of line 13 of LabBook

The concentration of about 0.26 ppm is therefore reaching the target range (60% of 0.5 ppm).

Autodilution

Autodilution is an automated process used to dilute one sample solution into a desired number of analytes with a specific concentration.

Experimental Setup

The setup is shown in Figure 14-19 and is therefore not different from the experimental setup used for intelligent dilution.

Calibration Curve created by Autodilution

An autodilutor creates a multi point standard calibration curve from one standard mix stock solution (which can contain multiple analytes) by the autodilution process. The following screenshots are taken from a demonstration LabBook.

❖ To create a calibration curve

1. For example, Y is selected as the Internal Standard analyte (IS) and Cd is selected as the quantification analyte, see Figure 14-24 and Figure 14-25.

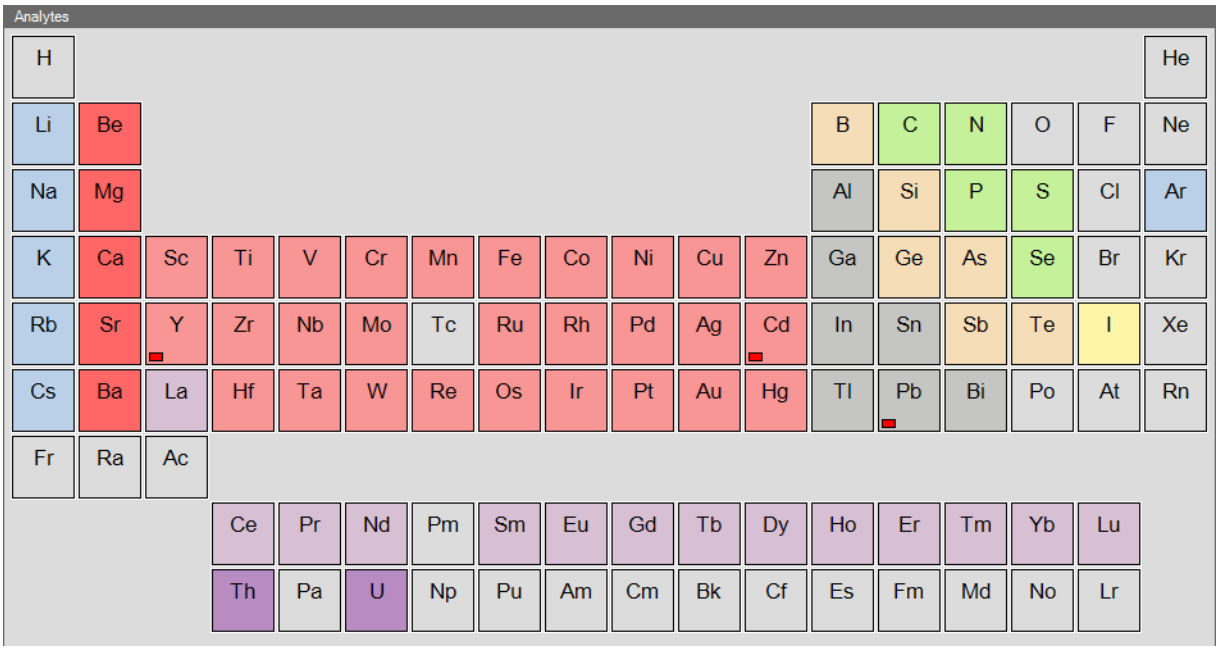
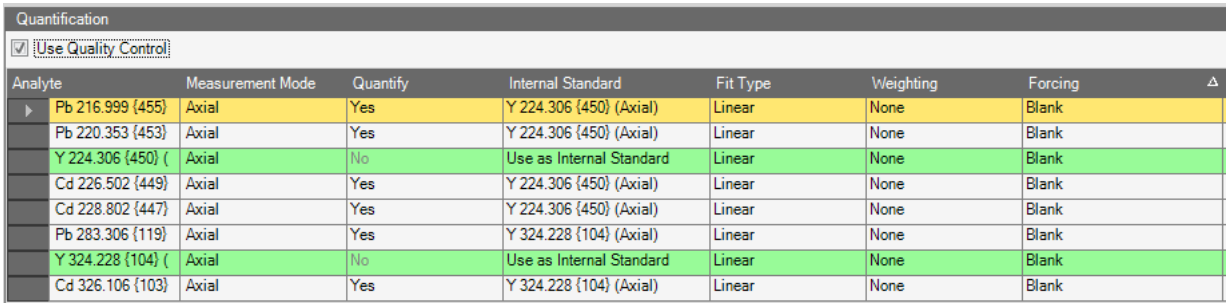


Figure 14-24. Selection of analytes from the periodic table of elements

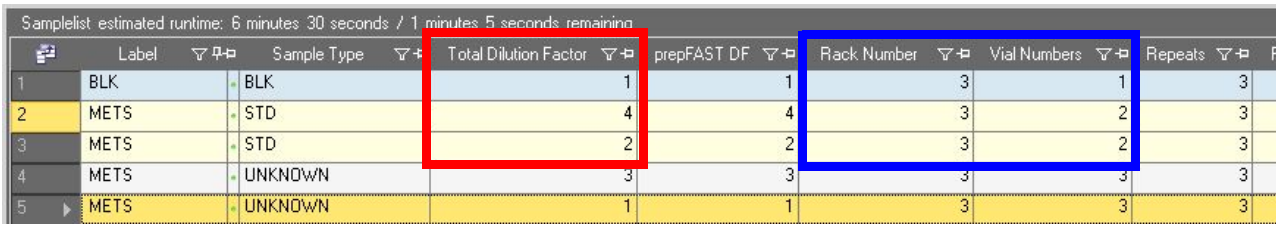


Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing
Pb 216.999 {455}	Axial	Yes	Y 224.306 {450} (Axial)	Linear	None	Blank
Pb 220.353 {453}	Axial	Yes	Y 224.306 {450} (Axial)	Linear	None	Blank
Y 224.306 {450} (	Axial	No	Use as Internal Standard	Linear	None	Blank
Cd 226.502 {449}	Axial	Yes	Y 224.306 {450} (Axial)	Linear	None	Blank
Cd 228.802 {447}	Axial	Yes	Y 224.306 {450} (Axial)	Linear	None	Blank
Pb 283.306 {119}	Axial	Yes	Y 324.228 {104} (Axial)	Linear	None	Blank
Y 324.228 {104} (	Axial	No	Use as Internal Standard	Linear	None	Blank
Cd 326.106 {103}	Axial	Yes	Y 324.228 {104} (Axial)	Linear	None	Blank

Figure 14-25. Presentation of quantification analytes in the LabBook

2. Set the blank solution (BLK) into rack 3, vial 1 and the standard stock solution (STD) METS into rack 3, vial 2, see blue rectangle in Figure 14-26. Make sure all solutions contain an IS.

3. To create the Sample List for the multi-point standard calibration curve, in the Sample List, select the BLK as first sample, the STD as second and third samples, see Figure 14-26.



Samplelist estimated runtime: 6 minutes 30 seconds / 1 minutes 5 seconds remaining

	Label	Sample Type	Total Dilution Factor	prepFAST DF	Rack Number	Vial Numbers	Repeats
1	BLK	BLK	1	1	3	1	3
2	METS	STD	4	4	3	2	3
3	METS	STD	2	2	3	2	3
4	METS	UNKNOWN	3	3	3	3	3
5	METS	UNKNOWN	1	1	3	3	3

Labeled Components: blue rectangle=selection of rack and vial, red rectangle=Total Dilution Factor for STD

Figure 14-26. Sort order of BLK and STD

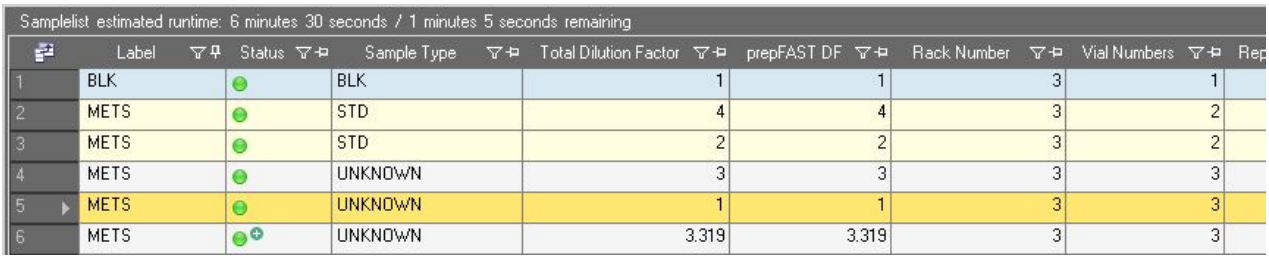
4. Type the *prepFAST DF (Dilution Factor)* for the STD entries. The autodilutor needs to dilute the 4- and 2-fold dilution to create the calibration curve for the standard mix solution, see the resulting *Total Dilution Factor* (red rectangle) in Figure 14-26.

5. The STD entries are prepared by autodilution from the same solution. Therefore, the rack and vial positions are the same for all standards, see blue rectangle in Figure 14-26.

6. Save this LabBook.

7. Schedule your LabBook.

8. The finished LabBook (see Figure 14-27) shows the calibration curve, see Figure 14-28.



Samplelist estimated runtime: 6 minutes 30 seconds / 1 minutes 5 seconds remaining

	Label	Status	Sample Type	Total Dilution Factor	prepFAST DF	Rack Number	Vial Numbers	Rep
1	BLK		BLK	1	1	3	1	
2	METS		STD	4	4	3	2	
3	METS		STD	2	2	3	2	
4	METS		UNKNOWN	3	3	3	3	
5	METS		UNKNOWN	1	1	3	3	
6	METS		UNKNOWN	3.319	3.319	3	3	

Figure 14-27. Sample List of finished LabBook

9. Double-click the STD entry to see the details of the calibration curve, see Figure 14-28.

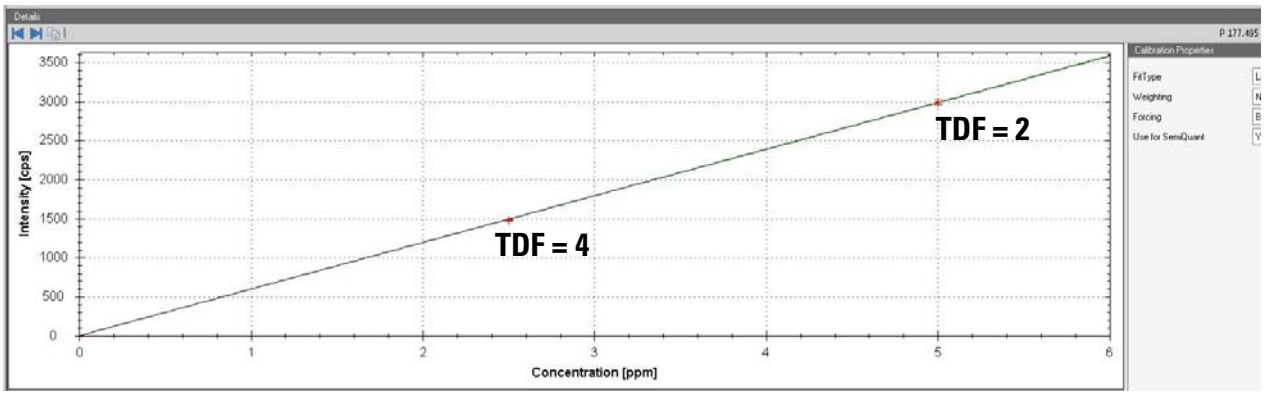


Figure 14-28. Calibration curve based on STD with 2 points of Total Dilution Factors (TDF)

Autodilution Using the ESI prep*FAST* II Method

The ESI prep*FAST* II Method is available as part of the ESI SC-2DX, ESI SC-4DX, ESI SC-8DX and ESI SC-14DX autosamplers. Several models are offered with different valves and vacuum pumps.

Tip This section describes actions to be performed in the Configurator tool, see "Configurator" on page 3-1.

❖ **To create an ESI prep*FAST* II Configuration**

1. From the **Configurator**, select **Experiment Configurator**.
2. Click **New** to create a new Configuration. Type a name and drag the instruments from the list of Available Items to the new Configuration on the left of the window to assign the instruments to the new Configuration. The new configuration should include the Thermo Scientific iCAP 7000 Plus Series ICP-OES as well as the ESI autosampler equipped with the prep*FAST* system, e.g., the ESI SC-2DX.

3. In the list of **Configurations**, right-click the Instrument you wish to edit the settings for, see Figure 14-29.

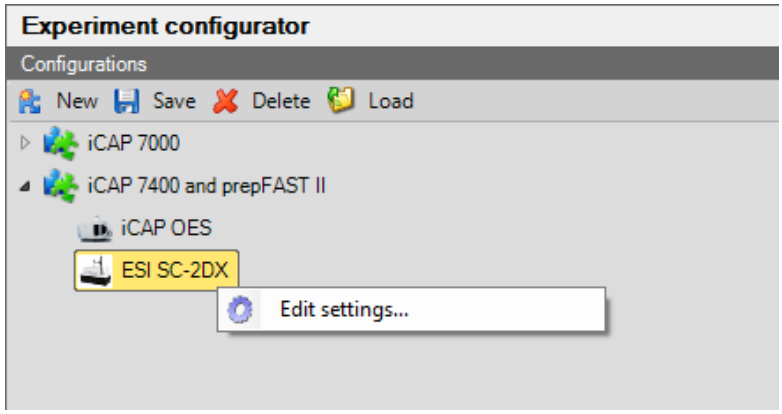
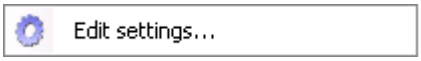


Figure 14-29. Shortcut menu to edit settings

4. Click 

to open the **Settings** window.

5. On the lower part, select the FAST Setup tab, see Figure 14-30.

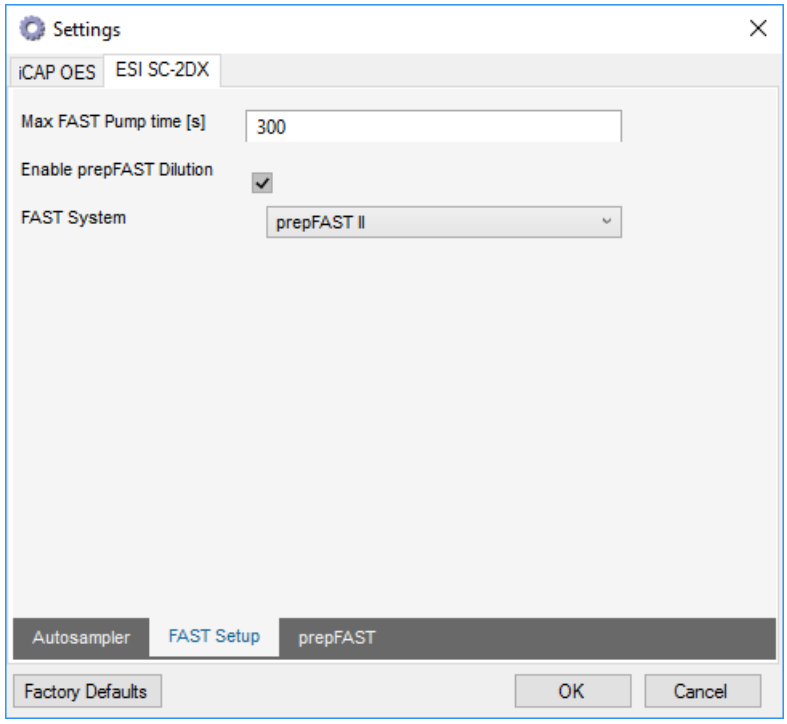


Figure 14-30. Settings window for FAST Setup

6. Select the **Enable prepFAST Dilution** check box.
7. From the **FAST System** list box, select *prepFAST II*.
8. Click **OK** to close the Settings window.

9. **Save** the Configuration.

Tip All other instrument settings of the Thermo Scientific iCAP 7000 Plus Series ICP-OES and the ESI autosampler provided inside the **Experiment Configurator** can be adjusted according to the demands of your analysis. However, Thermo Fisher Scientific recommends disabling the **FAST Uptake and Wash** option available for the iCAP 7000 Plus Series ICP-OES when using any FAST based sampling accessory. Additionally, the options **Optimization** and **Optimization Uptake Delay** should be disabled for the ESI autosampler in combination with the prep*FAST*.

❖ To create a prep*FAST* method

1. With a FAST System based Configuration loaded, on the Dashboard, select the ESI autosampler.

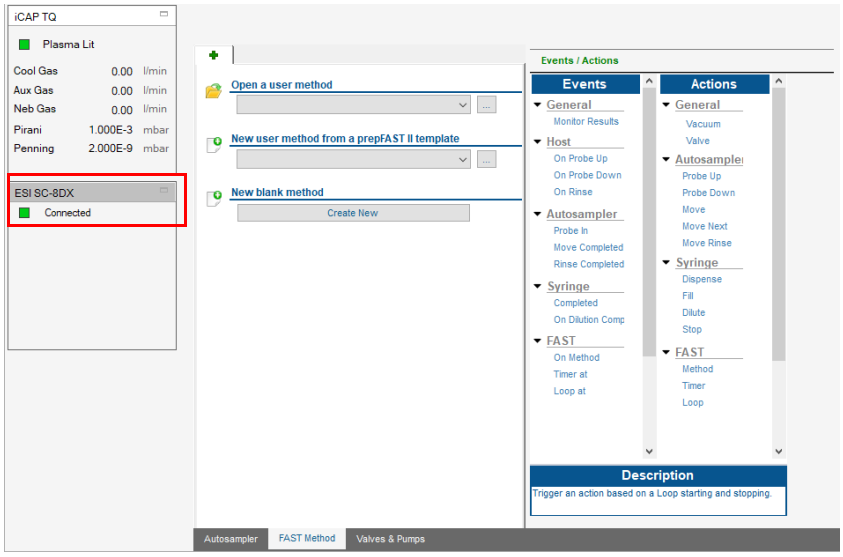


Figure 14-31. Initial Dashboard view of ESI autosampler

2. From the lower tabs, select **FAST Method** to display the initial view, see Figure 14-32.

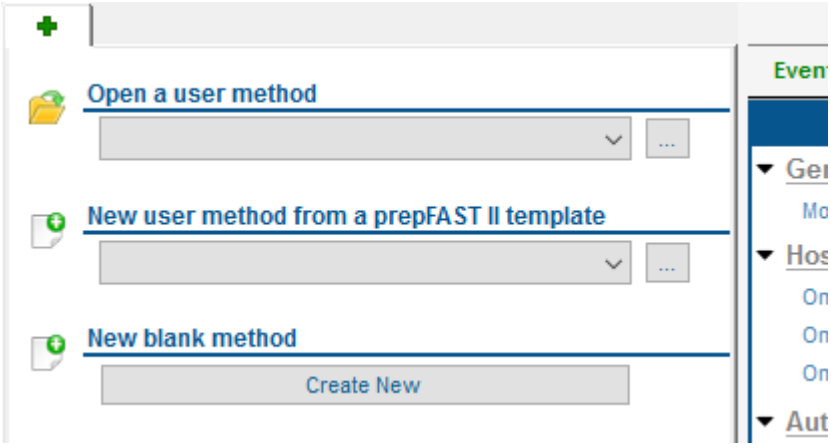
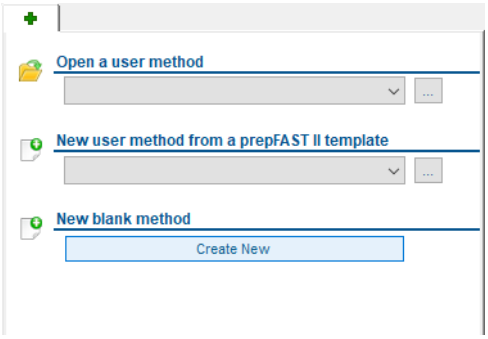


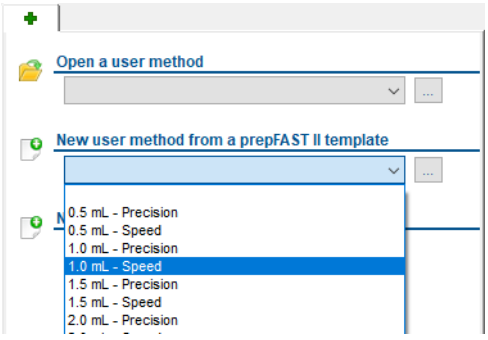
Figure 14-32. Initial view of ESI FAST method selection screen

3. Click **Create New** to create a new blank method.



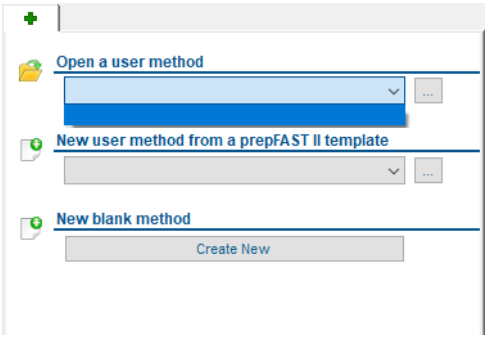
-or-

Create a new FAST method from a supplied template by selecting one from the **New user method from a prepFAST II template** drop-down list.



To keep the original method always unchanged, any modifications to this template are automatically saved to a user method when the **Save** button is clicked.

The modified template can then be selected from the **Open a user method** drop-down list (which initially is empty).



4. The FAST method tab initially shows the name *New Method* with an empty grid, see Figure 14-33. Each line of the grid can contain one action in the FAST method. All actions are carried out in order from top to bottom of the grid.

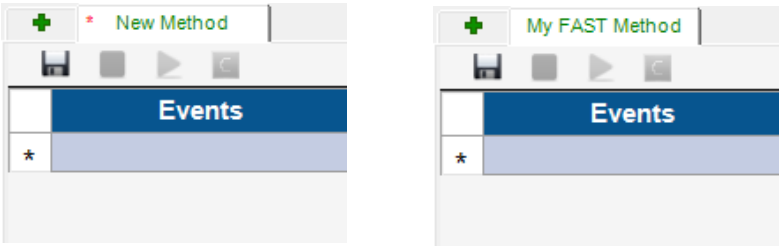


Figure 14-33. Blank ESI FAST template (left), once saved (right)

5. To build your FAST method, drag an Event from the list of **Events** and drop it to the first cell. Usually, *Method Start* is used as first sample line, that means,

   a. Select *On Method*.

   b. Drag this item to the first cell. This *On Method* event automatically changes to *On SubMethods: Completed*, see Figure 14-34.

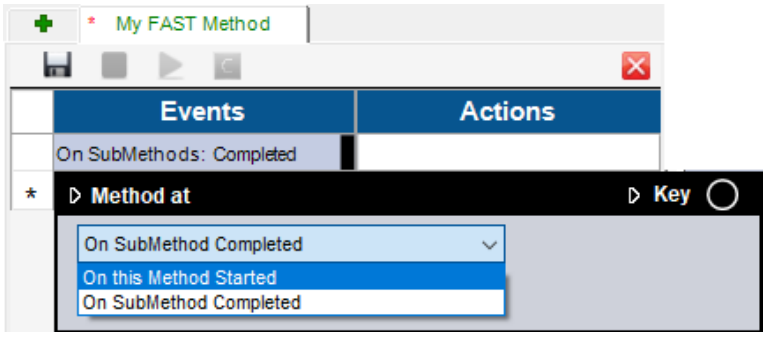


Figure 14-34. First ESI FAST Event

   c. In the pop-up dialog, specify the details, that means, select *On this Method Started* from the list box.

d. Click anywhere into your grid to close the pop-up dialog. *Method Start* is inserted as your first event.

6. Assign Actions steps in the same way, that means, drag the desired action from the list of Actions and drop it into the current line of your template.

7. Specify the details for the action by editing the pop-up dialog. The following screenshots show an example on how you can select several features from the pop-up dialog to specify the action, see Figure 14-35. Note that sub-menu items become visible when you click the triangle.

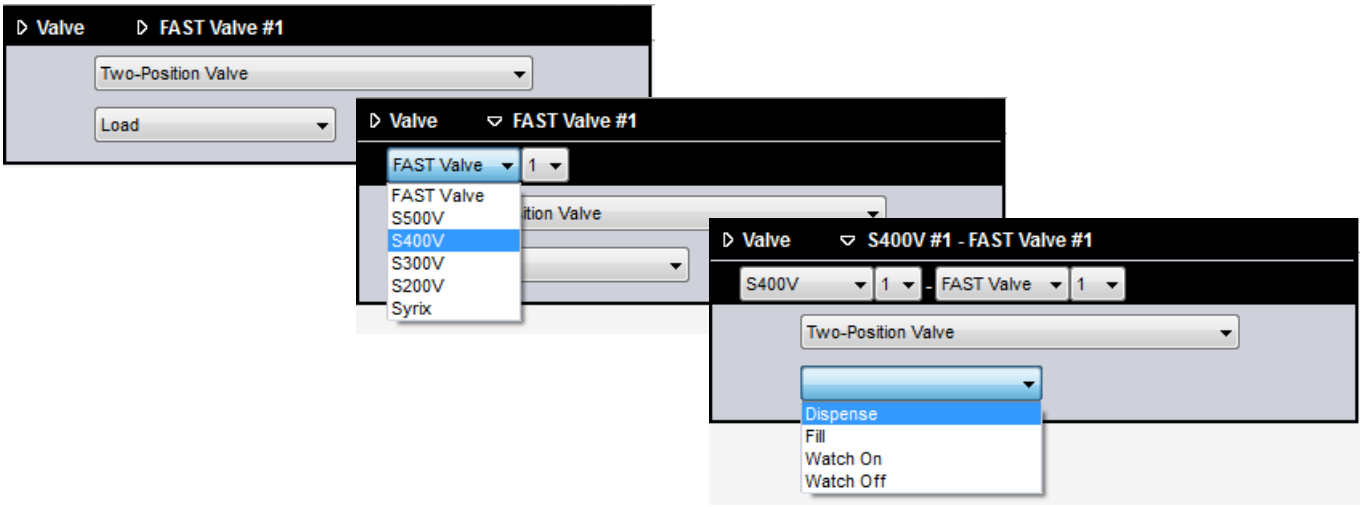


Figure 14-35. Pop-up Dialog with Detailed Specification of First Action Item

The example shown in Figure 14-35 creates *S400V-V1 Dispense* from the selected *FAST Valve 1 Load* Action.

8. Entries can be overwritten by selecting a new Event or Action item that is dropped into a currently used step.

   Tip Note that no confirmation message is shown while you overwrite the item.

9. Each step of your template is represented by its own line. By default, the lowest line is empty and may be filled with a new Event or Action. You can insert blank lines by use of the shortcut menu that is displayed when you right-click the left-most cell. Select **Insert Row** from the shortcut menu to insert a line below the selected line.

10. To remove a line, right-click the left-most cell of this line to open the shortcut menu and select **Delete Row**.
    Note that no confirmation message is shown while you remove the line.

    As the line completely is removed, you need to insert a new line to add an Event or Action on this step. Alternatively, just overwrite the current Event or Action as described above.

11. To link an Action and Event together, select a color from the pop-up dialog.

12. To change the detailed specification of an Event or Action, double-click the item to open the pop-up dialog.

    Finally, your FAST method could look like the example in Figure 14-36.

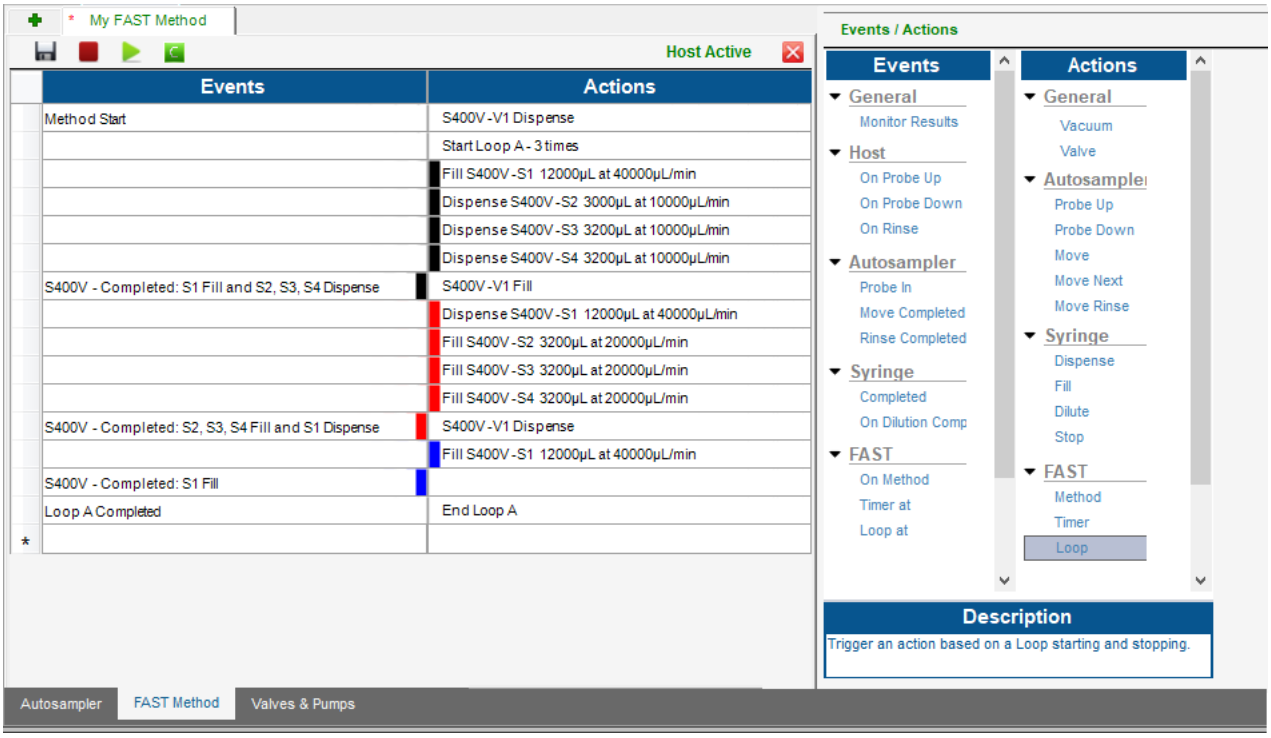
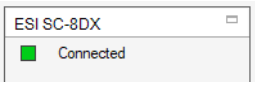


Figure 14-36. Final view of your FAST method

13. Save the completed FAST method.

Tip It may be easier to use the supplied FAST methods as templates to edit to meet your requirements rather than create new FAST method.

❖ To open ESI prep*FAST* settings



1. On the Qtegra Dashboard, select the ESI autosampler selector.

2. Open the FAST Methods view, see Figure 14-37.

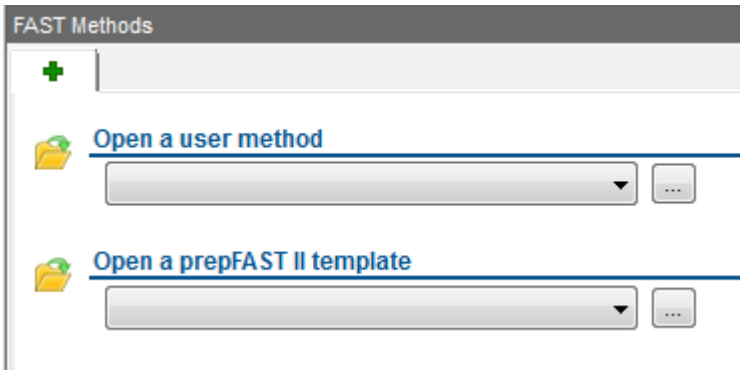


Figure 14-37. Opening a FAST Method from the FAST Methods tab

3. From the + tab, select one option to open the FAST Method.

   a. Select a **user method** from the drop-down list.
   -or-
   Click the **Browse** button to choose a user method.

   b. Select an original **prep*FAST* II template** from the drop-down list.
   -or-
   Click the **Browse** button to choose an original template.

4. The method settings open in a new tab and show a list of the Events and Actions, see Figure 14-38.

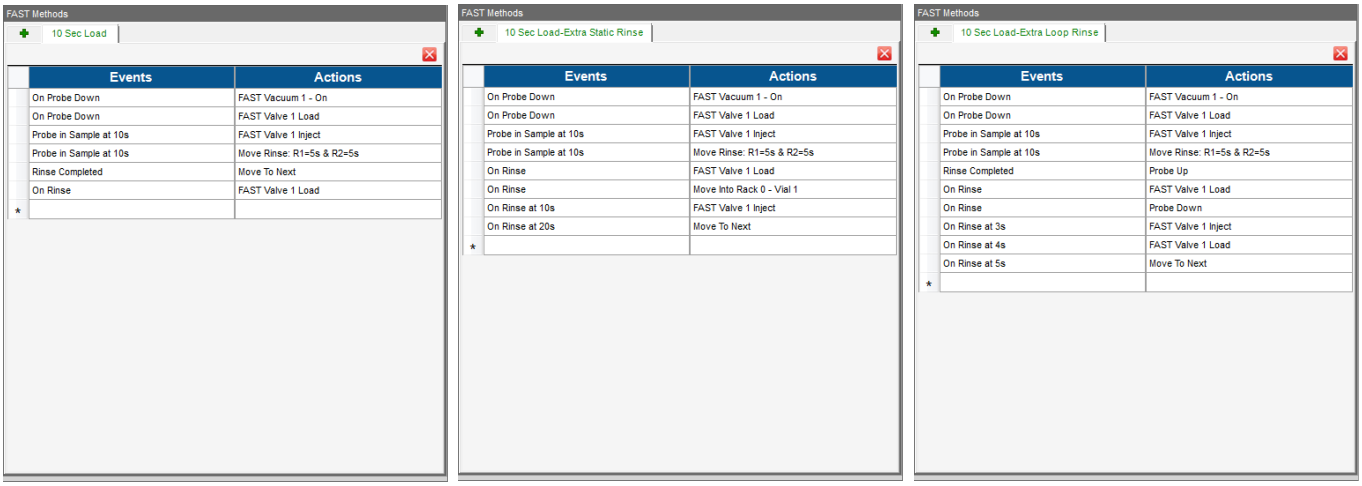


Figure 14-38. ESI FAST methods, loaded from templates delivered with Qtegra

Tip You can only change the settings via the Qtegra Dashboard.

❖ **To run an ESI prep*FAST* experiment**

1. Prepare your reagents. In case of ESI SC-2DX

a. Prepare the *prepFAST Carrier/Diluent* solution by filling the appropriately labeled bottle with nitric acid at a concentration that matches the matrix of your samples. Make the solution from acid and ultrapure water, which are suitable for trace elemental analysis by ICP-OES.

b. Place the tubing labeled *prepFAST Carrier/Diluent* in the bottle.

c. Prepare the *prepFAST Internal Standard* solution by filling the appropriately labeled bottle with nitric acid at a concentration that matches the matrix of your samples. Make the solution from acid and ultrapure water, which are suitable for trace elemental analysis by ICP-OES.

d. Place the tubing labeled *prepFAST Internal Standard* in the bottle.

e. Keep in mind that the Internal Standard is also diluted by a factor of 6, if the *FAST* methods are used, which were provided with the instrument.

2. On the Qtegra Dashboard, select the Configuration you saved in the Configurator tool.

   a. Open the autosampler display by clicking the headline, see Figure 14-39.

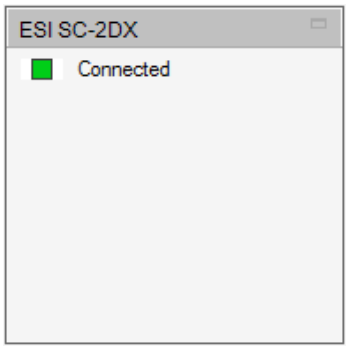


Figure 14-39. Opening the autosampler view

   b. From the lower tabs, select **FAST Method** to open a template of FAST Methods.

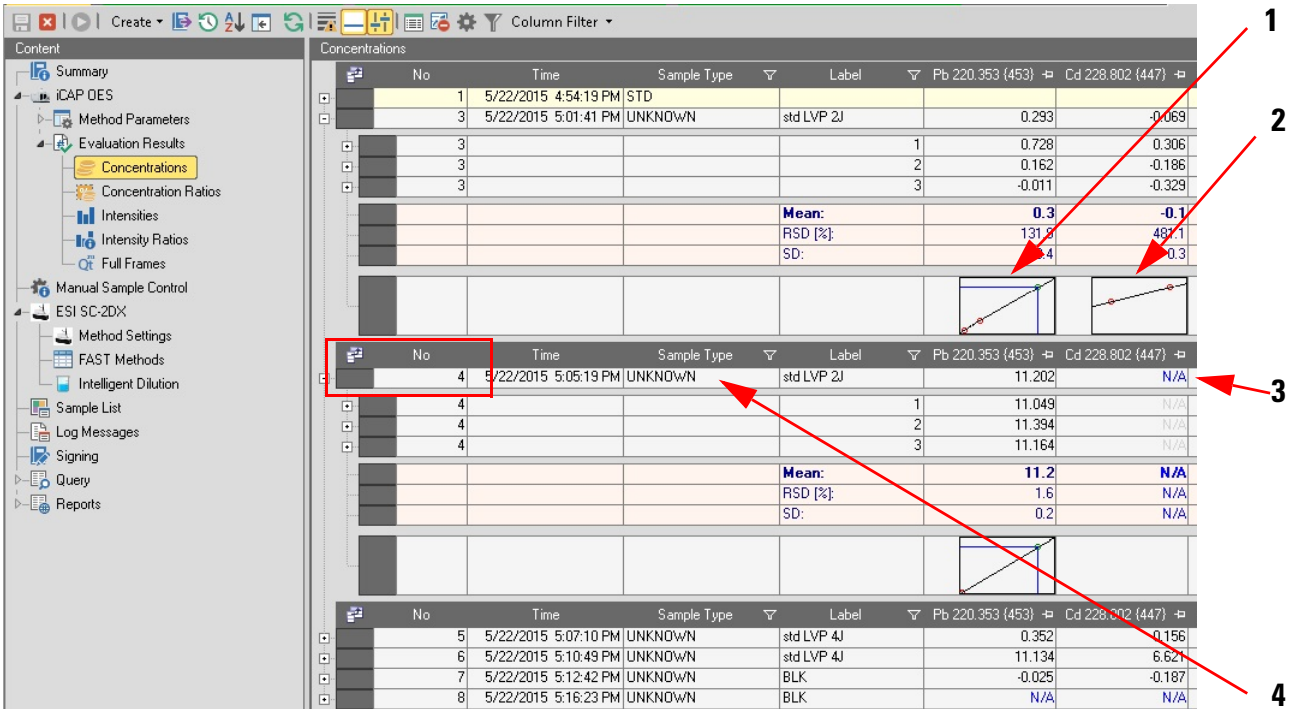
   c. From the **Template** listbox, select *prepFAST 2_Prime*.
   -or-
   Create a new Template. See "To create a prepFAST method" on page 14-26 for details.

3. Click the green **Play** button to prime the syringes.
   The peripheral will need to be primed a minimum of 3 times before analyses begin.

4. To run the performance checks, open **Qtegra** and click the **Get Ready** button.
5. Open and schedule the correct LabBook for the configuration being used.
6. Run the LabBook after the instrument has completed the Get Ready process.

N/A Indicator in Concentrations List

Intelligent Dilution is automatically performed if measured concentrations are outside the defined calibration range. This behavior may effect the Internal Standard as well as your sample solution, see Figure 14-40.



Labeled Components: 1=analyte 1 outside range, 2=analyte 2 inside range, 3=analyte 1 indicated by "N/A", 4=added new sample line

Figure 14-40. Indicating sample with N/A

The example displayed in Figure 14-40 shows a typical sample analysis. The concentration of the first analyte (Pb 220.353 nm) is outside the calibration range (**1** in Figure 14-40) while the concentration of the second analyte (Cd 228.802 nm) is within the calibration range (**2** in Figure 14-40).

As a result of the out of range concentration of Pb, a new sample line is added into the Sample List and the sample gets diluted in order to make it fit into the range. The analysis will only be evaluated for the analyte

that was previously out of range, Pb in this case (**4** in Figure 14-40). For the other analyte (Cd) no evaluation will be performed and N/A is displayed instead (**3** in Figure 14-40).

CETAC SDX High Performance Liquid Dilution System

This chapter describes how to use the Teledyne CETAC SDX_{HPLD} with the Qtegra ISDS Software. Once the SDX plug-in is installed and enabled, you need to select the appropriate settings in several places:

- ASX-560 autosampler settings in the Configurator tool.
- Sprint Valve settings in the Configurator tool.
- Instrument Controls.
- Method Editor.

Tip Do not operate the SDX syringe pump until the software has been configured. Software settings depend on the diameter of the probe. Incorrect settings will result in motor failure and valve damage.

The CETAC SDX_{HPLD} adds automated dilution to the capabilities of the ASX-560 autosampler. The autosampler draws a volume of sample from a sample vial, then injects it into a vortex mixing vessel along with a volume of diluent. After vortexing, the diluted sample is sent to the ICP-OES or other analytical instrument, and the sample probe and vortex vessel are thoroughly rinsed.

The SDX_{HPLD} system is often used along with the Teledyne CETAC *ASXPRESS PLUS* rapid sample introduction system, a 6-port valve system, which enables rapid sample loading and probe wash out. The *ASXPRESS PLUS* greatly improves throughput, by moving the sample close to nebulizer quickly, and then rinsing the sample line while the sample is being analyzed.

Reference Documentation

In addition to this *iCAP 7000 Plus Series ICP-OES Software Manual* it is recommended to read the *SDX_{HPLD} Operator's Manual* delivered with the CETAC peripheral.

Installing the Plug-in

You will need to have administrative privileges on the computer to install the software.

1. Run the ASX-560/Sprint Valve/SDX plug-in installation package, accepting all default options. For details on installing the plug-in, refer to the *Installation Guide*.
2. Patch the Microsoft .NET framework software, if necessary.

Up to version Qtegra 2.8 only the .NET 4.5 libraries are installed. There are several bugs in .NET 4.5, which will cause the ASX-560/SDX plug-in to be laid out oddly. Please install the .NET 4.5.1 patch, which can be acquired free from Microsoft.

3. In the **Configurator** tool, create a Configuration that includes the ASX-560 autosampler. Right-click the ASX-560 autosampler you wish to edit the settings for.

4. Click **Edit settings** to open the **Settings** dialog, see Figure 14-41.

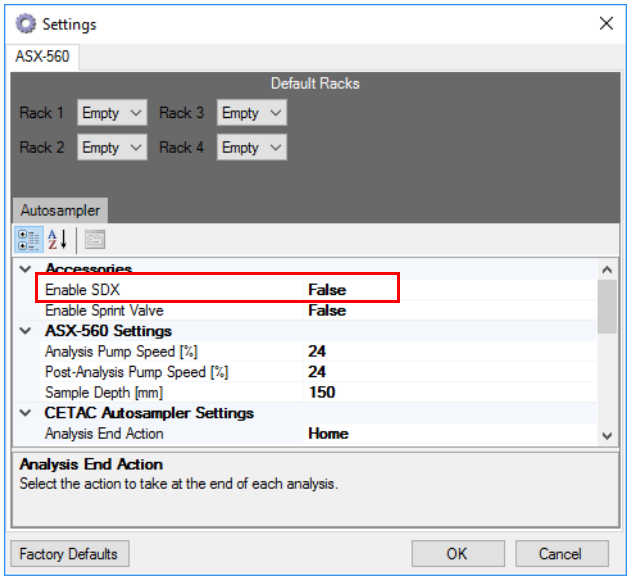


Figure 14-41. Settings dialog for the ASX-560 autosampler

5. In the **Accessories** section, select Enable SDX and double-click to set the value to *True*.

   The SDX tab is shown, see Figure 14-42.

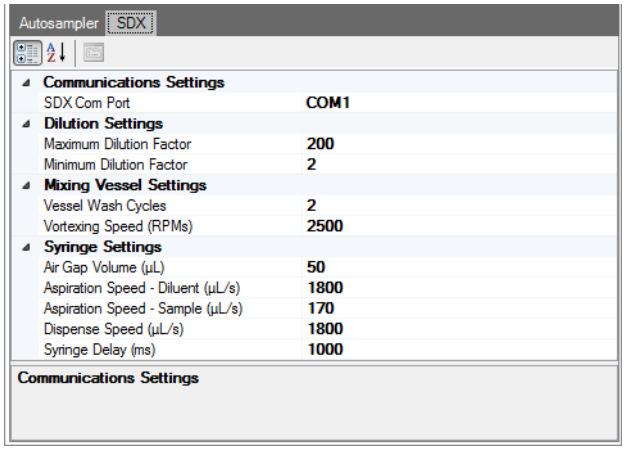


Figure 14-42. Initial settings for SDX

6. Set the values as described in Table 14-1.

Table 14-1. SDX setting parameters

Section	Description
Communications Settings	Apart from the SDX settings, make sure that the right COM port is set for communication. Refer to the *Operator's Manual* for details on how to detect the correct COM Port.
Dilution Settings	The dilution range that the SDX is capable of is a dilution of 2 up to 5000 fold. The minimum and maximum dilution factors have a large effect on the accuracy and speed of your analysis. High dilution factors require small quantities of the sample, therefore any error in the volume will be magnified in the dilution. Low dilution factors below 10 lead to long aspiration times. For dilution factors over 100, serial dilution is used. To provide the greatest accuracy throughout the dilution range, serial dilution always begins with a 50 fold dilution.
Mixing Vessel Settings	To reduce carryover between dilutions, up to four **Vessel Wash Cycles** can be prescribed. Each wash cycle takes about 10 seconds. For most quantitative analyses, 2 or 3 wash cycles should be sufficient. In general, optimal carryover results from using 3% nitric acid for the vortex rinse solution. The **Vortexing Speed** should always be 2500.
Syringe Settings	The syringe settings have a big impact on the accuracy and speed of the method and also on the correct functioning of the system. A pre-sample **Air Gap Volume** is always inserted between the solvent in the probe line and the sample being aspirated. For most applications a 50 µL gap is sufficient.

Table 14-1. SDX setting parameters, continued

Section	Description
	The **Aspiration Speed - Diluent** has a default setting of 1800 µL/s and can be left as is. The **Aspiration Speed - Sample** of 170 µL/s works well for most samples. For the 0.5 mm probe, use 50 µL/s. Note that slower sample aspiration speeds are more accurate, but lead to increase of the dilution time. The **Dispense Speed** depends on the diameter of the sample probe, which is indicated by different coloring of the probe bands. The 0.8 mm probe is used with ICP-OES and 600 µL/s dispense speed. When the Sprint Valve or *ASXPRESS PLUS* is coupled to the SDX and the instrument, the 1 mm probe can be used with a dispense speed of 1800 µL/s. If the dispense speed is too fast, the syringe pump may stall and the commonly acidic solvent may be forced out of the syringe valve, potentially causing damage and generate an error. The **Syringe Delay** parameter allows liquid and air pressure to equalize throughout all of the tubing after a syringe movement is complete. This pressure equalization improves the quantitative sample transfer accuracy. The optimum value depends on solvent viscosity and sample tubing diameter. If it is suspected there may be oscillations, increase the delay for maximum accuracy and repeatability.

7. Select the Autosampler tab for the final settings.

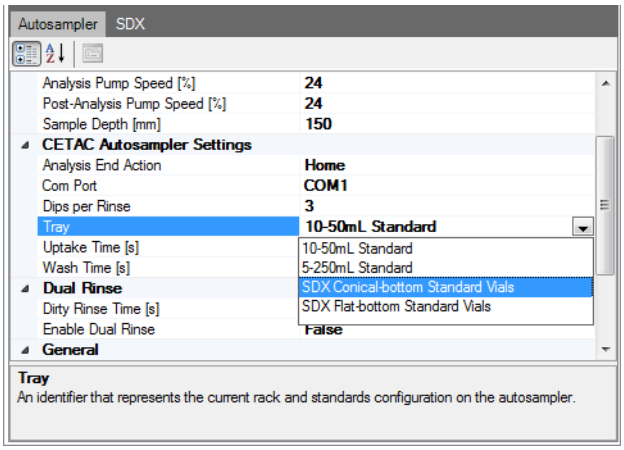


Figure 14-43. Tray settings for Autosampler

8. Set the values as described in Table 14-2. All other values may remain in the default status.

Table 14-2. Autosampler settings

Section	Description
CETAC Autosampler Settings	Select the correct **Com Port** for the autosampler. Refer to the *Operator's Manual* for details on how to detect the correct Com Port that is different from port number of the SDX.
	As the SDX_{HPLD} system comes with a specialized standards rack, there are two new options available under **Tray**: the *SDX Conical-bottom Standard Vials* and *SDX Flat-bottom Standard Vials*. Make the selection dependent on the type of vials used for your standards rack.

Configuration with Sprint Valve or *ASXPRESS PLUS*

In case the Sprint Valve or *ASXPRESS PLUS* is used together with the instrument and the SDX_{HPLD} system the following parameters should be set.

1. In the **Configurator** tool, create a Configuration that includes the ASX-560 autosampler. Right-click the ASX-560 autosampler you wish to edit the settings for.

2. Click **Edit settings** to open the **Settings** dialog, see Figure 14-44.

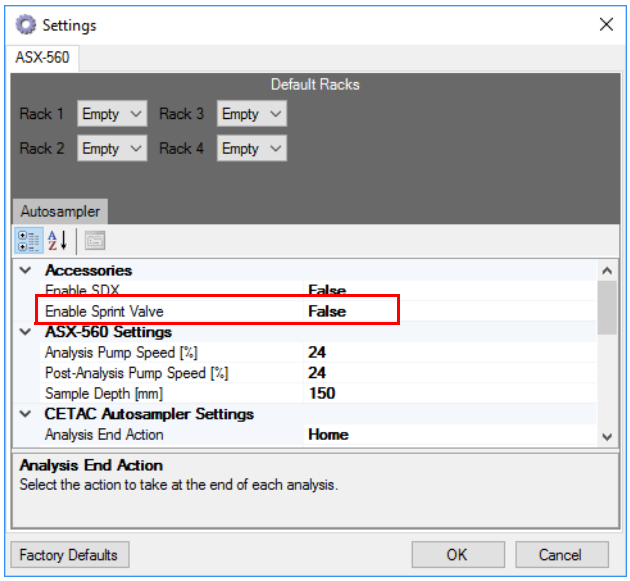


Figure 14-44. Settings dialog for the ASX-560 autosampler

3. In the **Accessories** section, select Enable Sprint Valve and double-click to set the value to *True*.

   The Sprint Valve tab is shown, see Figure 14-45.

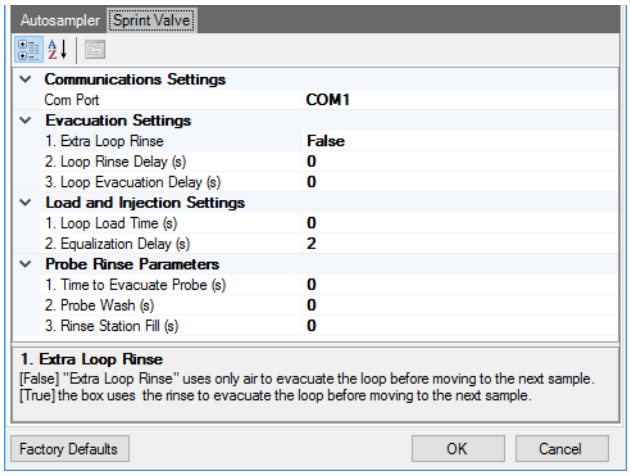


Figure 14-45. Typical settings for Sprint Valve

Refer to the *ASXPRESS PLUS Operator's Manual* for details on the Sprint Valve parameters.

Preparing the LabBook

In this section, examples are shown for demonstration purposes. For your measurements other values than shown here may be used. On the Qtegra ISDS Dashboard, load the SDX Configuration.

1. Click the **ASX-560** tile to show the rack layout, see Figure 14-46.

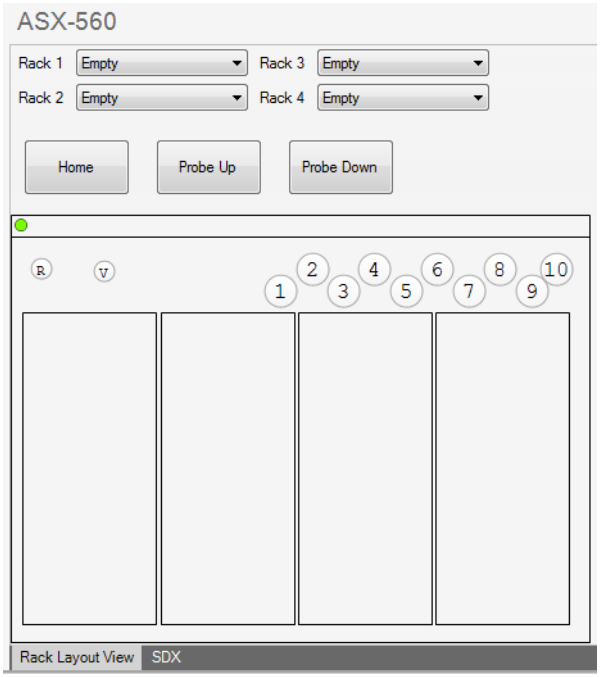


Figure 14-46. ASX-560 Rack Layout tab

The standard rack layout matches the layout used by the SDX_{HPLD} system.

2. Select the SDX tab to show the manual control parameters for the Syringe Pump, Mixing Vessel, and Operations, see Figure 14-47.

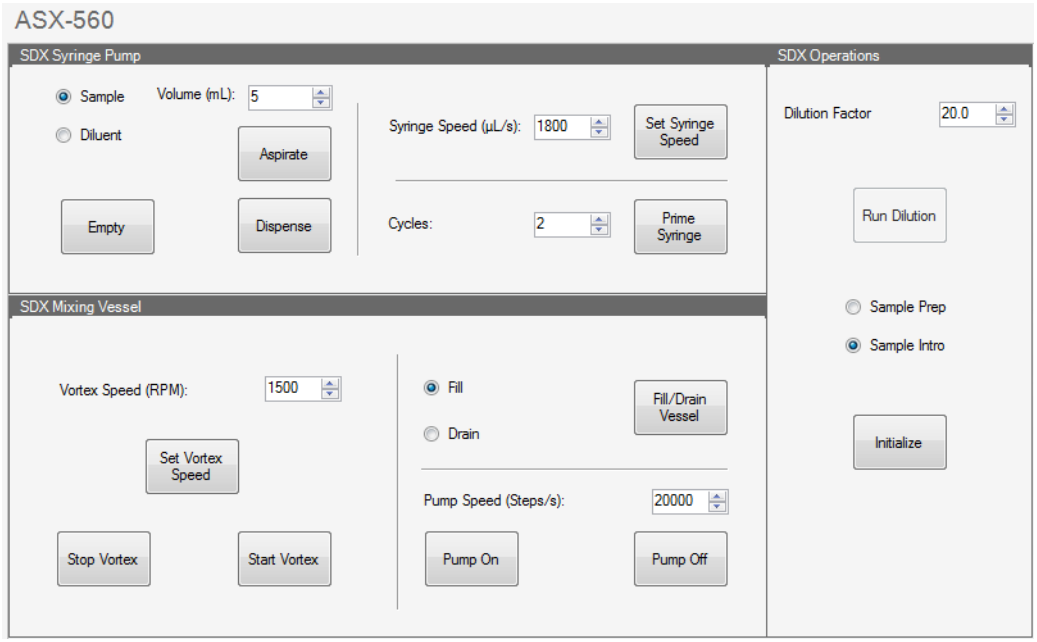


Figure 14-47. ASX-560 SDX tab

Most of the controls are for diagnostic purposes. However, some controls are relevant before and during routine usage and are described in Table 14-3.

Table 14-3. Manual control parameters

Section	Description
SDX Syringe Pump	Before using the SDX_{HPLD} system the first time, all lines of the SDX need to be filled with diluent. This is done by the **Prime Syringe** function.
SDX Operations	**Run Dilution** allows a test run of the dilution process, and can be used to verify that all fittings are properly tightened.
SDX Mixing Vessel	Use the **Fill/Drain Vessel** function to flush the vortex vessel and the SDX rinse tubing.

3. Select the Sprint Valve tab to show the manual control parameters for the Function Tests of the valve and the pump, see Figure 14-48.

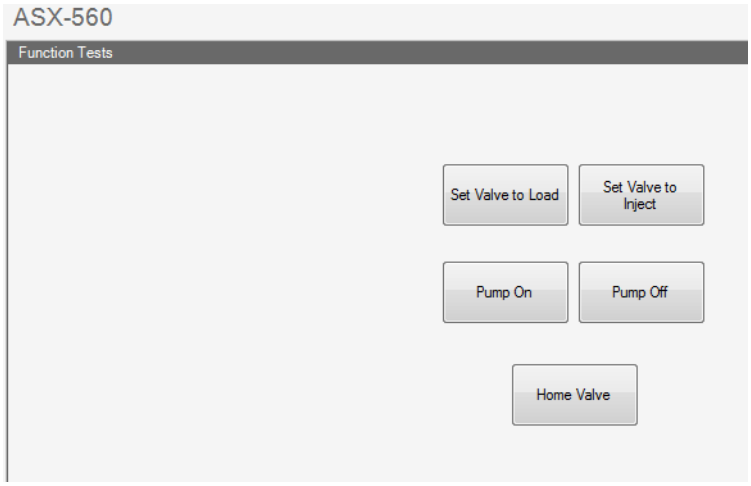


Figure 14-48. ASX-560 Sprint Valve tab

Tip When creating a LabBook with the SDX and the Sprint Valve, make sure the autosampler wash time is set to *0* (zero). To do so, open the ASX-560 view from the Content pane. Under **Time settings**, set **Wash Time** to *0*.

Prescriptive and Intelligent Dilution

The SDX has two main functions: prescriptive dilution and intelligent dilution due to certain parameters being outside specified ranges. In the following these functions are explained with an example LabBook.

1. The SDX example LabBook contains already preselected standards and analytes. For a better overview the Sample List only shows the following columns: Label, Status, Sample Type, Standard, Rack, Vial, Autodilution Factor.

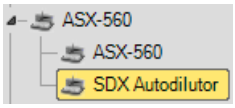
Samplelist estimated runtime: 8 minutes 25 seconds

	Label	Status	Sample Type	Autodilution Factor	Standard	Rack	Vial
1	Blank		BLK	1		Standard	1
2	Standard 1		STD	100	Stock	Standard	2
3	Standard 2		STD	50	Stock	Standard	2
4	Standard 3		STD	10	Stock	Standard	2
5	Standard 4		STD	2	Stock	Standard	2

Figure 14-49. Part of the example LabBook with focus on a few columns

The prescriptive dilution comes from the Autodilution factor column. Values between the minimum and maximum dilution factor set up in the Configuration can be entered here. The SDX will then do an autodilution on the sample in the position specified through Rack and Vial.

A calibration is defined though a blank and 4 standards. The standards have different autodilution factors (100, 10, 5, 2), but have the same stock solution and autosampler positions (Rack, Vial) defined.



2. In the **SDX Autodilutor** view, two sections are shown, the Internal Standard and the Calibration Range.

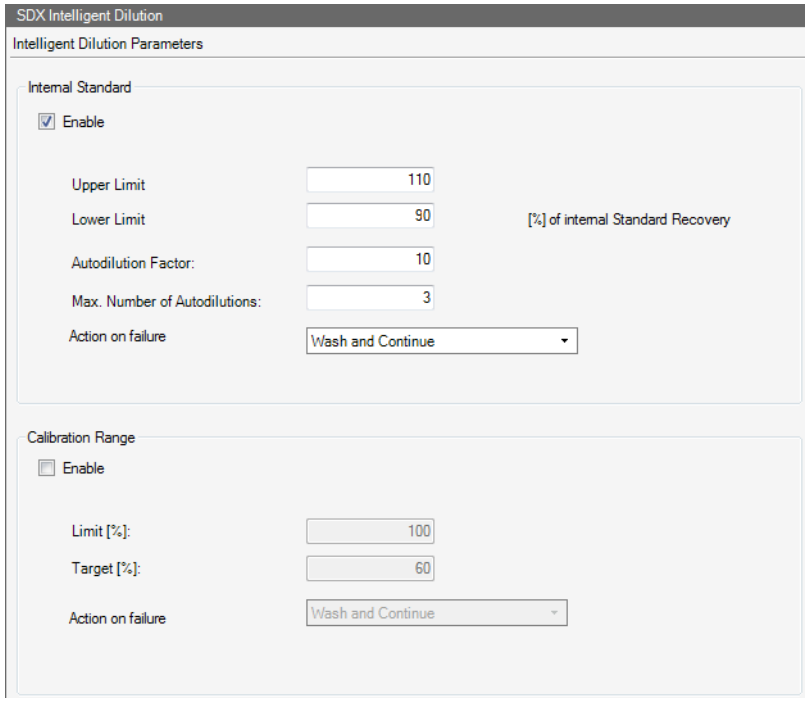


Figure 14-50. SDX Autodilutor view

If the Internal Standard is enabled (see Figure 14-50), a dilution is automatically performed when the Internal Standard recovery falls outside the prescribed range. The desired **Autodilution Factor** and the **Maximum Number of Autodilutions** can be entered.

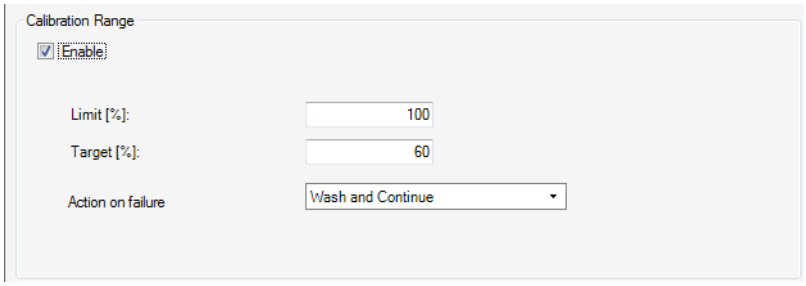


Figure 14-51. SDX Autodilutor view: Calibration Range

If the Calibration Range is enabled (see Figure 14-51), a dilution is performed when the sample concentration exceeds the **Limit [%]** of the concentration of the highest calibration standard. Qtegra will use the SDX to dilute the concentration to the level entered in **Target [%]**. The software will use the element, which is furthest from the range to calculate the dilution factor. The actual dilution performed may be constrained by the dilution limits specified in the Configurator settings.

3. Whenever a sample result triggers an Intelligent Dilution, a sample will be added to the Sample List. The intelligent addition is indicated by a green plus sign next to the status lamp.

❖ **Intelligent Dilution triggered by Internal Standard Recovery**

1. In the SDX Autodilutor view (see Figure 14-50), the limits are set to 110% and 90% of the Internal Standard Recovery.

2. The measured sample has an Internal Standard Recovery of 86%.

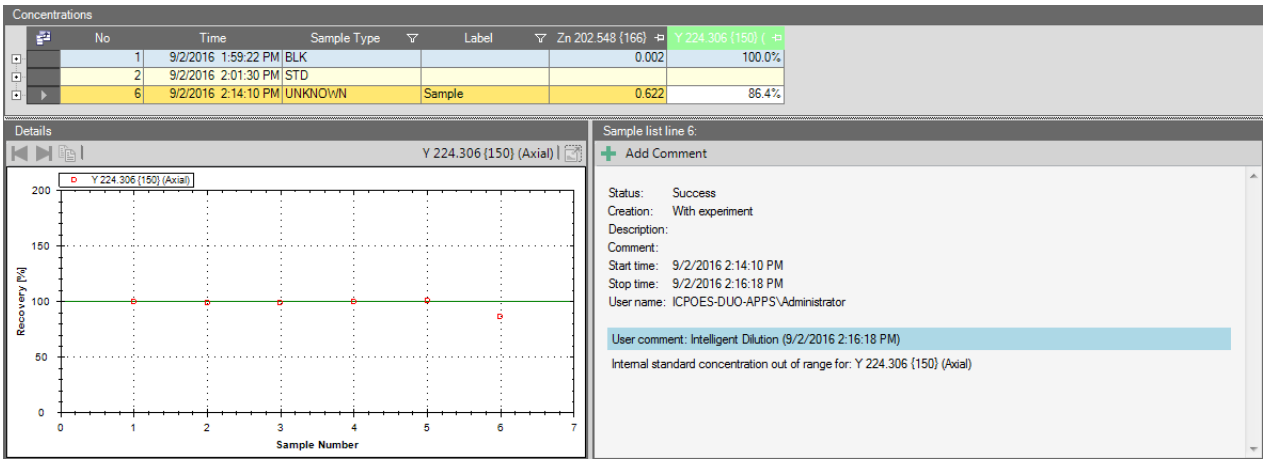


Figure 14-52. Details and Comments panes of Evaluation Results view for Internal Standard recovery

The Details pane and a Comments pane are shown. The reasons for trigger are written, for example, “Internal standard concentration out of range”, see Figure 14-52. All affected analytes are listed. In the Details pane, the used dilution factor for the diluted sample is shown, for example, “Measured with corrected dilution factor of 10.”

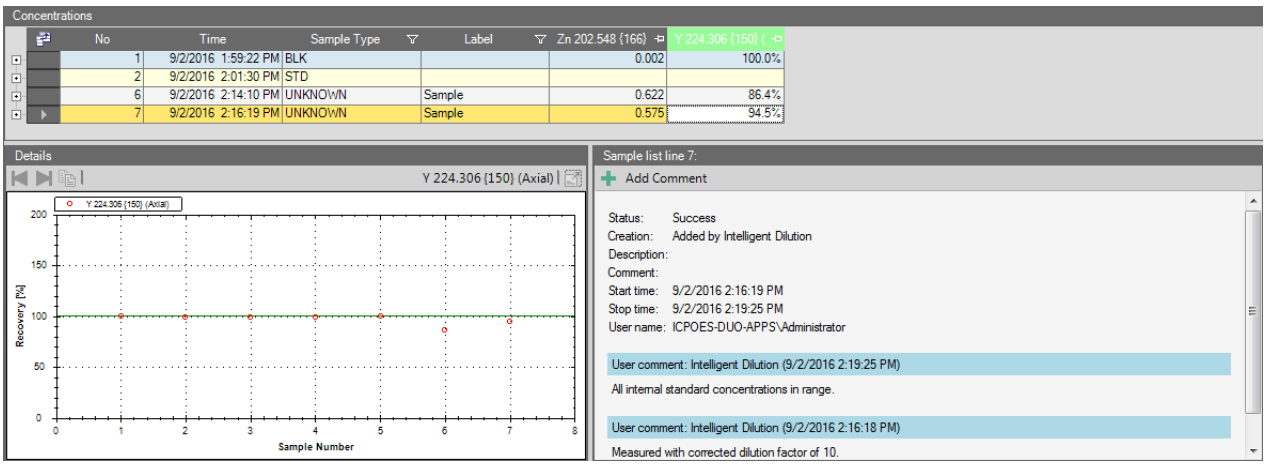


Figure 14-53. Details and Comments panes of Evaluation Results view for Internal Standard recovery with corrected dilution factor

❖ **Intelligent Dilution triggered by Calibration Range**

1. In the SDX Autodilutor view (see Figure 14-50), the limits are set to 100% and 60%.
2. The measured sample has a concentration outside these Calibration Range limits.

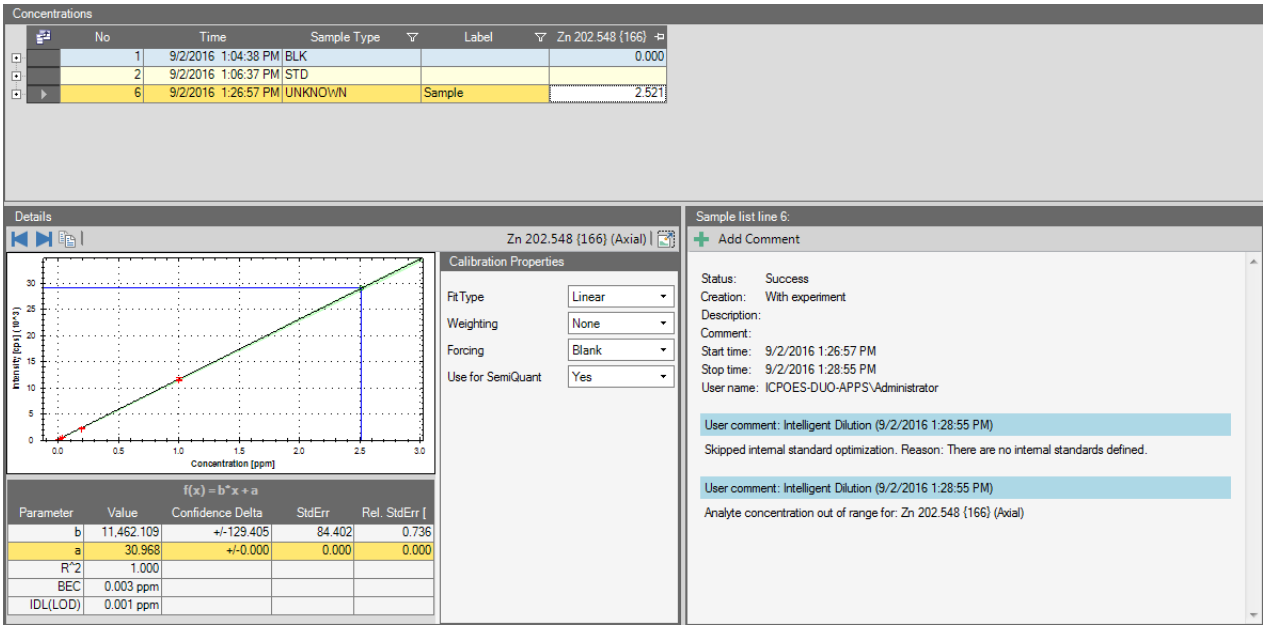


Figure 14-54. Details and Comments panes of Evaluation Results view for Calibration Range

The Details pane and a Comments pane are shown. In the Details pane, the calculated dilution factor used to dilute the analyte to its target value is shown. A message, for example, "Measured with corrected dilution factor of 4.201." summarizes the details, see Figure 14-55.

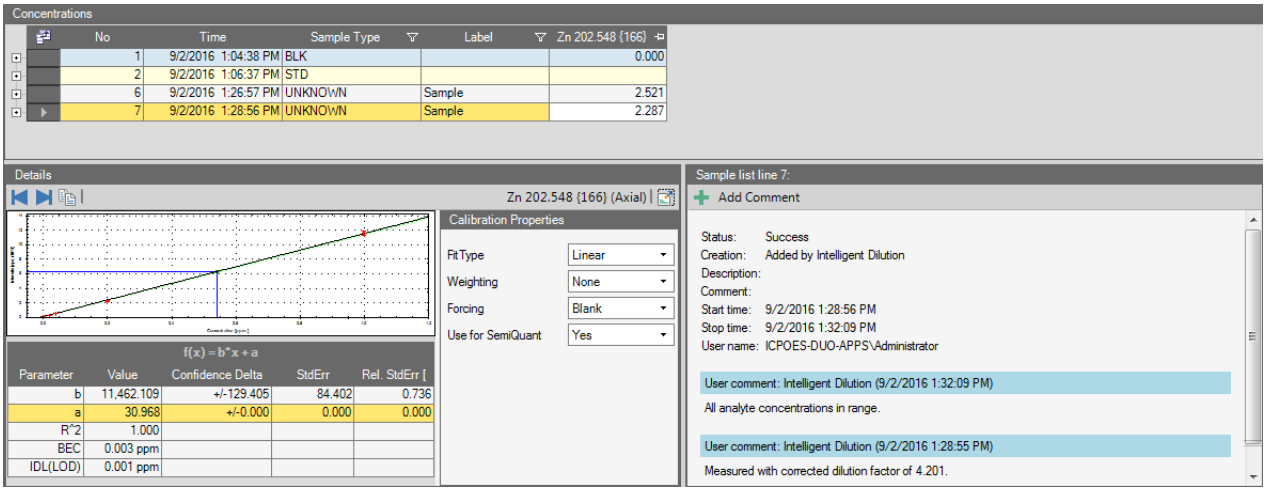


Figure 14-55. Details and Comments panes for a calculated dilution factor

The Sample List shows the autodilution factors in the Autodilution Factor column, see Figure 14-56.

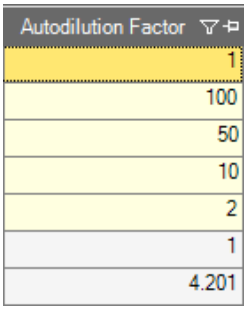


Figure 14-56. Autodilution Factor column of the LabBook

Manual Sample Control

Manual Sample Control can be added to your Configuration in the Configurator to enter samples without autosampler.

Tip Configurations are created by your Administrator or Thermo Fisher Scientific field service engineer, see "Experiment Configurator" on page 3-15.

In the Manual Sample Control view in Qtegra, Uptake and Wash Time can be defined, see Figure 14-57.

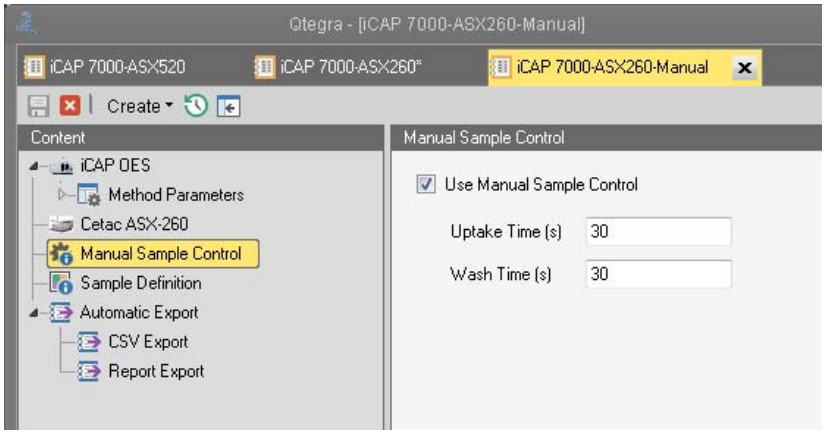
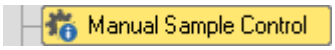


Figure 14-57. Manual Sample Control view

❖ **To define the Uptake and the Wash Time for manual sampling**

1. From the **Qtegra - [Home Page]** navigation pane, open a Template as described in "Opening a Template" on page 4-37.
   Be sure to open a Template with a Configuration including Manual Sample Control.
2. Click 

to open the Manual Sample Control view of the Template.

3. Select **Use Manual Sample Control**.
4. Type the values for **Uptake Time (s)** and **Wash Time (s)**.
   While the setting for the Uptake Time mainly depends on the length of the probe capillary and the uptake rate, the value of the Wash Time should be increased when going for high analyte concentrations or tough matrices to avoid carry-over effects.

Designing the LabBook Table

There are several ways to adapt the table layout according to your needs as a User. Dependent from your current selection in the Content tree, not all shortcut menu items are available on all LabBook tables.

Resizing the Width of the LabBook Table

The shortcut menu offers a fast way to execute design commands for your LabBook table. Select the desired command from the shortcut menu that opens when you right-click an item in the first column.

The description is explained in Table 14-4.

Tip The commands effect on the line above, when you insert items. You can only modify sample actions, when the current sample line is yet not finished (green indicator in Status column).

Table 14-4. Shortcut menu of a LabBook Sample List

Command	Description
Insert Rows	Inserts a number of blank lines above the current cursor position. A dialog opens to type the number of lines you wish to add. Select the desired label from the shortcut menu to fill the cells as far as possible.
Delete Selected Rows	In some cases you may modify existing LabBooks to adapt them to your needs. To delete actions, select the desired line and then select this shortcut menu item. Confirm the message dialog.
Fit Cells To Grid	The table consists of several columns that use space according to their width. Depending on your screen the table extends outside the program window. A slider below that table indicates that you will find additional columns to the right. Select this shortcut menu item, when you need all columns to fit the current screen. This command can help to get an overview but most of the columns are cut!
Fit Cells To Content	In some cases, you may need to enlarge the table with regard to their content. Select this shortcut menu item, when you want to resize all columns to display the whole content and column header.
Cut Selected Rows **<Ctrl> + <X>**	When you want to move an action to another position of your LabBook, then select the desired lines and cut them with this shortcut menu item, before you insert or paste the lines. Lines that are currently cut, are indicated with a light gray frame.

Table 14-4. Shortcut menu of a LabBook Sample List, continued

Command	Description
Copy Selected Rows **<Ctrl> + <C>**	❖ **To duplicate the selected actions** 1. Click and drag the left most column to select the desired source lines. Your selection is highlighted. 2. Select this shortcut menu item to copy the selected lines. 3. Select the destination lines and paste your selection.
Paste Copied Rows **<Ctrl> + <V>**	You can overwrite the current line with the currently copied action. Use this shortcut menu item to paste the action into the currently selected line. Note that you will never get a warning message, when overwriting existing lines.
Insert Copied Rows	To finalize a copy procedure, select this shortcut menu item. The copied lines are inserted above the currently selected line.
Append Copied Rows	In cases you need to add actions at the end of the current LabBook, copy existing lines and then select this shortcut menu item to append the lines.
Export To Excel	For presentation or documentation purposes it may be helpful to run further calculations in an Excel spreadsheet. Use this shortcut menu item to export the table into an *.xls format. The resulting file includes the column header as well as the colored indicators of the Status column.
Jump To Evaluation Results	To quickly navigate into the details of the evaluation results, select this shortcut menu item. The target grid already focuses the desired item.
Suspend Before The Measurement Of This Sample	In cases you need to interrupt or pause the measurement process, you may add this suspend marker that is displayed next to the current line number of the grid. When the action above this selection is finished, the measurement process will stop and is awaiting your interaction. Proceed with clicking the **Run** button of the **Scheduler** tab.

Fixing Columns in the LabBook Table

When your LabBook table extends the Qtegra program window, a bottom slider helps to navigate to hidden columns. To keep the desired line you can freeze the left column(s).

❖ **To fix a column**

1. On the header, click the pin icon to move the selected column to the next free position on the left. The pin rotates into an upright position to indicate the frozen state. All frozen columns are grouped on the left side. See Figure 14-58.

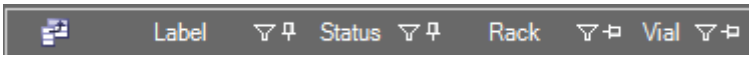


Figure 14-58. Two Fixed Columns of a LabBook Sample List

2. Click that pin again to remove the desired column from the frozen state. When you click a column within the frozen group it is moved to the next free position right from this group. The pin rotates back to its horizontal position.

When columns of the LabBook table are frozen, you can scroll the grid and display hidden columns by simultaneously seeing the frozen columns.

Moving Columns in the LabBook Table

When you want your LabBook table to be displayed in another order you can move a selected column to the desired position.

❖ **To move a column**

1. Click the column header you want to move. The column then is highlighted to indicate the focus.
2. Click and hold your mouse button and drag the column to the desired position. A black line indicates the current insert position.
3. Release your mouse button to insert the column on the selected position.

Tip When moving a column into the frozen group, the currently selected column also gets frozen.

Sample Definition and Sample List

The columns and functionality in the Sample List is dependent on both the evaluation method defined in the LabBook/Template and the accessory plug-ins defined in the loaded Configuration. All columns that may be shown in Sample Definition and Sample List are listed in Table 14-5, Table 14-6, Table 14-7, Table 14-8, and Table 14-9. Depending on the evaluation method selected for the Template, the columns of the components may differ.

Table 14-5. General columns of Sample Definition/Sample List

Column Header	Description
Index	Line number to indicate the sample position in the Sample List. Click the index to select the entire sample line. **<Ctrl> + click** or **<Shift> + click** to select a range of sample lines.
Label	User defined identification (name) for the sample line.

Table 14-5. General columns of Sample Definition/Sample List, continued

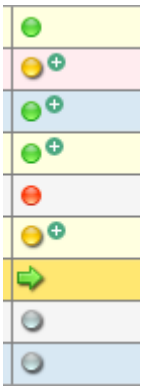
Column Header	Description
Status 	Column in Sample List of a LabBook. Colored lamps indicate the status of this sample line. • green arrow: Currently running sample line. • gray: Analysis has not been scheduled yet. • green: Analysis was executed as defined in the LabBook/Template and did not trigger a QC warning or failure. • yellow: Analysis was executed with measured values in the warning range. • red: Analysis was aborted. Plus sign: Indicates a sample line automatically added by a QC rule or Intelligent Dilution. Helps you to identify samples also when QC is not enabled.
Comment	Double-click the cell to enter user definable text.
Evaluate (check box)	Column in Sample List of a LabBook. Clear the Evaluate box to hide samples from display. If the Evaluate box is cleared, the sample line will be hidden in the Evaluation Results as well as in Exports, Queries and Reports. This function is useful when a sample has to be remeasured, for example, when the concentration exceeds the calibration range and has to be diluted. The faulty sample can then be hidden.
Standard	To select a standard from the drop-down list if the sample type is a standard or a certain type of a quality control sample. See also Method Parameters view "Standards" on page 9-25.
Special Blank	Column in Sample List of a LabBook. Used in eQuant evaluation. Value is selected from a drop-down list. Refer to "Special Blank" on page 13-11.
Repeats	The number of times that a given sample should be analyzed. Typically 3 repeats are sufficient.
Full Frame	Full Frame option as defined in "Measure Modes" on page 9-12.

Table 14-6. Dilution factor columns in Sample Definition/Sample List

Column Header	Description
Dilution Factor	Dilution of sample independent from the sample type. Used to define different calibration concentrations. The Dilution Factor (DF) of the Sample List view is automatically applied to any value displayed in the Concentrations view. For example, when you change the DF for an UNKNOWN in the Sample List from 1 into 10, the concentration shown for the selected analysis automatically changes from 2 ppb to 20 ppb. DF is one component used in the calculation of the TDF. **Tip** When you open a LabBook from older versions the DF automatically is recalculated from the ADF and is therefore changed.

Table 14-6. Dilution factor columns in Sample Definition/Sample List, continued

Column Header	Description
Total Dilution Factor	This column is only displayed if your Configuration includes an autodilution system. The Total Dilution Factor (TDF) is the total dilution factor applied to an analysis. It is calculated as a product of Dilution Factor (DF) and Autodilution Factor (ADF). The value shown here is calculated automatically and can not be edited. $TDF = DF \times ADF$ TDF displays the cumulative dilution factor. It is dynamically updated to reflect any changes (automatically or by user input) in the dilution factor used. TDF does not take into account any dilution generated from Sample Weight and Final Quantity however.
Autodilution Factor	This column is only displayed if your Configuration includes an autodilution system. Set the Autodilution Factor (ADF) to let the autodilutor automatically dilute your STD to get several points on the calibration curve. For example, a STD solution of 50 ppm gets an ADF of 2 to run the calibration according a 25 ppm solution. Type an ADF of *5* to run the calibration according a 10 ppm solution. In all these cases, the same rack and vial with your STD may be selected. ADF is one component used in the calculation of the TDF.
Amount only in combination with Final Quantity	The Amount and Final Quantity define any additional dilution performed during sample preparation. For example, the dilution of one solution by another or the digestion/dissolution of a solid into a solution. In a completed LabBook, the Amount and Final Quantity defined in the Sample List view are automatically applied to any value displayed in the Concentrations view. If Final Quantity *q*, Amount *a,* and Dilution Factor *df* are specified in the Sample List, any concentration value displayed in the Concentrations view is corrected by a combination of all factors: $c_{corr} = c \cdot \frac{1}{df} \cdot q / a$ Any unspecified values are set to *1*.

Table 14-7. Evaluation specific columns of Sample Definition/Sample List

Column	Description
Survey Runs	The number of survey runs (scans of the mass spectrum) performed. The number of runs can be set from *0* to *100*. By default, the number is set to *0*. The spectral regions to be acquired during a survey run are defined in the method parameters view. **Recommended settings:** It is recommended to run at least one survey run per sample when eQuant was selected as evaluation method. **Tip** High concentration matrix components that may be scanned as part of the survey run leading to unnecessary exposure of the detector to high count rates, shortening its lifetime. Choose the skip mass ranges and detector mode used in Survey Scans accordingly.
Main Runs	Number of main runs (peak jumping acquisition) performed. The number of runs can be set from *1* to *1000000*. By default, the number is set to *1*. **Recommended settings:** It is recommended to run at least three main runs per sample. **Tip** Sweeps are defined in the Advanced Parameters section of the Acquisition Parameters view. See "Acquisition Parameters" on page 9-14.
Sample Type	Definition of the sample type, e.g., *BLK*, *STD*, *UNKNOWN*, *QC*. See Table 13-1 for sample types supported.
Internal Standard	To select a previously defined Internal Standard from drop-down list, which should be used to correct the signal of the corresponding sample. See also Method Parameters view "Standards" on page 9-25. If the Internal Standard column in the Sample List is empty, all analyses (BLKs, STDs, UNKNOWNs, QCs, etc.) are assumed to have the same IS created as 'Internal Standard (Isotopical)' in the LabBook. Alternatively, Qtegra allows the use of analysis specific Internal Standards at different concentrations. This can be useful, for example, when the calibration standard used contains one or more of the elements used as Internal Standard.

Table 14-8. QC columns of Sample Definition/Sample List

Column Header	Description
QC Action	Used in eQuant evaluations. QC test type. Value is selected from drop-down list. Relates sample to set of rules defined for this QC test type. See method parameters view "Quality Control" on page 10-5.
QC Restart	Used in eQuant evaluations. Defines restart point in a Sample List for certain QC tests. Value is selected from a drop-down list.
QC Reference	Used in eQuant evaluations. If QC test type, for example, *DUP* or *SER* (see Table 10-5) is selected in a Template, a <*unique ID*> can be entered and used to connect the linked analyses.

Table 14-9. Autosampler columns of Sample Definition/Sample List

Column Header	Description
Rack (Teledyne CETAC) -or- Rack Number (ESI)	Rack number specifies autosampler rack of the solution in the autosampler.
Vial (Teledyne CETAC, Accela) -or- Vial Number (ESI)	Vial number specifies autosampler vial of the solution in the autosampler.
Block/Tray (Accela)	Block and tray numbers specify Accela autosampler block and tray of the solution in the Accela autosampler.

Individual columns in the Sample List

Qtegra ISDS Software provides an option to add individual columns to the Sample List. By default, the Label column is used to type sample information. Additional columns may be used to show more sample information, which then also is accessible in Query and Reports. The following sections describe how to set up Qtegra ISDS.

- In the Configurator, create a Configuration with a Generic Instrument.
- With the Windows Explorer, navigate to the new folder and create the XML file.
- In Qtegra, load the new or updated Configuration.
- Create a LabBook and check the Sample List for the new columns.
- Under LabBook > Automatic Export, the new columns are available for Query.

- Under LabBook > Reports, the new columns are available.

Configuration using a Generic Instrument

Additional columns become part of your Configuration.

❖ **To create a Configuration using a Generic Instrument**

1. Open the Configurator tool and select the Experiment Configurator applet.
2. In the pane of Available Items > Instruments, right-click and select **Add Generic Instrument** from the shortcut menu.
   A box “GenericInstrument” is appended to the list.

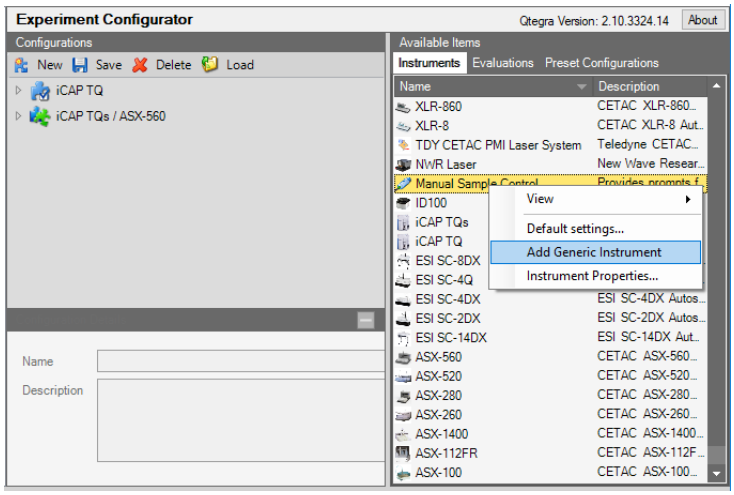


Figure 14-59. Adding a Generic Instrument

3. In the box, type a name, for example, “AdditionalColumns”.
4. Create a new Configuration or select an existing Configuration to change its settings.

5. Drag the Generic Instrument “AdditionalColumns” to your Configuration.

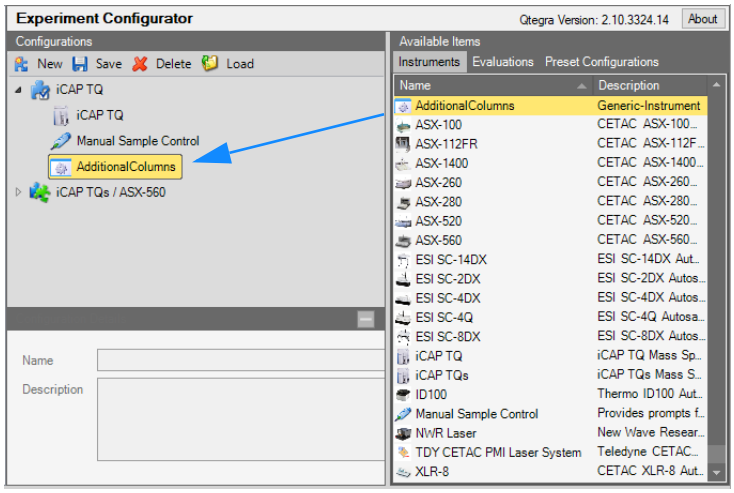


Figure 14-60. Configuration with “AdditionalColumns”

6. Save the Configuration.

XML File providing Layout Information

The name and optional parameters of the individual columns are controlled by an XML file.

❖ To edit the XML file

1. When creating a new Generic Instrument (see step 2 above), a folder is automatically created under `_Application Data\PluginData`. The new folder name is created from the name you have typed for the Generic Instrument, for example `AdditionalColumns`. Blanks are removed.

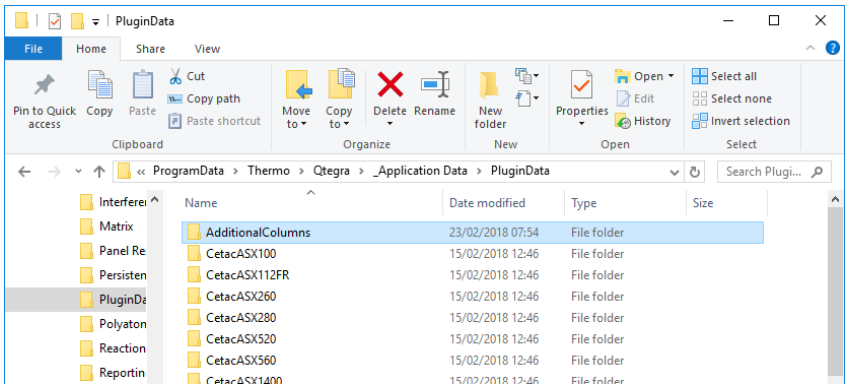
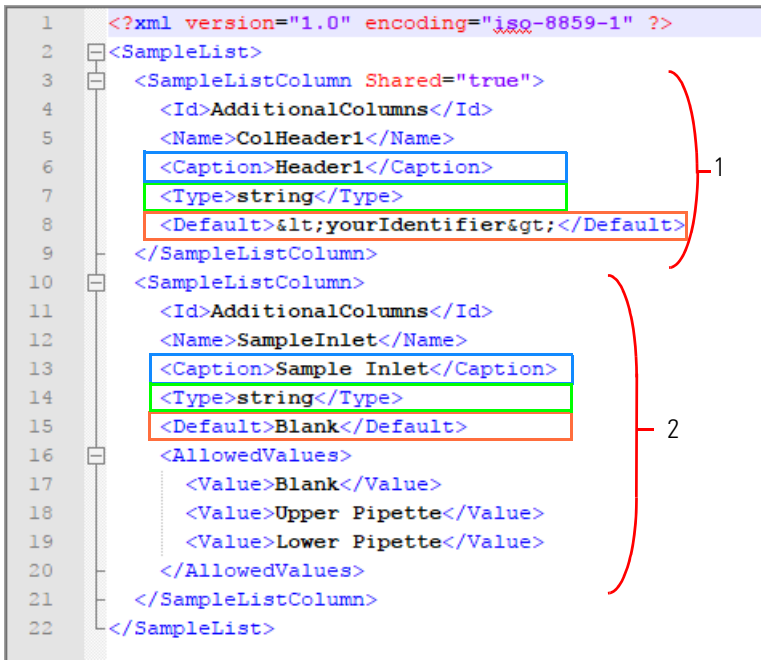


Figure 14-61. New “AdditionalColumns” folder under PluginData

2. Create your XML file within this new folder. The name of the XML file must match the folder name. In this example, the file is named

`AdditionalColumns.SampleList.xml`. Note the prefix ".SampleList", which is essential.

Figure 14-62 shows the structure of the XML file with some highlighted sections.



Labeled Components: 1=definition for column #1, 2=definition for column #2.

Figure 14-62. Structure of the AdditionalColumns.SampleList.xml

3. Change the <Caption> text (for each column) to change the column header name displayed in the Sample List.

4. Change the <Type> (for each column) to define what type of entry is allowed, for example, 'string' can be anything but 'int' will only allow integer values to be accepted.

5. Change the <Default> (for each column) to define the default value displayed in the cells of the column. Use XML code for special characters, like "<" to display "<".

6. Optionally, add a list of allowed values (as shown in the definition for column #2 in Figure 14-62). If such a list is defined, the user can not add a value, but only select one item from a list.

Loading the Configuration

❖ To load the Configuration

1. Open Qtegra and click the currently loaded Configuration or the instrument image on the Dashboard page.

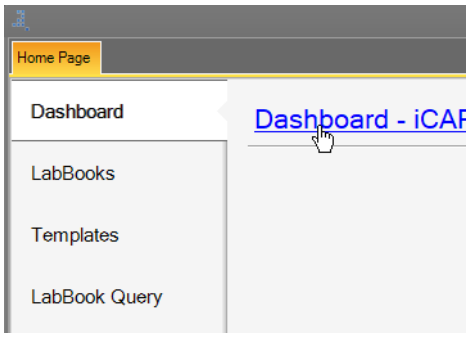


Figure 14-63. Clicking dashboard to select another Configuration

2. From the dialog, select the new or updated Configuration and click **OK**.

Creating a new LabBook

❖ To create a LabBook with the additional columns

1. On the LabBooks page of Qtegra, create a LabBook.
2. In the Content pane of the LabBook, navigate to Sample List.
3. See the new columns appended to the Sample List.

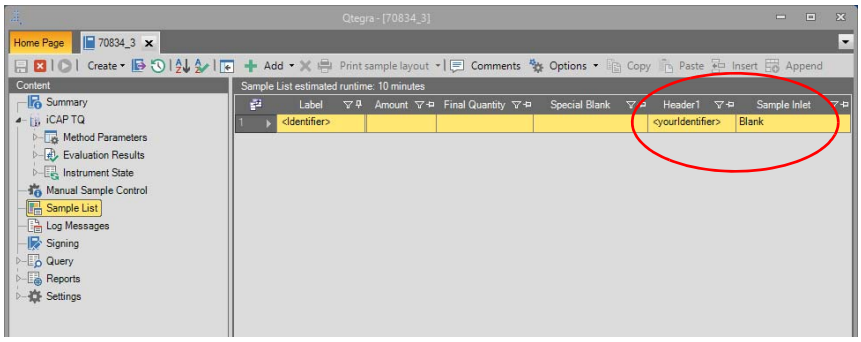


Figure 14-64. LabBook Sample List with new columns

Querying the new columns

The additional columns are available in all Qtegra export formats Automatic Export (see "Automatic Export - Template" on page 5-10), Export (see "To export LabBook data" on page 6-3), Query (see "Query" on page 6-44), and Reports (see "Reports" on page 6-52). Some examples are sown below.

❖ To query the new columns

1. After a LabBook is completed, several query options allow to read the data of the additional columns. For example, select Query from the Content pane, and then select the Categories and least the new columns from the Columns pane, see Figure 14-65.

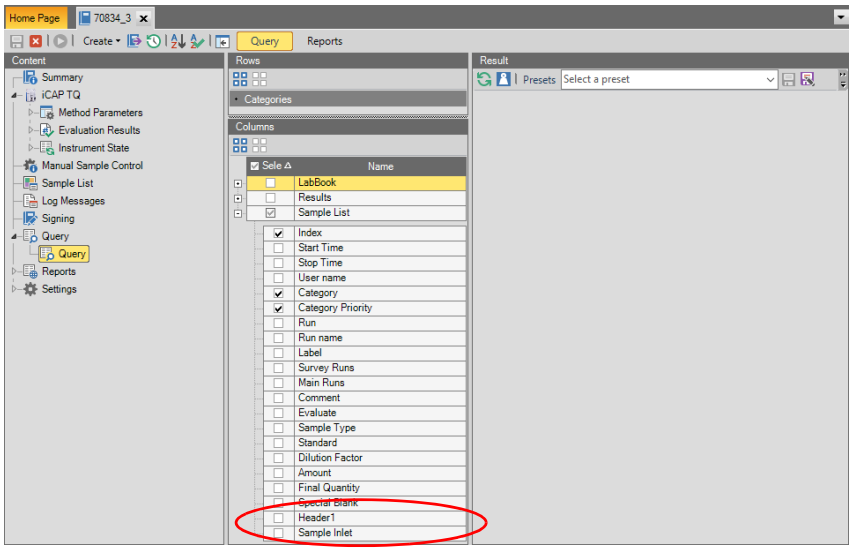


Figure 14-65. LabBook Query with new columns

2. Click **Refresh** or press **<F5>** to see the result of your query.

-or-

3. If the LabBook has not been measured, select Automatic Export from the Content pane to see the new columns provided for CSV Export or SpreadsheetML Export.

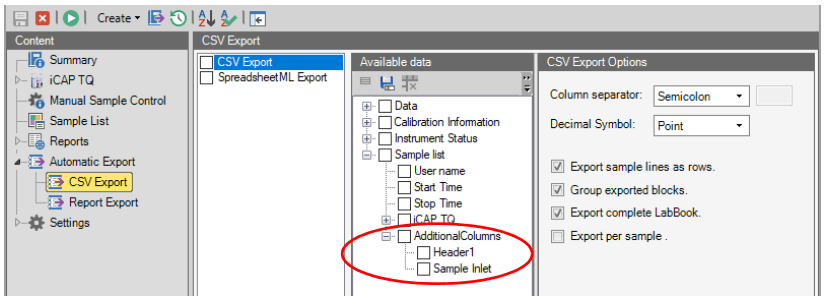


Figure 14-66. LabBook Automatic Export with new columns

-or-

4. Click **Export** or press **<Ctrl> + <E>** to open the Export data dialog. The Export function provides the new columns.

5. In the Export data dialog, select the Exporter (*SpreadsheetML Export* or *CSV Export*). From the Available data area, expand Sample List > AdditionalColumns to select the new columns for the exported file.

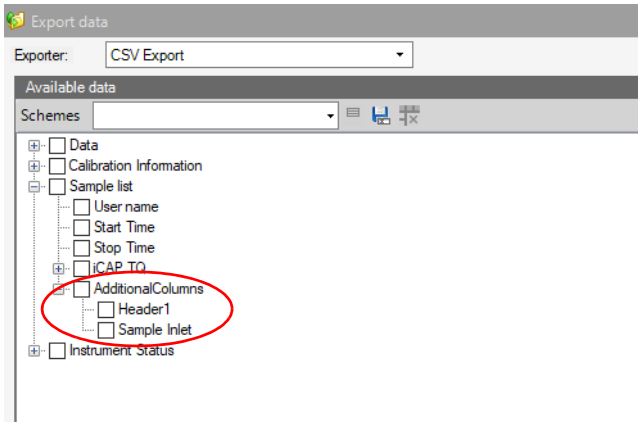


Figure 14-67. LabBook Export with new columns

Displaying the new columns in a Report

❖ To display the new columns in a Report

1. As shown for the queries, the new columns are also available in Reports. For example, under Reports, edit the Sample List Summary Report. The new columns are available in the Table: Sample Summary as shown in Figure 14-68. Add the new columns to the Result columns table.

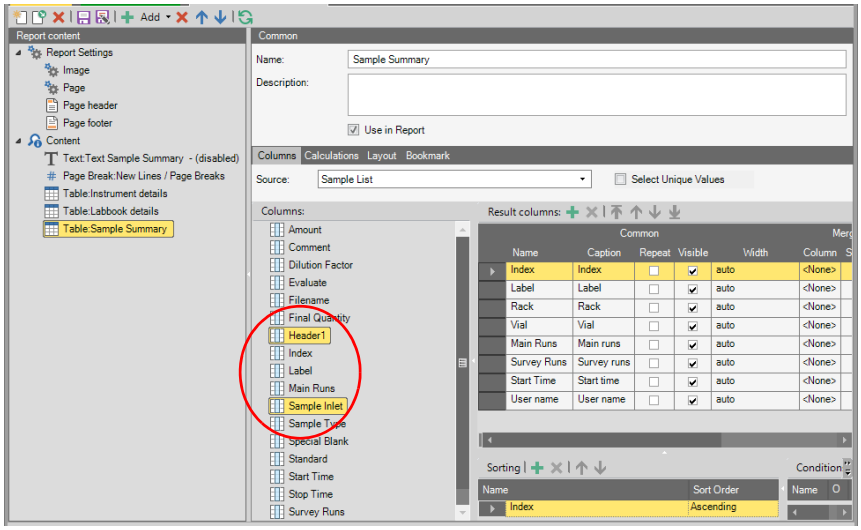
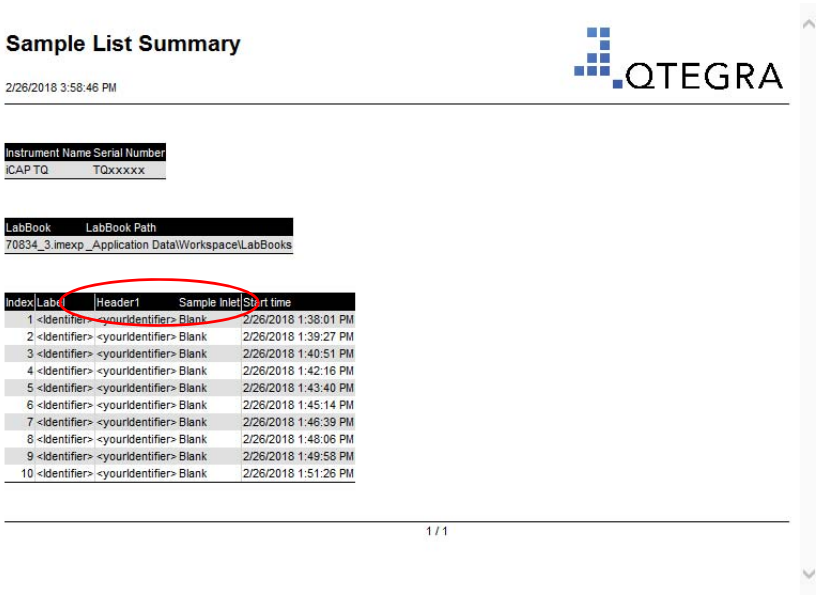


Figure 14-68. LabBook Reports with new columns available

2. Click **Execute Report** to see the new columns in your Report.



Sample List Summary

2/26/2018 3:58:46 PM

QTEGRA

Instrument Name	Serial Number
iCAP TQ	TQxxxxx

LabBook	LabBook Path
70834_3.imexp	_Application Data\Workspace\LabBooks

Index	Label	Header1	Sample Inlet	Start time
1	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:38:01 PM
2	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:39:27 PM
3	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:40:51 PM
4	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:42:16 PM
5	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:43:40 PM
6	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:45:14 PM
7	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:46:39 PM
8	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:48:06 PM
9	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:49:58 PM
10	<Identifier>	<yourIdentifier>	Blank	2/26/2018 1:51:26 PM

1 / 1

Figure 14-69. LabBook Report example with new columns

Color Scheme of the Periodic Table

The periodic table of elements, see Figure 14-70, is part of the Analytes section of the Method Parameters in Qtegra, independent from the Evaluation defined for the Template. Qtegra offers several different, colored presentations of the periodic table. Each color scheme represents specific characteristics of the elements.

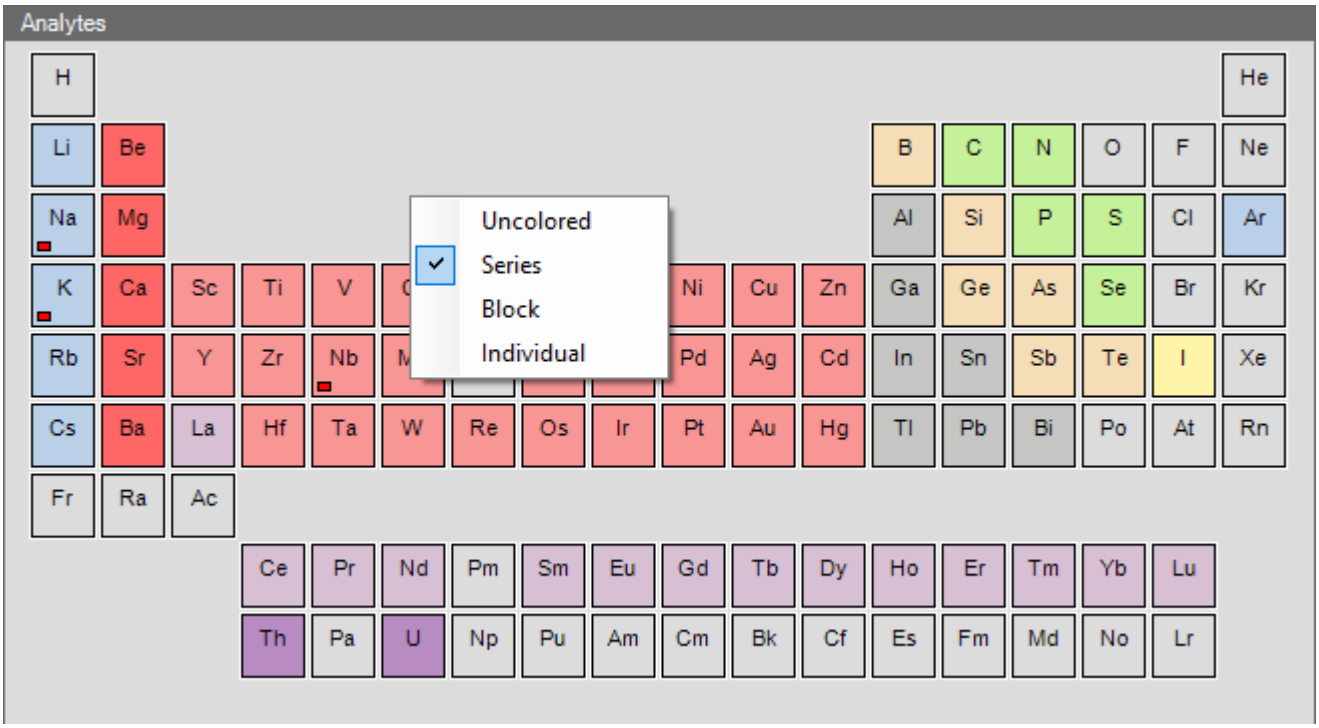


Figure 14-70. Periodic table with shortcut menu

Selected analytes are indicated by red colored squares.

❖ **To change the color scheme of the periodic table**

1. From the **Qtegra - [Home Page]** navigation pane, open a Template as described in "Opening a Template" on page 4-37.
2. Expand the Method Parameters and select the **Analytes** view.
3. Right-click next to the periodic table (but not on the table itself) to open the shortcut menu, see Table 14-10.

Table 14-10. Color scheme of periodic table

Scheme	Description
Uncolored	All elements in the periodic table are displayed as gray boxes.
Series	The elements are color-coded in groups according to their chemical properties or series.

Table 14-10. Color scheme of periodic table, continued

Scheme	Description
Block	The elements are color-coded in blocks, where the respective highest-energy electrons in each element in a block belong to the same atomic orbital type. Use this scheme to distinguish between s, p, d, and f-electrons.
Individual	All elements are marked individually, for example, each showing a different color.

4. Select a scheme from the shortcut menu.
The color in the periodic table changes accordingly.

The Qtegra Backup Tool

A separate tool for managing automatic backups of LabBooks was introduced with Qtegra ISDS Software version 2.8 SR3. The Qtegra Backup tool runs as a service in the background and is set up in the Configurator tool.

During the installation of Qtegra ISDS Software, you can activate the automatic startup of this Qtegra Backup tool, see the wizard page in Figure 14-71.

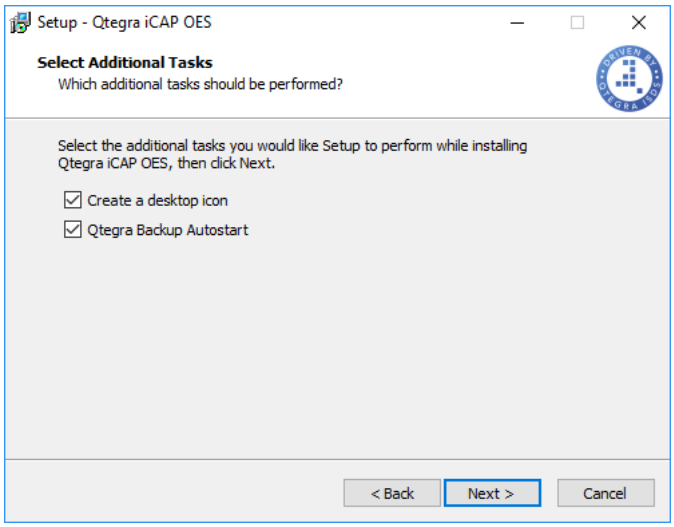
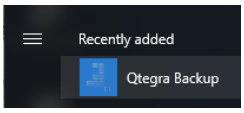


Figure 14-71. Qtegra installation wizard page

The Qtegra Backup tool runs in the background and is shown as a service in the notification area of Windows.

❖ **To set the Qtegra Backup parameters**



1. If the Qtegra Backup tool is not automatically started, select the entry from the **Start** menu.

The empty window is shown. Monitoring is not started and yet not necessary to be started.

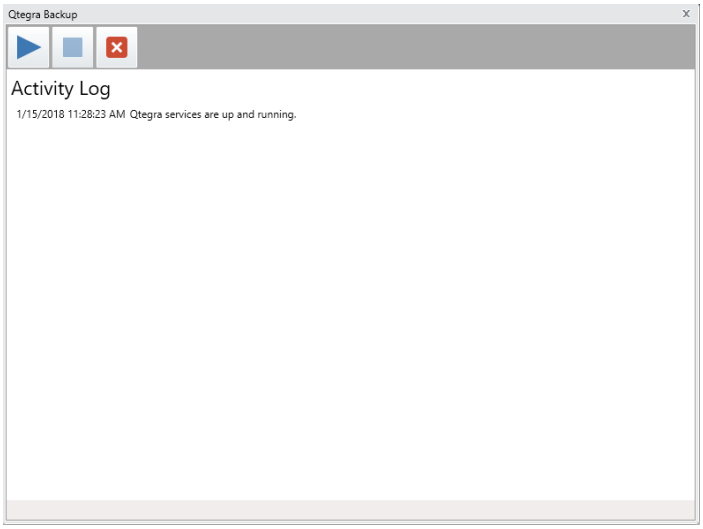


Figure 14-72. Qtegra Backup window

2. Open the Configurator tool and select the Settings applet.

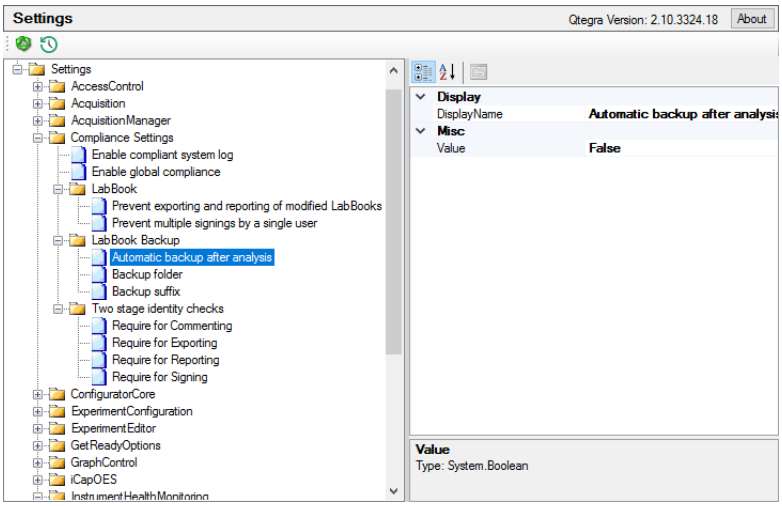


Figure 14-73. Configurator Settings for Automatic LabBook backup

3. If desired, change the **Value** entry as described in Table 14-11.

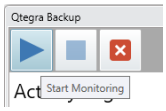
Table 14-11. Automatic LabBook backup settings

Setting parameter	Description
Automatic backup after analysis	Select *True* to activate the Qtegra Backup tool, that means, the LabBook is copied after acquisition to the specified backup folder. Select *False* to disable this function.
Backup folder	Initially, the Qtegra path to the LabBooks is shown as `C:\ProgramData\Thermo\Qtegra\_Application Data\Workspace`. Enter the new path to the folder, where the backup files are stored. Any folder or linked folder can be set that is used by the Qtegra File Manager.
Backup suffix	The backup files always are named with the current date and time stamp as a prefix. Type the suffix that is appended to the backup name if required.

4. After setting parameters have been changed, the Qtegra Backup tool must be stopped and restarted to make the parameters available.

❖ **To start monitoring**

1. Open the Qtegra Backup tool from the notification area of Windows.



2. On the toolbar, select **Start Monitoring**.
The Qtegra Backup tool checks the Workspace > LabBooks folder and all subfolders for changes and is waiting for LabBooks to backup.

3. In Qtegra, create or select a LabBook and drag it into the Scheduler. Run the Scheduler.

4. After the LabBook is finished, open the Qtegra Backup tool to check the Activity Log.
Log entries in bold letters give a hint for errors. Log entries like "Successfully copy file from _Application Data\Workspace\LabBooks\MyLabBook.imexp to <Backup folder>\<Date>_<Time>_MyLabBook.imexp" show a successful backup process.

❖ **To stop monitoring**

1. Open the Qtegra Backup tool from the notification area of Windows.

2. On the toolbar, select **Stop Monitoring**.
   The Windows service of the Qtegra Backup tool is stopped. The Qtegra Backup tool may be restarted for monitoring. With a Windows restart, monitoring is automatically started once the Qtegra Backup Autostart (see Figure 14-71) was ticked.

❖ **To close the Qtegra Backup application**

1. Open the Qtegra Backup tool from the notification area of Windows.

   If the **Close** button is disabled, first stop monitoring.

2. On the toolbar, select **Close Application**.
   The Qtegra Backup tool stops running and is removed from the notification area.

3. After a Windows restart, the Qtegra Backup application is automatically started again.

❖ **To permanently stop the Qtegra Backup tool**

1. Open the Configurator tool and select the Settings applet.
2. Expand the LabBook Backup tree view item and select Automatic backup after analysis, see Figure 14-73.
3. Change the **Value** to *False* to disable the backup function.

Alternatively, you can stop the Qtegra Backup tool via the Task Manager.

1. Press **<Ctrl> + <Shift> + <Esc>** to open the Task Manager.
2. Select the **Startup** tab.
3. From the list of automatically started programs, select Qtegra Backup and right-click to select **Disable** from the shortcut menu.

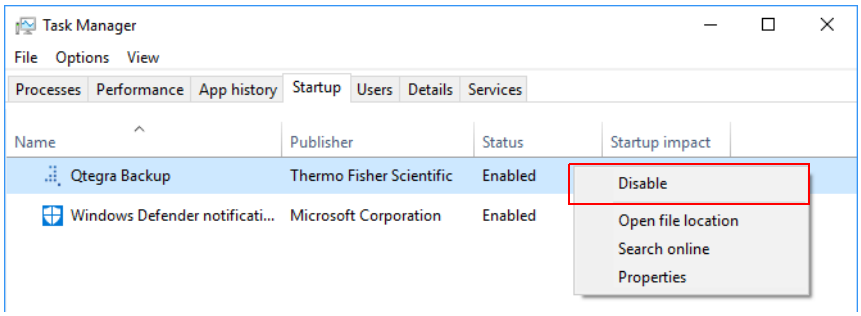


Figure 14-74. Qtegra Backup tool in the Task Manager

4. After a Windows restart, Qtegra Backup remains disabled.

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