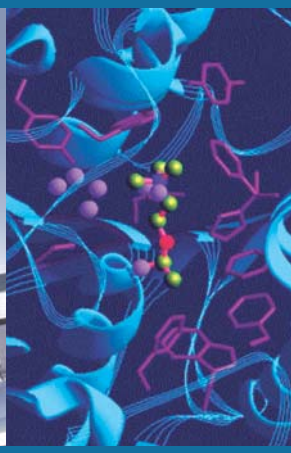
Thermo Fisher Scientific

iCAP™ Q
Software Manual

Revision B - 1288010





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Contacting Us

There are several ways to contact Thermo Fisher Scientific.

Assistance

For technical support and ordering information, **visit us on the Web**:

www.thermoscientific.com/ms

Service contact details for customers are available under:

www.unitylabservice.com

Customer Information Service

The Customer Information Service site cis.thermo-bremen.com is aimed at providing instant access to latest software updates and manuals, application reports, and brochures.

Thermo Fisher Scientific recommends that you register with the site as soon as the instrument is installed. To register, visit register.thermo-bremen.com/form/cis and fill in the registration form. Once your registration has been finalized, you will receive confirmation by e-mail.

Suggestions to the Manual

❖ **To suggest changes to this manual**

- Please send your comments (in German or English) to:
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- Send an e-mail message to the Technical Editor at documentation.bremen@thermofisher.com

You are encouraged to report errors or omissions in the text or index. Thank you.

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Chapter 1 Using This Manual

This *iCAP Q Software Manual* introduces the software suite Qtegra and describes the configuration and operation of the iCAP™ Q instrument with Qtegra. For information about the operating procedures for the iCAP Q MS system, we recommend that you read the *iCAP Q Operating Manual*.

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:

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

Viewpoint Orientation

Left and *right* used in this manual always refer to the viewpoint of a person facing the front side of 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**".

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

Reference Documentation

In addition to this guide, Thermo Fisher Scientific provides the following documents for the iCAP Q instrument:

- *iCAP Q Preinstallation Requirements Guide*
- *iCAP Q Operating Manual*

The *iCAP Q Operating Manual* represents the Original Operating Instructions. Thermo Fisher Scientific provides this iCAP Q Software Manual as additional reference documents for the iCAP Q mass spectrometer.

The Qtegra software also provides Help.

A printed version of the *iCAP Q Operating Manual* is shipped with the instrument. A printed version of the *iCAP Q Preinstallation Requirements Guide* is part of the Preinstallation Kit. This kit is sent to your laboratory before the arrival of the iCAP Q mass spectrometer.

Chapter 2 Introduction to Qtegra

Qtegra is a configurable software package for elemental analyses. It 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 frameworks introduced in this chapter are:

Contents

- Configurator Overview
- Instrument Control Overview
- Experiment Editor Overview

Configurator Overview

The Configurator tool is used by the Administrator of your network and the Manager of your laboratory. Different applets are provided to edit general settings of the hardware and software and to configure and adjust the Thermo Scientific Qtegra framework for your laboratory.

The user interface of the Configurator tool is shown in Figure 2-1:

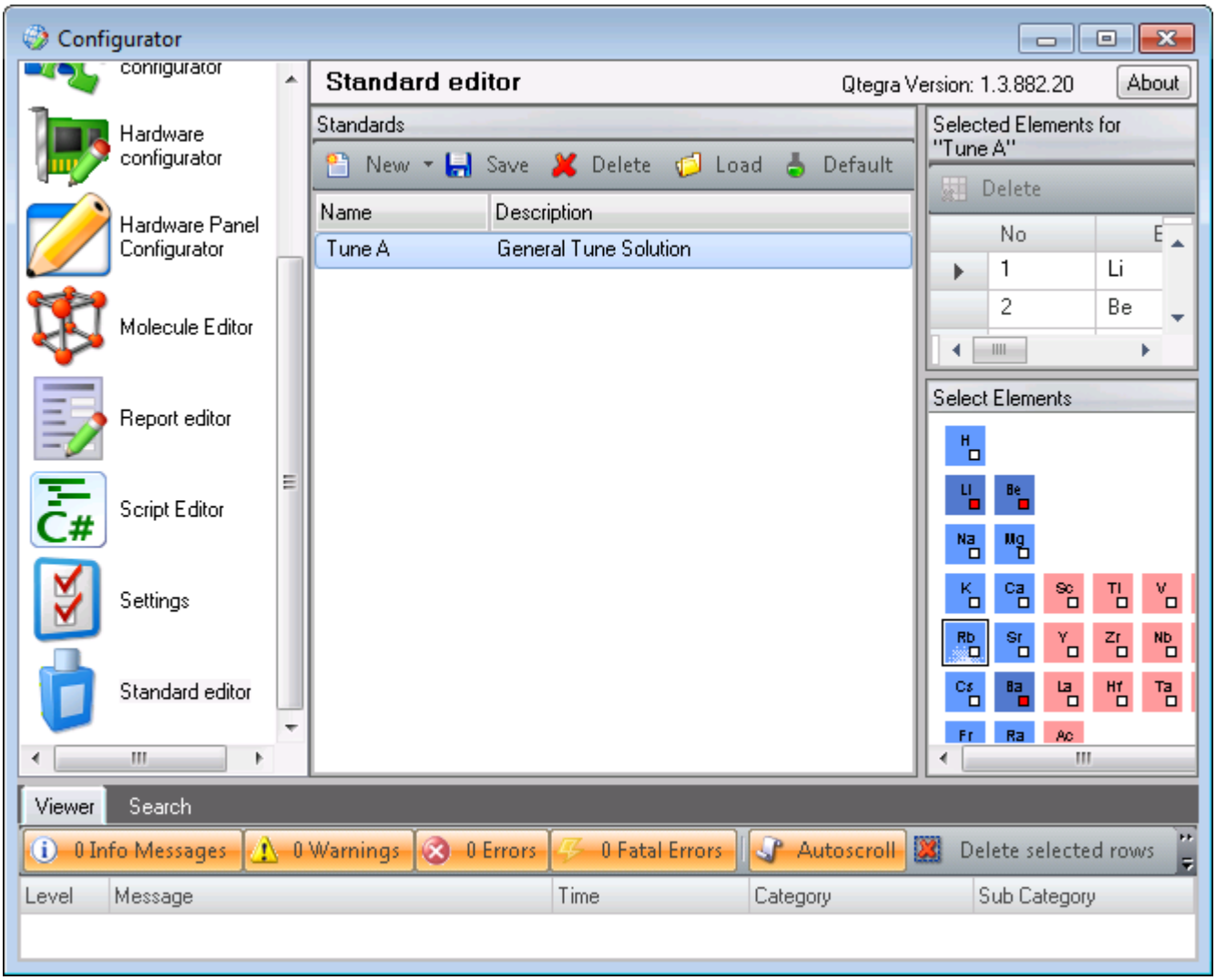


Figure 2-1. User interface of Configurator

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

Table 2-1. Applets of the Configurator

Applet		Description
	Access Control Editor	Allows the Administrator/Manager to define the access permissions for the different programs and applications in the user interface.
	Element Editor	Element and isotope properties and the default isotopes are listed. The default isotope set to TRUE in the database is either the most abundant isotope or the most abundant isotope which is likely to have the least interferences. The properties can be changed here and are applied throughout the Qtegra framework.
	Experiment Configurator	Allows the Administrator/Manager to define instrument settings, communication ports, and combine instrument sets and evaluation strategies for a specific Experiment Configuration. These combinations can be selected in the Experiment Configuration tab of Instrument Control for direct control of the hardware instruments associated with the Experiment Configuration. Templates created in Experiment Editor are based upon these Configurations.
	Hardware Configurator	Gives access to hardware databases where instrument control and other hardware parameter ranges or settings can be defined.
	Hardware Panel Configurator	Defines how the Hardware Panel in Instrument Control is displayed for each of the devices or instruments set associated with the Configuration.
	Molecule Editor	Allows the Administrator/Manager to create polyatomics and doubly charged ions that can then be viewed and selected within the Analytes view of Instrument Control and Experiment Editor.
	Report Editor	Allows the Administrator/Manager to create new and to edit existing report templates.
	Script Editor	Allows the Administrator/Manager to create and edit C# scripts that can then be loaded and run in Instrument Control.
	Settings	Gives access to the settings database (Registry) and controls default settings such as the default directory path for Experiment Editor or default settings for dwell time. The settings stored here should not normally need any modifications.
	Standard Editor	Central database editor for stock solutions and standards.

NOTICE For details on the Configurator tool, see "Configurator" on page 3-1. ▲

❖ To open the Configurator tool

1. Click 

to open **Configurator**.

Instrument Control Overview

Instrument Control is used by the Manager to switch on, optimize and calibrate the iCAP Q instrument.

To run a measurement the appropriate Experiment Configuration has to be loaded. The Experiment Configuration is created by the Manager, see "Experiment Configurator" on page 3-13.

An Experiment Configuration selected in the ribbon tab of Instrument Control enables tabs in the data view for each instrument defined in the Experiment Configuration. The iCAP Q data view contains an analyte table and real-time display where time-resolved and mass spectral data can be observed.

The ribbon tabs of Instrument Control change dynamically upon selecting a different peripheral tab in the data view region.

The user interface of Instrument Control is shown in Figure 2-2:

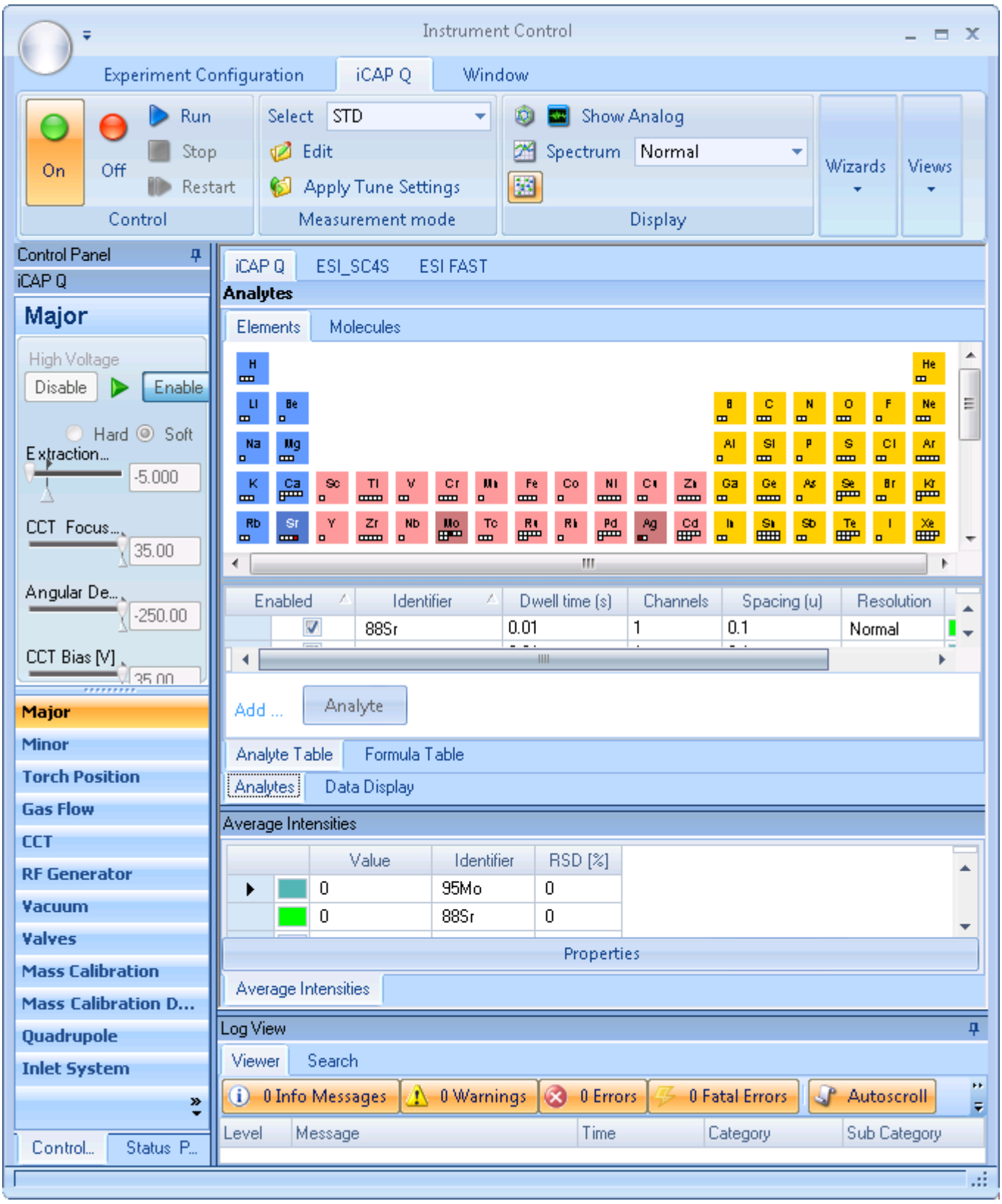


Figure 2-2. User interface of Instrument Control

In the ribbon tab iCAP Q, user-definable Wizards for instrument calibration, autotunes and performance reports can be run, edited, stored and viewed. Optimized tune parameter sets to be used throughout the Qtegra framework are stored in Instrument Control.

NOTICE For details on the Instrument Control tool, see "Instrument Control" on page 4-1. ▲

❖ To open the Instrument Control tool

1. Click 

to open **Instrument Control**.

Experiment Editor Overview

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

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 appropriate Template.

The user interface of the Experiment Editor tool is shown in Figure 2-3:

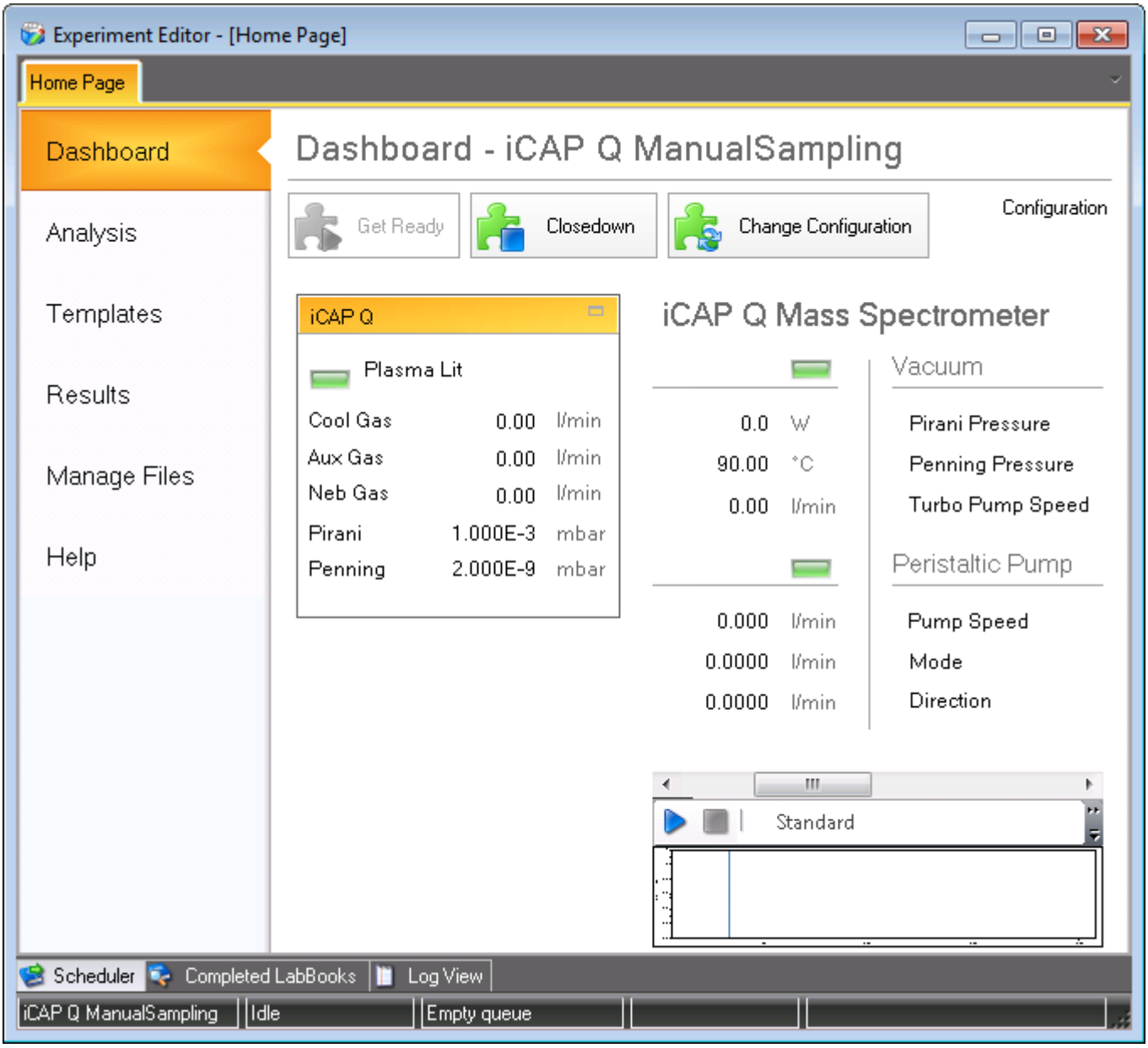


Figure 2-3. User interface of Experiment Editor

NOTICE For details on the Experiment Editor tool, see "Experiment Editor" on page 5-1. ▲

❖ To open the Experiment Editor tool

1. Click 

to open **Experiment Editor**.

Chapter 3 Configurator

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

Contents

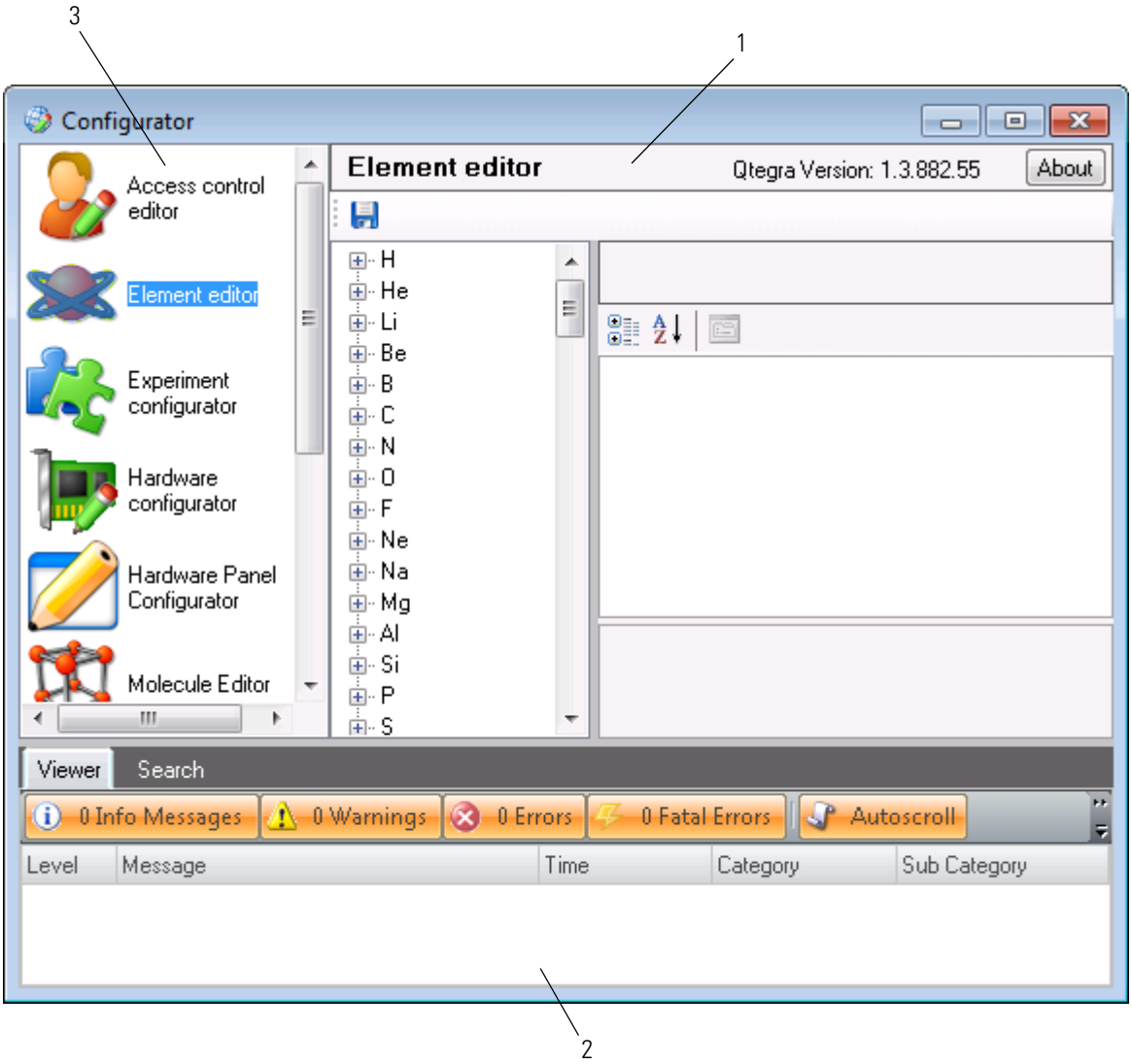
- User Interface of the Configurator Tool
- Viewer Region
- Access Control Editor
- Element Editor
- Experiment Configurator
- Hardware Configurator
- Hardware Panel Configurator
- Molecule Editor
- Report Editor
- Script Editor
- Settings
- Standard Editor

❖ **To open the Configurator tool**

1. Click Configurator to open **Configurator**.

User Interface of the Configurator Tool

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



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

Figure 3-1. User interface of Configurator

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

The **Viewer** region displays a list of log files, such as messages, errors and warnings.

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 Configurator

NOTICE The Viewer tab is also shown in "Experiment Editor" on page 5-1 and "Instrument Control" on page 4-1. ▲

❖ To open the Viewer

1. Click Configurator to open **Configurator**.
2. Click the tab **Viewer**.

Access Control Editor

The **Access control editor** applet of the Configurator tool allows the Administrator and Manager to control the access permissions by granting or denying access to the different programs and applications of Qtegra.

With Access control editor (see Figure 3-3), the Administrator or Manager defines who has access to programs or parts of programs and what type of access permission is granted or denied to a user or user group.

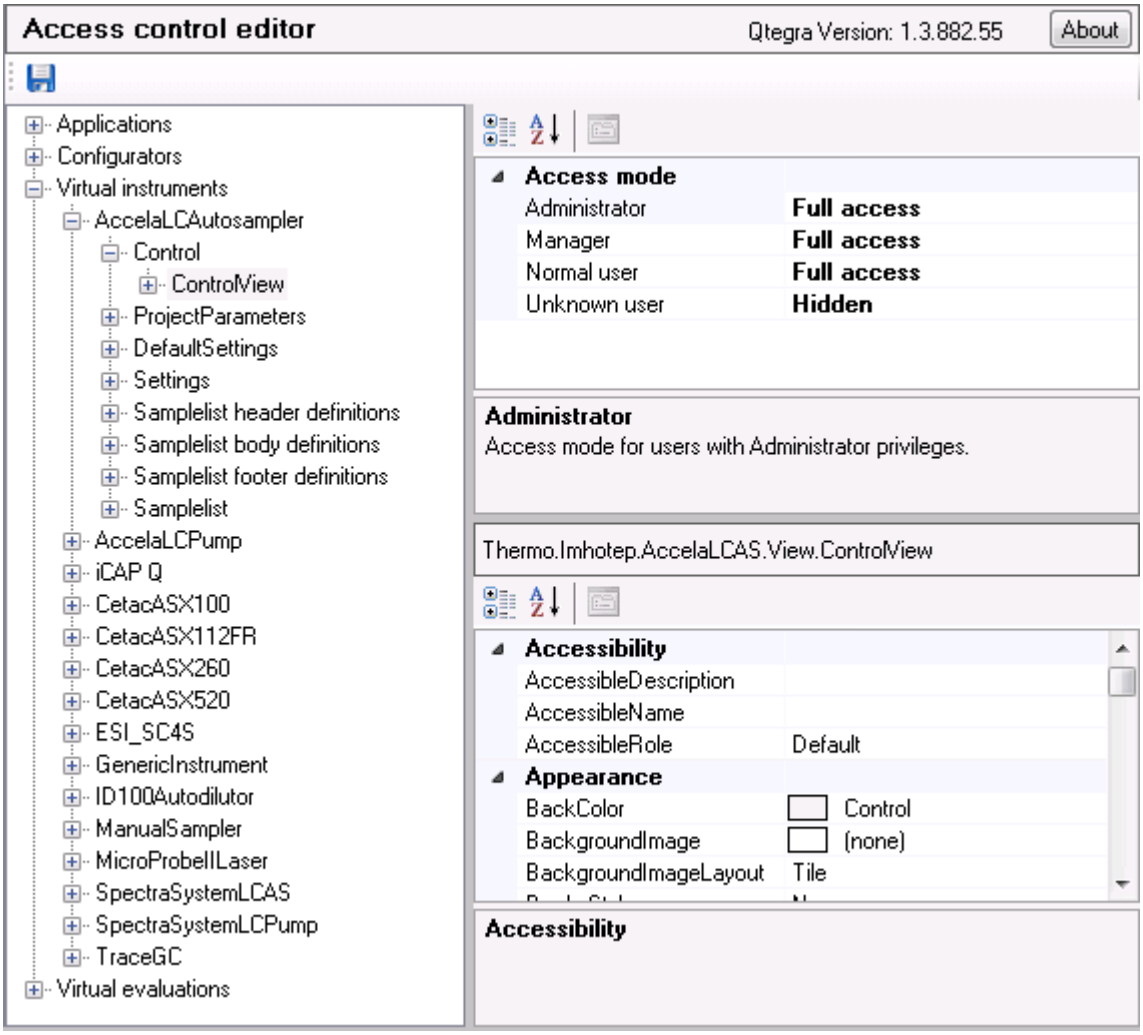


Figure 3-3. Layout Access control editor

During Setup of Qtegra, Thermo Fisher Scientific provides the user groups shown in Table 3-1. The Windows™ user installing Qtegra is added to the group Administrator.

Table 3-1. User roles provided by Qtegra

Name	Description
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.
Manager	The Manager is responsible for method setup/creation and instrument maintenance. By default, the Manager has full access to all programs and applications available. However, access rights of the Manager can be changed by the Administrator.
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 or Manager.

NOTICE By default, the minimum user level for **Applications** and **Configurators** is defined as Administrator. Other user groups cannot open these programs. ▲

Types of access rights that can be granted or denied are listed in Table 3-2.

Table 3-2. Access rights for Qtegra

Name	Description
Full Access	The user can both see the certain program or application and edit the settings.
Read Only	The user can only see the certain program or application; changes are not allowed.
Hidden	The program or parts of the program are hidden for this user.

NOTICE **Full Access** rights by default are granted to the groups **Administrator**, **Manager**, **Normal user**. Users that have not been assigned (by the Windows™ administrator) to a Qtegra group belong to the group **Unknown user**. For this group everything is **Hidden**. ▲

❖ **To open Access control editor**

1. Click 

to open **Configurator**.

2. Click  **Access control editor**.

How to Set User Levels

You set the minimum user level to define which user group is allowed to start a program in the **Access control editor** applet of the Configurator tool.

❖ **To set the minimum user level for access to Applications and Configurators**

1. Click 

to open **Configurator**.

2. Click  **Access control editor**.

3. Select the **Applications** or **Configurators** from the browser view.

4. Click on the item below **Applications** or **Configurations** to open the **Access mode** view on the right.

5. Click  to display the list of defined access groups, see Figure 3-4.

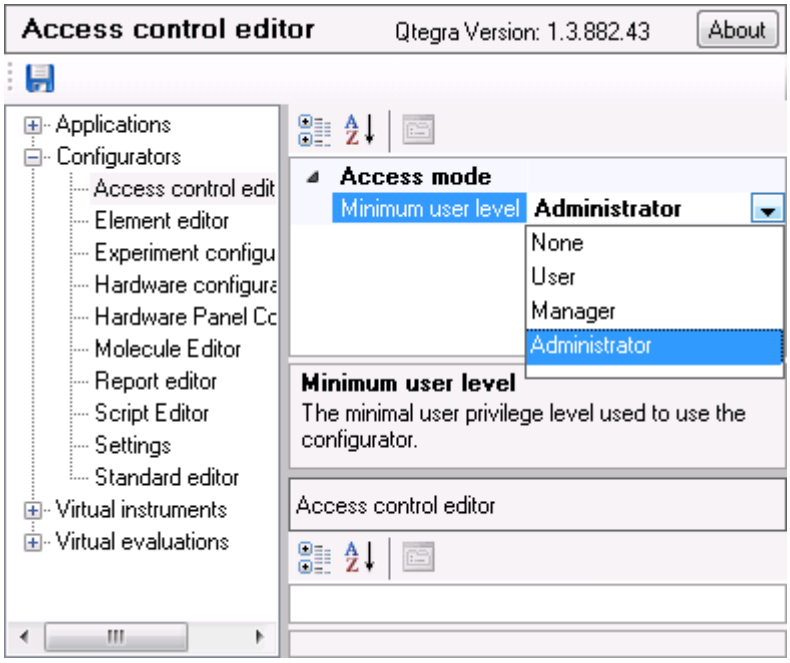


Figure 3-4. List of access groups for minimum user level

6. Click to select the new **Minimum user level**, for example, **Administrator**.
   The minimum access level for the selected item of Applications or Configurators is now defined.
   In this example, only the group Administrator is allowed to open Access control editor.

7. Click  to save the changes.

How to Grant Access Rights

For each user group, you can define which buttons and controls are visible and activated in the **Access control editor** applet of the Configurator tool.

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

1. Click 

to open **Configurator**.

2. Click  **Access control editor**.

3. Select an item from **Virtual instruments** or **Virtual evaluations** in the browser view.
   The **Access mode** settings are shown on the right.

4. Click the user group for which you wish to change the access rights, for example, **Normal user**.

5. Click  to display the list of access rights, see Figure 3-5.

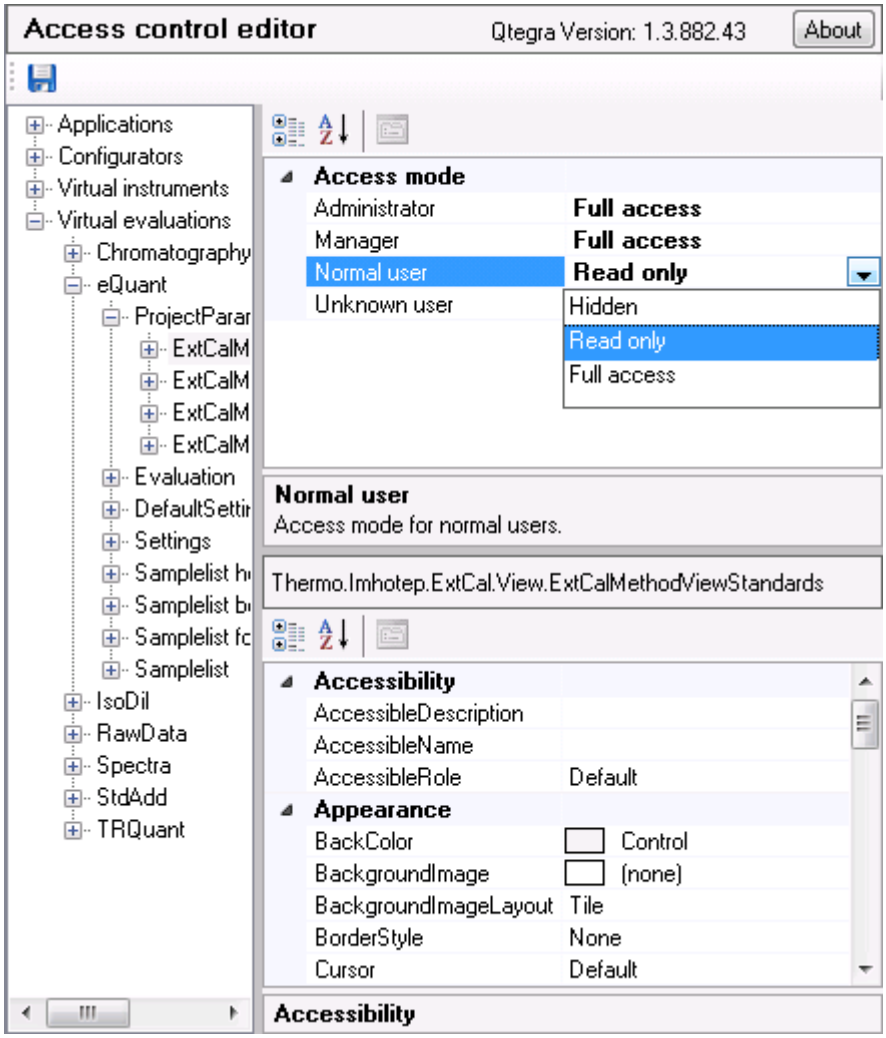


Figure 3-5. List of access rights for user group

6. Select the new access right for the user group, for example, **Read only**.
   The new access rights are defined for this **Virtual instruments** or **Virtual evaluations** item.

7. Click  to save the changes.

Element Editor

The **Element editor** applet of the Configurator tool gives access to the properties of the element and isotope table.

Element editor contains a list of all elements and their properties sorted in the order of their atomic number, see Figure 3-6. The information listed here will be used for all experiments.

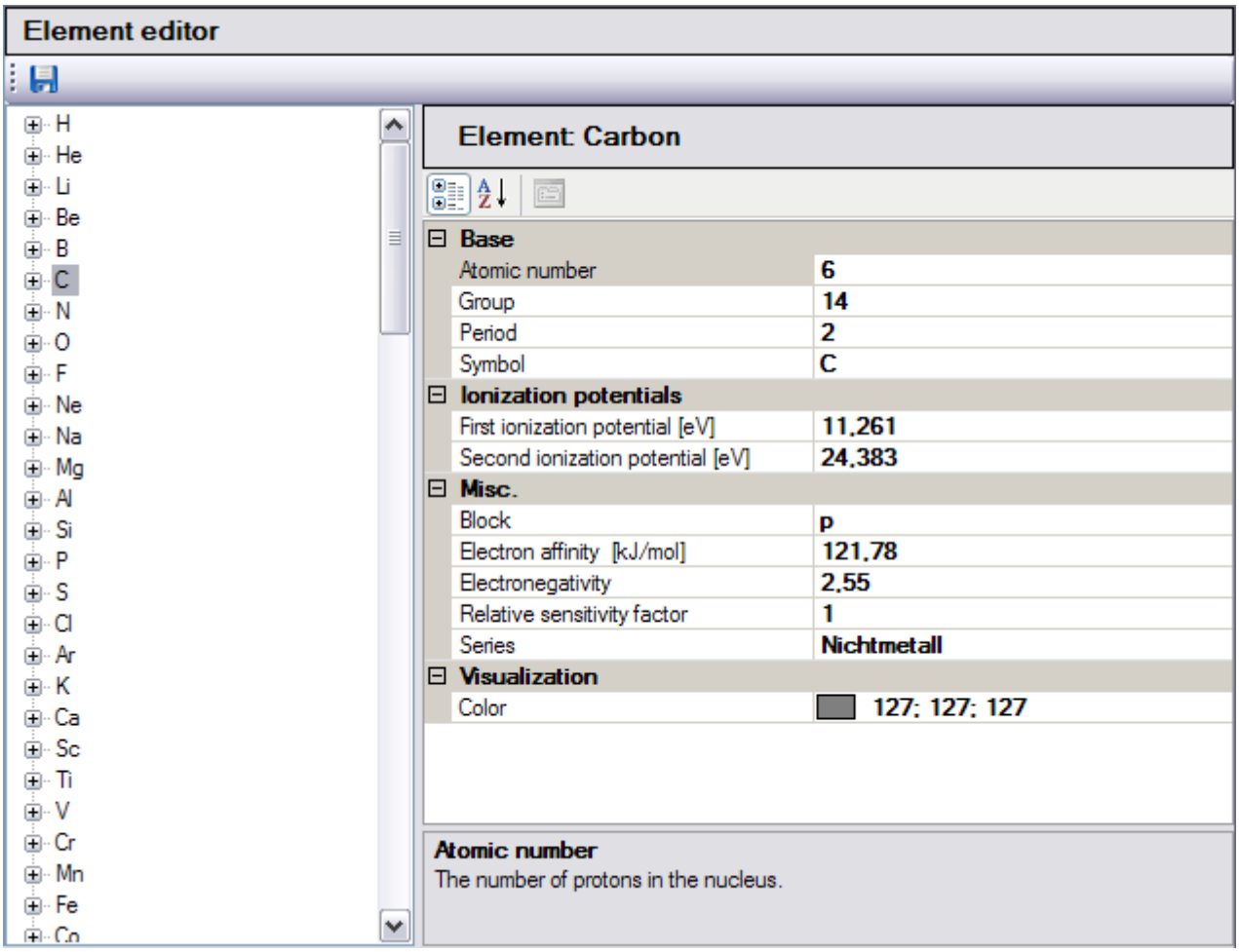


Figure 3-6. Layout Element editor

❖ **To open Element editor**

1. Click Configurator to open **Configurator**.
2. Click **Element editor**.

How to Change the Properties of an Element or Isotope

It might be necessary to add or change an element or isotope in the **Element editor** applet of the Configurator tool. Usually, these settings would only be changed by the Manager.

❖ **To change the properties of an element or isotope**

1. Click 

to open **Configurator**.
2. Click  **Element editor**.
3. Select an element or click  to display the list of isotopes and select an isotope to display the element or isotope properties.
4. Click in the respective field to edit a property and click  to save the changes.

❖ **To add an isotope to the table**

1. Click 

to open **Configurator**.
2. Click  **Element editor**.
3. Select the element of interest and right-click anywhere next to it to open the context menu.
4. Select **Add isotope**.
The **Add isotope** window opens, see Figure 3-7.

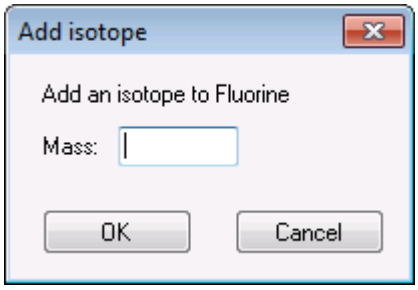
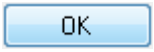


Figure 3-7. Element editor - add isotope

5. Enter the **Mass** of the isotope and click 

to exit the window.

6. Click  to save the changes in the database.

How to Change the Default Isotope

It might be necessary to change a default isotope in the **Element editor** applet of the Configurator tool. Usually, these settings would only be changed by the Manager.

❖ **To change the default isotope**

1. Click 

to open **Configurator**.

2. Click  **Element editor**.

3. Select an element and click  to display the list of isotopes.

4. Click an isotope to display the isotope properties.

5. Click in the cell next to **Is default**.

   The button appears, see Figure 3-8.

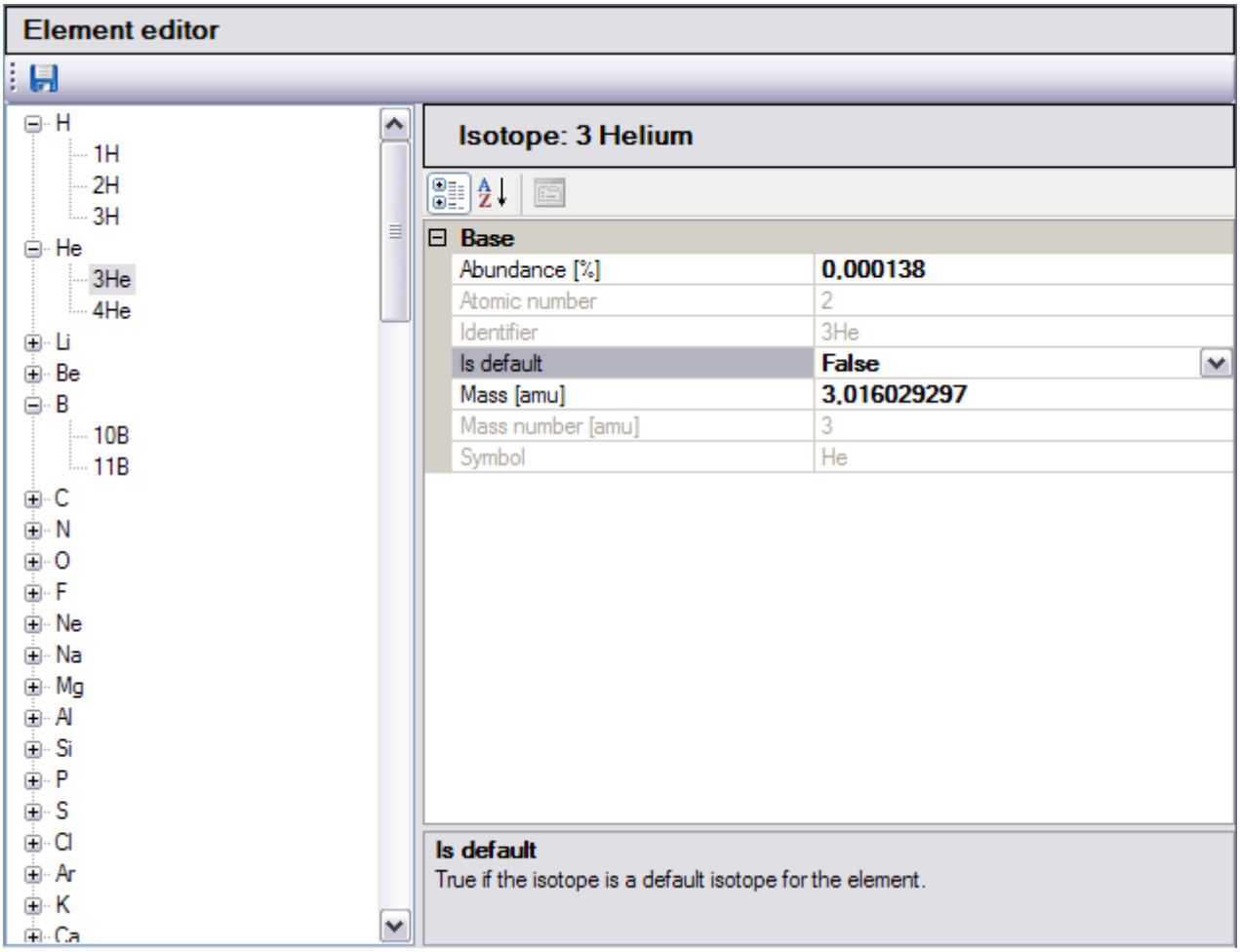


Figure 3-8. Default isotope properties

6. Click and select **True** or **False** for this isotope, as appropriate.

7. Click to save the changes in the database.

Experiment Configurator

The **Experiment configurator** applet of the Configurator tool combines instrument sets. Each combination is saved as specific Experiment Configuration for later use in the Experiment Editor tool when creating a Template, and in Instrument Control.

NOTICE Access to this module is defined in the "Access Control Editor" on page 3-4. Generally, only the Administrator and the Manager have full access to this module. ▲

In Experiment configurator, all virtual instruments, virtual evaluation types and preset configurations are listed on tabbed pages, see Figure 3-9.

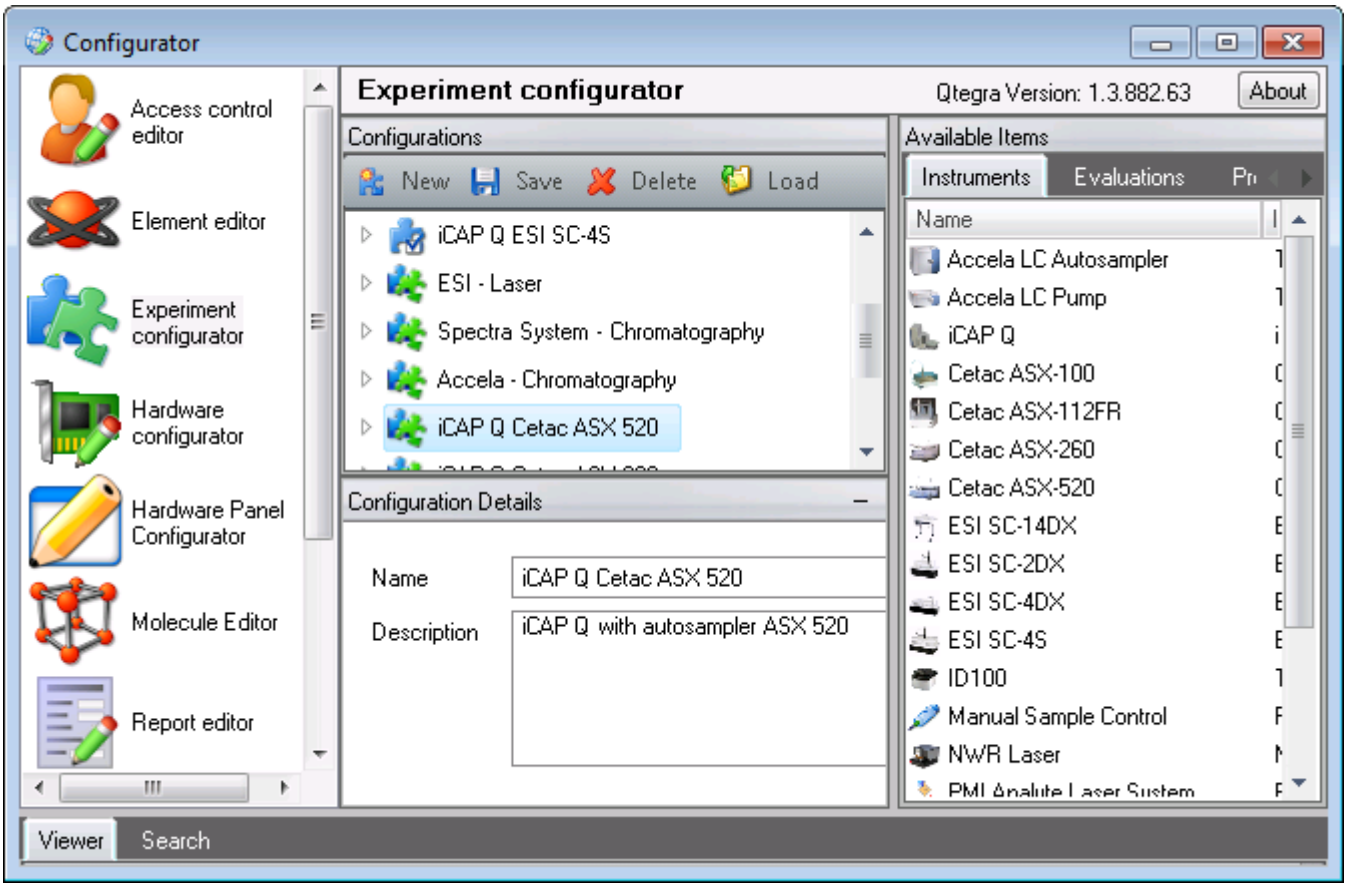


Figure 3-9. Layout Experiment Configurator

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

Table 3-3. Experiment configurator commands

Commands	Description
	To create a new Configuration. Adds **New Experiment Configuration** to be renamed.
	To load all Configurations saved in the configurations data base.
	To save the current Configuration.
	To delete the current Configuration.

❖ **To open Experiment configurator**

1. Click 

to open **Configurator**.

2. Click  **Experiment configurator**.

How to Create a New Experiment Configuration

In the **Experiment configurator** of the Configurator tool, Configurations are created for each of your instrument setups.

❖ **To create a new Experiment Configuration**

1. Click 

to open **Configurator**.

2. Click  **Experiment Configurator**.

3. Click **New** to add a new Experiment Configuration, see Figure 3-10.

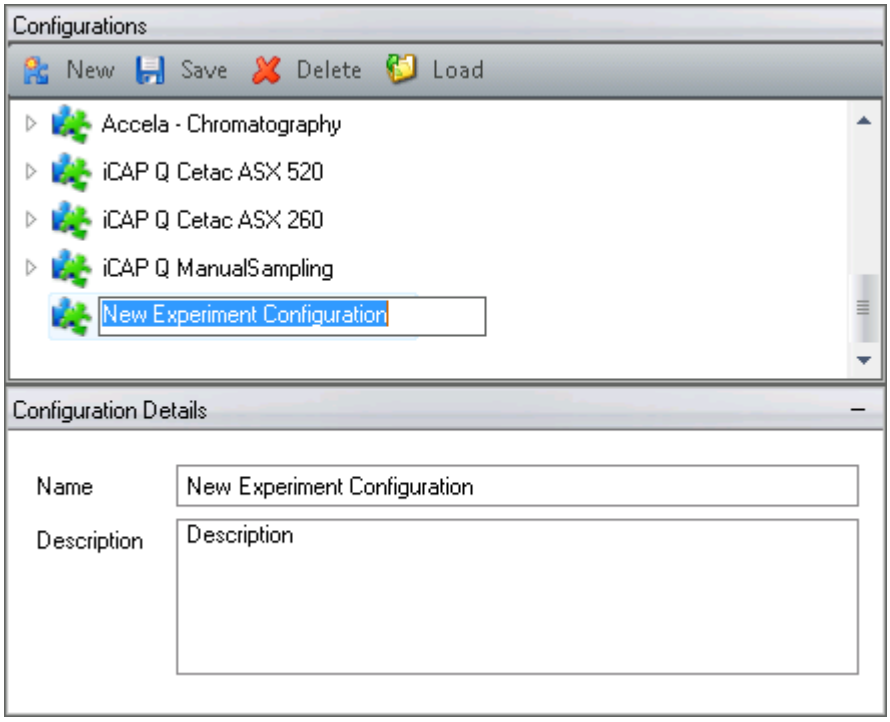


Figure 3-10. Add new Experiment Configuration

4. Enter a name and click anywhere outside the field to confirm. The name is accepted and displayed in the **Configuration Details** view.

5. Enter a **Description** in **Configuration Details**.

6. Click the tab **Instruments** on the right, see Figure 3-11.

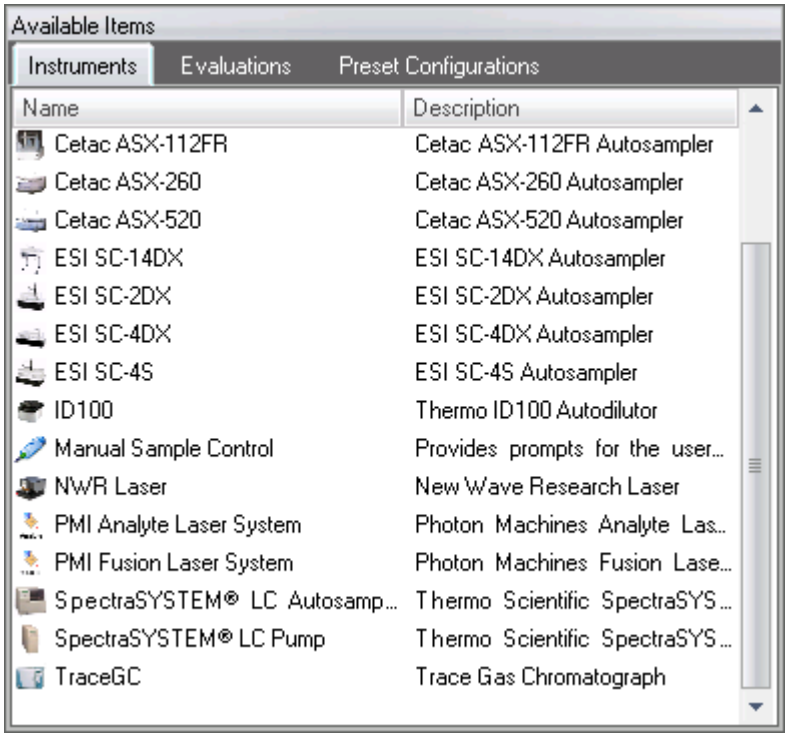


Figure 3-11. Available instruments and peripherals

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

7. Drag and drop **iCAP Q** from the tab **Instruments** to your new Configuration.

Drop when  is shown, see Figure 3-12.

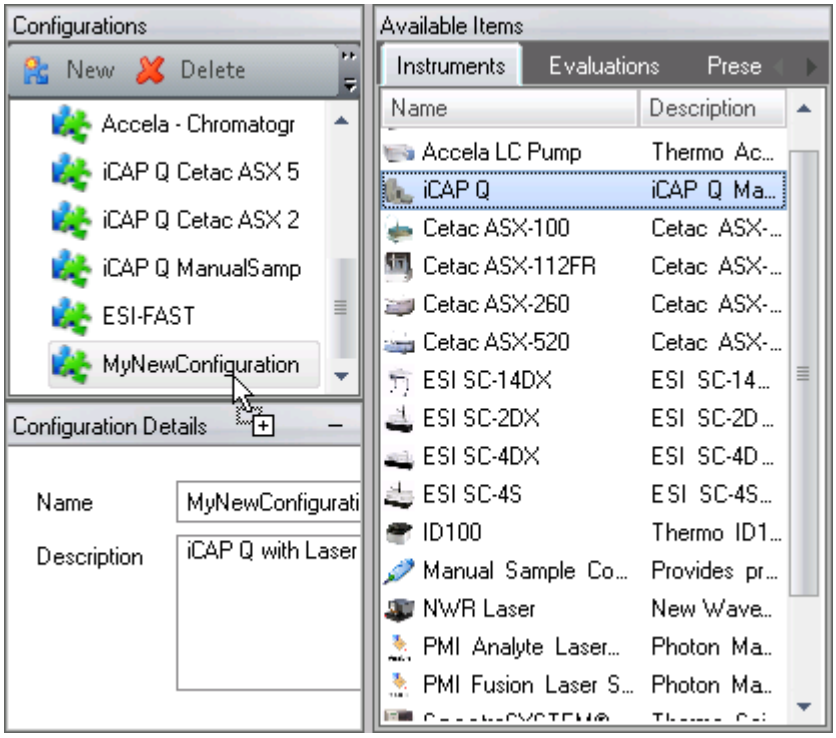


Figure 3-12. Add iCAP Q to your Configuration

8. Drag and drop the peripheral you wish to add from the tab **Instruments** to your new Configuration, see Figure 3-13.

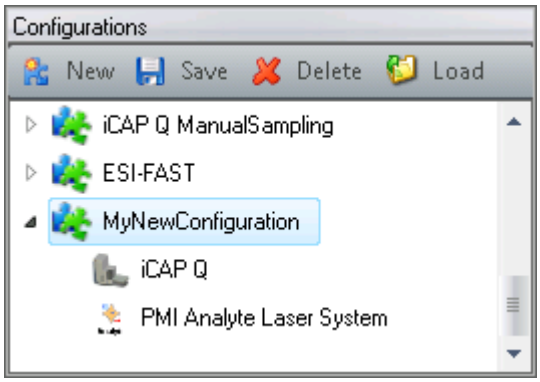


Figure 3-13. Instrument and laser system added to your Configuration

9. Click  to save the **Configuration**.

How to Edit the Settings of Instruments

In the **Experiment configurator** of the Configurator tool, your Administrator edits the settings for the Instrument in the Configurations field.

❖ **To edit Instrument settings**

1. Click 

to open **Configurator**.

2. Click  **Experiment Configurator**.

3. In the list of **Configurations**, right-click the Instrument you wish to edit the settings for, see Figure 3-14.

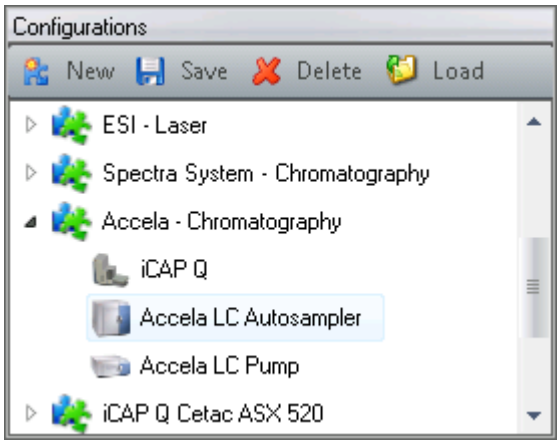
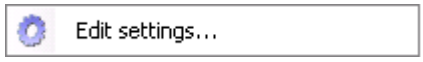


Figure 3-14. Right-click Instrument to edit settings

4. Click 

to open the **Settings** window, see Figure 3-15.

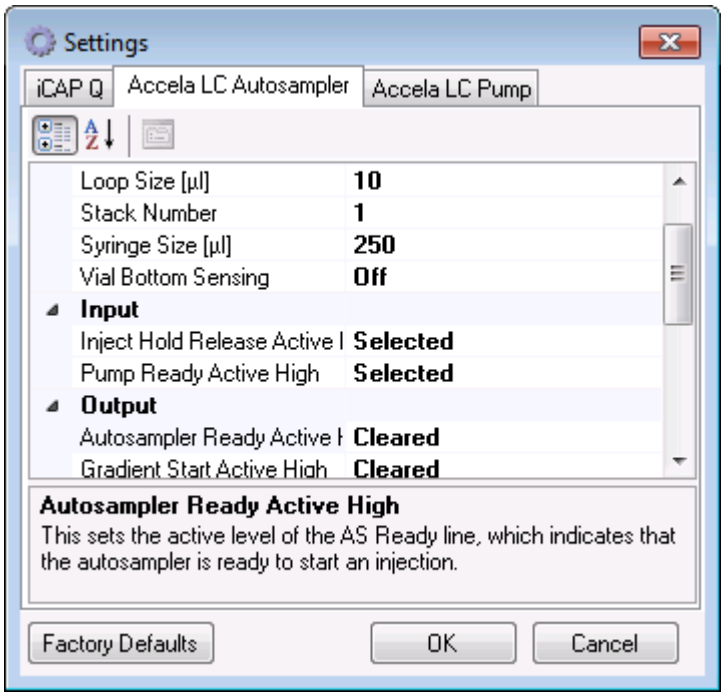


Figure 3-15. Settings window for Instrument in Configurator

All Instruments of the current Configuration are presented in tabs.

5. In the **Settings** window, select the tab for the Instrument you wish to edit, for example, **Accela LC autosampler**.

6. Click in a cell to change the value.
If a drop-down menu is available for this cell, the drop-down arrow  is shown.

7. Change the value or click the arrow to display the drop-down menu if available, see Figure 3-16.

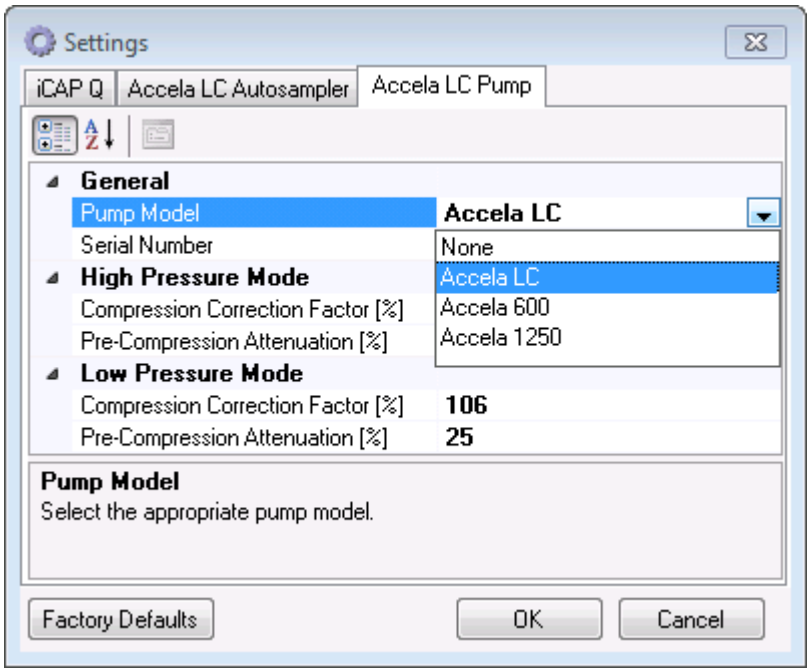
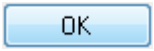


Figure 3-16. Drop-down menu of Settings in Configurator

8. Select an item from the list.
9. Click  .
10. Click  to save the **Configuration**.

How to Load Experiment Configurations

In the **Experiment configurator** of the Configurator tool, Configurations are loaded from the configurations database.

❖ **To load an Experiment Configuration from configuration database**

1. Click 

to open **Configurator**.
2. Click  **Experiment Configurator**.
3. Click  to load the Experiment Configurations from the configurations database.

How to Create a Preset Configuration

In the **Experiment configurator** of the Configurator tool, Configurations can be saved as preset configurations.

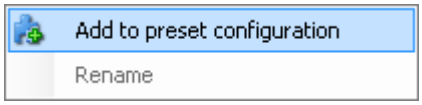
❖ **To create a Preset Configuration**

1. Click 

to open **Configurator**.

2. Click  **Experiment Configurator**.

3. In the list of **Configurations**, right-click the Configuration you wish to add to the list of Preset Configurations.

4. Select 

from the context menu to add the Configuration to the list of Preset Configurations.

5. Click  to save the **Configuration**.

How to Delete a Configuration

In the **Experiment configurator** of the Configurator tool, Configurations can be deleted from the configurations database.

❖ **To delete a Experiment Configuration**

1. Click 

to open **Configurator**.

2. Click  **Experiment Configurator**.

3. In the list of **Configurations**, right-click the Configuration you wish to delete.

4. Click  to delete the selected Configuration.
   The **Delete Configuration** dialog opens, see Figure 3-17.

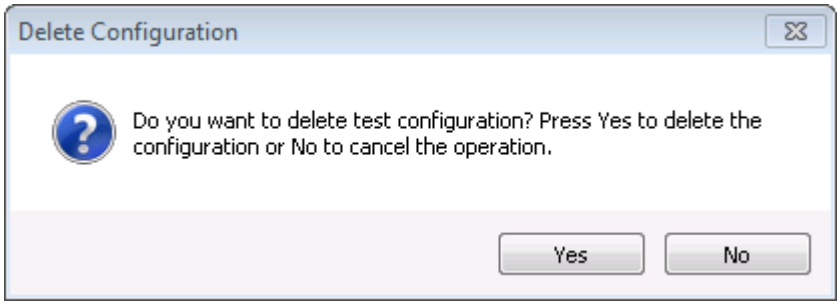
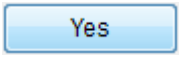


Figure 3-17. Delete Configuration dialog

5. Click  to delete the Configuration.

6. Click  to save the **Configurations** to the database.

Hardware Configurator

The **Hardware configurator** applet of the Configurator tool gives access to hardware databases on electrotechnical items level.

NOTICE Generally, these settings are factory-set and do not need to be modified. ▲

Hardware configurator (see Figure 3-18) comprises all settings of interfaces and hardware devices.

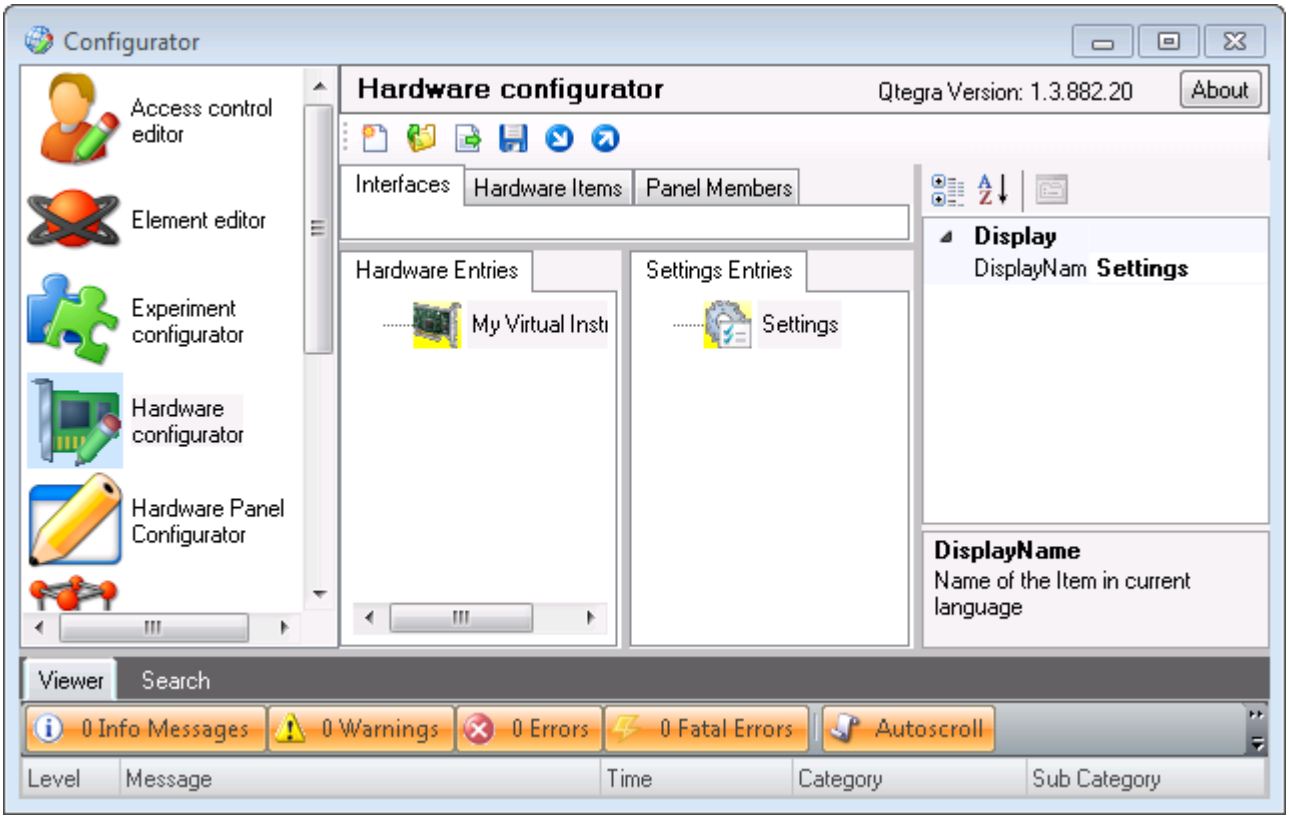


Figure 3-18. Layout Hardware configurator

The commands available in Hardware configurator are summarized in Table 3-4.

Table 3-4. Hardware configurator commands

Commands	Description
	To create a new Hardware configuration.
	To open Hardware configurations saved in the configurations data base in the file format *.imhwd.
	Import *.csv file.

Table 3-4. Hardware configurator commands

Commands	Description
	To save the current Hardware configuration.
	To import settings.
	To export settings.

❖ **To open Hardware configurator**

1. Click 

to open **Configurator**.

2. Click  **Hardware configurator**.

Hardware Panel Configurator

The **Hardware Panel Configurator** applet of the Configurator tool defines how the hardware panels of the devices or instrument sets are displayed.

Hardware Panel Configurator (see Figure 3-19) assigns graphical views or panels to Virtual Instruments and Hardware Items and aligns scripts to these.

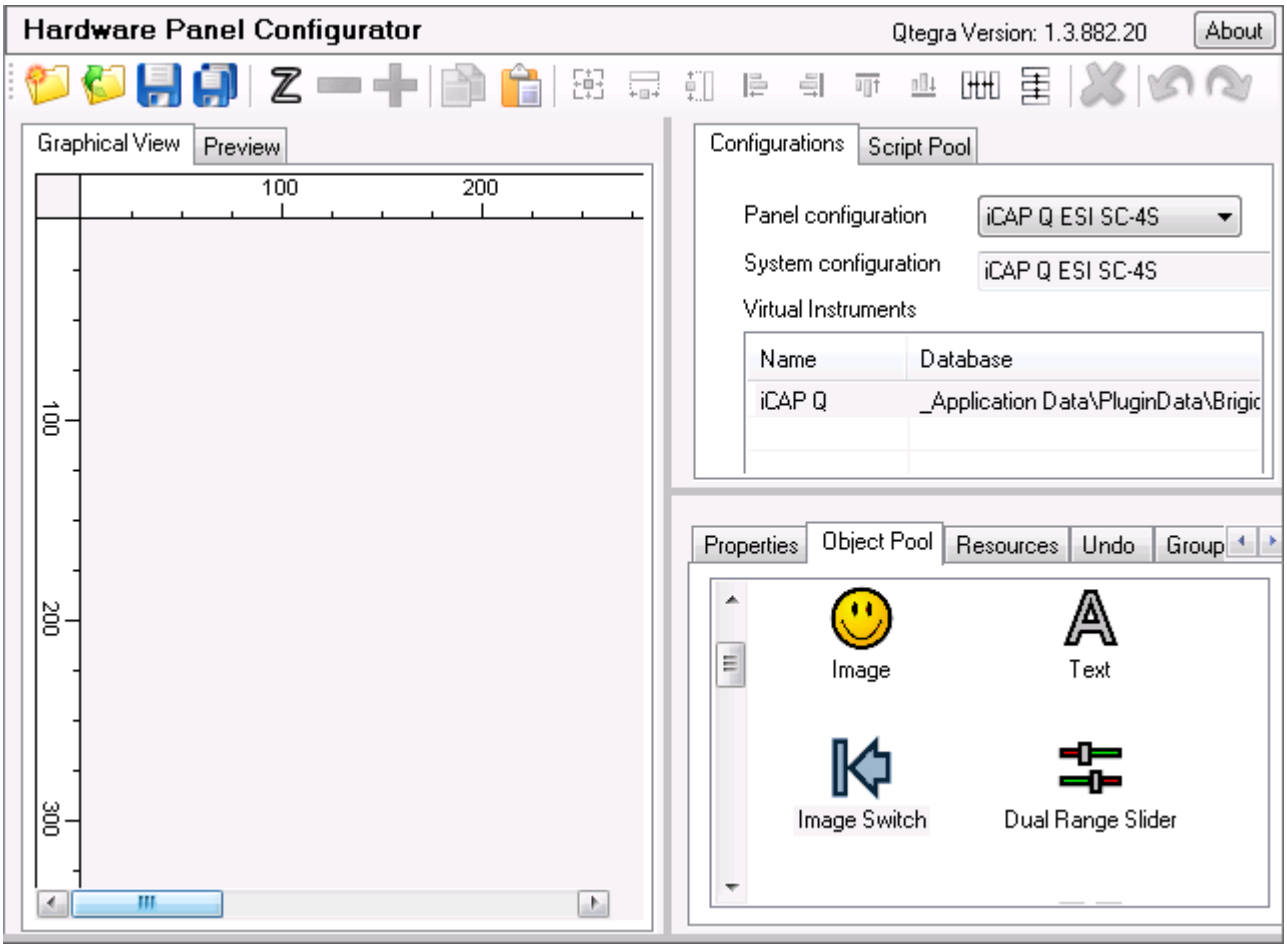


Figure 3-19. Layout Hardware Panel Configurator

The commands available in Hardware Panel Configurator are summarized in Table 3-5.

Table 3-5. Hardware Panel Configurator commands

Commands	Description
	To create a new Hardware Panel Configuration.
	To open a Hardware Panel Configurations saved in the configurations data base in the file format *.panel.

Table 3-5. Hardware Panel Configurator commands

Commands	Description
	To save the current hardware panel configuration.
	To save as the current hardware panel configuration.

❖ **To open Hardware Panel Configurator**

1. Click 

to open **Configurator**.

2. Click  **Hardware Panel Configurator**.

Molecule Editor

The **Molecule Editor** applet of the Configurator tool allows the Administrator and Manager to create molecules (or polyatomics) which are automatically added to the Molecules tab of the Method Parameter Analytes (see "Analytes" on page 6-15) and in Instrument Control (see "Analytes Tab" on page 4-6).

Molecule Editor, see Figure 3-20, shows the periodic table as well as the fields to enter elements and molecules.

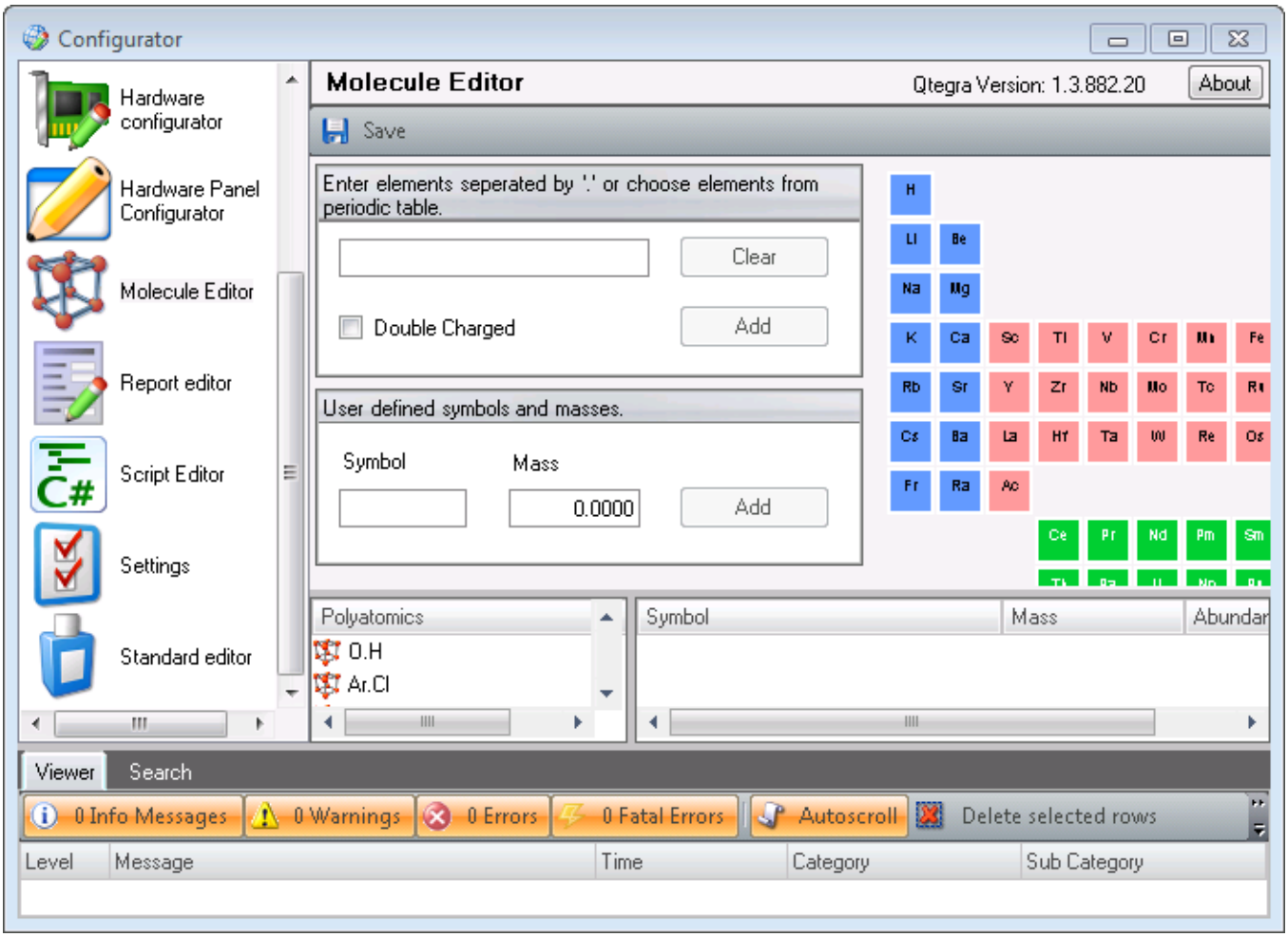


Figure 3-20. Layout Molecule Editor

Molecules and doubly charged ions created can subsequently be selected in Instrument Control and for acquisition in Experiment Editor. Creating molecules, often based on the matrix components expected in samples, can help the analyst visualize where interferences can occur and help correct for the interferences.

NOTICE Molecules are usually created by the Administrator or Manager. ▲

❖ **To open Molecule Editor**

1. Click 

to open **Configurator**.

2. Click  **Molecule Editor**.

❖ **To create molecules**

1. Click 

to open **Configurator**.

2. Click  **Molecule Editor**.

3. Click the elements in the periodic table to select the elements for the molecule to be created.
   Alternatively, type in the relevant symbols for the elements of the molecule, separated by a period <.>, see Figure 3-21.

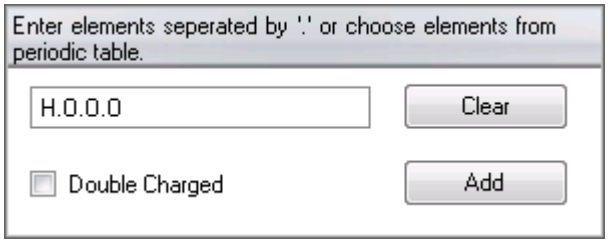


Figure 3-21. Elements entered for new molecule in Molecule Editor

4. If an element exists more than once in the molecule, click or enter the element the equivalent number of times.

5. If the molecule is doubly charged, select the **Double Charged** check box before you add the molecule to the list.

6. Click 

next to the check box **Double Charged** to add the molecules to the list **Polyatomics**.
   The distribution of ions in the newly created molecule and the

masses are displayed in the lower right panel, see Figure 3-22.

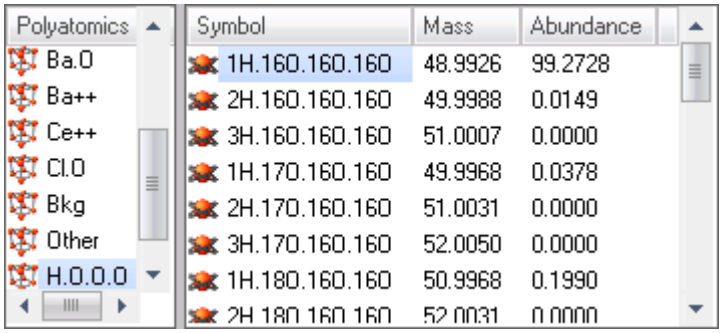


Figure 3-22. Polyatomics list in Molecule Editor

7. Click Clear before you enter the elements for another molecule.
8. For user-defined elements, enter **Symbol** and **Mass**, see Figure 3-23.

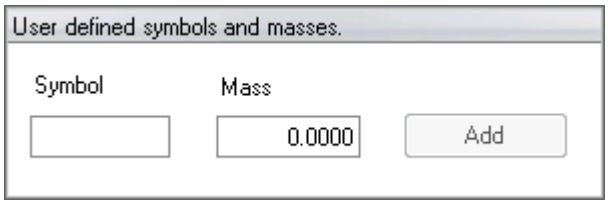


Figure 3-23. User-defined element in Molecule Editor

9. Click Add.
   The user-defined element is added to the **Polyatomics** list.
10. To delete a molecule of the **Polyatomics** list, right-click the molecule in the column **Polyatomics** and select Delete.
11. Click to save the changes in the database.

Report Editor

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

Report editor (see Figure 3-24) determines the layout of the reports.

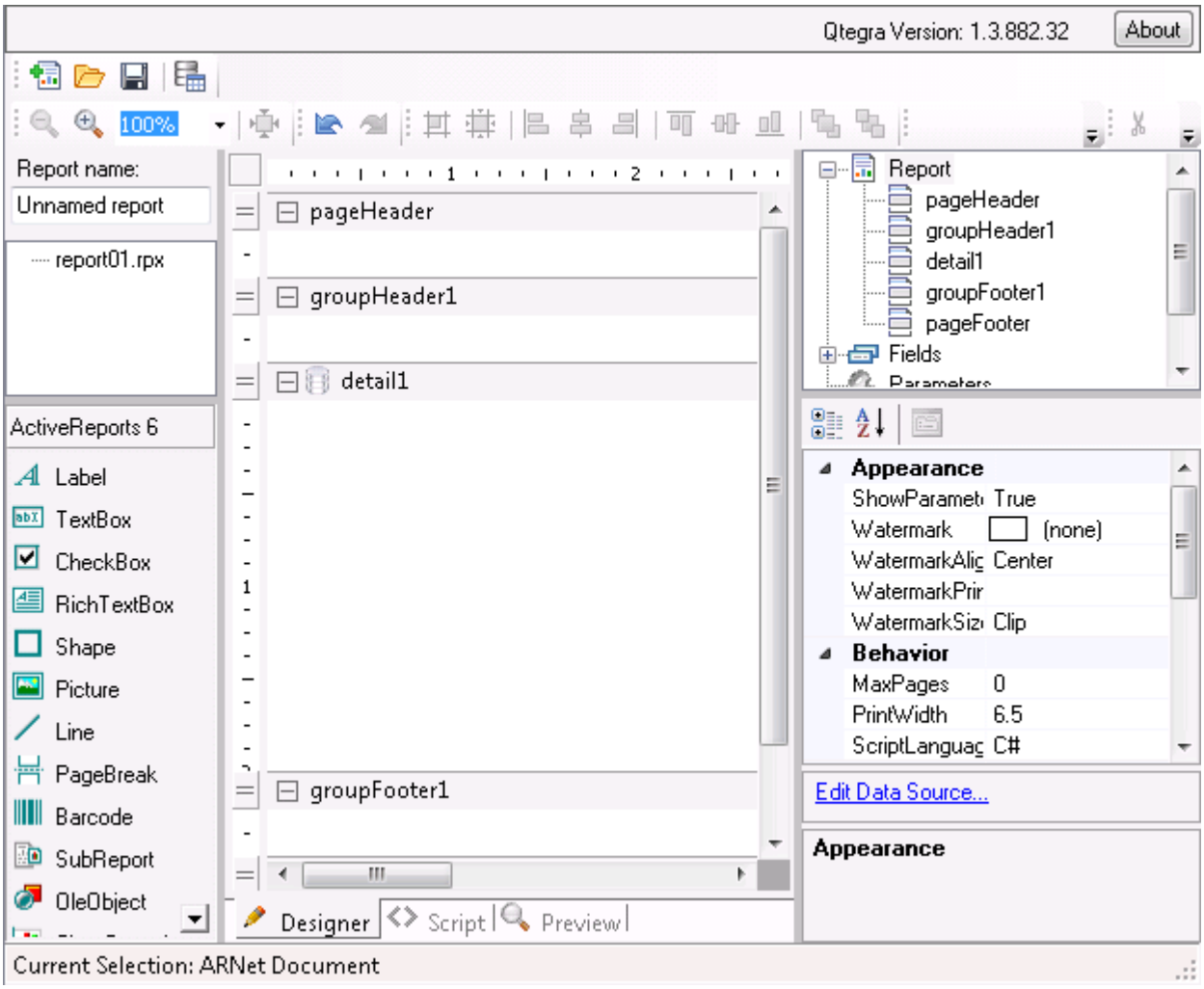


Figure 3-24. Layout Report editor

The commands available in Report editor are summarized in Table 3-6.

Table 3-6. Report editor commands

Commands	Description
	To create a new Report template.
	To open/load a Report in the file format *.imrep.

Table 3-6. Report editor commands

Commands	Description
	To save the current Report template.
	To load a Template from the XDML database.

❖ **To open Report editor**

1. Click 

to open **Configurator**.
2. Click  **Report editor**.

❖ **To create a new report template**

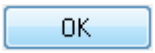
1. Click 

to open **Configurator**.
2. Click  **Report editor**.
3. Click  to create a new Report template.
4. Enter a **Report name**.
5. Configure the layout.
6. Click  to save the Report template.
The file is saved in the file format *.imrep.

❖ **To edit an existing report template**

1. Click 

to open **Configurator**.
2. Click  **Report editor**.
3. Click  and browse for the report file.
4. Select the report file you wish to edit.

5. Click 

to open the file.
6. Edit the file.
7. Click  to save the Report template.

Script Editor

The **Script Editor** applet of the Configurator tool allows you to create and compile C# scripts for virtual instruments.

Script Editor (see Figure 3-25) is designed to be used by persons experienced with C# scripts.

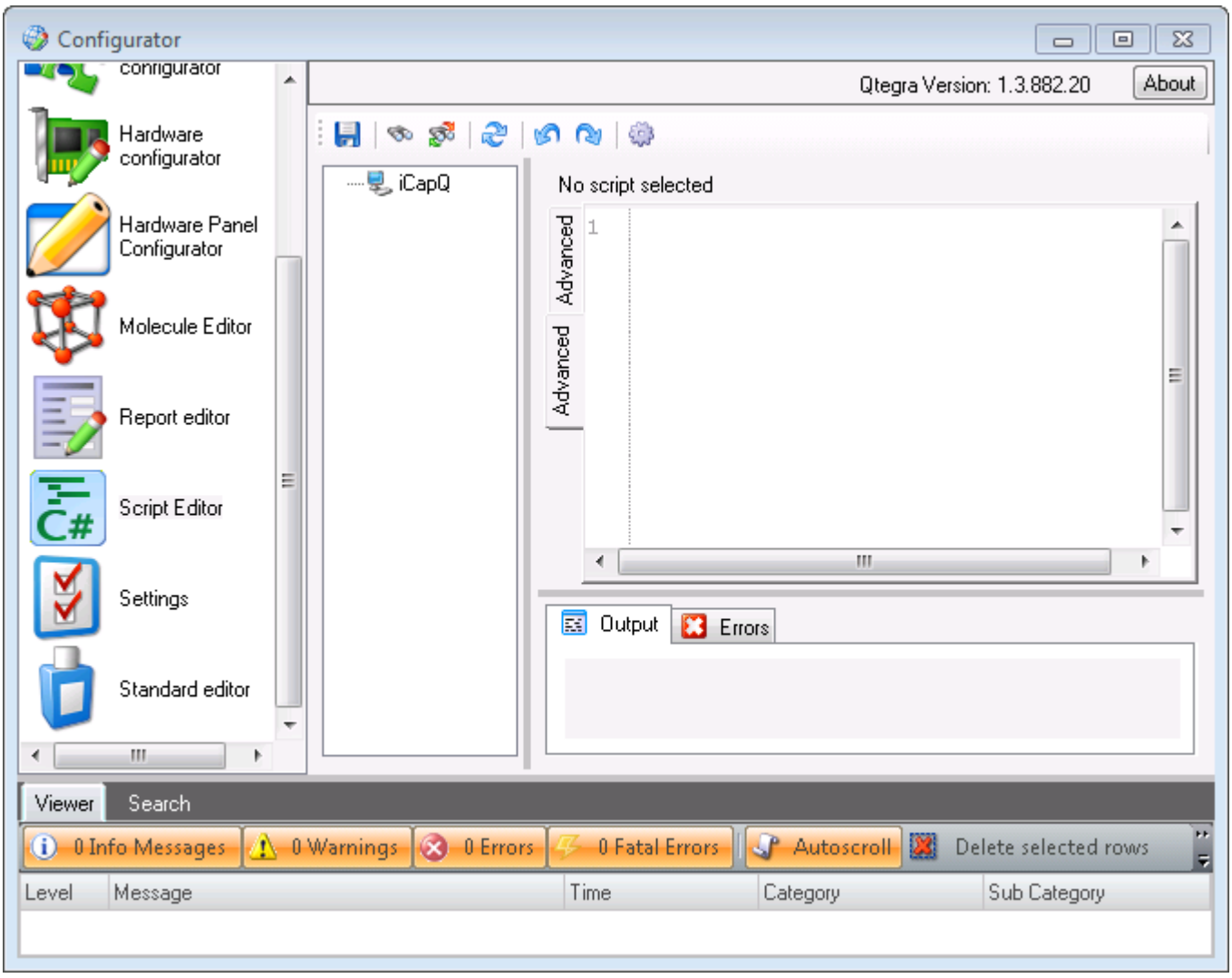


Figure 3-25. Layout Script Editor

❖ **To open Script Editor**

1. Click 

to open **Configurator**.

2. Click  **Script Editor**.

Settings

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

Settings (see Figure 3-26) gives access to the settings database (registry).

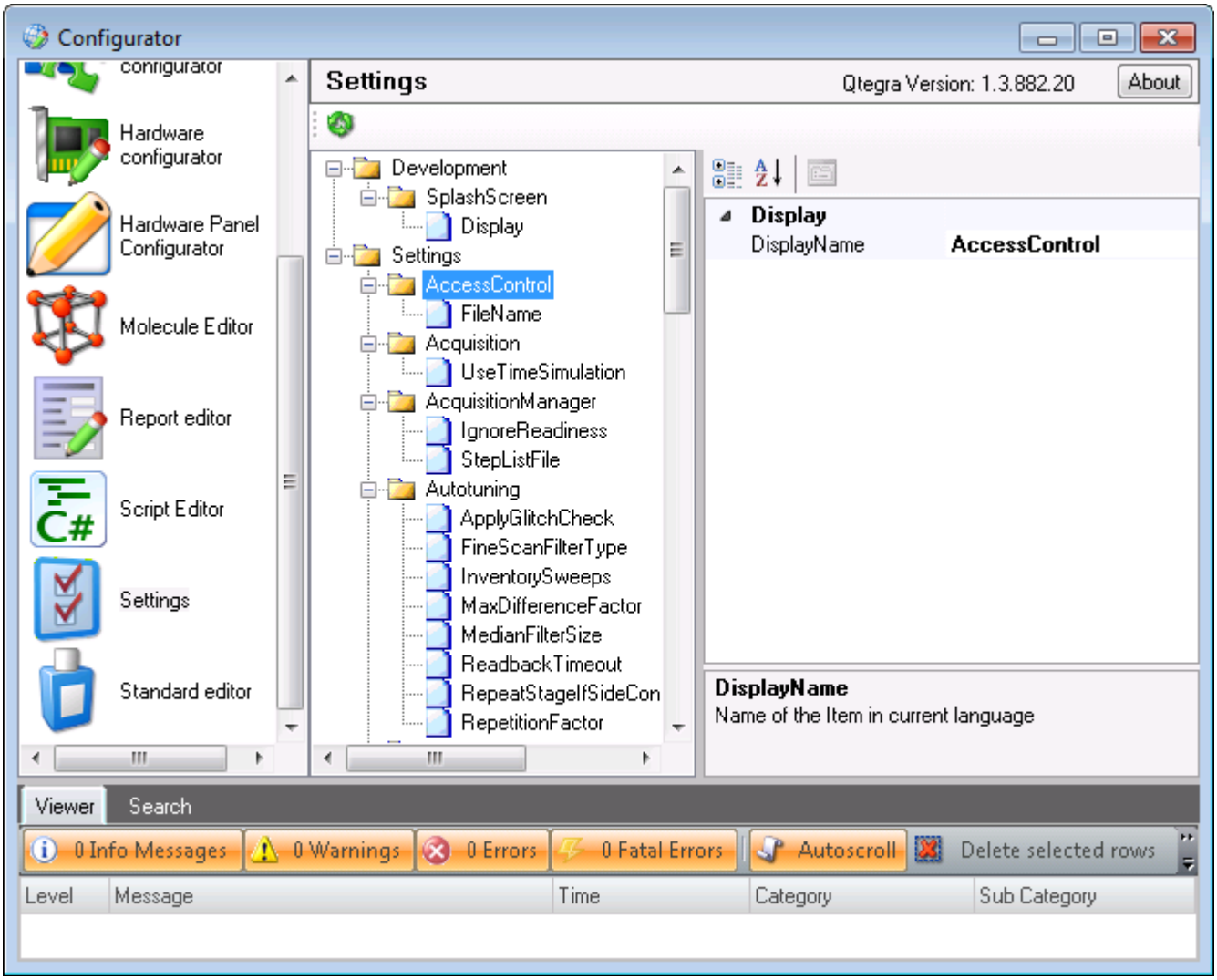


Figure 3-26. Layout Settings

❖ **To open Settings**

1. Click 

to open **Configurator**.

2. Click  **Settings**.

Standard Editor

The **Standard editor** 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.

Standard editor (see Figure 3-27) shows a list of standards on the left. On the right the associated elements and their concentration in the standard solution are displayed as well as the periodic table.

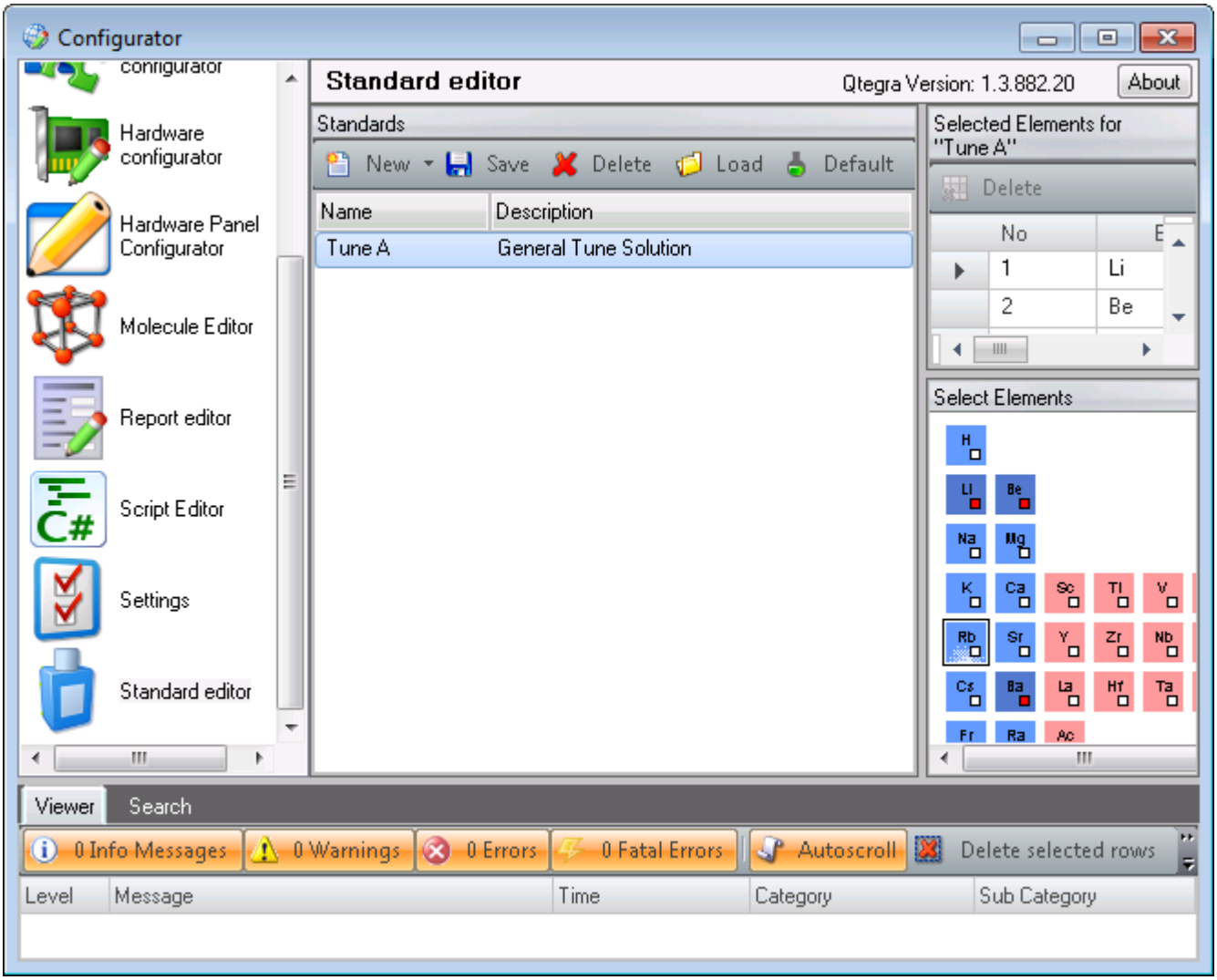


Figure 3-27. Layout Standard editor

The Standard editor commands are summarized in Table 3-7.

Table 3-7. Standard editor commands

Commands	Description
	To create a new Standard, Internal Standard or Isotope Dilution Standard.
	To delete the selected standard(s).
	To load all standards from the preset standard database.
	To save the standard files to the database.
	To edit the default concentration. The **Default Concentration** of the isotopes in the solutions is set to 10 ppm.

❖ **To open Standard editor**

1. Click 

to open **Configurator**.
2. Click  **Standard editor**.

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

1. Click 

to open **Configurator**.
2. Click  **Standard editor**.
3. Click  .
All standards are loaded from the database.

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

1. Click 

to open **Configurator**.
2. Click  **Standard editor**.

3. Change or add standards to your needs.

4. Click  .
   The standards are saved to the database.

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

1. Click 

to open **Configurator**.

2. Click  **Standard editor**.

3. In the list, click the standard you wish to delete.

4. Click  .
   The **Delete Standard** dialog opens, see Figure 3-28.

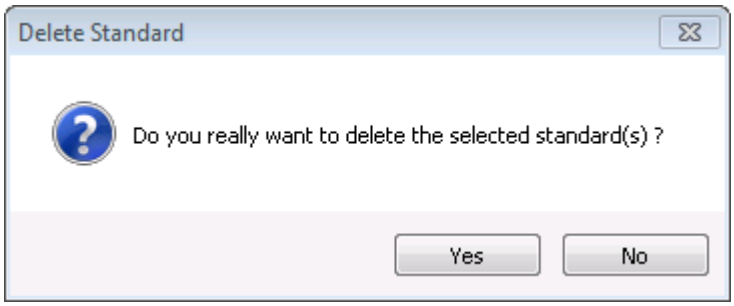
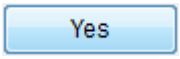


Figure 3-28. Delete Standard dialog

5. Click 

   The standard is deleted from the database.

6. Click  to save the changes.

Changing the Default Concentration

You can change value and unit of the default concentration for the elements that are newly added to a standard in the **Standard editor** applet of the Configurator tool.

❖ **To change the default concentration**

1. Click 

to open **Configurator**.

2. Click  **Standard editor**.

3. Click  to open the **Set Default Concentration** window, see Figure 3-29.

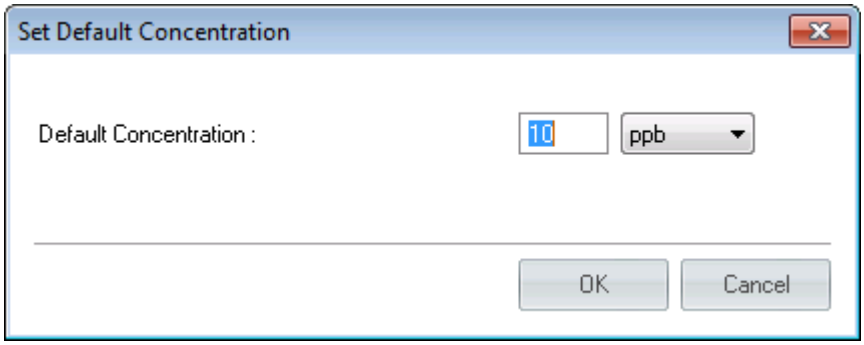
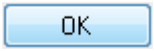


Figure 3-29. Set Default Concentration window

4. Change the default concentration and unit as required.

5. Click  to exit the window.

The new default concentration will be used when adding, creating or editing standard files.

6. Click  to save the changes.

Creating a New Standard

Database standards are created in the **Standard editor** applet of the Configurator tool.

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.

❖ **To create a new standard file**

1. Click 

to open **Configurator**.

2. Click **Standard editor**.

3. Click New.
   The drop-down menu opens, see Figure 3-30.

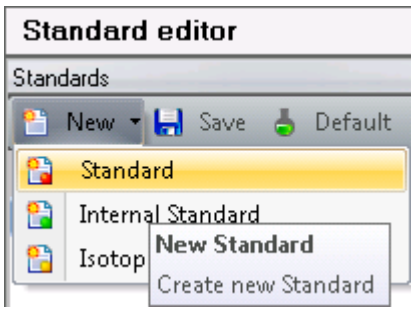


Figure 3-30. Creating a new standard

4. Click **Standard** to open the **Add New Standard** window.

5. Click to check the default concentration.
   Change if appropriate as described in "Changing the Default Concentration" on page 3-37.

6. Enter a **Standard Name** and a **Standard Description**.

7. Click OK to add the file.
   The new standard is added to the list on the left. An empty page opens containing the table columns **No**, **Element**, **Concentration** and **Unit** and the periodic table of elements with all available isotope information.

8. Add elements to the standard table by clicking on the element in the periodic table.
   The default isotope of the element is added to the table. Concentration and Unit are added according to the default concentration.

9. To remove the element, click the respective element in the periodic table again.

10. Repeat until all elements have been added.

11. Click to add the standard file to the database.

Creating a New Internal Standard

Database internal standards are created in the **Standard editor** applet of the Configurator tool.

Internal standards 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.

❖ **To create a new internal standard file**

1. Click 

to open **Configurator**.

2. Click  **Standard editor**.

3. Click 

.
The drop-down menu opens, see Figure 3-31.

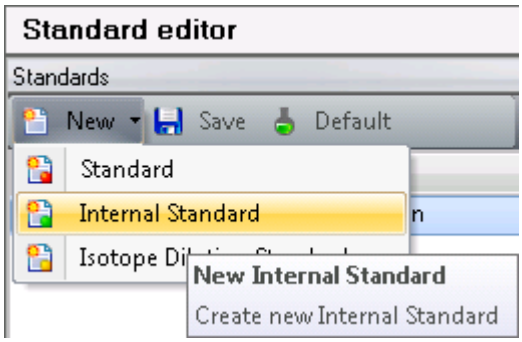
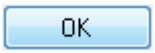


Figure 3-31. Creating a new standard

4. Click  **Internal Standard** to open the **Add New Standard** window.

5. Enter the **Standard Name** and a **Standard Description**.

6. Click 

to add the file.
The new internal standard is added to the list on the left. An empty page opens containing the table columns **No**, **Isotope**, **Concentration** and **Unit**, and the periodic table of elements with all available isotope information.

7. Add the isotope to the table by clicking on the element in the periodic table.
   The most abundant isotope is added to the table.
8. To add more than one isotope of the element, right-click the element to open the list of isotopes and select the check boxes of the isotopes you wish to add.
9. Click anywhere next to the table to confirm the selection.
10. To remove the isotope, click the respective element in the periodic table again or right-click and deselect the check box.
11. Repeat until all isotopes are added.
12. Click  to add the internal standard file to the database.

Creating a New Isotope Dilution Standard

Database isotope dilution standards are created in the **Standard editor** applet of the Configurator tool.

Isotope dilution is used for quantification. For example, an isotope dilution standard with enriched isotopes and a certified isotopic abundance can be added.

❖ **To create a new isotope dilution standard file**

1. Click 

to open **Configurator**.
2. Click  **Standard editor**.
3. Click 

.
   The drop-down menu opens, see Figure 3-32.

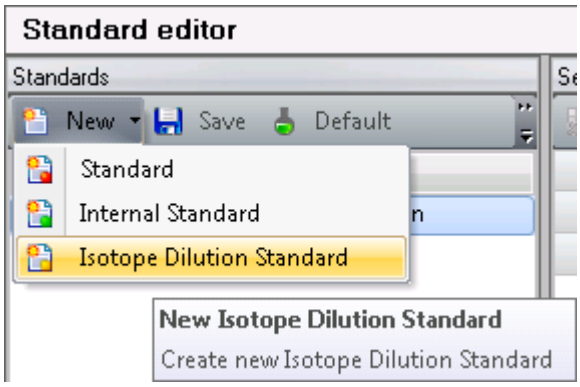
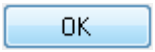


Figure 3-32. Creating a new standard

4. Click  **Isotope Dilution Standard** to open the **Add New Standard** window.
5. Enter the **Standard Name** and a **Standard Description**.
6. Click  to add the file.
   The new isotope dilution standard is added to the list on the left. An empty page opens containing the table columns **No**, **Element**, **Concentration**, **Unit**, **Isotope 1**, **Isotope 2**, **Abundance 1**, **Abundance 2** and **Atomic Weight**, and the periodic table of elements with all available isotope information.
7. Click an element in the periodic table to add it to the table.
8. Select the isotope of interest from the drop-down list of column **Isotope 1**.
9. Select the isotope of interest from the drop-down list of column **Isotope 2**.
10. To remove the element, click the respective element in the periodic table again.
11. Repeat for all elements you wish to add to or remove from the standard file.
12. Click  to add the isotope dilution standard file to the database.

Chapter 4 Instrument Control

The Instrument Control tool is used to perform instrument calibrations and to edit general instrument controls such as tune settings and measurement modes or change stabilization times.

Contents

- User Interface of the Instrument Control Tool
- Data View Region
- Experiment Configuration Ribbon Tab
- The iCAP Q Ribbon Tab
- Window Ribbon Tab
- Control Panel
- Status Panel
- Log View Region

❖ **To open Instrument Control**

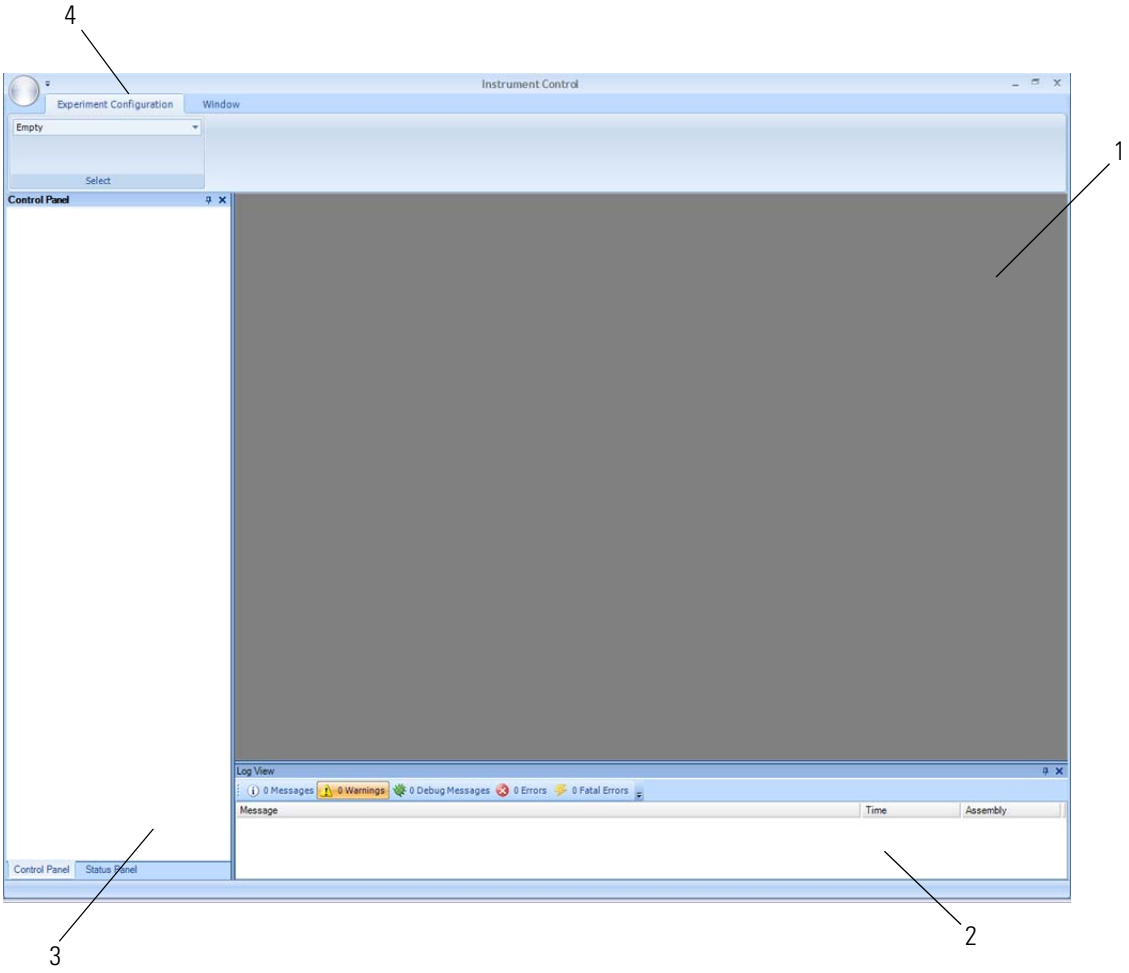
1. Click 

to open **Instrument Control**.

User Interface of the Instrument Control Tool

The Instrument Control tool gives quick access to system controls and log messages for the instrument and peripherals loaded with the Configuration.

The Instrument Control tool (see Figure 4-1) shows four regions.



Labeled Components: 1=data view region, 2=Log View region, 3=Control and Status Panel region, 4=ribbon tabs

Figure 4-1. User interface composition of Instrument Control

The data view region (**1** in Figure 4-1) displays tabs with instrument parameters and data being acquired in real time according to the Configuration loaded.

The **Log View** (**2** in Figure 4-1) displays the log files, such as messages, errors and warnings.

The **Control Panel** and **Status Panel** (**3** in Figure 4-1) display the controls of the iCAP Q instrument and the status of the scripts of the Configuration loaded.

The ribbon tabs (**4** in Figure 4-1) are displayed in accordance with the Configuration loaded. By default the **Experiment Configuration** and the **Window** tab are displayed. Additional tabs are added for each instrument.

❖ **To maximize and minimize the ribbon**

1. Click 

to open **Instrument Control**.
2. Select the **Window** ribbon, for example.
3. Right-click anywhere in the ribbon to display the context menu, see Figure 4-2.

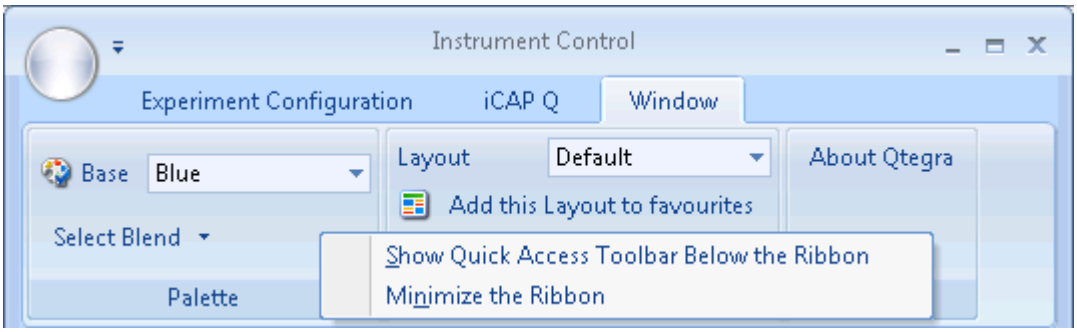


Figure 4-2. Window ribbon of Instrument Control tool

4. Select **Minimize the Ribbon**.
   A check mark is shown before **Minimize the Ribbon** and the ribbon is minimized.

Data View Region

The data view region of Instrument Control displays all configurable data of the iCAP Q system and of all configured peripherals. The different instrument data is provided on tabbed pages and can be accessed by clicking on the appropriate tab.

By default, the data view region is empty when no configuration is loaded. When a configuration is loaded, this pane displays the settings available for the selected instrument, for example, autosampler rack information, see Figure 4-3.

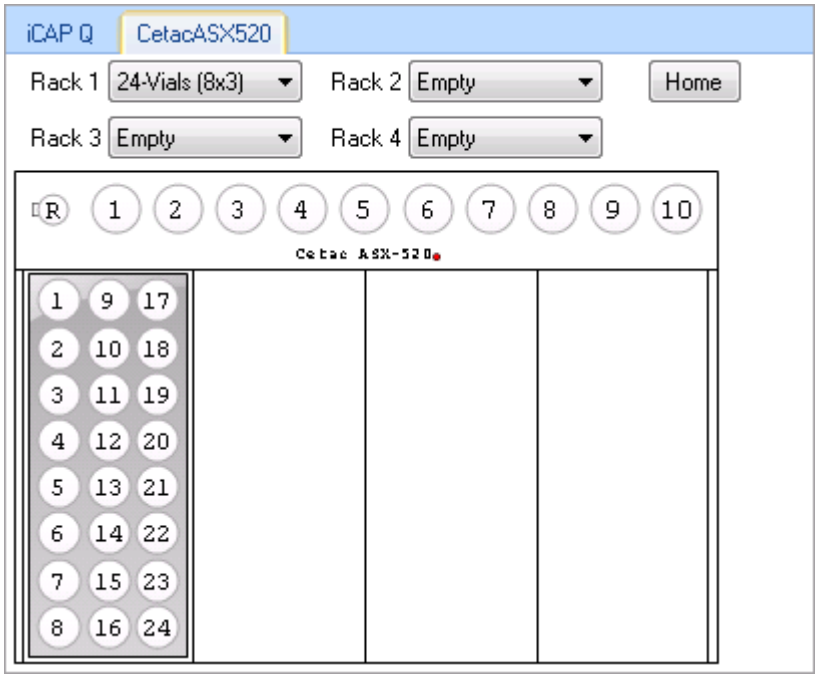


Figure 4-3. Example of data view region in Instrument Control

❖ **To display the data view region of an instrument component**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the tab you wish to display.

Instrument Settings in the Data View Region

In the data view region of Instrument Control, the **iCAP Q** tab offers two main views on tabbed pages, the **Analytes** and the **Data Display** page, see Figure 4-4.

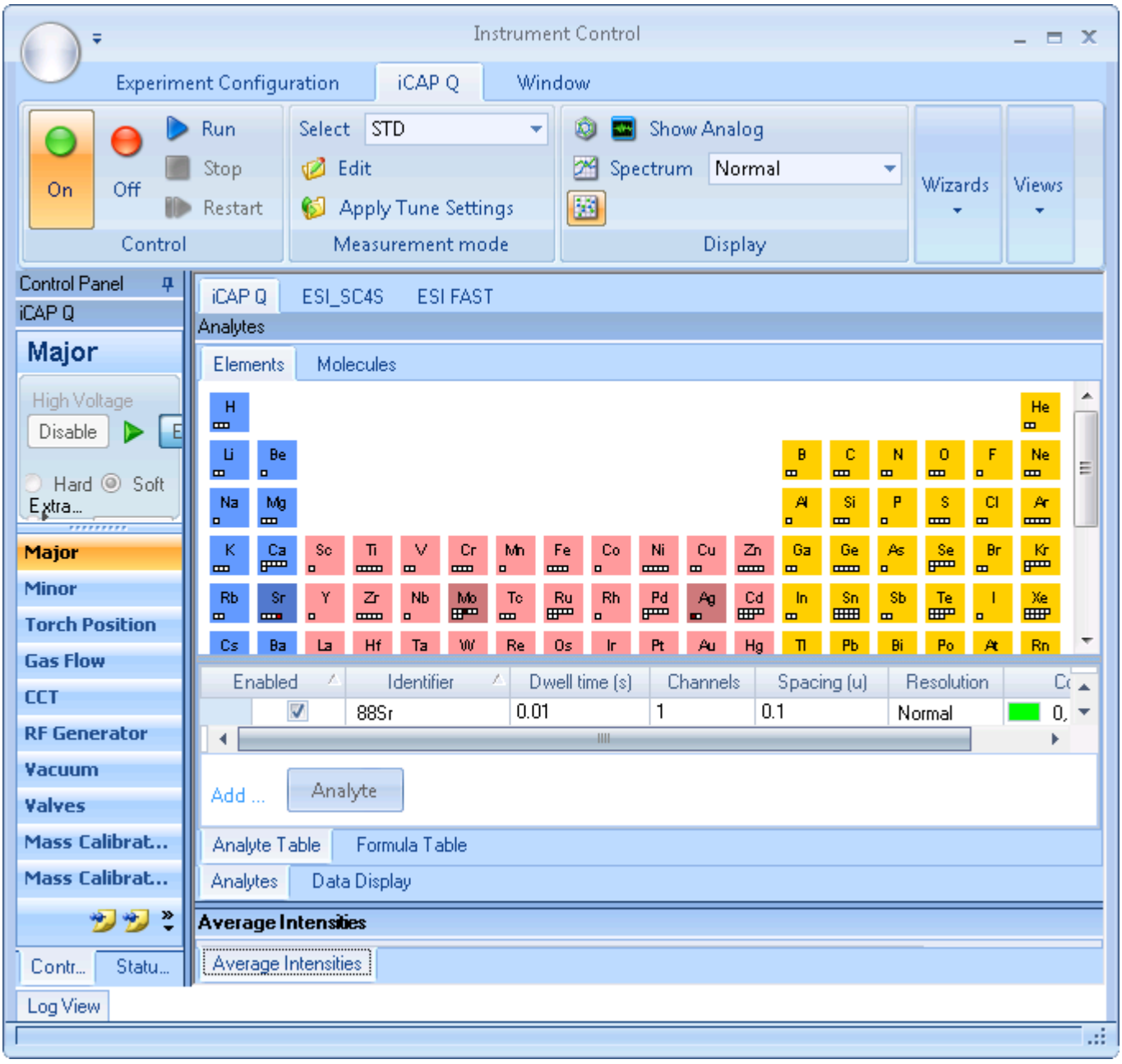


Figure 4-4. Instrument Control with periodic table in the data view region

❖ **To display the iCAP Q settings view region**

1. Click 

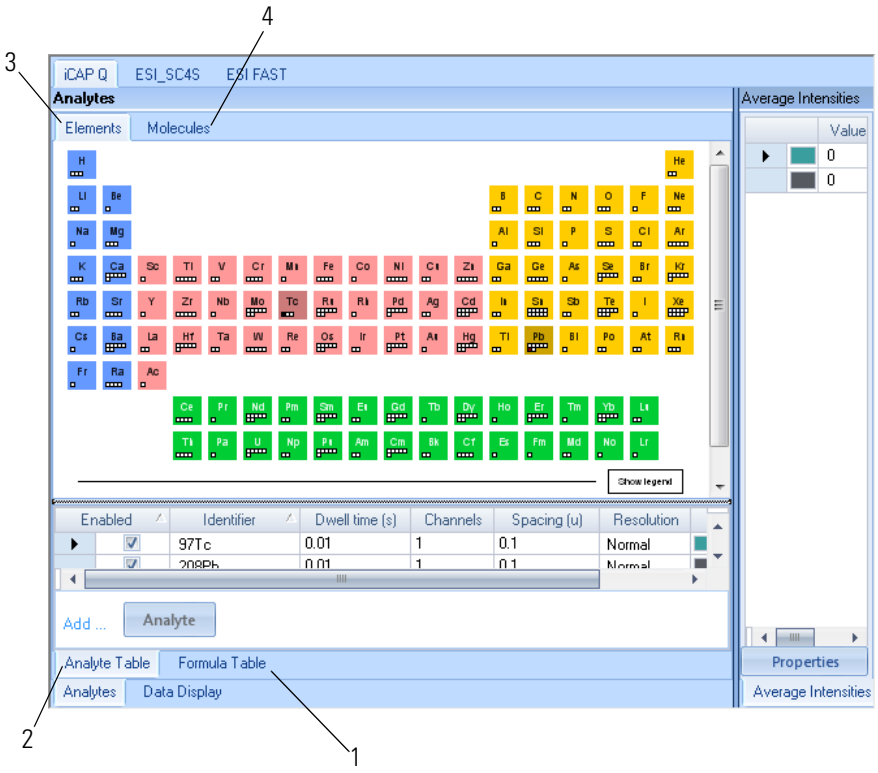
to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The data view region **iCAP Q** is displayed and the ribbon **iCAP Q** is activated.

Analytes Tab

The **Analytes** view in the **iCAP Q** tab of the data view region in Instrument Control is divided into an upper and a lower part.

The upper part shows the periodic table on the tabbed page **Elements**, see Figure 4-5, and Polyatomics on the tabbed page **Molecules**. The lower part shows the **Analyte Table** and **Formula Table** on tabbed pages. Each can be edited as required.



Labeled Components: 1=tab Formula Table, 2=tab Analyte Table, 3=tab Elements, 4=tab Molecules

Figure 4-5. iCAP Q tab Analytes showing Elements page

❖ To open the Analytes view

1. Click to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The data view region **iCAP Q** is displayed and the ribbon **iCAP Q** is activated.

3. In the data view region, click the **Analytes** tab.
   The upper tabbed pages **Elements** (**3** in Figure 4-5) and **Molecules** (**4** in Figure 4-5) and lower tabbed pages **Analyte Table** (**2** in Figure 4-5) and **Formula Table** (**1** in Figure 4-5) are now accessible.

Data Display Tab

The **Data Display** view in the **iCAP Q** tab of the data view region in Instrument Control, see Figure 4-6, presents the chromatogram and the spectrum of data. Toggling between the views is possible.

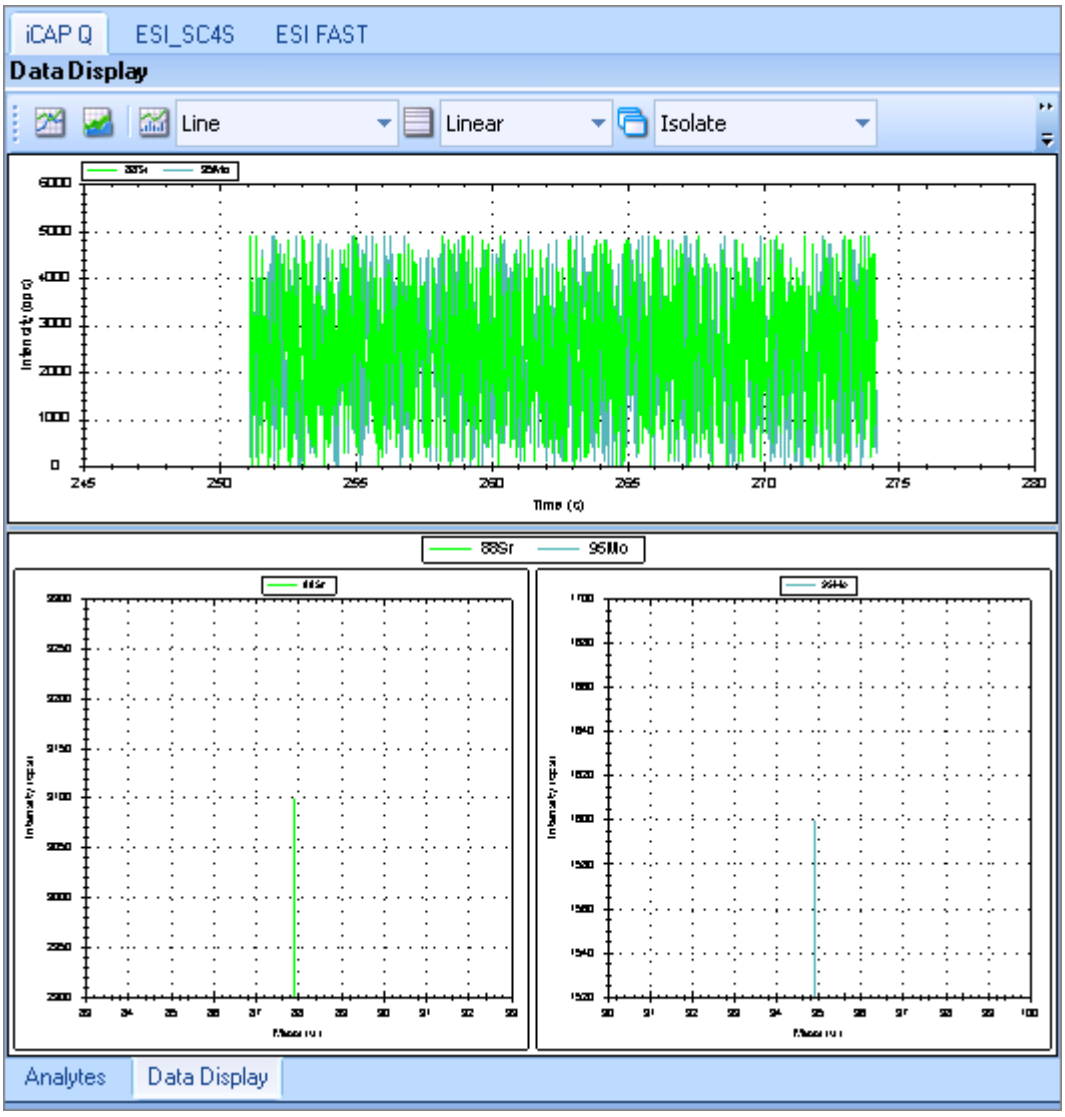


Figure 4-6. iCAP Q tab Data Display showing spectrum and chromatogram

The graphical presentation can be adjusted to your needs, see Table 4-1.

Table 4-1. Data display options

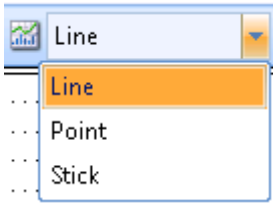
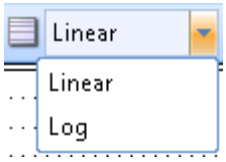
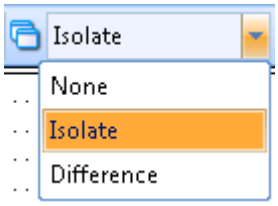
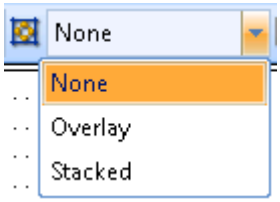
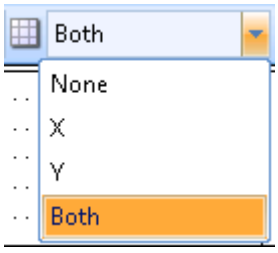
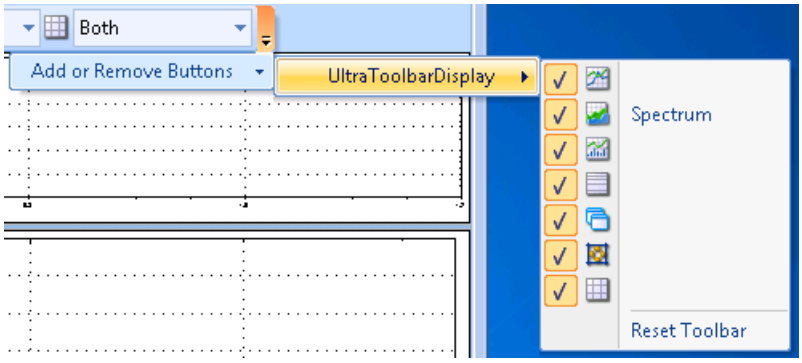
Icon	Description
	Button to toggle the chromatogram window.
	Button to toggle the spectrum window.
	Options for the presentation of data series display within spectrum window.
	Options for the scale of data series display in spectrum window.
	Options for the segmentation strategy of data series in spectrum window.
	Options for the stacking strategy of data series in chromatogram window.

Table 4-1. Data display options

Icon	Description
	Options for the type of grid for data series display.
	Toolbar Options to add or remove buttons.

NOTICE The ribbon group "Display Group" on page 4-21 is dedicated to the data view region. ▲

❖ To open the Data Display tab

1. Click to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
   The data view region **iCAP Q** is displayed and the ribbon **iCAP Q** is activated.
3. In the data view region, click the **Data Display** tab.

Peripheral Settings in Data View Region

Peripherals such as the ESI SC-4S autosampler are shown in their own tabs, see Figure 4-7. The settings can be edited here.

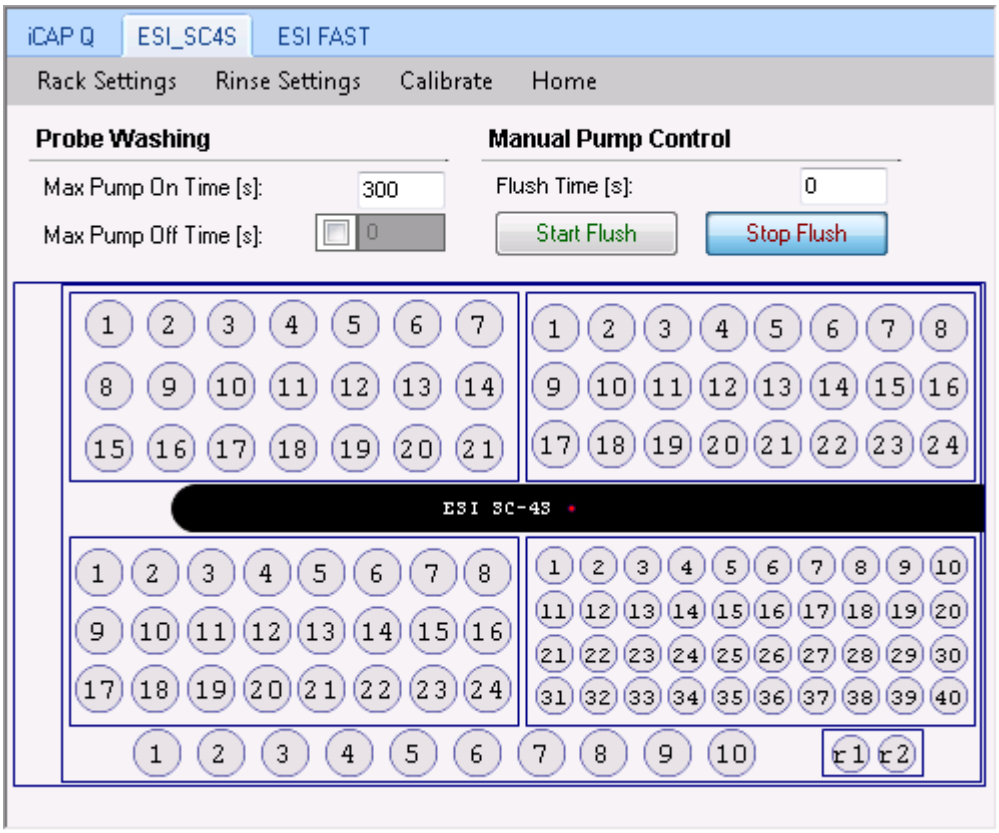


Figure 4-7. Instrument Control with integrated autosampler tab showing

❖ **To open the peripheral tab**

1. Click to open **Instrument Control**.
2. In the tab **Experiment Configuration**, load your configuration with a peripheral, for example, an autosampler.
3. In the data view region, select the tab of the peripheral, for example, **ESI_SC4S** for the integrated autosampler.

Experiment Configuration Ribbon Tab

In the ribbon tab **Experiment Configuration** of the Instrument Control tool, see Figure 4-8, you select a Configuration created in the Configurator tool to display the associated instrument controls.

Figure 4-8. Experiment Configuration tab

❖ **To load a Configuration**

1. Click 

to open **Instrument Control**.
2. Select the **Experiment Configuration** ribbon tab.
3. In the group **Select**, click  to display the list of available Configurations.
4. Select the Configuration of your iCAP Q system.
   The controls of the Configuration for your instrument are loaded into Instrument Control.

The iCAP Q Ribbon Tab

The Instrument Control tool opens the **iCAP Q** ribbon tab (see Figure 4-9) if a Configuration is loaded that includes the iCAP Q instrument.

Figure 4-9. The iCAP Q tab

❖ **To open the iCAP Q ribbon**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

Control Group

The Control group of the **iCAP Q** ribbon tab in Instrument Control, see Figure 4-10, offers basic commands to switch the iCAP Q system on and off and to start and stop the scanning of the instrument. The results are displayed in real time.

Figure 4-10. Control group of the iCAP Q ribbon tab

The buttons to control the iCAP Q instrument are summarized in the **Control** group of the **iCAP Q** ribbon tab, see Table 4-2.

Table 4-2. Control buttons for iCAP Q instrument

Icon	Meaning	Description
	On	Switches the instrument on.
	Off	Switches the instrument off.
	Run	Starts an acquisition in the real-time display.
	Stop	Stops the real-time display acquisition.
	Restart	Restarts the real-time display acquisition.

NOTICE To start the plasma, see also Experiment Editor chapter "Getting Ready" on page 5-7. ▲

❖ To start the plasma

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. Click  in the group **Control** of the **iCAP Q** tab.
The confirmation window opens, see Figure 4-11.

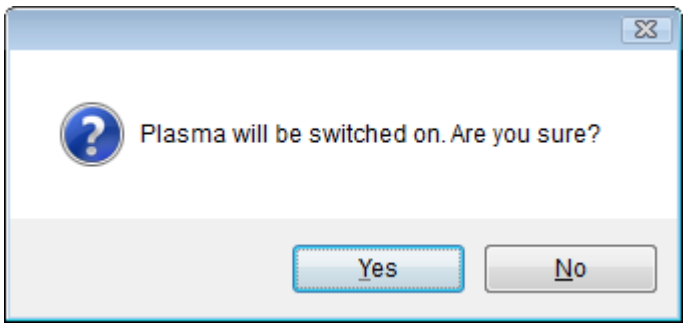
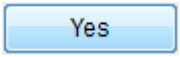


Figure 4-11. Confirm switching on plasma

4. Click 

.
The plasma is switched on.

❖ **To start data acquisition in the real-time display**

1. Click to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.
3. Click  in the group **Control** of the **iCAP Q** tab.
   The acquisition is started.

❖ **To stop data acquisition in the real-time display**

1. Click to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.
3. Click  in the group **Control** of the **iCAP Q** tab.
   The acquisition is stopped.

❖ **To restart data acquisition in the real-time display**

1. Click to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.
3. Click  in the group **Control** of the **iCAP Q** tab.
   The acquisition is restarted.

❖ **To switch off the plasma**

1. Click to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. Click  in the group **Control** of the **iCAP Q** tab.
   The confirmation window opens, see Figure 4-12.

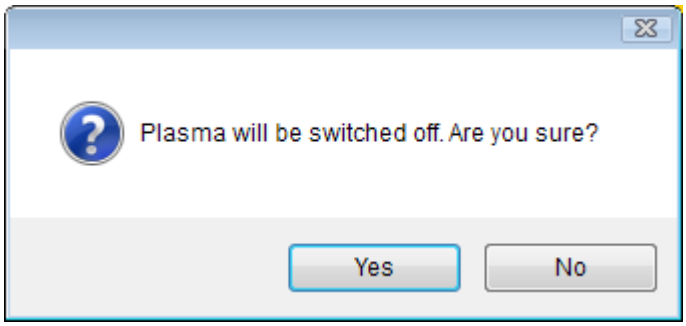
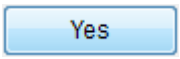


Figure 4-12. Confirm switching off plasma

4. Click  .
   The plasma is switched off.

Measurement Mode Group

Measurement modes are managed in the **Measurement mode** group of the **iCAP Q** ribbon tab in Instrument Control, see Figure 4-13. KED/KEDS and CCT/CCTS are the modes of operation that can be employed for a quadrupole iCAP Q instrument fitted with a collision/reaction cell (QCell).

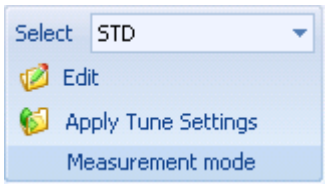


Figure 4-13. Measurement mode group of the iCAP Q ribbon

The iCAP Q Measurement modes pre-configured for samples with potentially high matrix load are:

- STD - standard mode, the mode of operation where the cell is not pressurized
- KED - collision cell mode with kinetic energy discrimination and
- CCT - reaction cell mode

Additionally, these modes are made available in Sensitivity Mode for samples without high matrix load.

The buttons of the **Measurement mode** group of the **iCAP Q** ribbon tab are summarized in Table 4-3.

Table 4-3. Buttons of Measurement mode group

Item	Settings	Description
Select	CCT	The CCT measurement mode pressurizes the cell with gas which may lead to a chemical reaction of the generated ions.
	KED	The KED measurement mode pressurizes the cell with gas and applies an energy discrimination barrier.
	STD	The STD measurement mode is the standard mode of operation (and does not pressurize the cell).
	CCTS	CCT Sensitivity Mode.
	KEDS	KED Sensitivity Mode.
	STDS	STD Sensitivity Mode.
	Edit	Displays Measurement Mode settings in the data view region. Measurement Mode settings can be viewed and edited in the data view region.
	Apply Tune Settings	Saves tune settings modified in the Control Panel to the current measurement mode.

❖ **To load a Measurement mode into Instrument Control**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the group **Measurement mode**, click  next to **Select** and select a mode from the drop-down menu.
The settings last saved for this Measurement mode are loaded into Instrument Control.

Change Tune Settings of a Measurement Mode

All tune settings can be adjusted to your needs in Instrument Control. See also "Control Panel" on page 4-117.

❖ **To change the Tune Settings of a Measurement mode**

1. Click 

to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.
3. In the group **Measurement mode**, click  next to **Select** and select a mode you wish to change from the drop-down menu.
The settings last saved for this Measurement mode are loaded into Instrument Control.
4. Adjust the settings of the Control Panel as needed.
5. Click  **Apply Tune settings** to store the current settings to the selected Measurement mode.

Editing a Measurement Mode

In the **Measurement mode** group of the **iCAP Q** ribbon in Instrument Control, the button **Edit** opens the new tab **Measurement Modes** in the data view region, see Figure 4-14. Here, new measurement modes

can be changed, created or deleted. The newly created Measurement modes are based on the pre-configured Measurement modes and can be modified to suit the needs of your application.

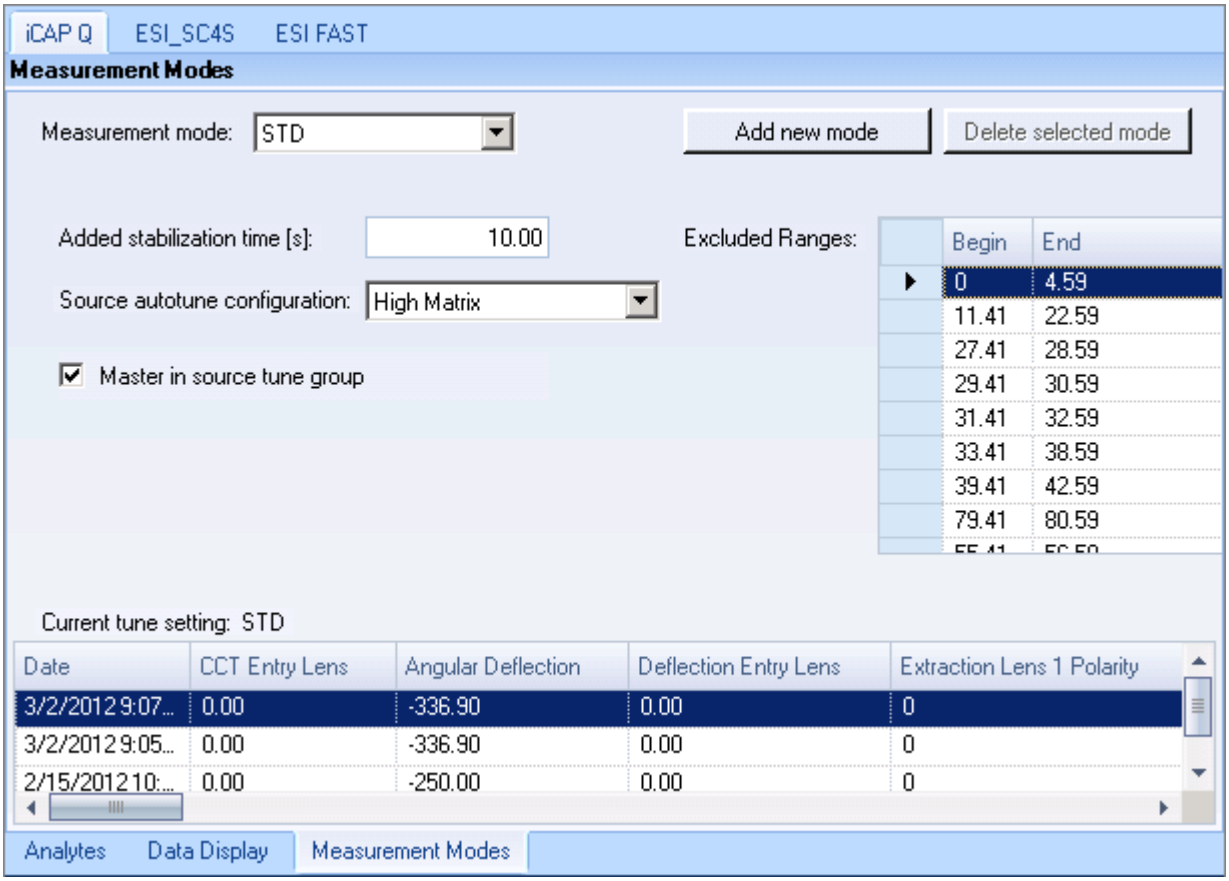


Figure 4-14. Edit Measurement mode in data view region

The drop-down list **Measurement mode** lists all modes defined. For each Measurement mode you can define the **Added stabilization time [s]**, a delay time that is used when switching from one mode to another within an analysis. The table **Excluded Ranges** shows the **Begin** and **End** range for each excluded range. The excluded ranges refer to protected zones of the mass spectrum which are not scanned in a survey run.

The table **Current tune setting** lists a history of tune settings defined for this Measurement mode, according to the date they were created.

All changes are automatically applied to the selected mode in the Edit view of the data view region, no extra saving is necessary. The changes have no effect on the currently loaded settings.

❖ **To open Edit mode for a Measurement mode**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. In the group **Measurement mode**, click **Edit**.
   A new tab **Measurement Modes** opens in the data view region.

❖ **To edit a Measurement mode in the Edit mode**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. In the group **Measurement mode**, click **Edit**.
   A new tab **Measurement Modes** opens in the data view region.

4. Select the mode you wish to edit from the drop-down list **Measurement mode** in the new tab **Measurement Modes** in the data view region.

5. Change the values for **Added stabilization time** as appropriate.
   The changes are automatically applied to the measurement mode selected. The changes have no effect on the currently loaded settings.

6. Change the values for **Excluded Ranges** as appropriate.
   The changes are automatically applied to the measurement mode selected. The changes have no effect on the currently loaded settings.

7. Select the **Source autotune configuration** from the drop-down menu, see Figure 4-15.

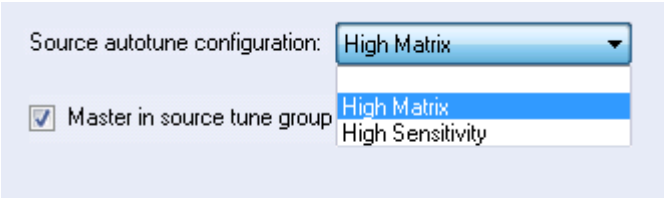


Figure 4-15. Source autotune settings

NOTICE The Source autotune configuration available is mainly dependent on the hardware adopted for your iCAP Q system. ▲

8. Select the check box **Master in source tune group** to use these settings for the selected source autotune configuration.
   This check box is by default selected for STD and STDS.

❖ **To add a new Measurement mode in the Edit mode**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the group **Measurement mode**, click  **Edit**.
A new tab **Measurement Modes** opens in the data view region.

4. Click 

.
The **Add Measurement Mode** dialog opens, see Figure 4-16.

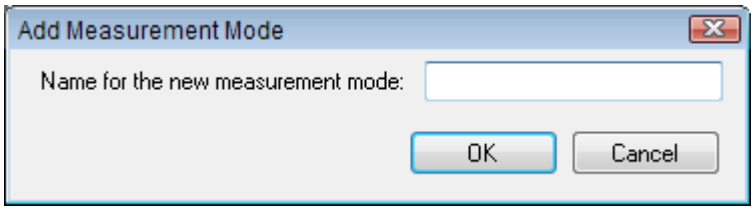


Figure 4-16. Add Measurement Mode dialog

5. Enter a **Name for the new measurement mode**.

6. Click 

.
The new measurement mode is added to the list.

❖ **To delete a new Measurement mode in the Edit mode**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the group **Measurement mode**, click  **Edit**.
A new tab **Measurement Modes** opens in the data view region.

4. Select the mode you wish to delete from the drop-down list **Measurement mode** in the new tab **Measurement Modes** in the data view region. Default Measurement modes cannot be deleted.

5. Click Delete selected mode.
   The **Delete measurement mode** dialog opens, see Figure 4-17.

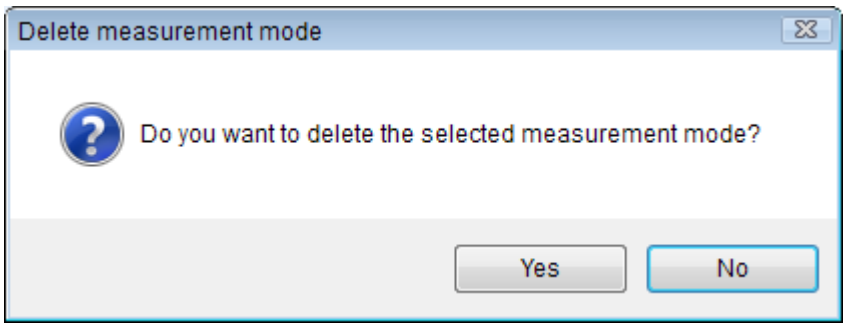


Figure 4-17. Delete measurement mode dialog

6. Click Yes.
   The selected measurement mode is deleted from the list.

❖ **To close the Edit mode**

1. Click Instrument Control to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.
3. In the group **Measurement mode**, click Edit.
   The tab **Measurement Modes** in the data view region closes.

Display Group

The **Display** group of the **iCAP Q** ribbon tab in Instrument Control, see Figure 4-18, allows you to select different views for the real-time display data in both the Data Display tab and the Average Intensities view of the data view region.

Figure 4-18. Display group of the iCAP Q ribbon

The buttons of the **Display** group are summarized in Table 4-4. They take effect in all modes.

Table 4-4. Buttons of Display group

Item	Meaning	Description
	Calibrated	The real-time display analytes are cross calibrated. These are the analytes which are selected in the Analyte View and which are shown in both the graphic and tabulated RTDs. Analytes are acquired in the appropriate detector mode depending on the absolute count rate for the respective analyte signal. The calibrated intensity is shown in cps.
	Analog	The ion counting section of the detector is switched off and real-time display analytes are acquired with the analog section of the detector only.
	Ion Counting	The analog section of the detector is disabled and real-time display analytes are acquired in ion-counting only. If the signal is sufficient to trip and gate the detector, the signal reads -33.
	Show Analog	Displays the analog signal as well as the calibrated signal in the Average Intensities view and in the Spectrum window of the Data Display. The Chromatogram window of the Data Display still only displays calibrated signals.
Spectrum	Normal	Sets mode in the iCAP Q tab Data Display to Normal. Each scan is shown individually.
	Average	Sets mode in the iCAP Q tab Data Display to Average. From the moment Average is selected, scans are averaged where the number of averaged scans is displayed in red in the top left corner of the spectra.
	History	Sets mode in the iCAP Q tab Data Display to History. The latest scan is shown in full color and preceding scans are shown in gradually fading color.

The **Spectrum** display is modified and presented according to the mode selected from the **Spectrum** drop-down list.

For details on the data view region display, see "Data Display Tab" on page 4-7.

❖ **To switch between different detector modes**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. Click  **Calibrated**,  **Analog** or  **Ion Counting** to select the desired detector mode.
The data in the Data Display tab of the data view region is presented according to the selection. The Average Intensities list changes respectively.

❖ **To set the real-time display**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. Click  next to **Spectrum** and select a mode from the drop-down menu, for example, **Average**.
The data in the Data Display tab of the data view region is presented according to the selection.

Wizards Group

The wizards available in the **Wizards** group of the **iCAP Q** ribbon tab in Instrument Control, see Figure 4-19, help tuning the system. It is possible to run these wizards in different measurement modes.

Figure 4-19. Wizard group of the iCAP Q ribbon

The buttons of the **Wizards** group are summarized in Table 4-5.

Table 4-5. Buttons of Wizard group

Icon	Meaning	Description
	Performance Report	Opens the Performance Report wizard. The Report wizard guides you through the steps necessary to create, edit or run a performance report.
	Autotune	Offers direct access to Source Autotune. Opens the Autotune Wizard via the drop-down list. The wizard guides you through the steps necessary to create, edit or run an autotune sequence for the instrument.
	Detector Setup	Opens the Detector Setup wizard. The wizard guides you through the steps necessary to set up the detector and carry out a cross calibration.
	Mass Calibration	Opens the Mass Calibration wizard. The wizard guides you through the steps necessary to carry out a mass calibration of the quadrupole.

Performance Report Wizard

The **Wizards** group of the **iCAP Q** ribbon tab in Instrument Control gives access to the **Performance Report** wizard.

Performance reports are normally performed every day before analysis takes place. This ensures that the instrument is operating consistently and is delivering the desired sensitivity and performance characteristics.

❖ **To edit an existing Performance Report with the Performance Report Wizard**

1. Click 

to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the **Wizard** group, click 

.
The **Performance Report** wizard opens, see Figure 4-20.

Figure 4-20. Welcome to the Performance Report Wizard

4. Click **Edit an existing Performance report**.
5. Click **Next**.

6. Select a **Performance Report**, see Figure 4-21.

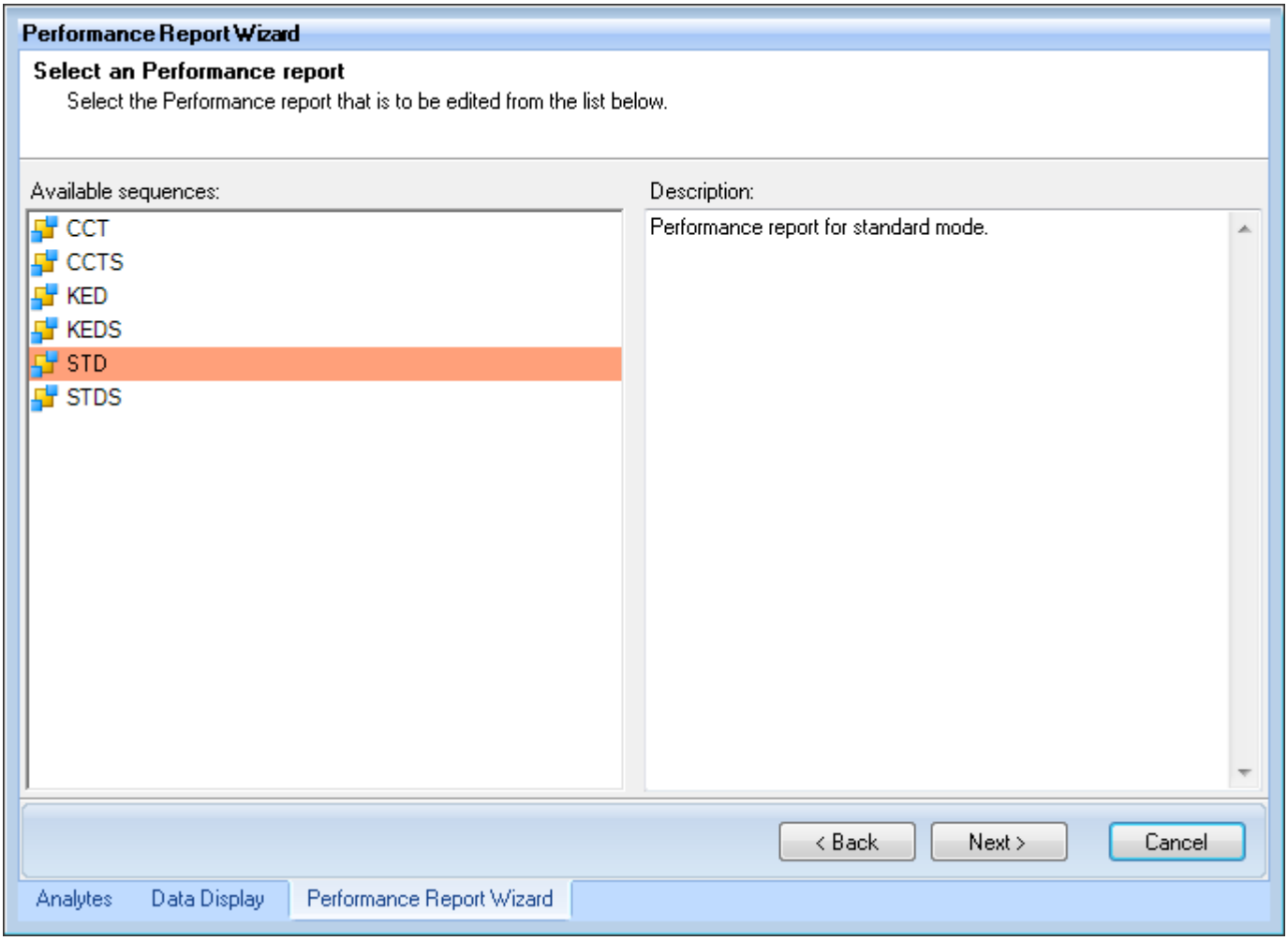


Figure 4-21. Selecting Performance Report

7. Click **Next**.

8. In the tab **Elements**, select the analytes for the Performance report selected in the periodic table, see Figure 4-22.

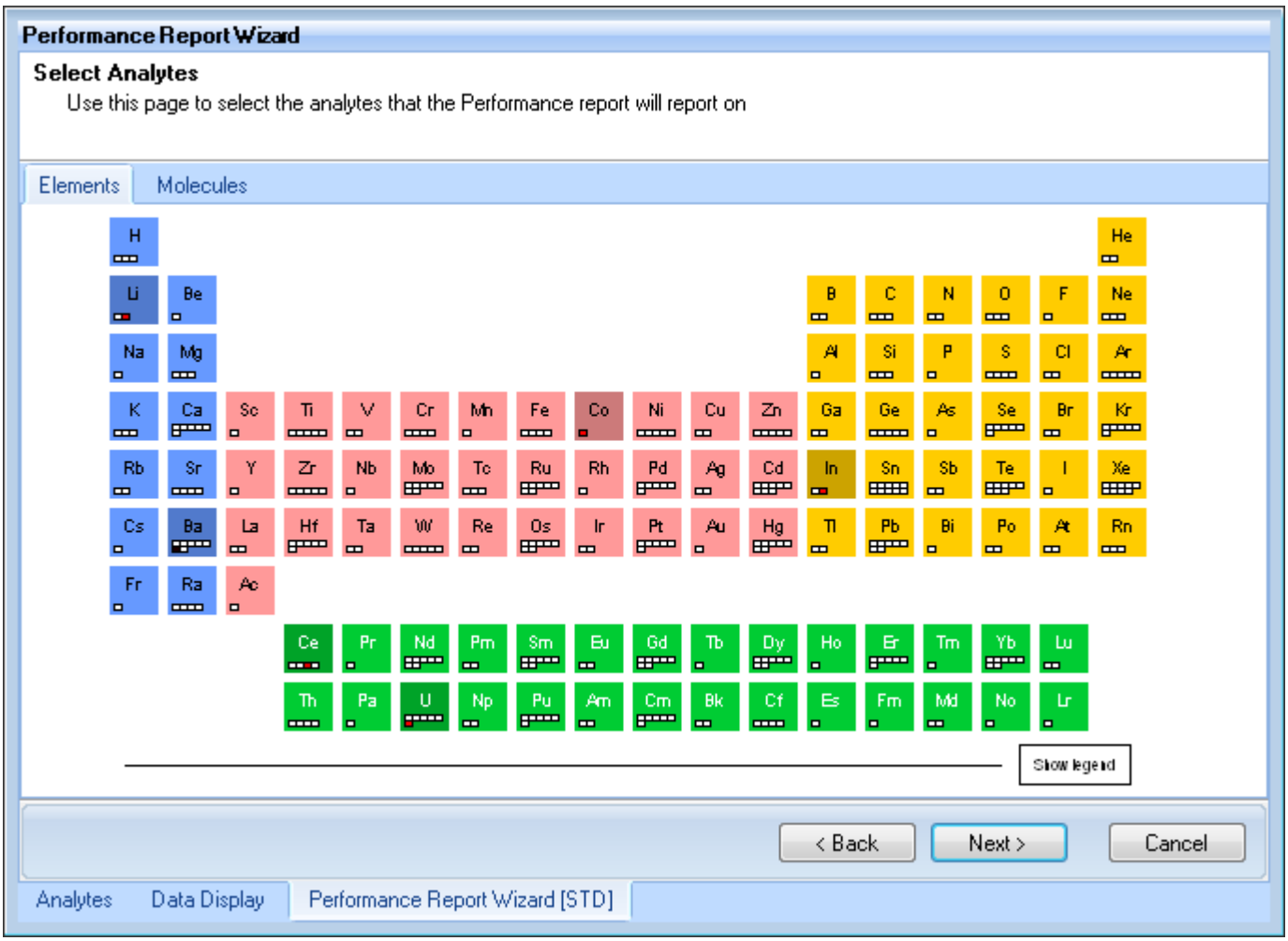


Figure 4-22. Selecting Analytes in the periodic table

9. Click the **Molecules** tab and select molecules, if appropriate, see Figure 4-23.

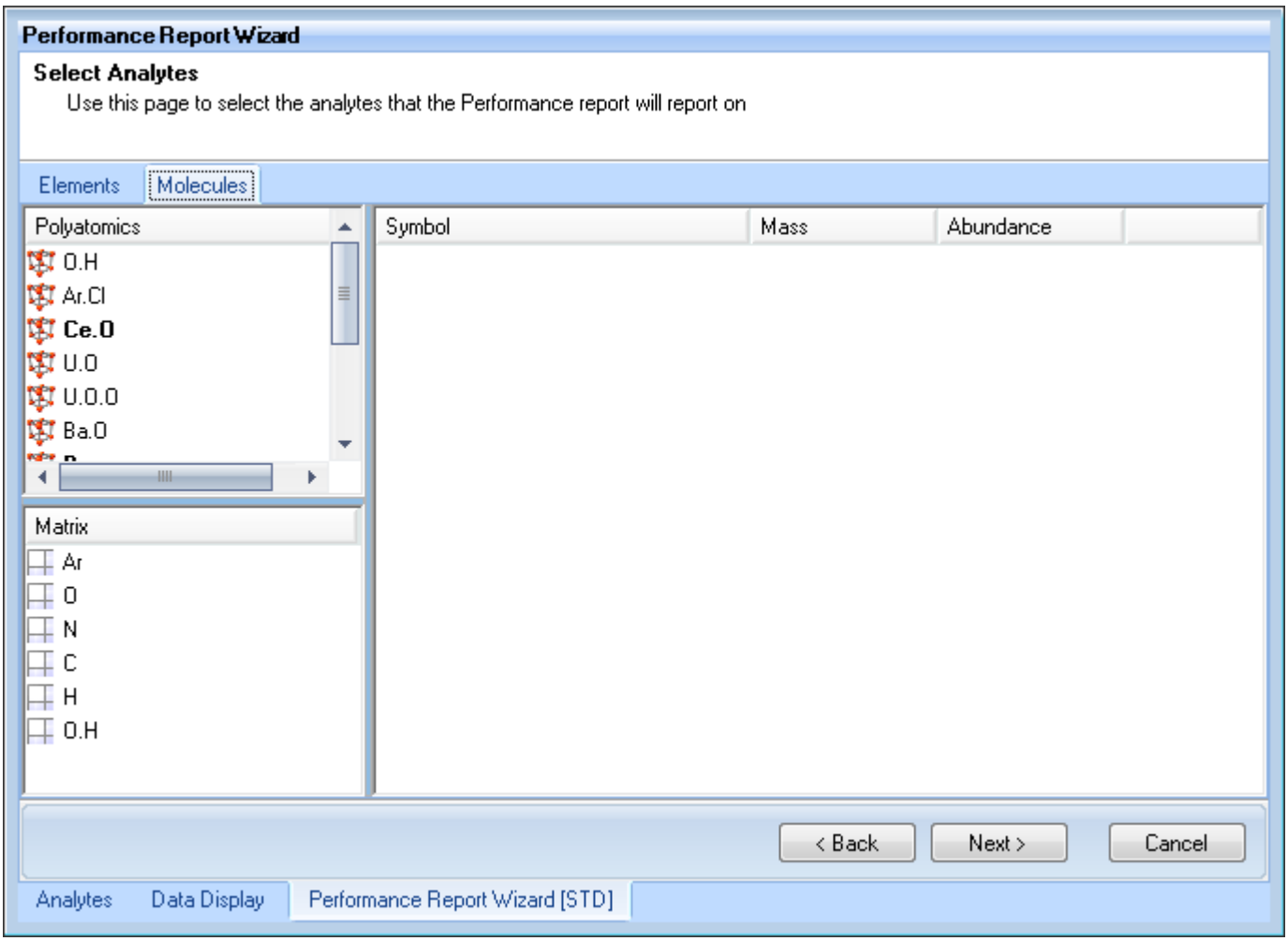


Figure 4-23. Selecting molecules

10. Click **Next**.

11. Drag and drop analytes from **Selected analytes** to **Defined ratios** to define the ratios for the analytes needed to determine, for example, the oxide ratio or the ratio of doubly charged ions, see Figure 4-24.

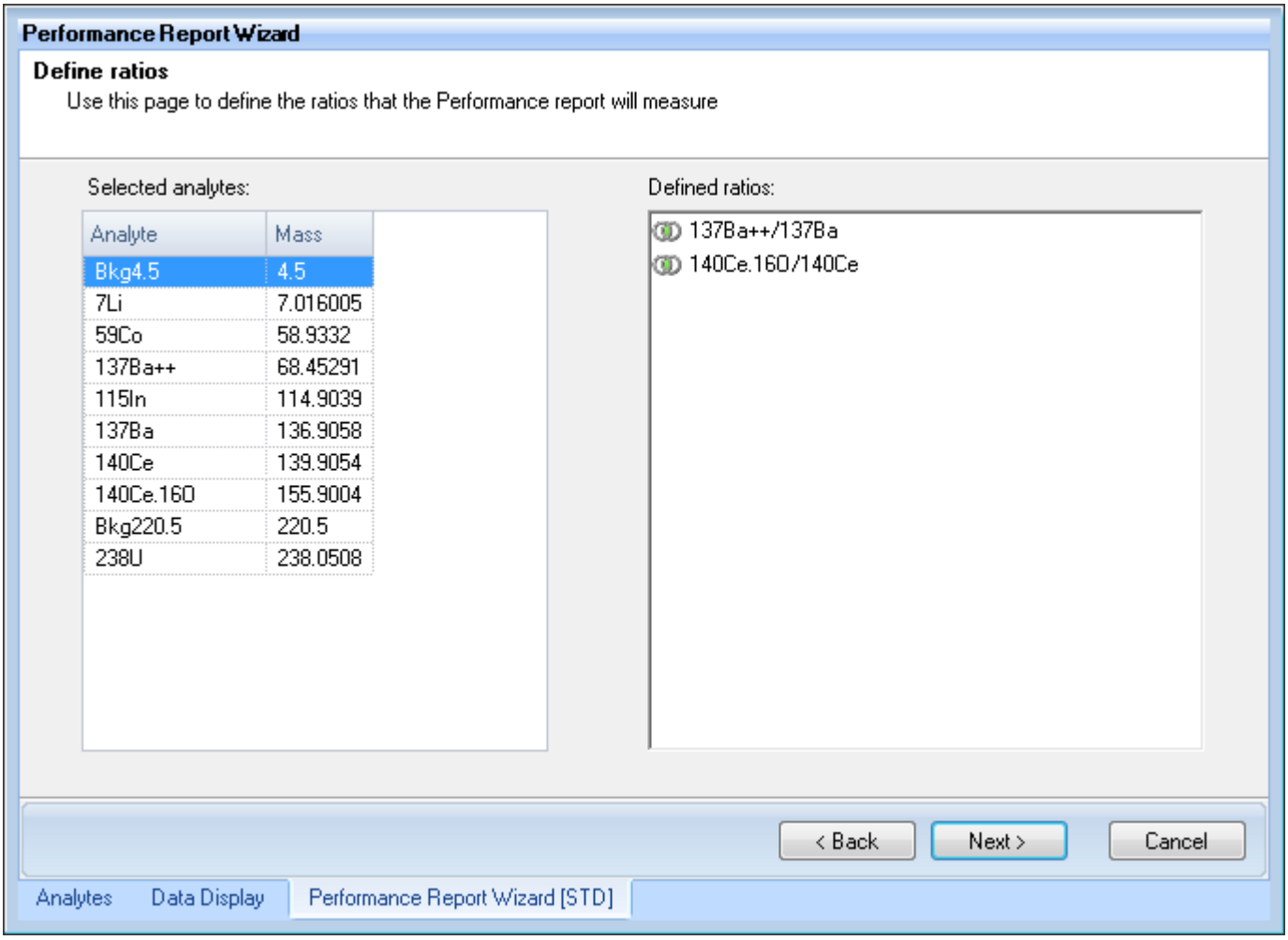


Figure 4-24. Defining ratios for the Analytes

12. Click **Next**.

13. Define the tests, see Figure 4-25.

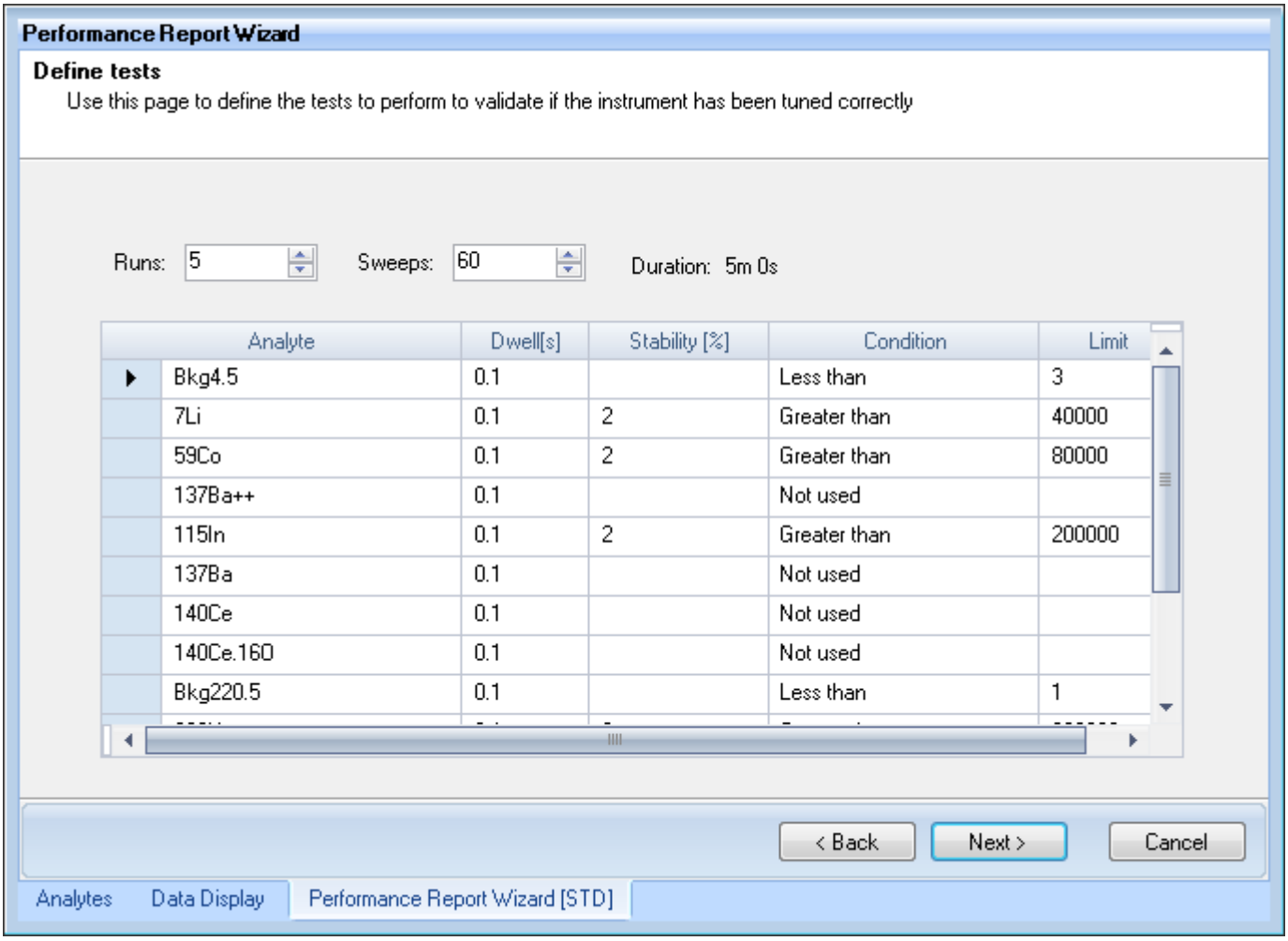


Figure 4-25. Defining tests

14. Click **Next**.

15. Define the mass calibration tests, see Figure 4-26.

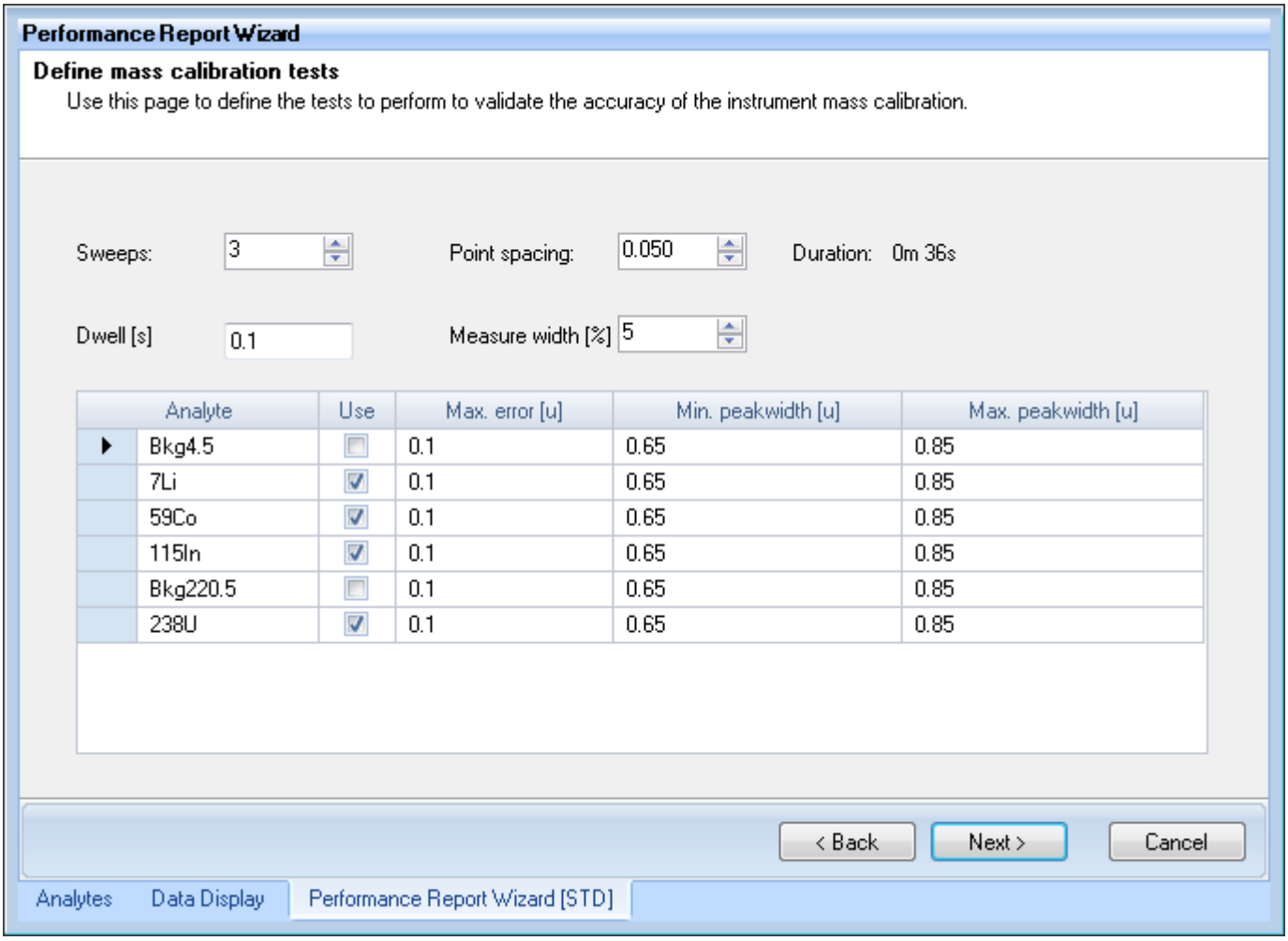


Figure 4-26. Defining mass calibration tests

16. Click **Next**.

17. Select a **Performance Report** from the list.
    For **Name**, you can also enter a new name for the report, see Figure 4-27.

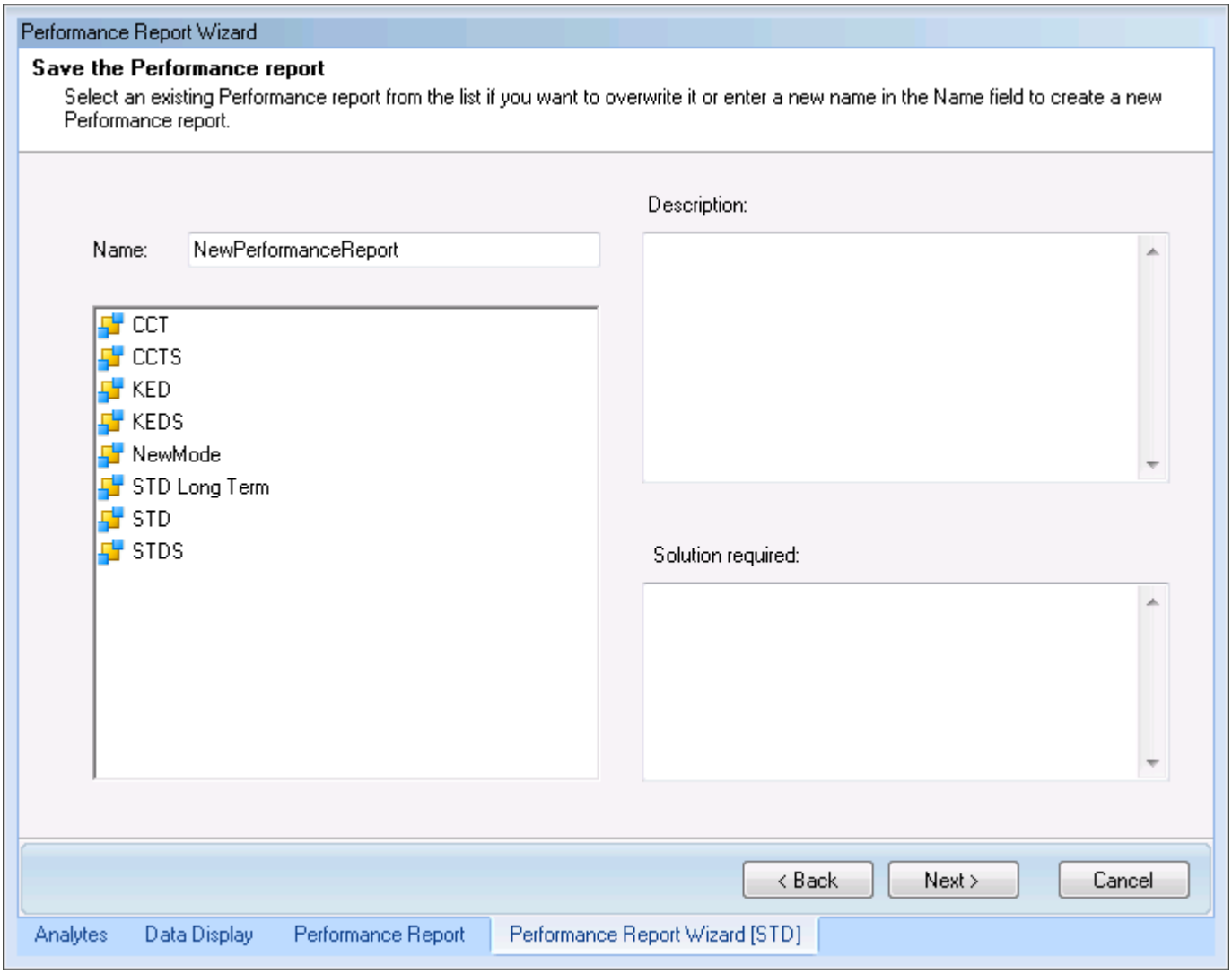


Figure 4-27. Selecting Performance Report name

18. Click **Next** to save the Performance Report.

19. Click **Finish** to end the Performance Report Wizard, see Figure 4-28.

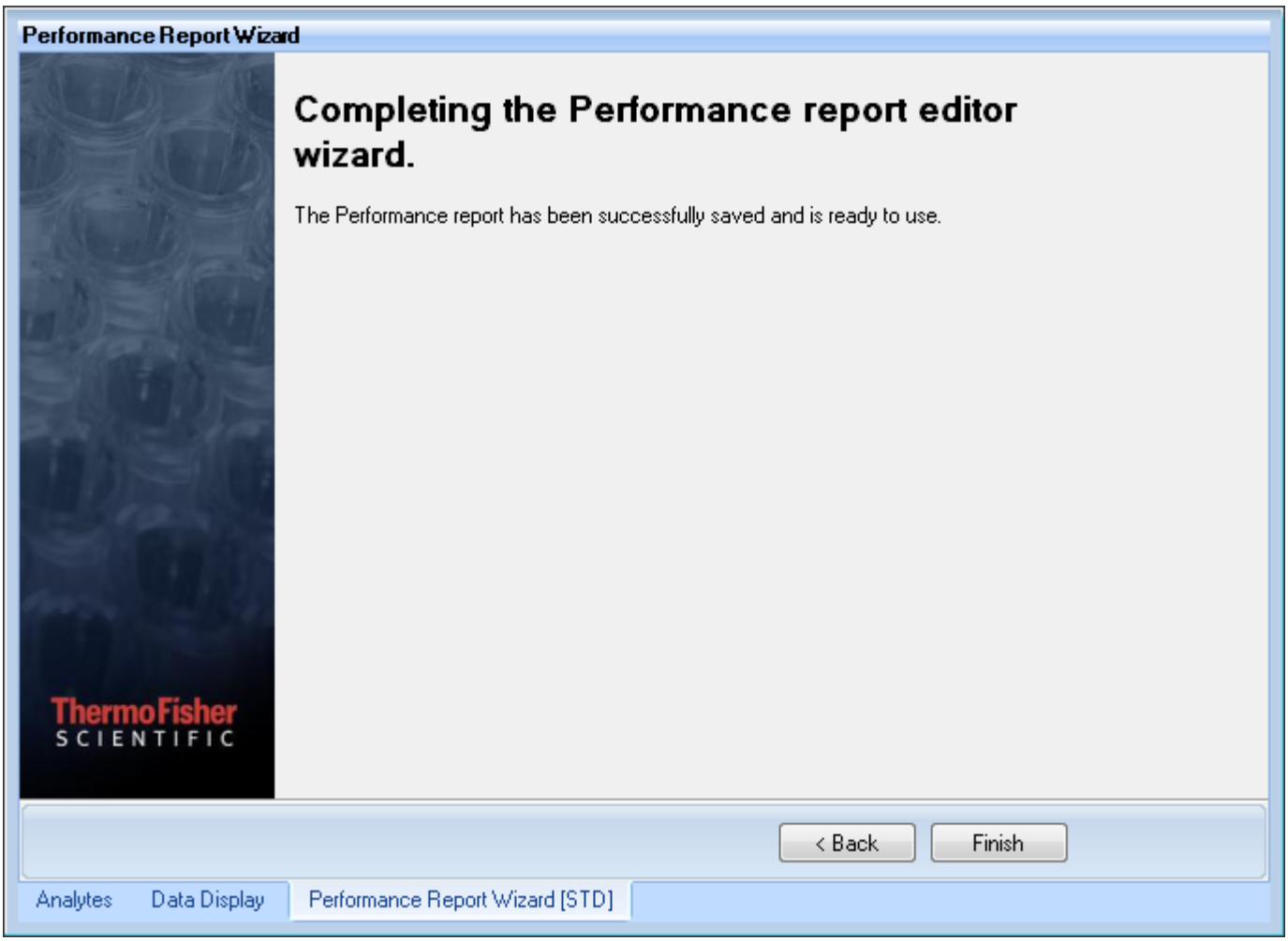


Figure 4-28. Completing Performance Report wizard

❖ **To create a new Performance Report with the Performance Report Wizard**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab. The ribbon **iCAP Q** is activated.

3. In the **Wizard** group, click 

.
The **Performance Report** wizard opens, see Figure 4-29.

Figure 4-29. Welcome to the Performance Report Wizard

4. Select **Create a Performance report**.
5. Click **Next**.

6. In the tab **Elements**, select the analytes for the Performance report, see Figure 4-30.

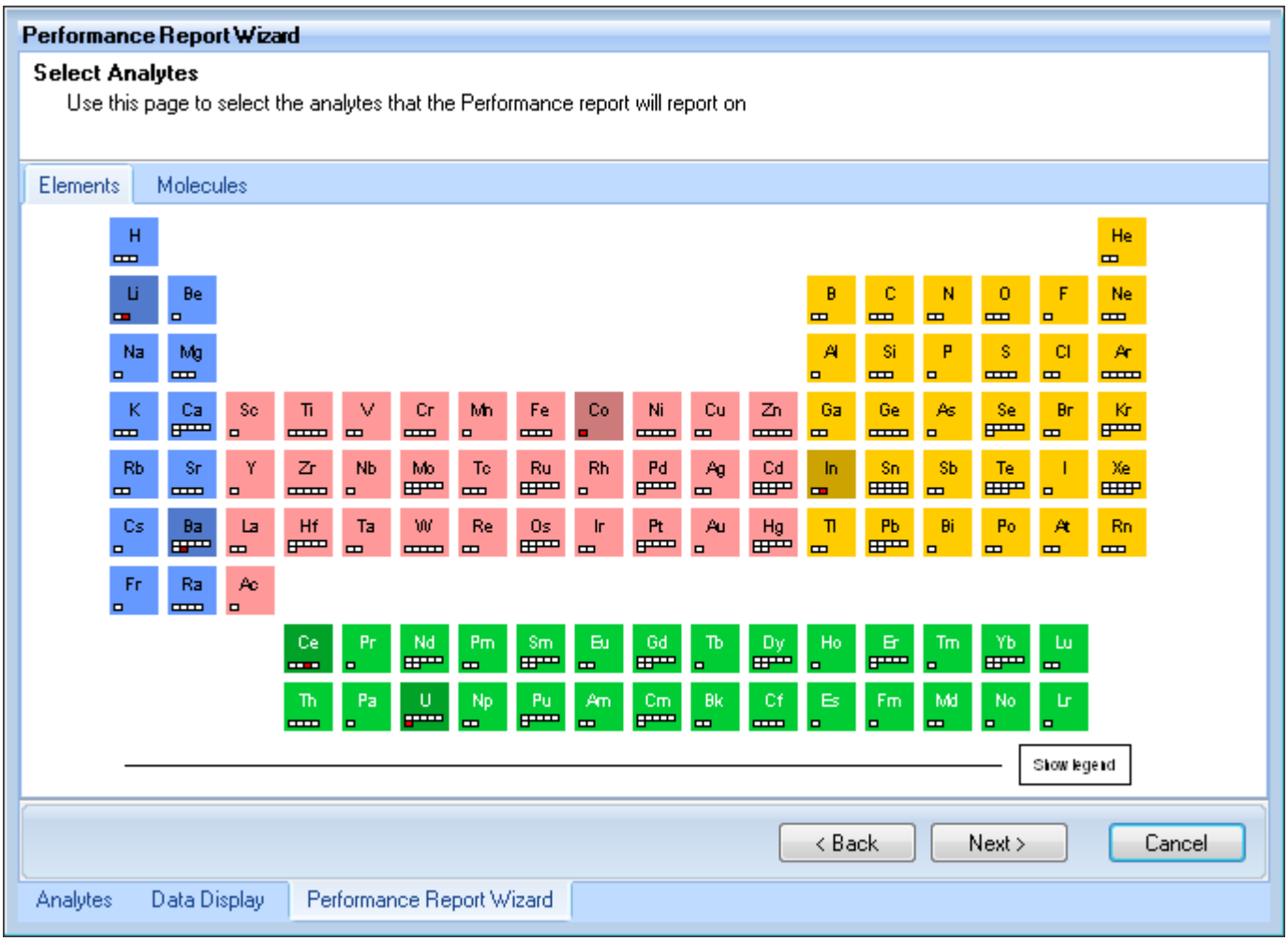


Figure 4-30. Selecting analytes for the Performance Report Wizard

7. Click the **Molecules** tab and select molecules, if appropriate, see Figure 4-31.

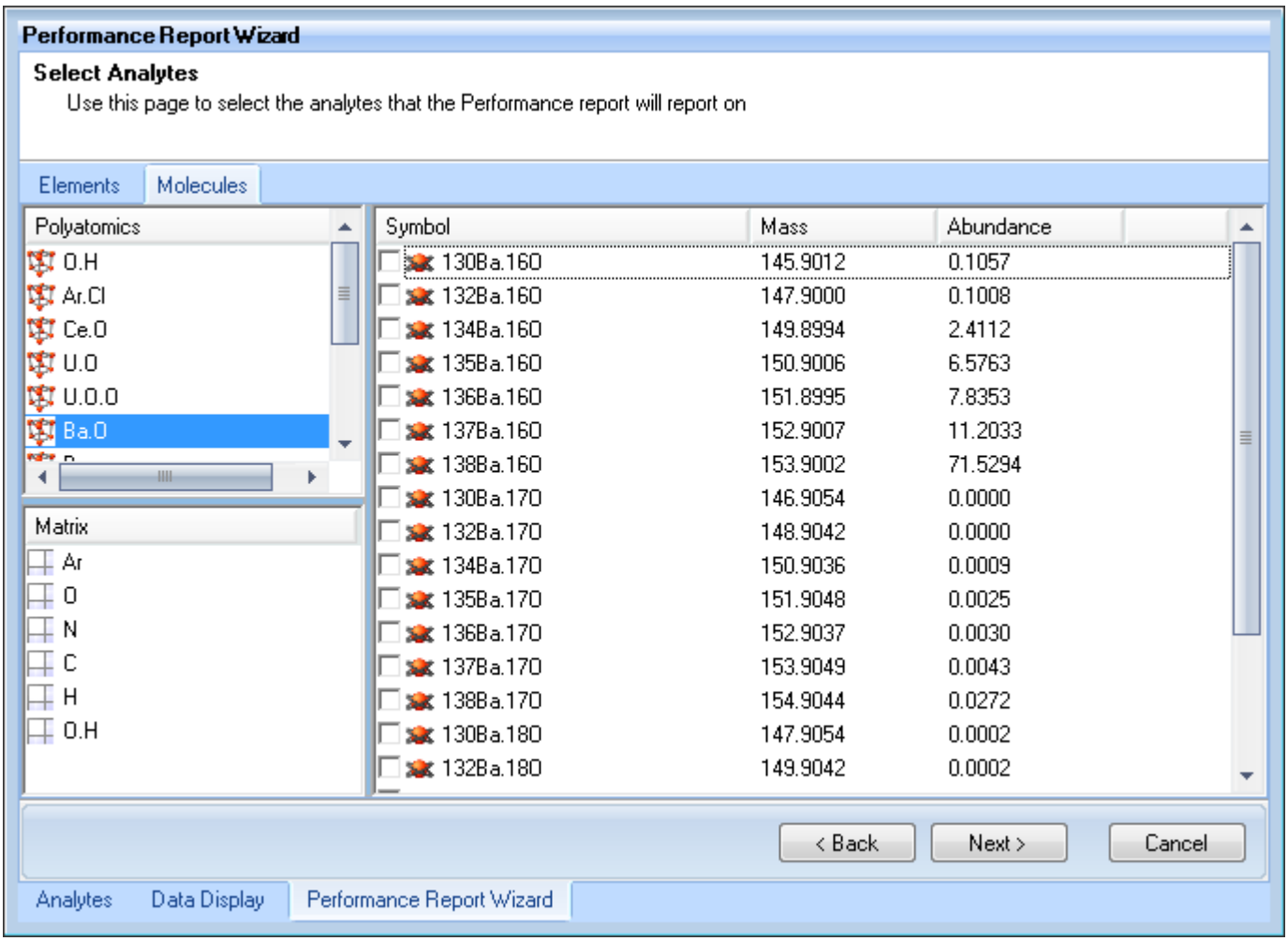


Figure 4-31. Selecting molecules for the Performance Report Wizard

8. Click **Next**.

9. Drag and drop analytes from **Selected analytes** to **Defined ratios** to define the ratios for your analytes, see Figure 4-32.

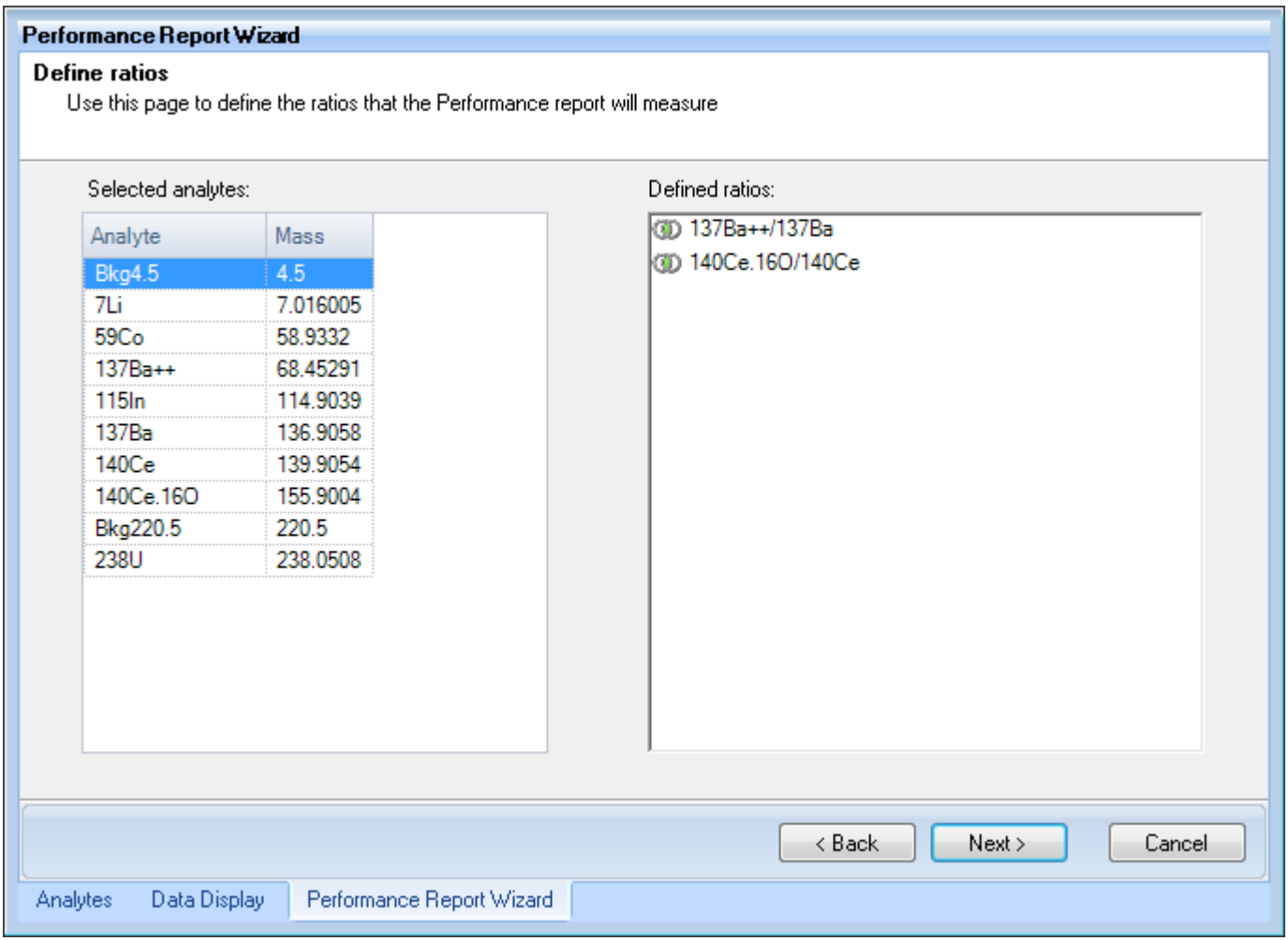


Figure 4-32. Defining ratios for the Performance Report Wizard

10. Click **Next**.

11. Define the tests for the Performance report, see Figure 4-33.

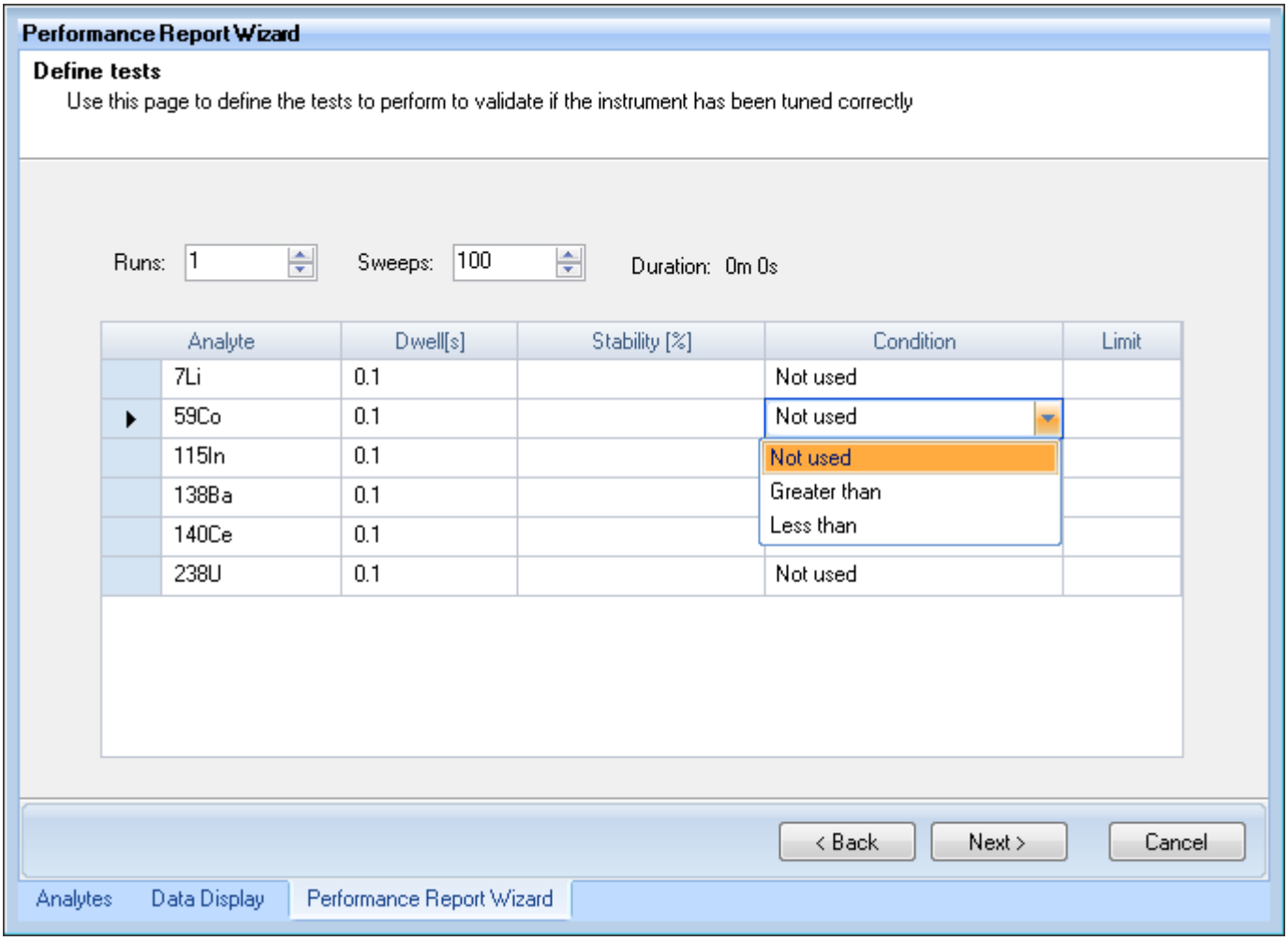


Figure 4-33. Defining tests for the Performance Report Wizard

12. Click **Next**.

13. Define the mass calibration tests for the Performance report, see Figure 4-34.

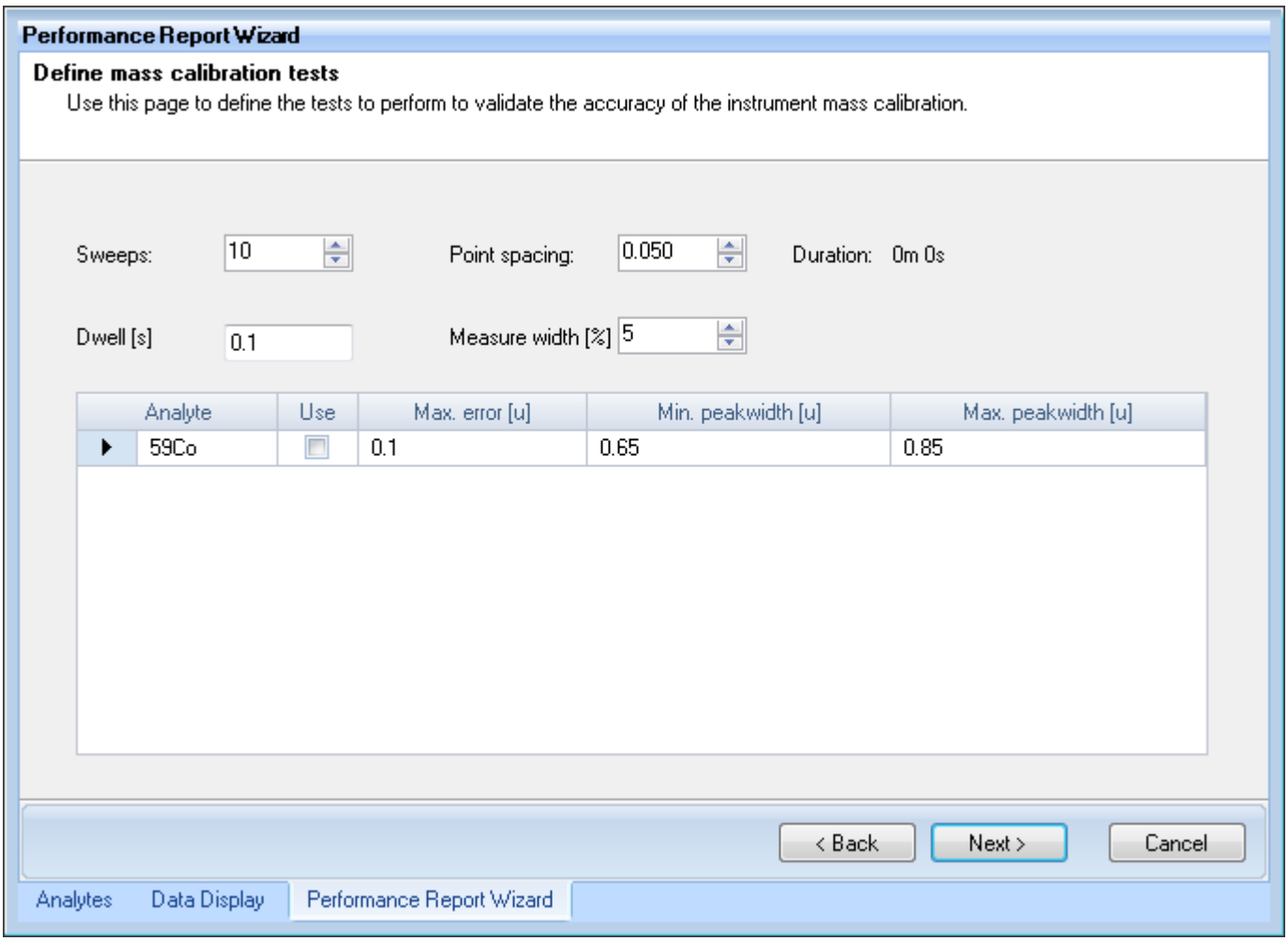


Figure 4-34. Defining mass calibration tests for the Performance Report Wizard

14. Select a report from the list or enter a new **Name**, see Figure 4-35.

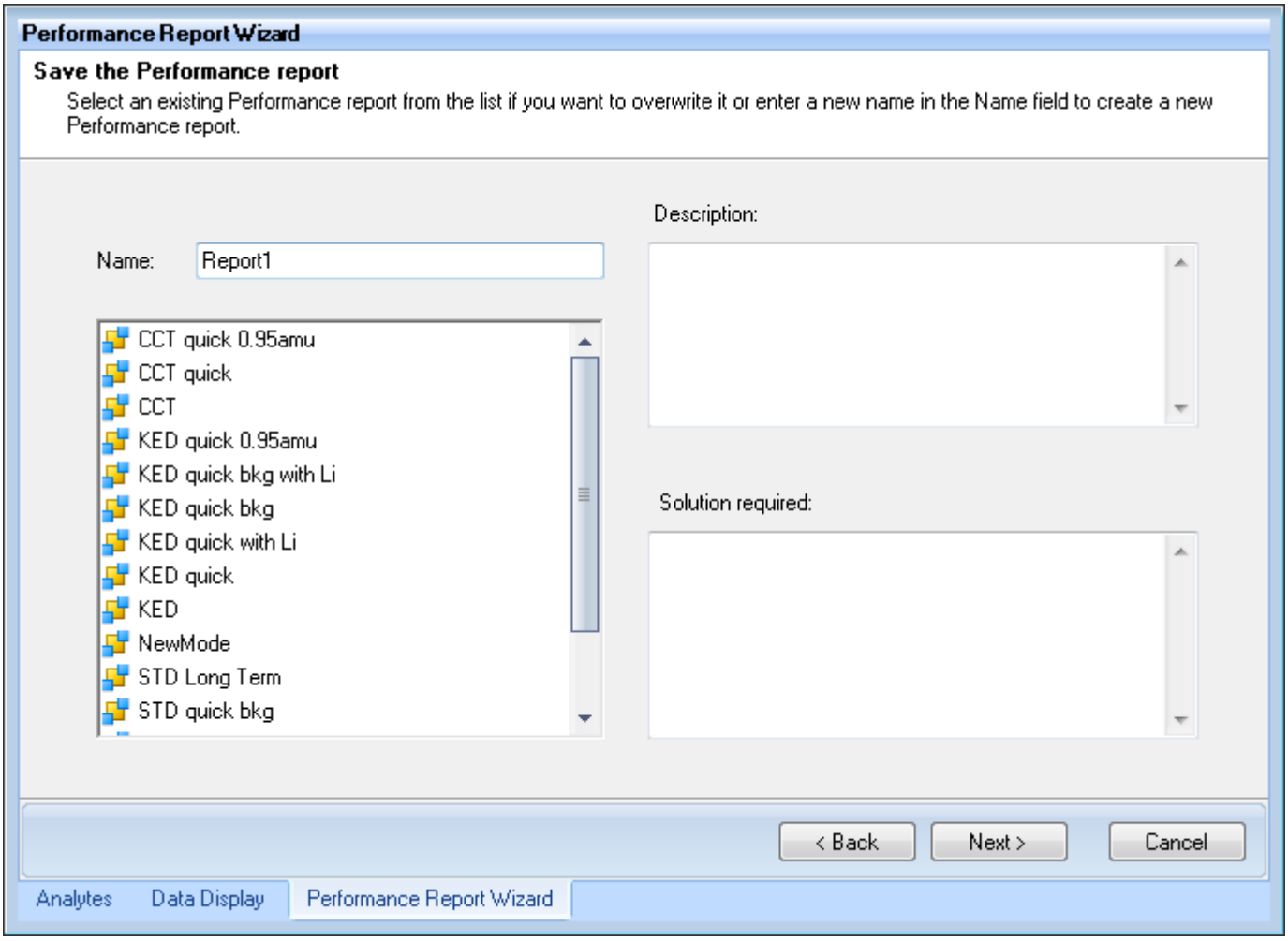


Figure 4-35. Selecting Performance Report name for the new report

15. Click **Next** to save the Performance Report.

16. Click **Finish** to complete the Performance Report Wizard, see Figure 4-36.

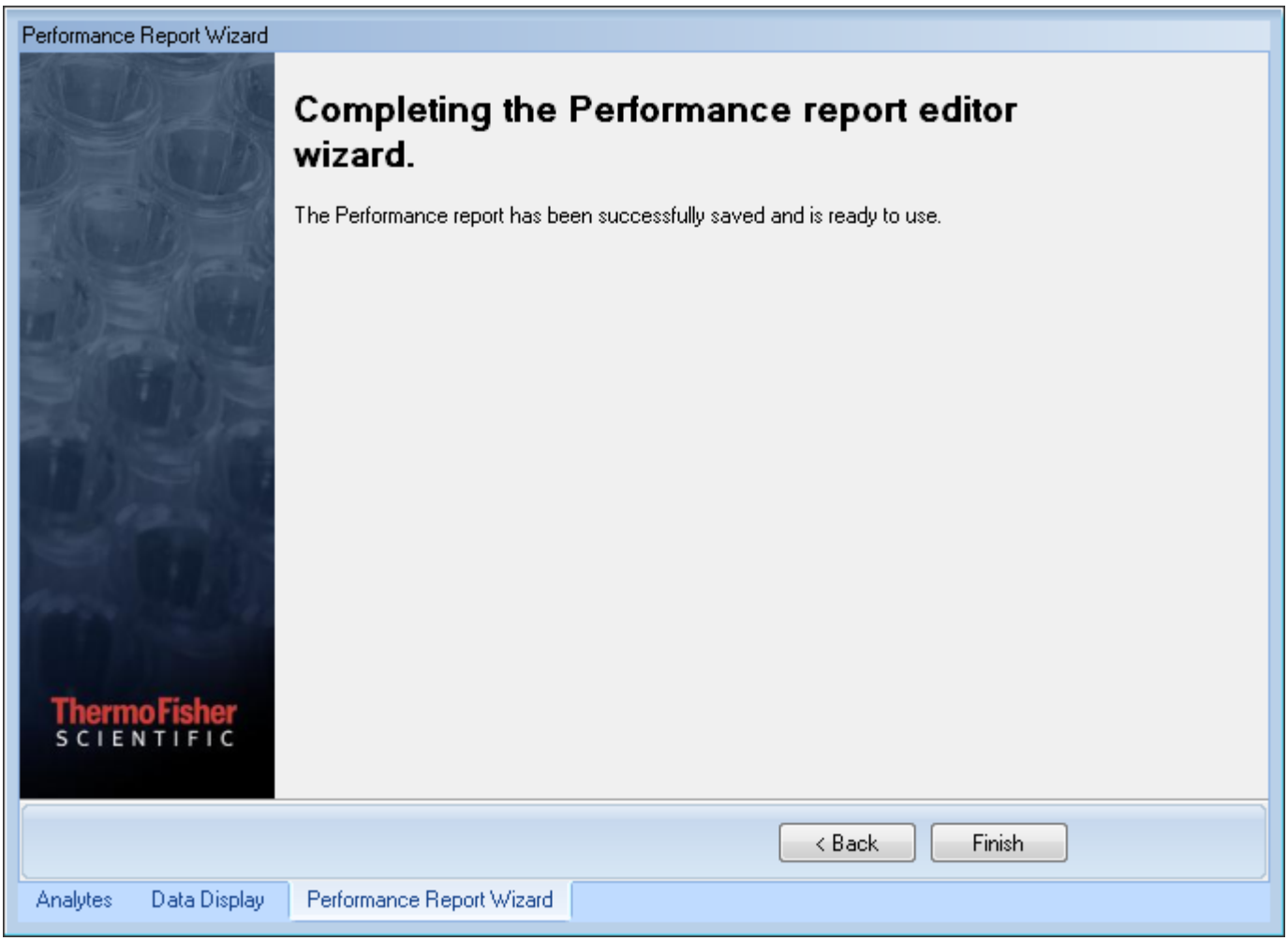


Figure 4-36. Completing the Performance Report wizard

❖ **To run an existing Performance Report with the Performance Report Wizard**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the **Wizard** group, click 

.
The **Performance Report** wizard opens, see Figure 4-37.

Figure 4-37. Welcome to the Performance Report Wizard

4. Select **Run an existing Performance report**.
5. Click **Next**.

6. Select a **Performance Report**, see Figure 4-38.

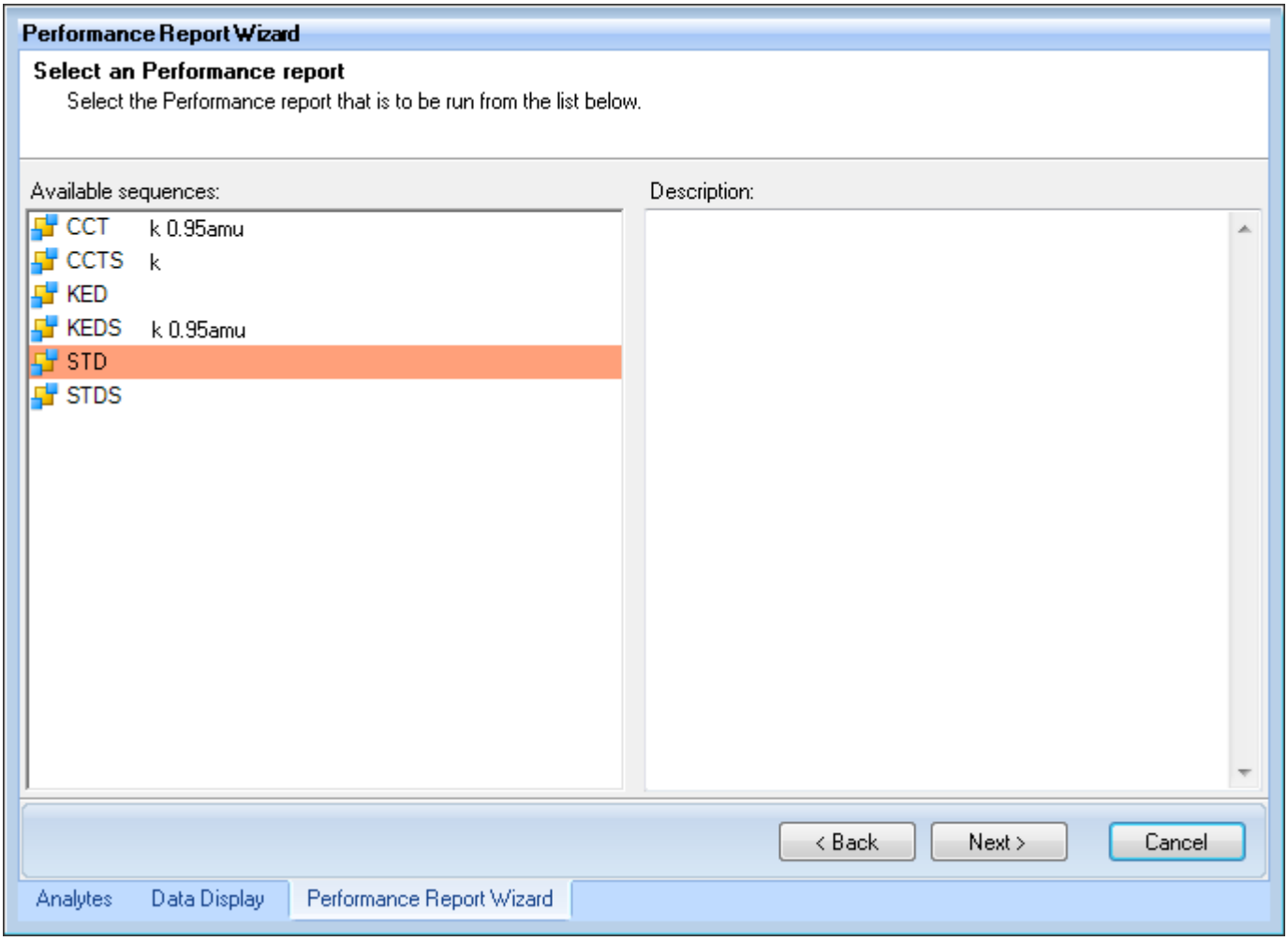


Figure 4-38. Selecting Performance Report

7. Click **Next**.
   The performance report requires the samples to be placed, see Figure 4-39.

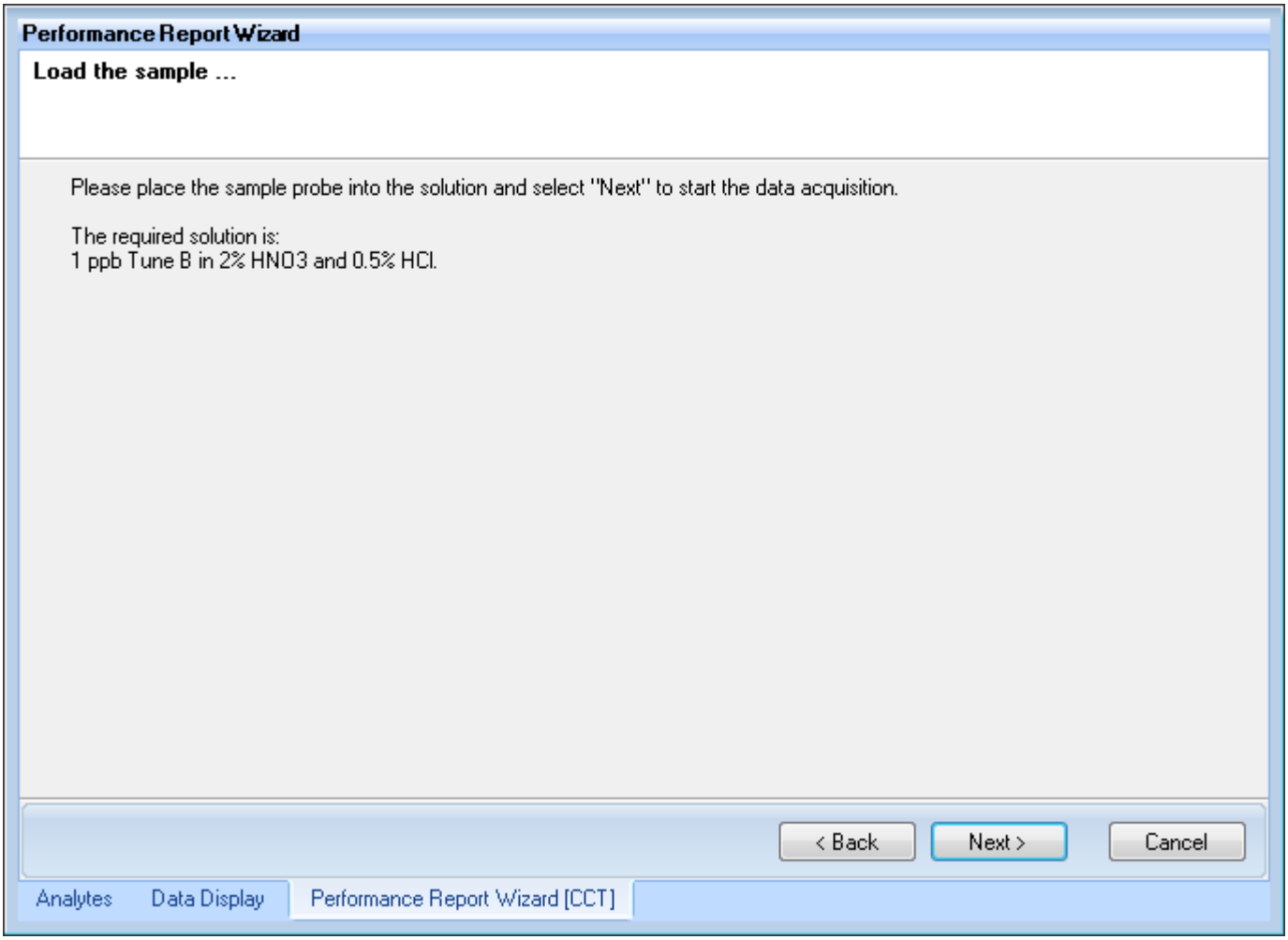


Figure 4-39. Performance Report Wizard loads samples

8. Place the probe into the solution and click **Next**.
   The acquisition status is shown, see Figure 4-40.

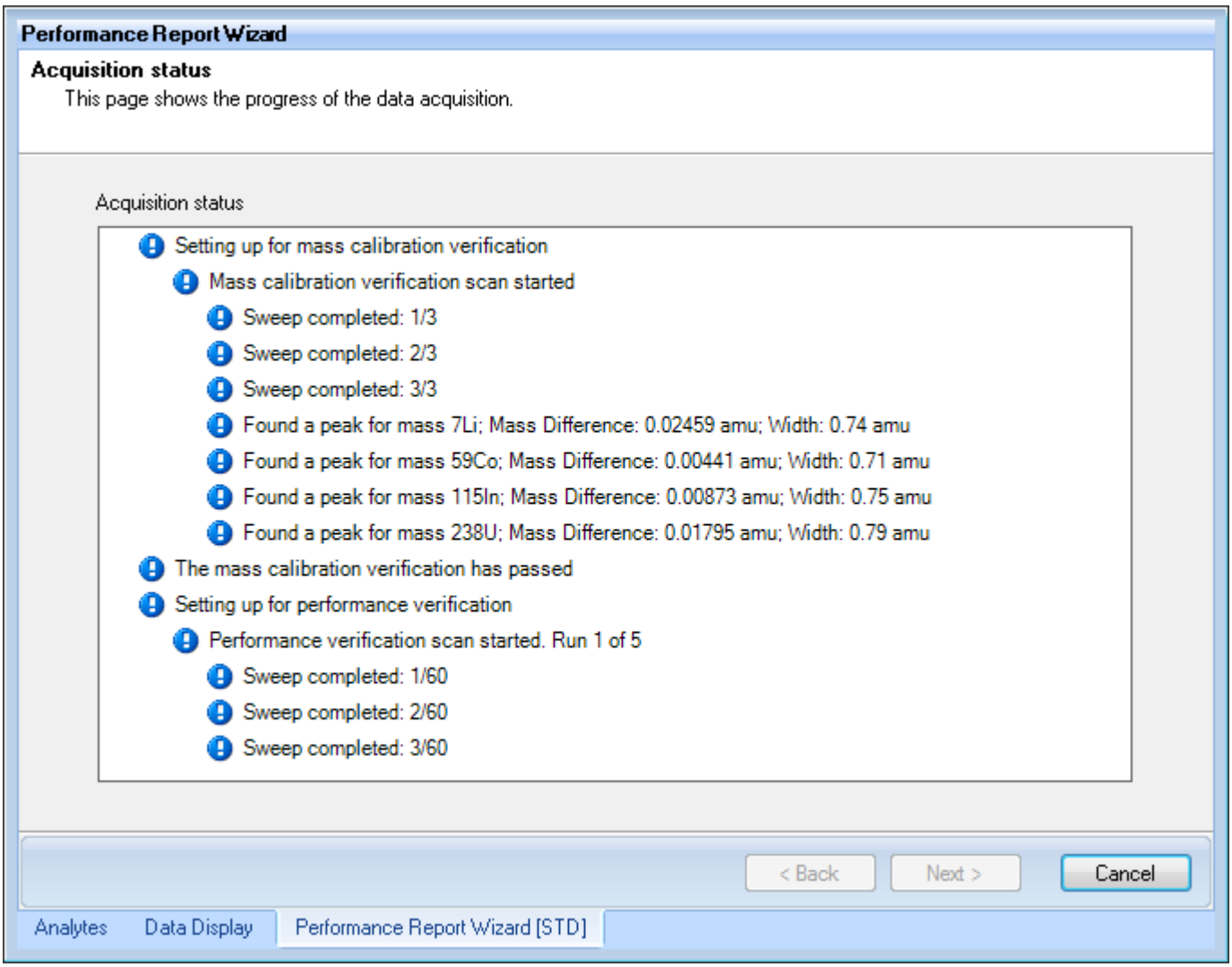


Figure 4-40. Status of acquisition for the Performance Report Wizard

When the acquisition is completed, the Next button is activated, see Figure 4-41.

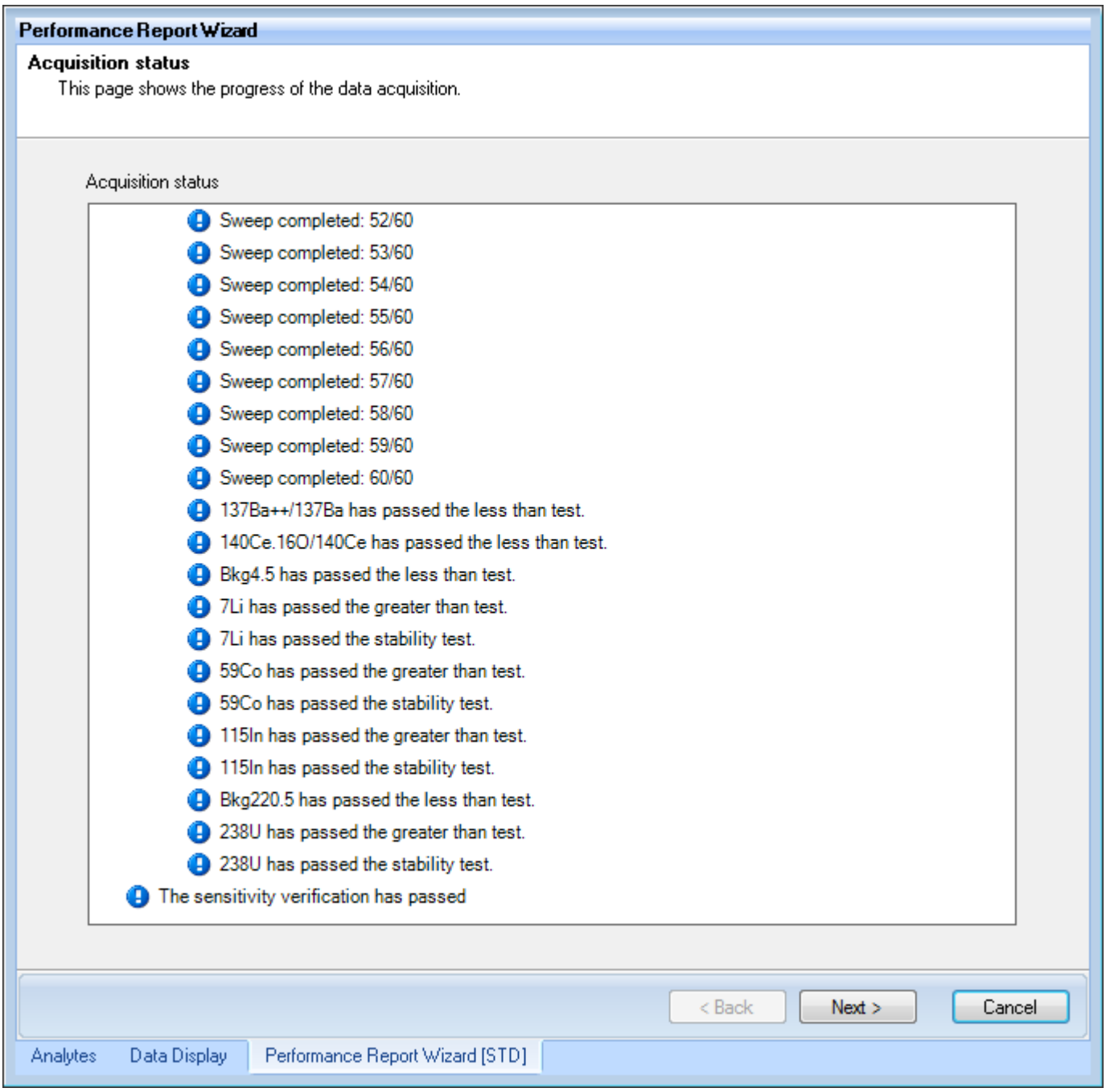


Figure 4-41. Acquisition completed for the Performance Report Wizard

9. Click **Next**.

10. Click **Finish** to complete the Performance Report Wizard, see Figure 4-42.

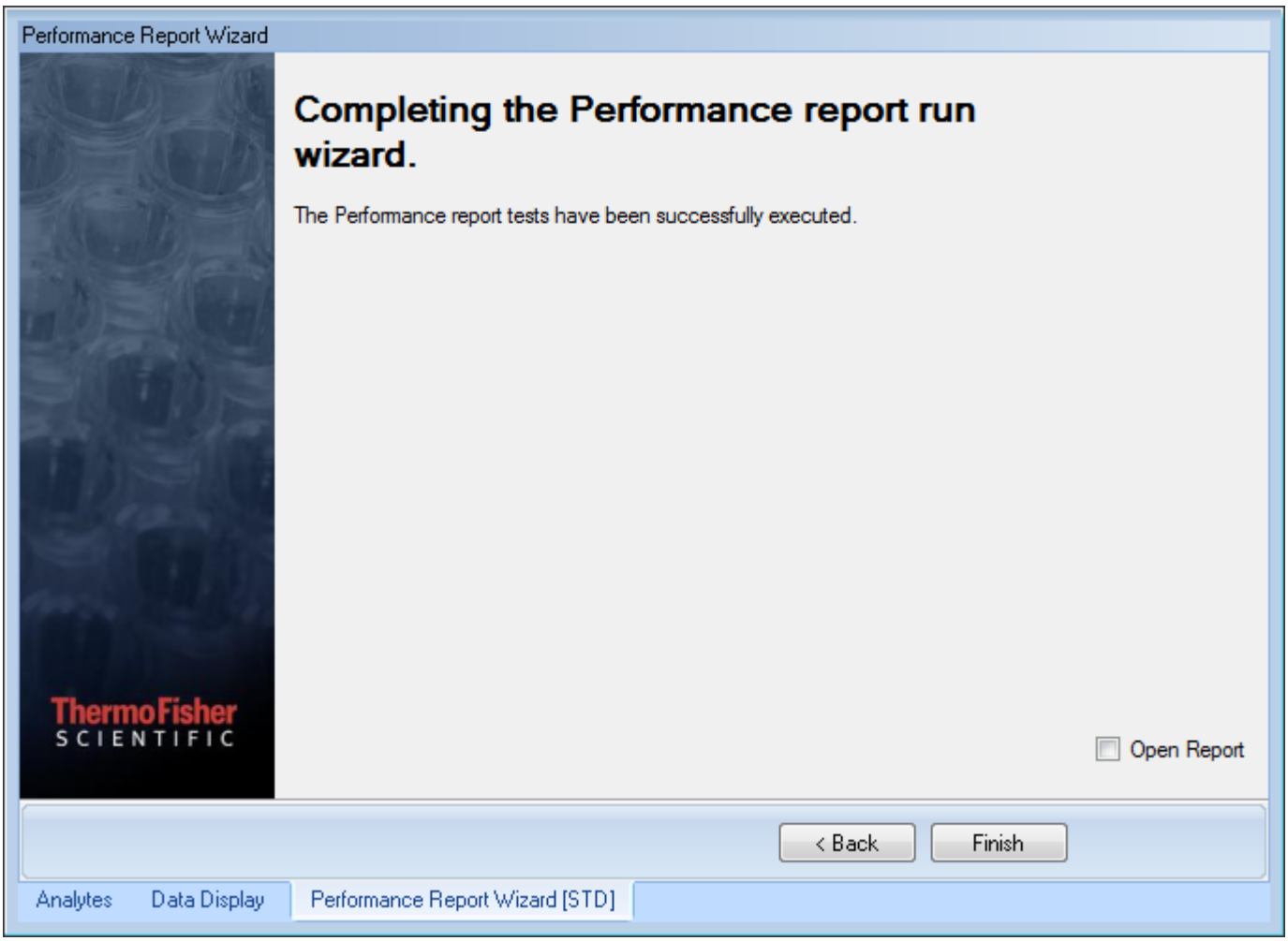


Figure 4-42. Completing the Performance Report wizard

❖ **To run a Performance Report from the active Measurement mode with the Performance Report Wizard**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the **Wizard** group, click 

.
The **Performance Report** wizard opens, see Figure 4-43.

Figure 4-43. Welcome to the Performance Report Wizard

4. Select **Run a Performance Report from the active Measurement mode**.

5. Click **Next**.
   The performance report requires the samples to be placed, see Figure 4-44.

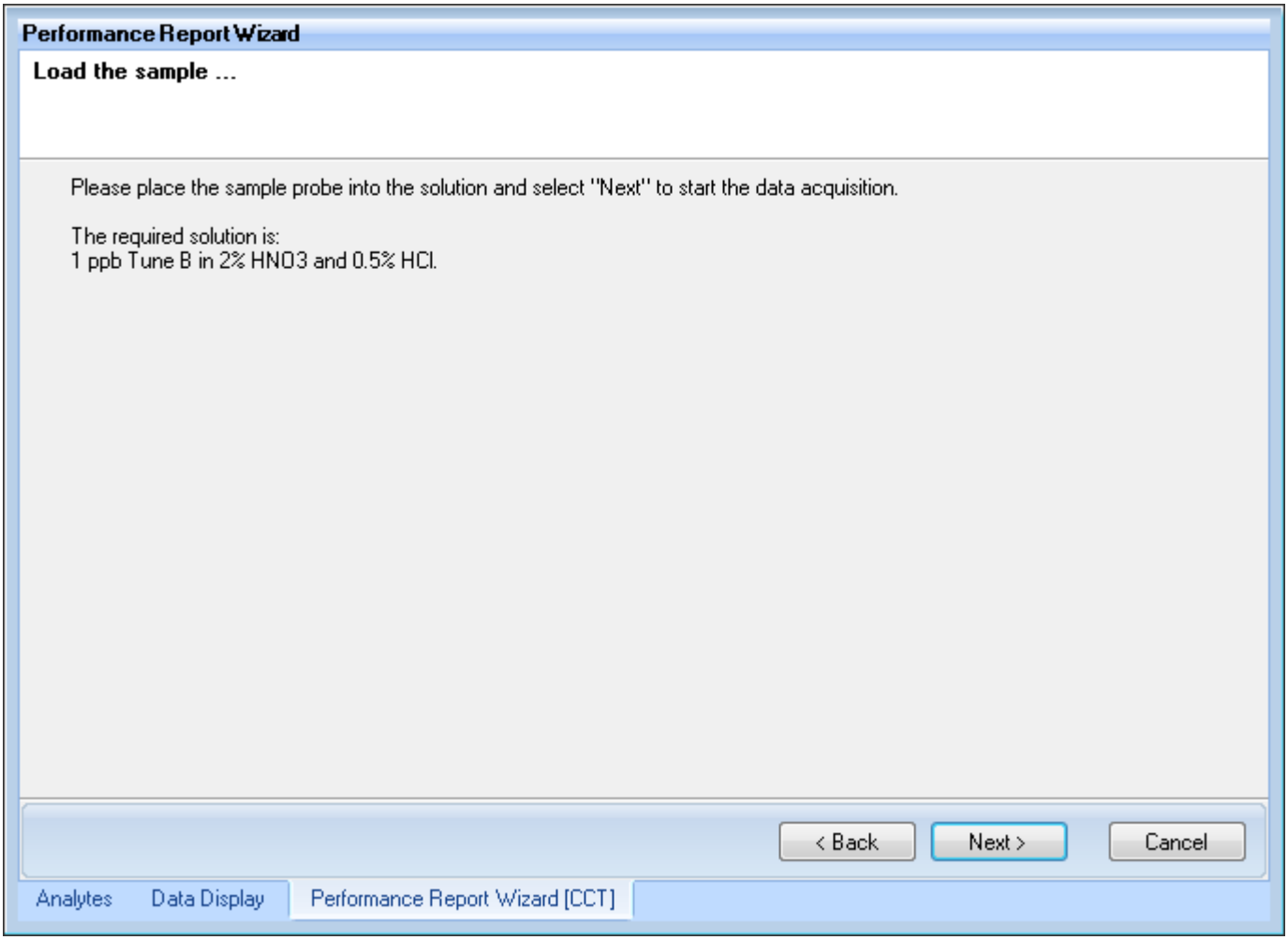


Figure 4-44. Performance Report Wizard loads samples

6. Place the probe into the solution and click **Next**.
   The acquisition status is shown, see Figure 4-45.

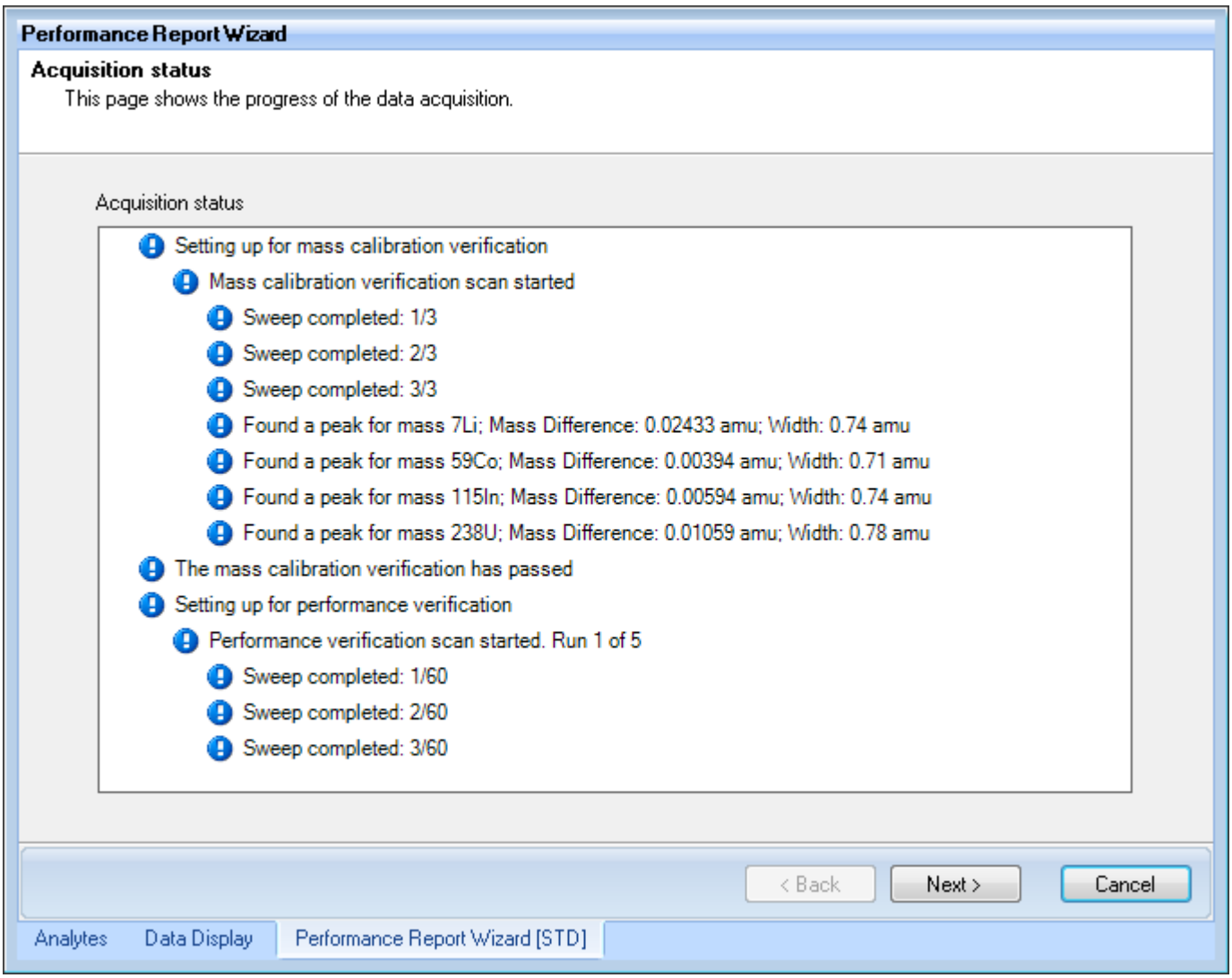


Figure 4-45. Status of acquisition for the Performance Report Wizard

When the acquisition is completed, the Next button is activated, see Figure 4-46.

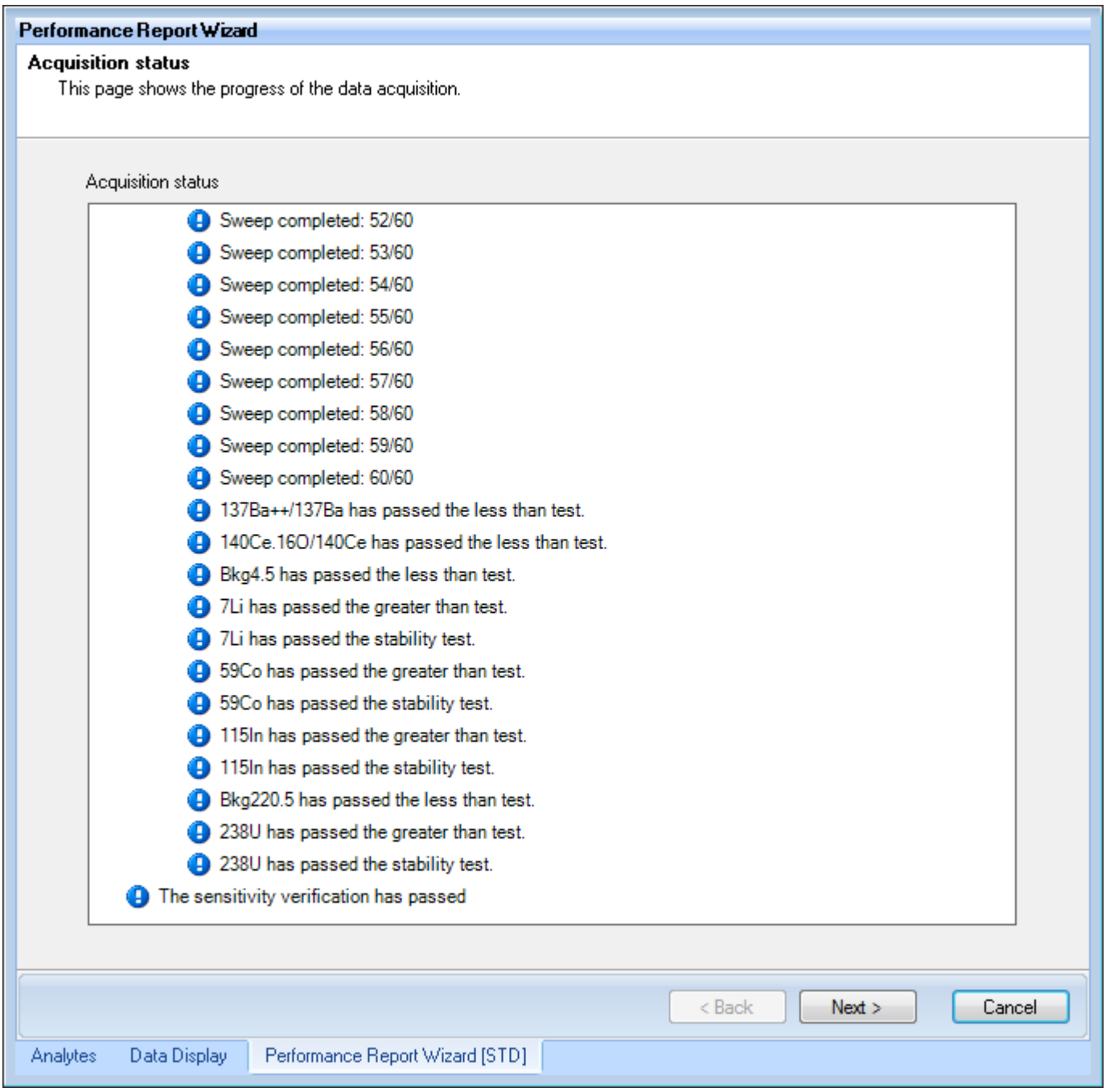


Figure 4-46. Acquisition completed for the Performance Report Wizard

7. Click **Next**.

8. Select the check box **Open Report** if you wish to open the report, see Figure 4-47.

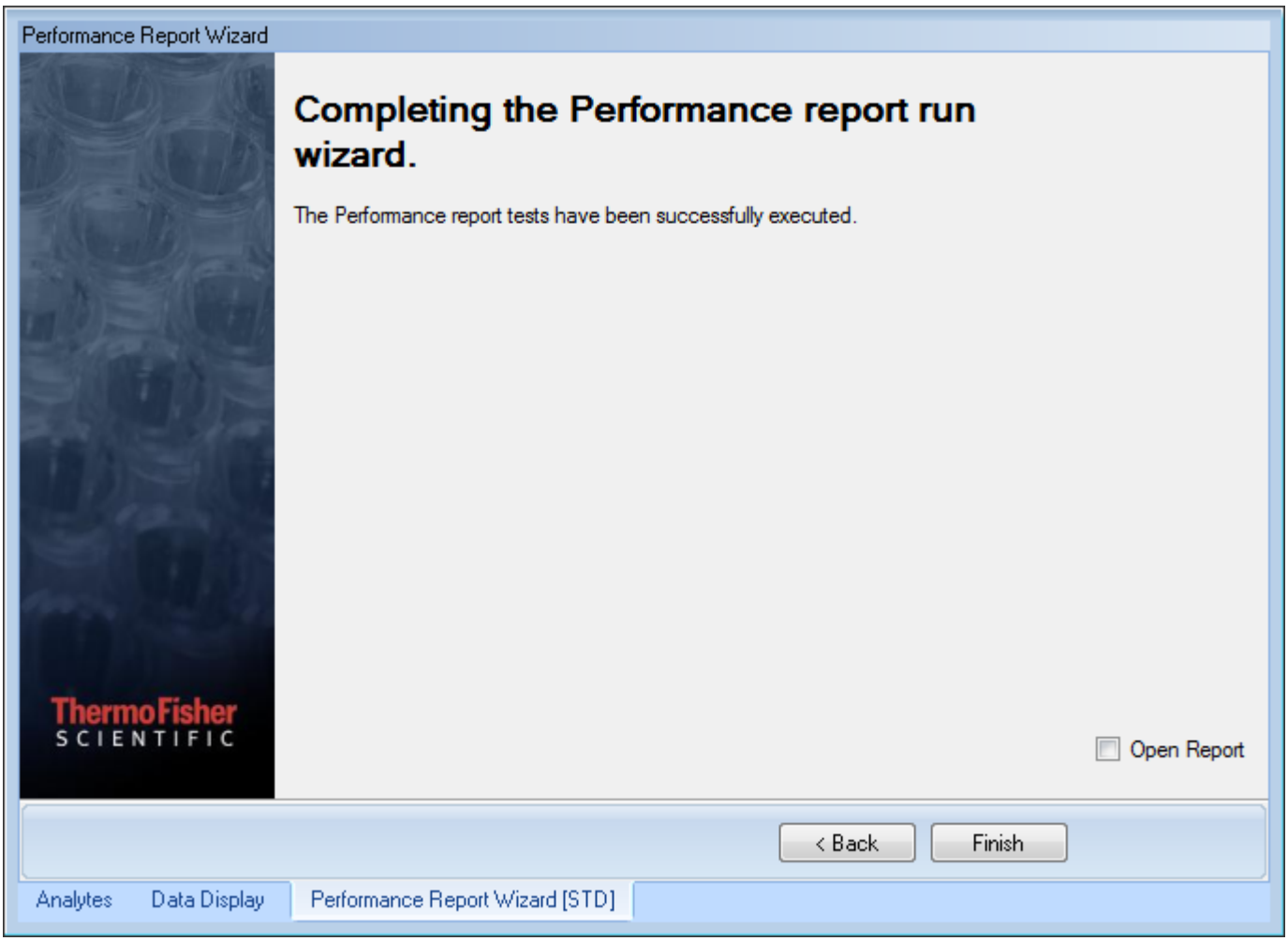


Figure 4-47. Completing the Performance Report wizard

9. Click **Finish** to complete the Performance Report Wizard.

Autotune Wizard

The **Wizards** group of the **iCAP Q** ribbon tab in Instrument Control gives access to the **Autotune Wizard**.

An autotune procedure is only necessary when the performance of the instrument falls below the limits specified in the performance report, although they can be performed more regularly if desired. Each Measurement mode has a defined autotune (with the same name) which you can modify.

The **Autotune Wizard** guides you through creating, editing or running an autotune sequence.

❖ **To edit an existing Autotune sequence with the Autotune Wizard**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the **Wizard** group, click 

(arrow next to or below Autotune) to open the drop-down menu, see Figure 4-48.

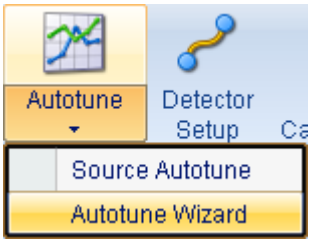


Figure 4-48. Autotune drop-down menu

4. Click **Autotune Wizard**.
   The **Autotune** wizard opens, see Figure 4-49.

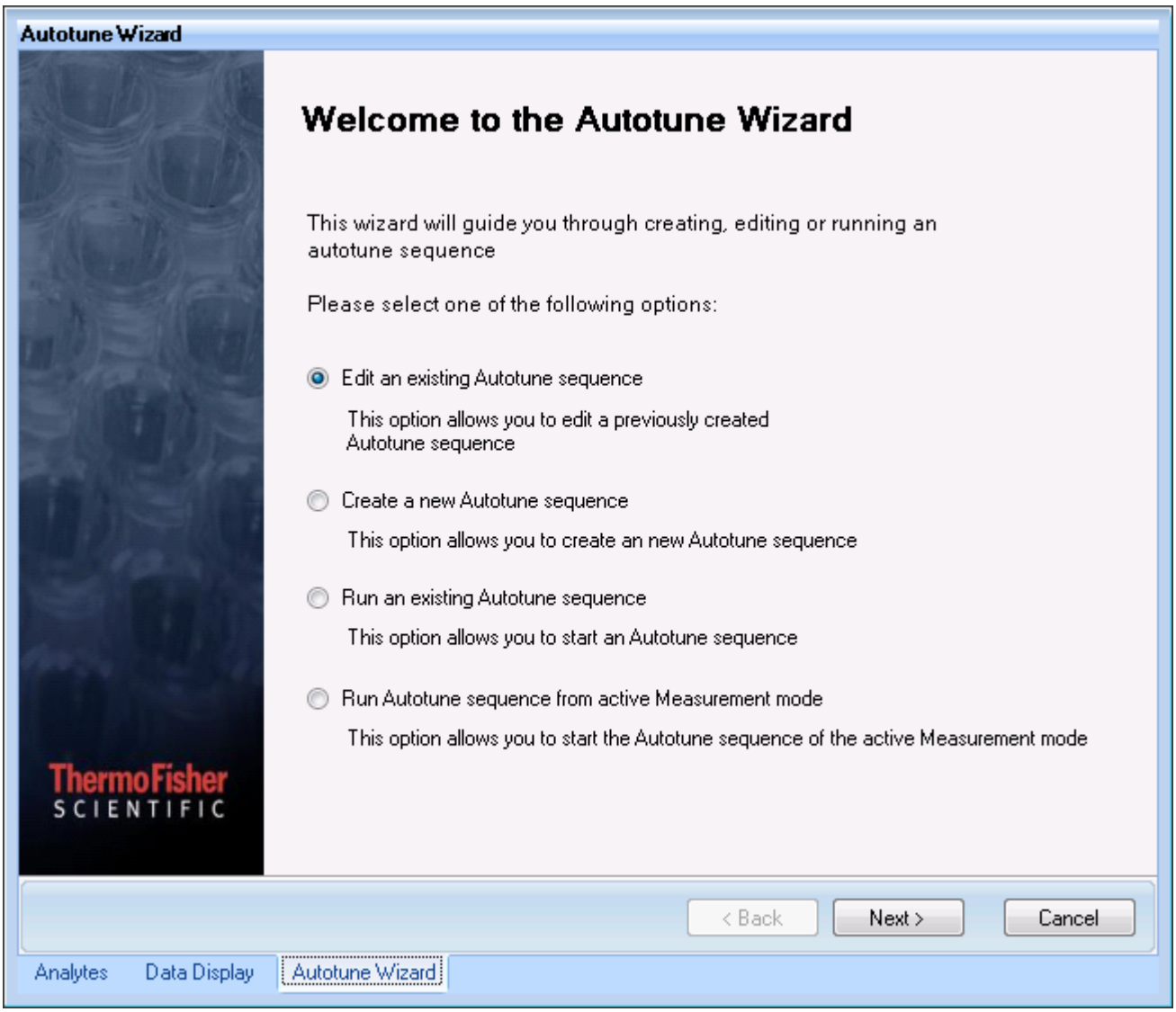


Figure 4-49. Welcome to the Autotune wizard

5. Select **Edit an existing Autotune sequence**.
6. Click **Next**.

7. Select the autotune sequence to be edited from the list, see Figure 4-50.

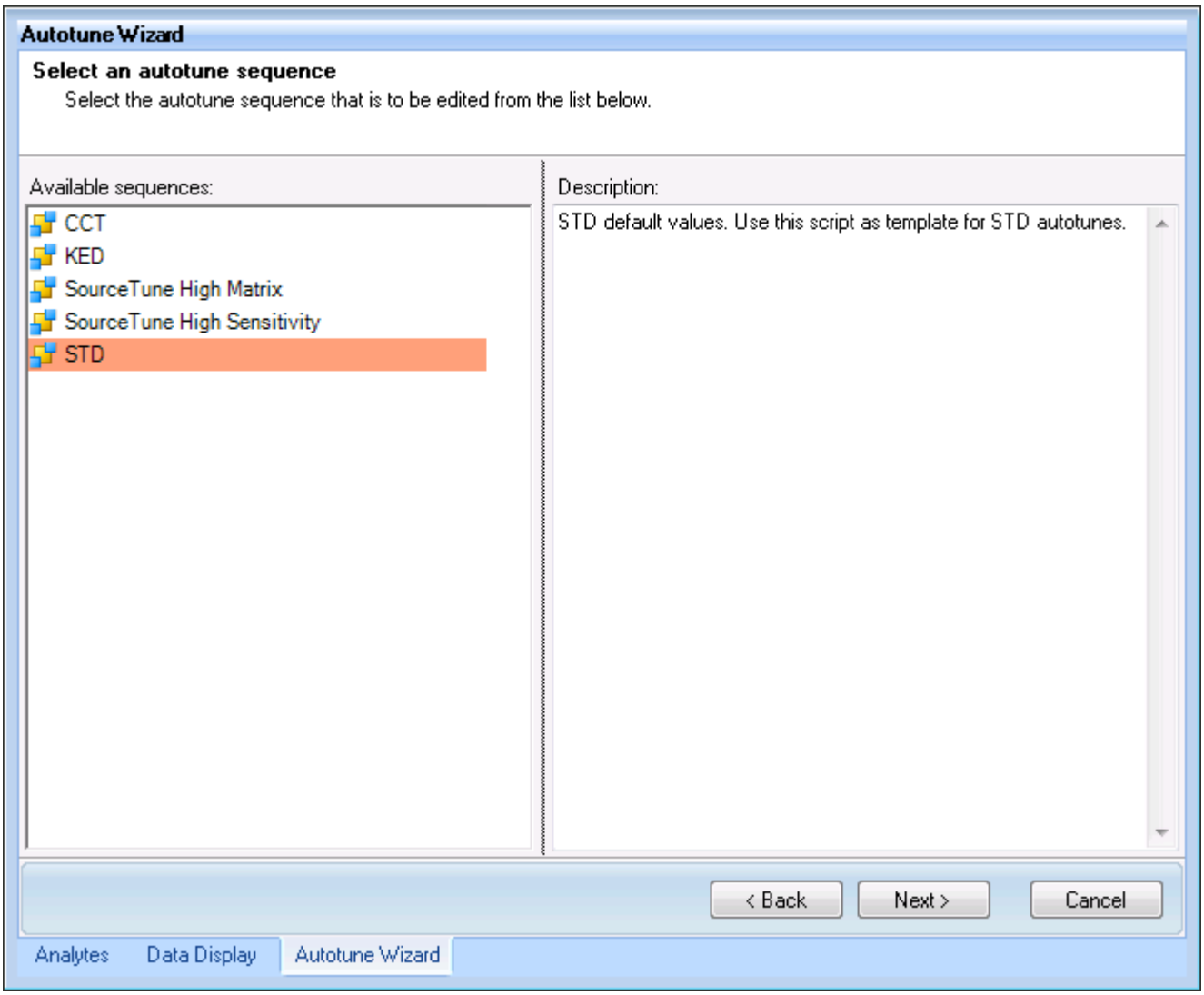


Figure 4-50. Select Autotune sequence in Autotune wizard

8. Click **Next**.

9. Select the controls and ranges for the autotune sequence, see Figure 4-51.

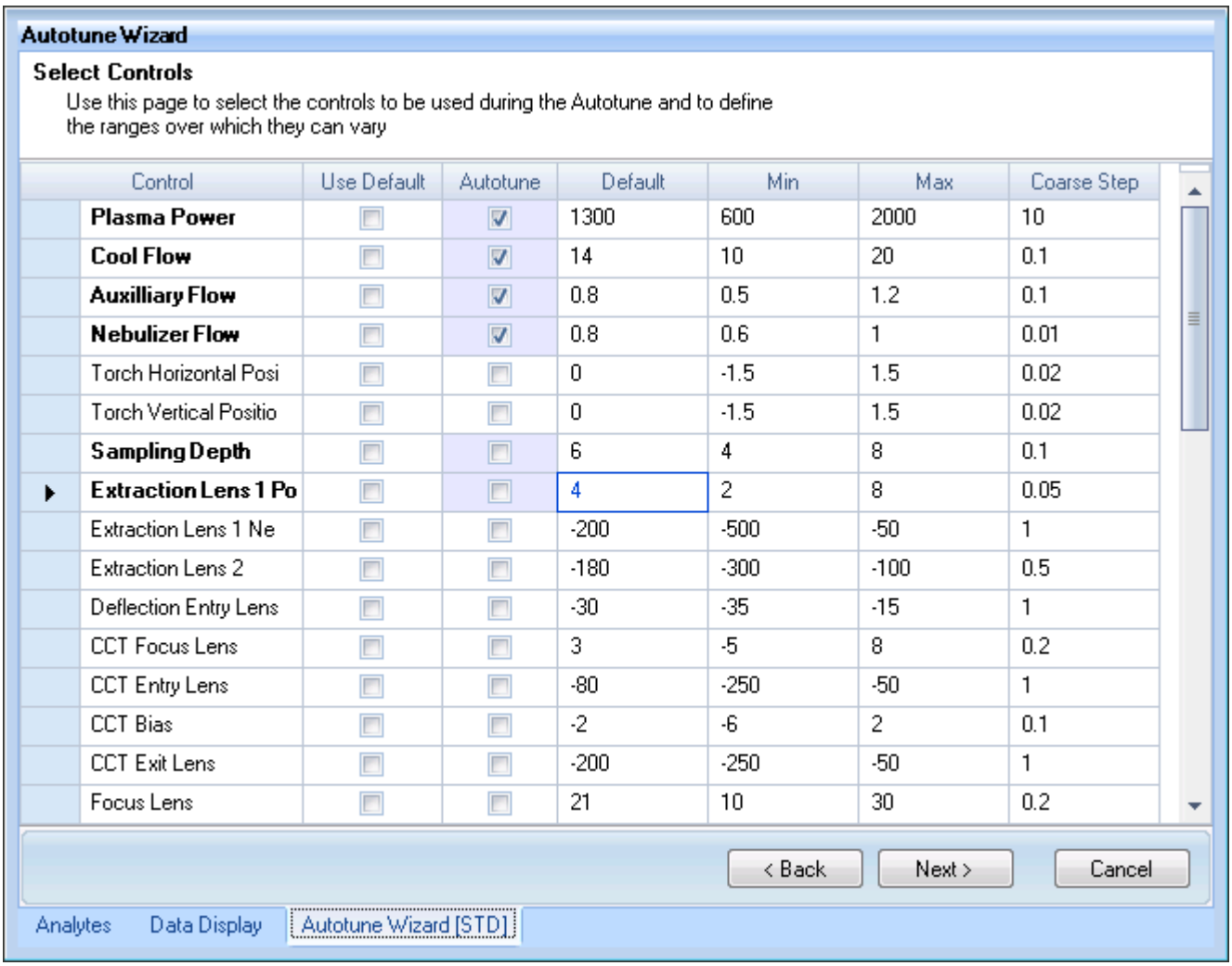


Figure 4-51. Select controls and ranges of sequence in Autotune wizard

10. Click **Next**.

11. Select the analytes to tune the instrument and select the dwell time for each, see Figure 4-52.

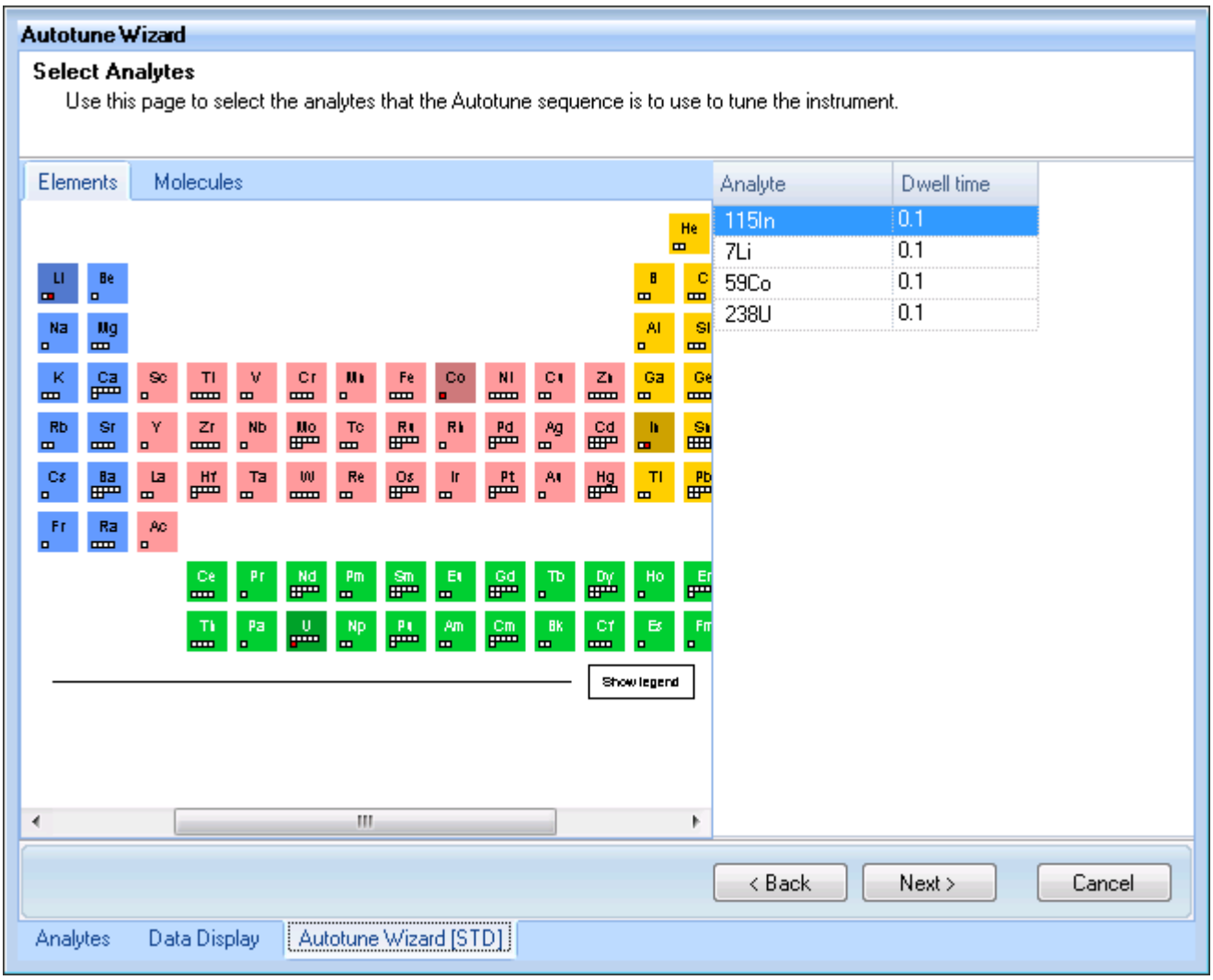


Figure 4-52. Select dwell time for analytes in Autotune wizard

12. Click **Next**.

13. Define ratios, see Figure 4-53.

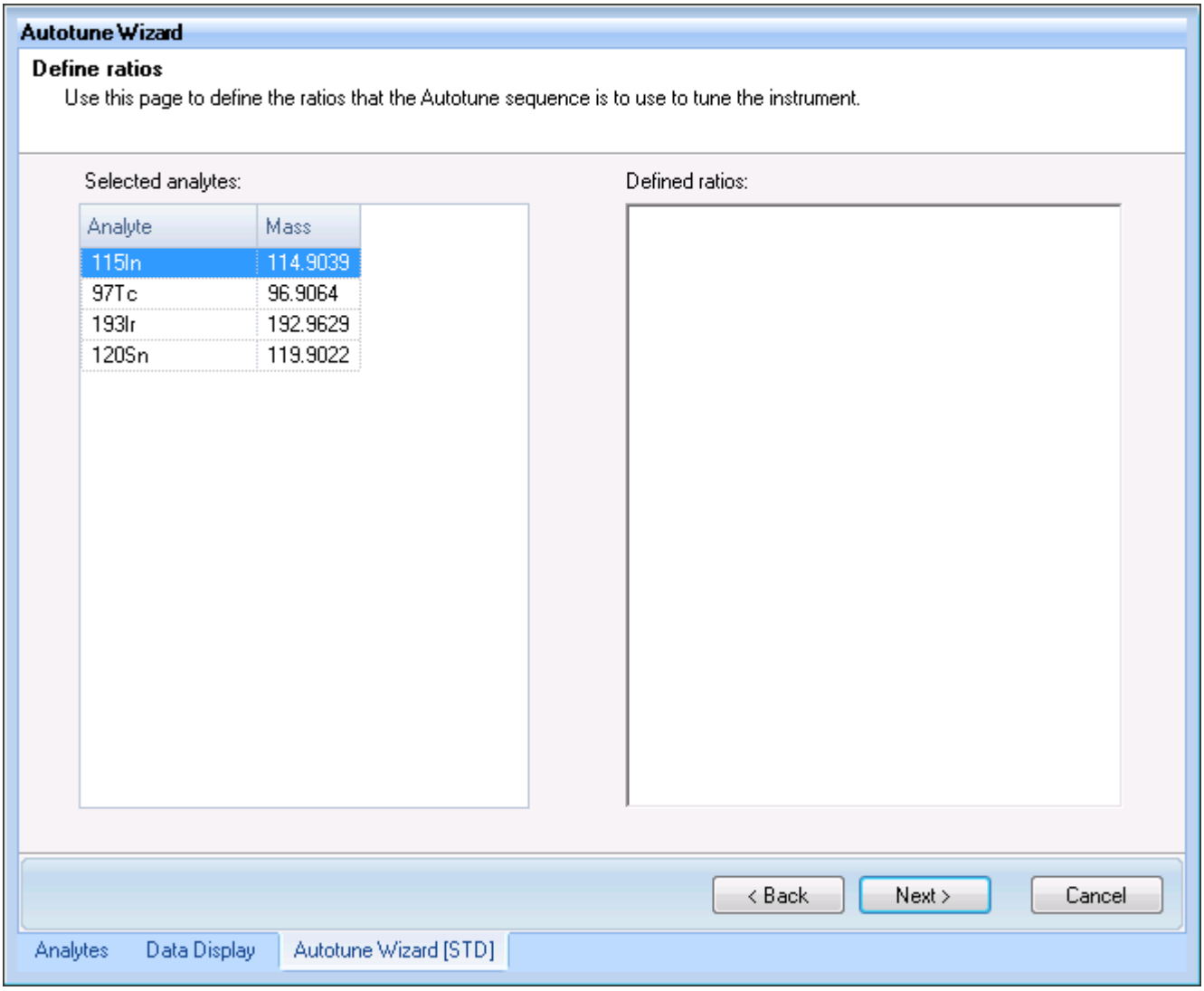


Figure 4-53. Define ratios in Autotune wizard

14. Click **Next**.

15. Define conditions for all stages and click **Next** each time, see Figure 4-54.

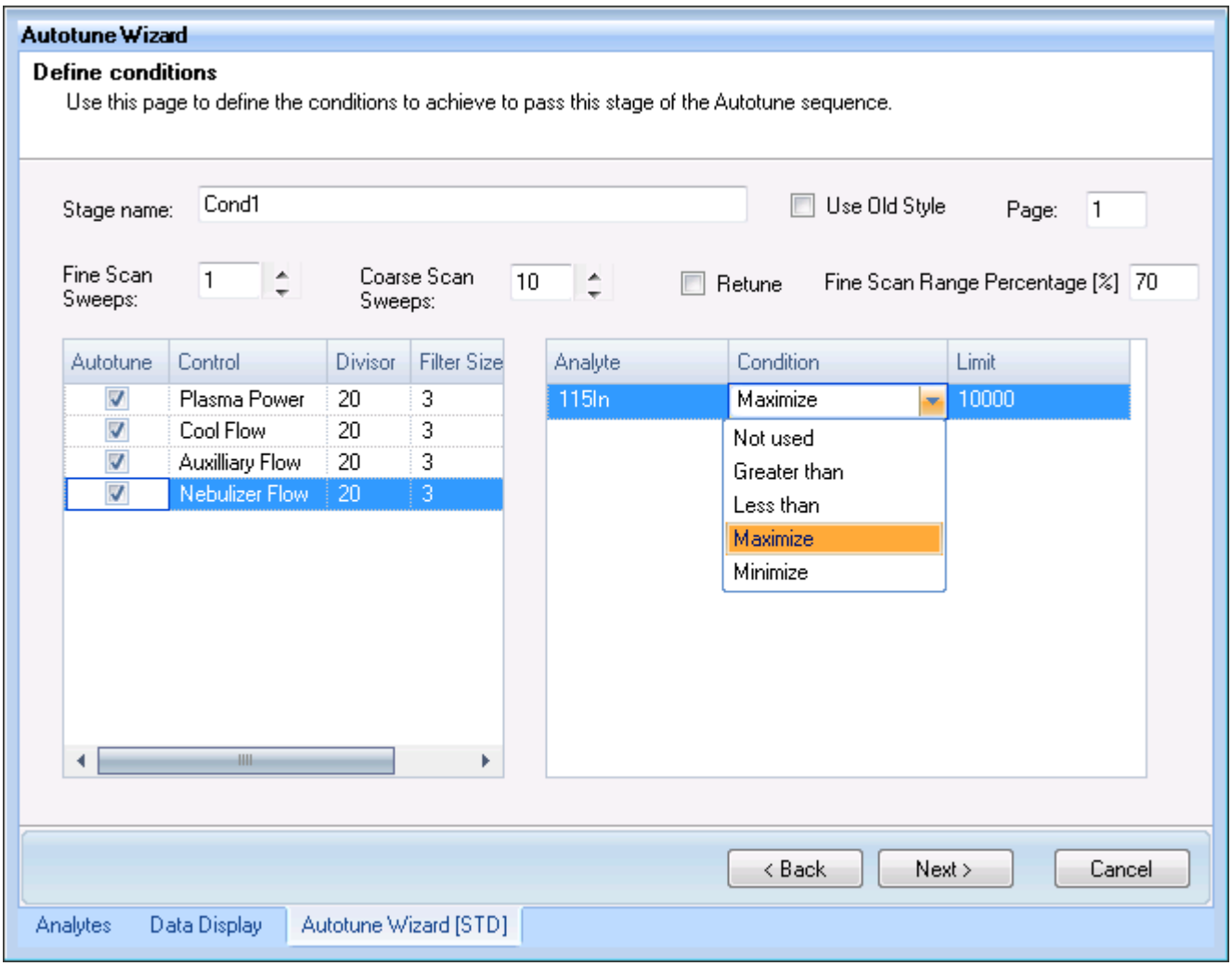


Figure 4-54. Define conditions for autotune sequence in Autotune wizard

16. Select an existing Autotune sequence from the list if you wish to overwrite it or enter a new name, see Figure 4-55.

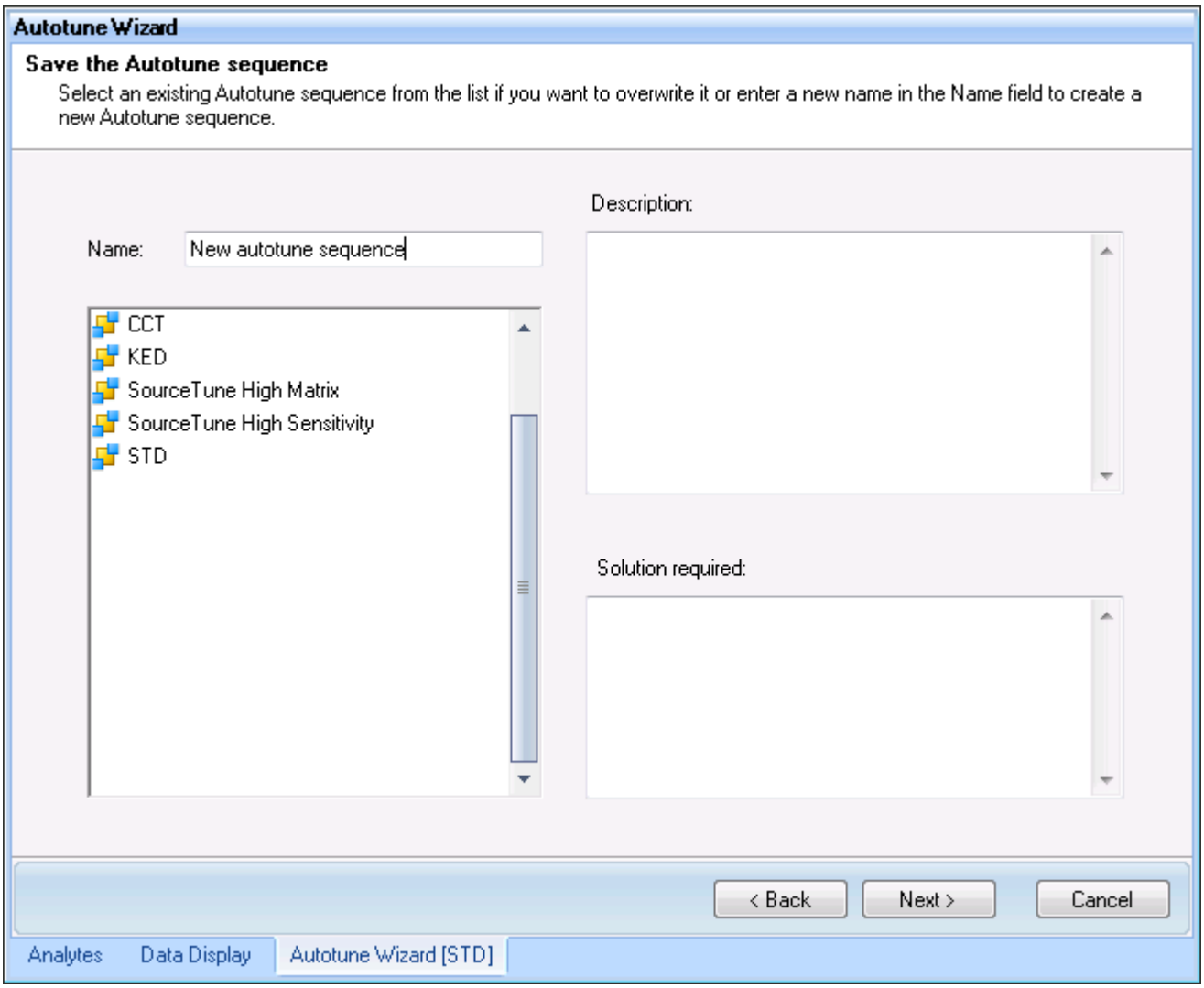


Figure 4-55. Define name for autotune sequence in Autotune wizard

17. Click **Next**, see Figure 4-56.

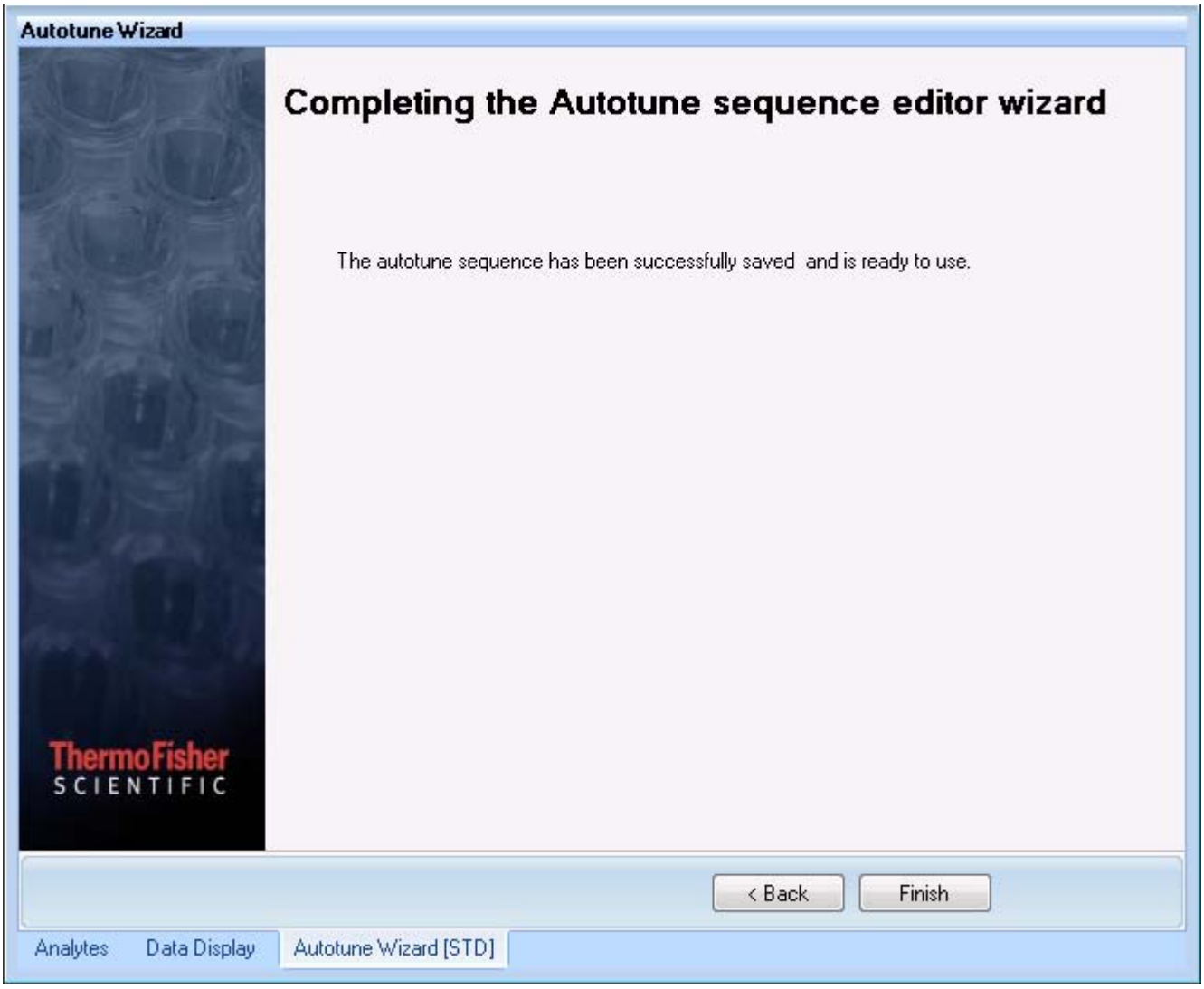


Figure 4-56. Autotune sequence is saved in Autotune wizard

18. Click **Finish** to close the wizard.

Source Autotune

The **Wizards** group of the **iCAP Q** ribbon tab in Instrument Control gives access to the **Source Autotune** wizard.

For the modi STD, CCT and KED, Source Autotune will be started with High Matrix, for STDS, CCTS and KEDS with High Sensitivity, or as defined, see "Editing a Measurement Mode" on page 4-17.

A source autotune is executed every time the Performance Report of the "Getting Ready" on page 5-7 function fails, that is, the performance of the instrument falls below the limits specified in the performance report,

although they can be performed more regularly if desired. Each Measurement mode has a defined autotune (with the same name) which you can modify.

❖ **To run the Source Autotune Wizard**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the **Wizard** group, click 

(arrow next to or below Autotune) to open the drop-down menu, see Figure 4-57.

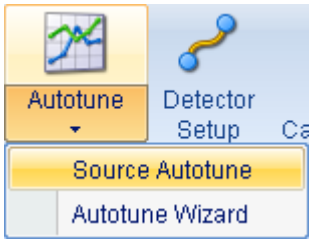


Figure 4-57. Drop-down Source Autotune

You can also directly click  to open the Source Autotune wizard.

4. Click **Source Autotune**.
   The **Source Autotune** wizard opens, see Figure 4-58.

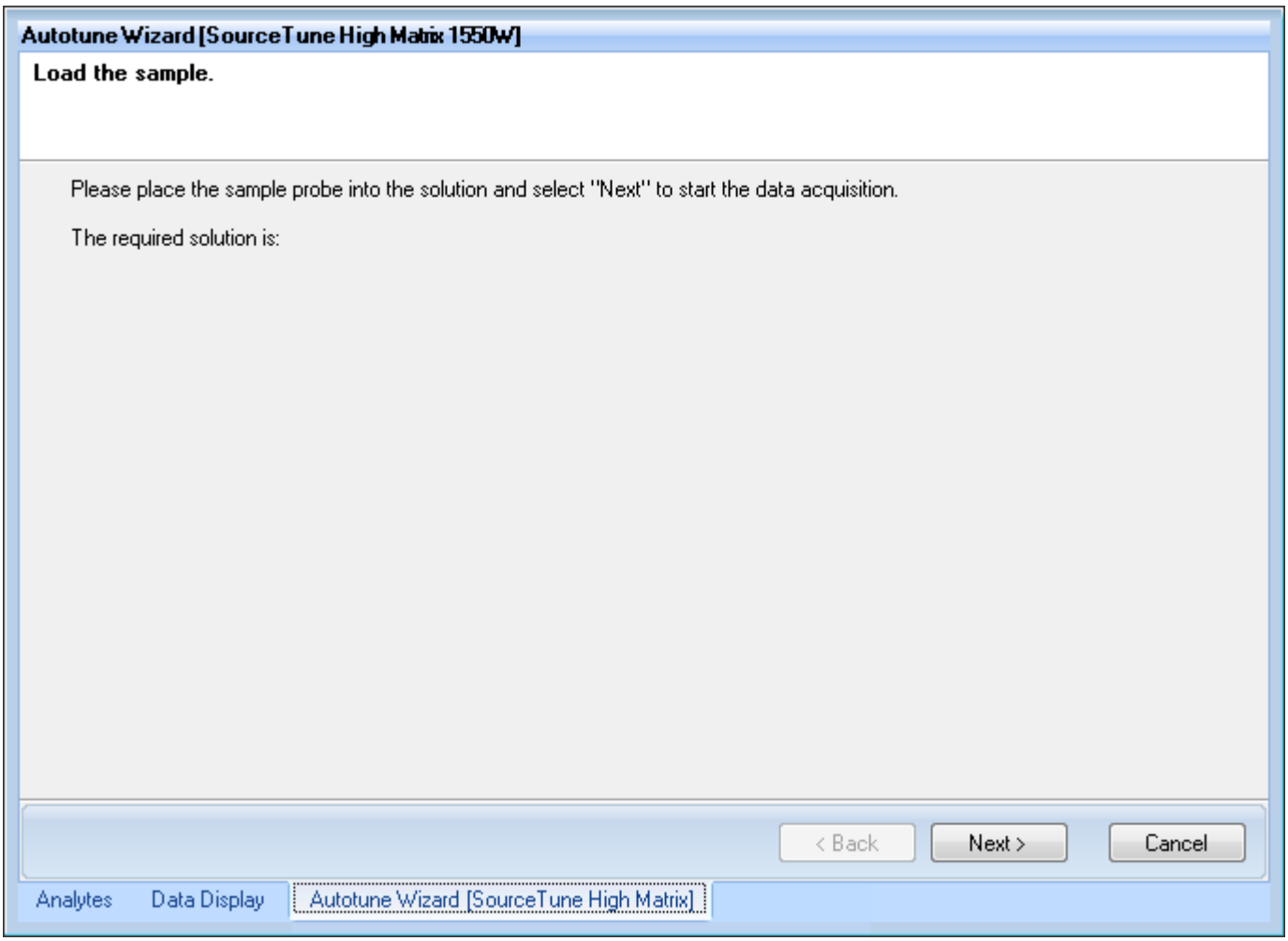


Figure 4-58. Start Source Autotune wizard

5. Load the tuning solution and click **Next**.
   The **Tune Data View** opens, see Figure 4-59.

Figure 4-59. Tune Data View Source Autotune wizard

The next **Tune Data View** is shown, see Figure 4-60.

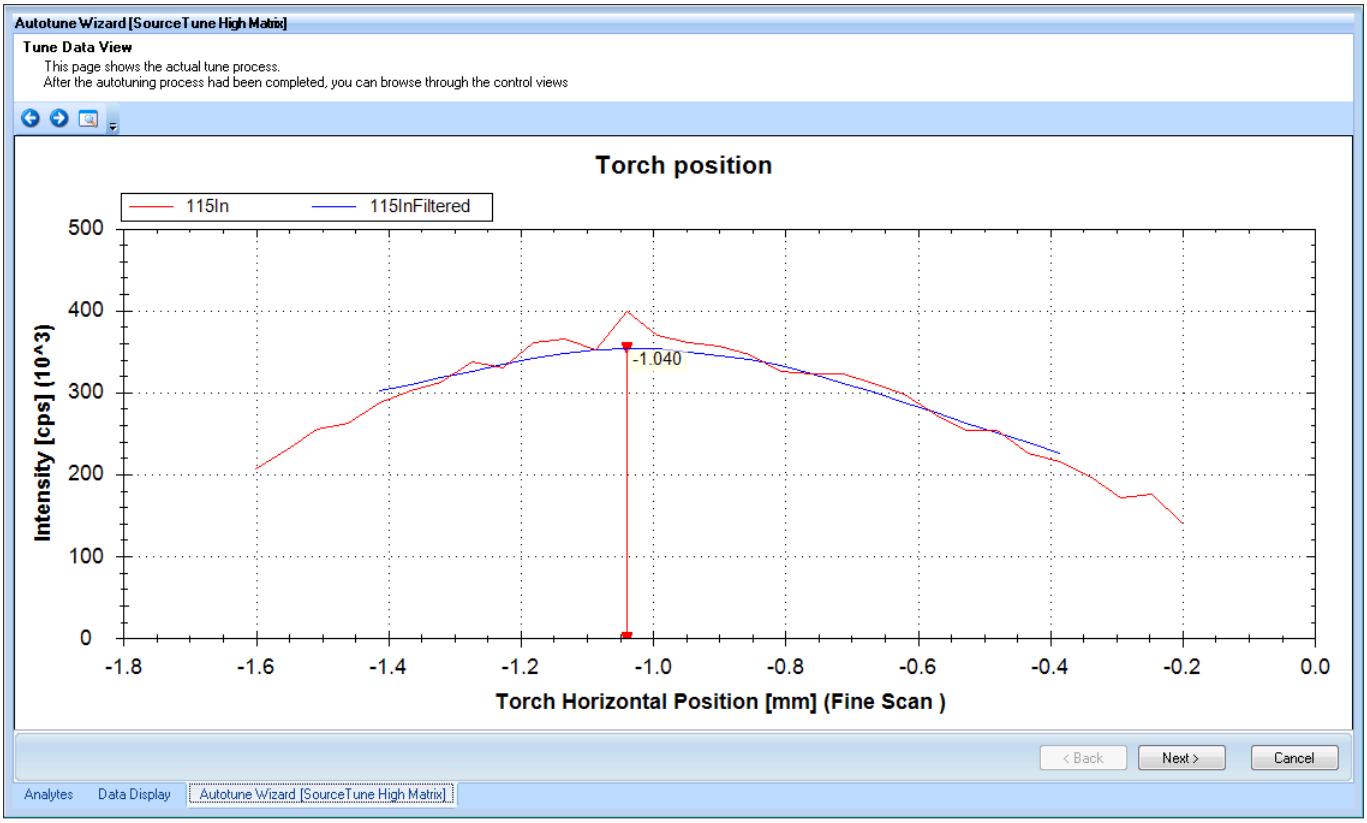


Figure 4-60. Tune Data View Source Autotune wizard

6. Click **Next**.
   The Acquisition Status window opens, see Figure 4-61.

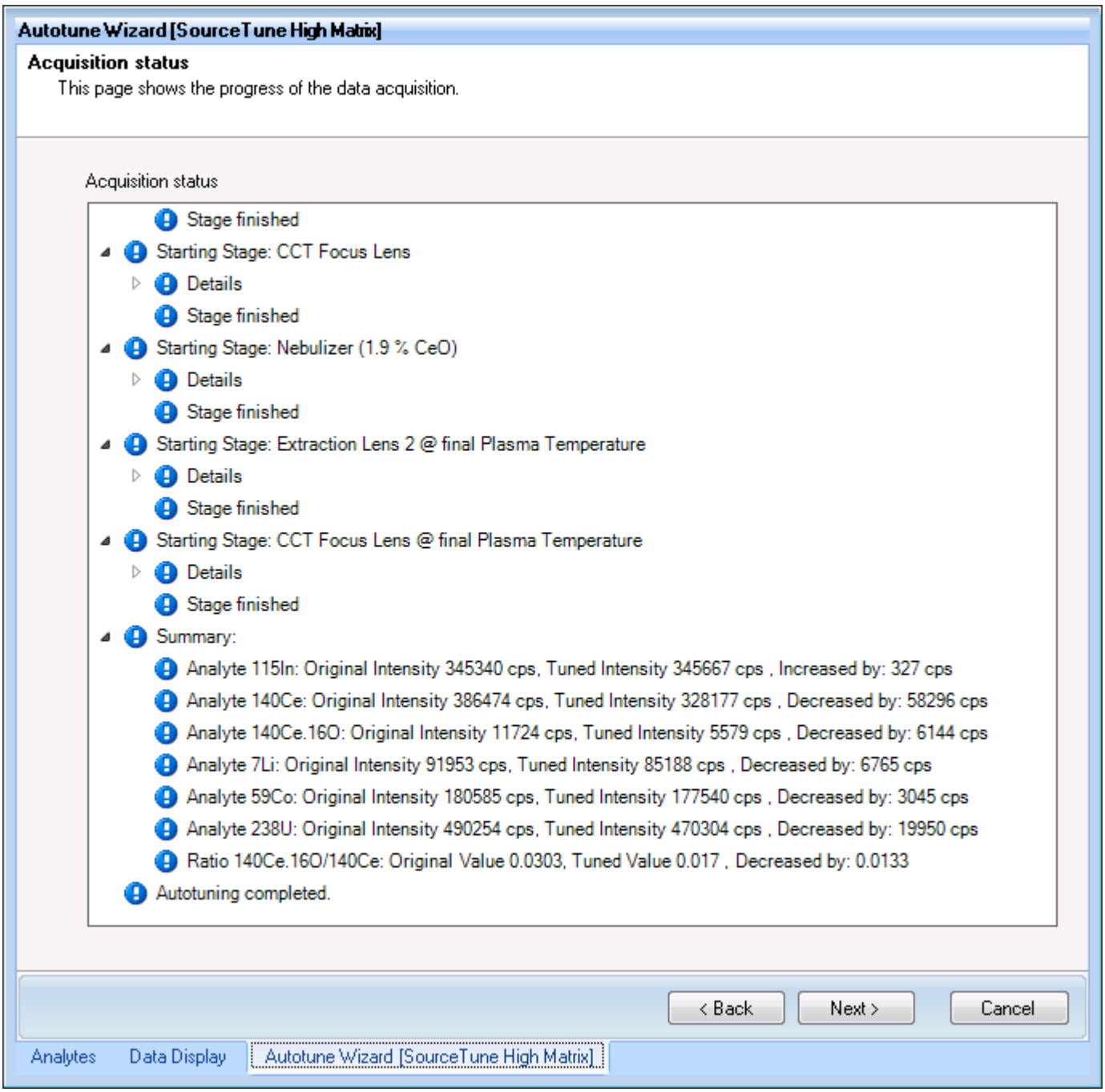


Figure 4-61. Acquisition Status Source Autotune wizard

7. Click **Next**.
   The Acquisition Status window opens, see Figure 4-62.

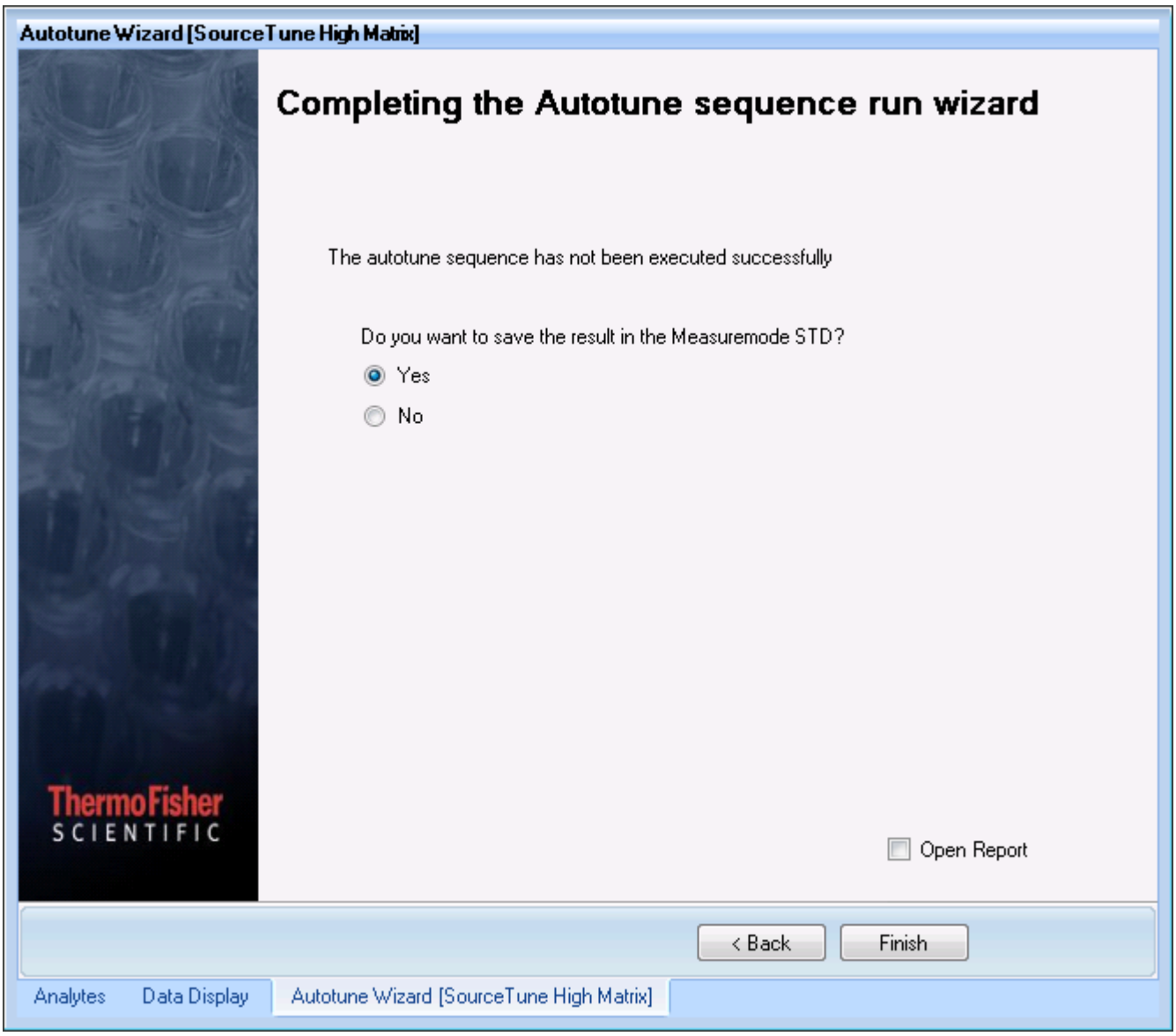


Figure 4-62. Completing Source Autotune wizard

8. Select **Yes** to save the results.
9. Select the check box **Open Report** if you wish to open the report.
10. Click **Finish**.

Detector Setup Wizard

The **Wizards** group of the **iCAP Q** ribbon tab in Instrument Control gives access to the **Detector Setup** wizard.

The detector set-up should only be performed when the instrument sensitivity is starting to decline. The procedure is performed on average once a month and typically, the automated procedure will increase the voltage applied to the pulse section of the detector so that it just lies on the plateau of a detector gain curve. The voltage of the analog section of the detector is normally also increased to ensure the cross calibration is accurate and maintained at a defined level.

❖ **To perform a detector cross calibration with the Detector Setup Wizard**

1. Click 

to open **Instrument Control**.
2. Be sure to change to STD/STDS mode before starting the wizard.
3. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

4. In the **Wizard** group, click 

.
The **Detector Setup Wizard** opens, see Figure 4-63.

Figure 4-63. Welcome to the Detector Setup Wizard

5. Select **Detector Cross Calibration**.

6. Click **Next**.
   The periodic table window opens, see Figure 4-64.

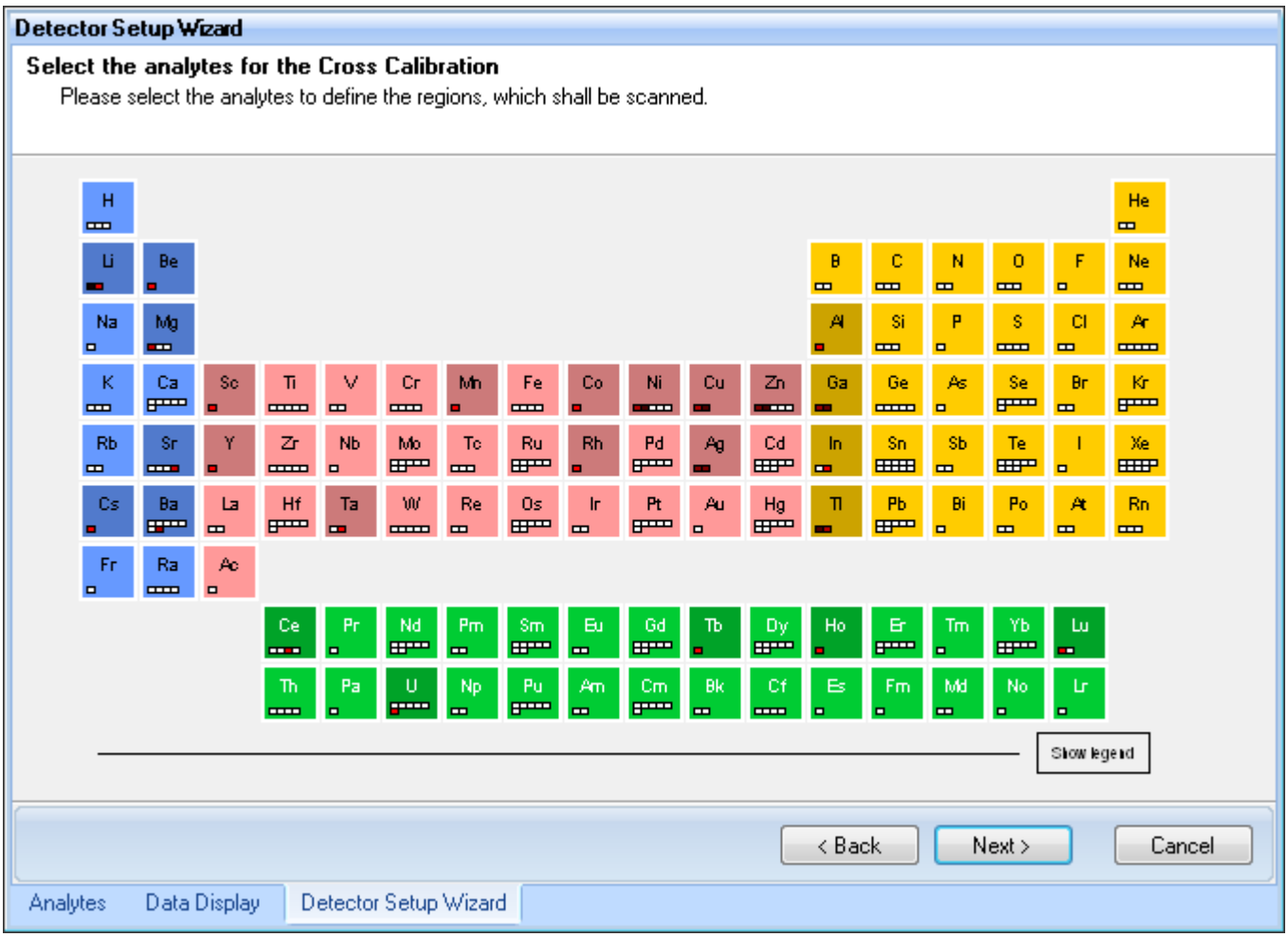


Figure 4-64. Select analytes for Detector Setup Wizard

7. Select your analytes.

8. Click **Next**.
   The Load the Sample window opens, see Figure 4-65.

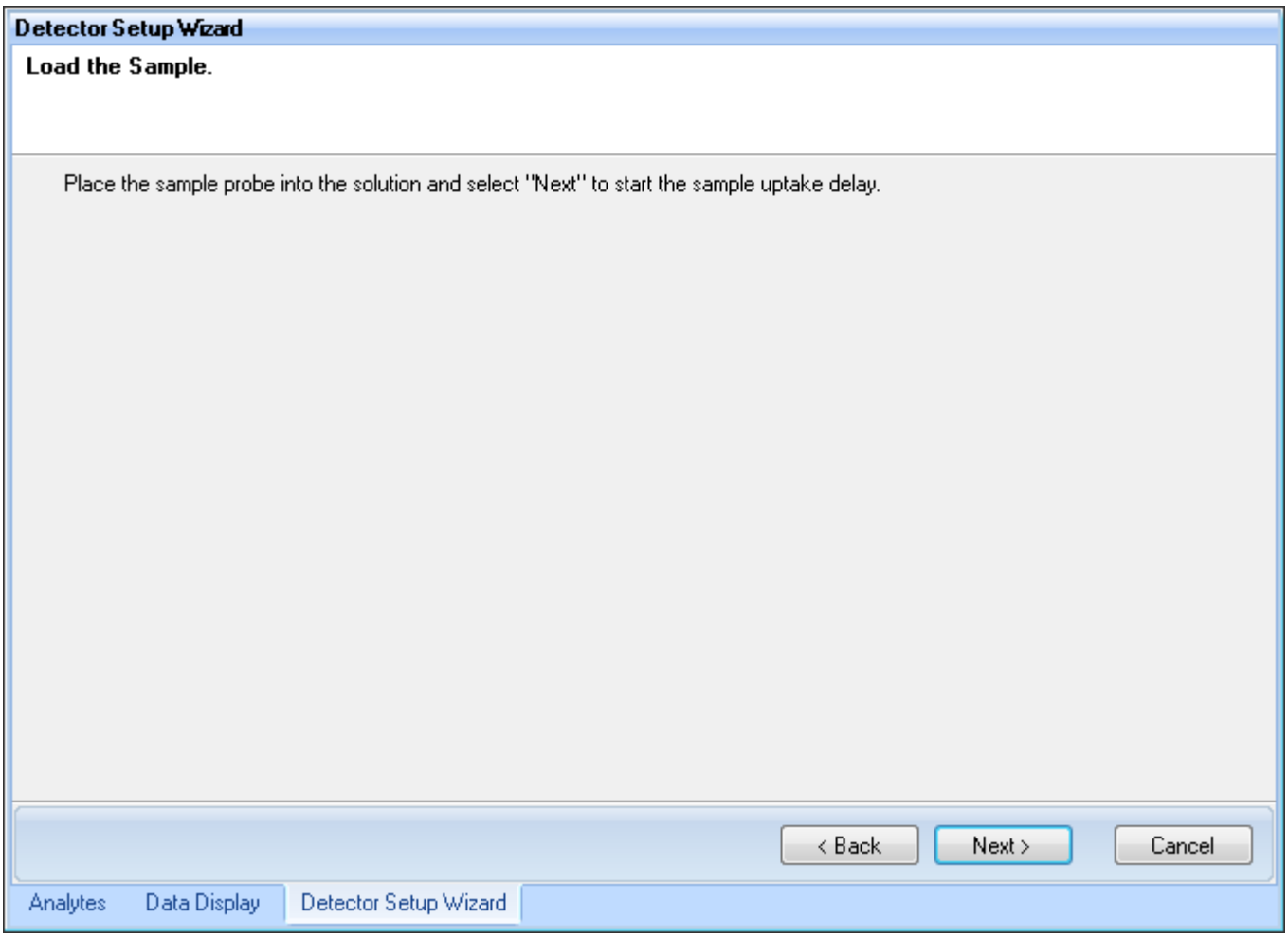


Figure 4-65. Load sample for Detector Setup Wizard

9. Place the probe into the setup solution.

10. Click **Next**.
    The **Waiting for sample uptake** window opens, see Figure 4-66.

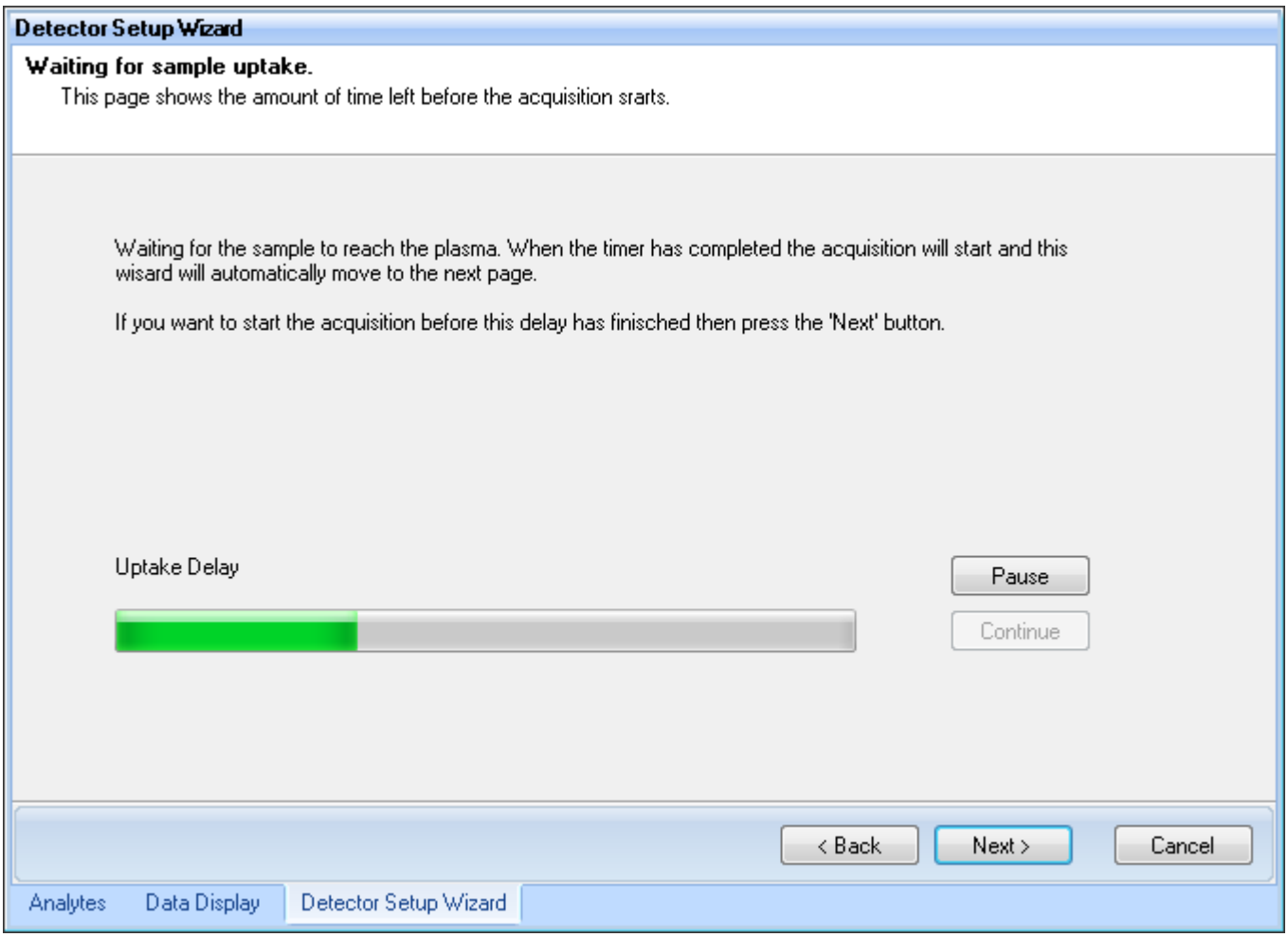


Figure 4-66. Waiting for sample uptake in Detector Setup Wizard

The Detector Setup wizard applies a minimum delay time for sample uptake in order to assure that enough sample has entered the plasma.

11. Click **Pause** to delay further if more time is needed.
    Click **Continue** when ready.

12. To begin the setup before the delay time elapsed, click **Next**.
    The Analog Offset Determination starts, see Figure 4-67.

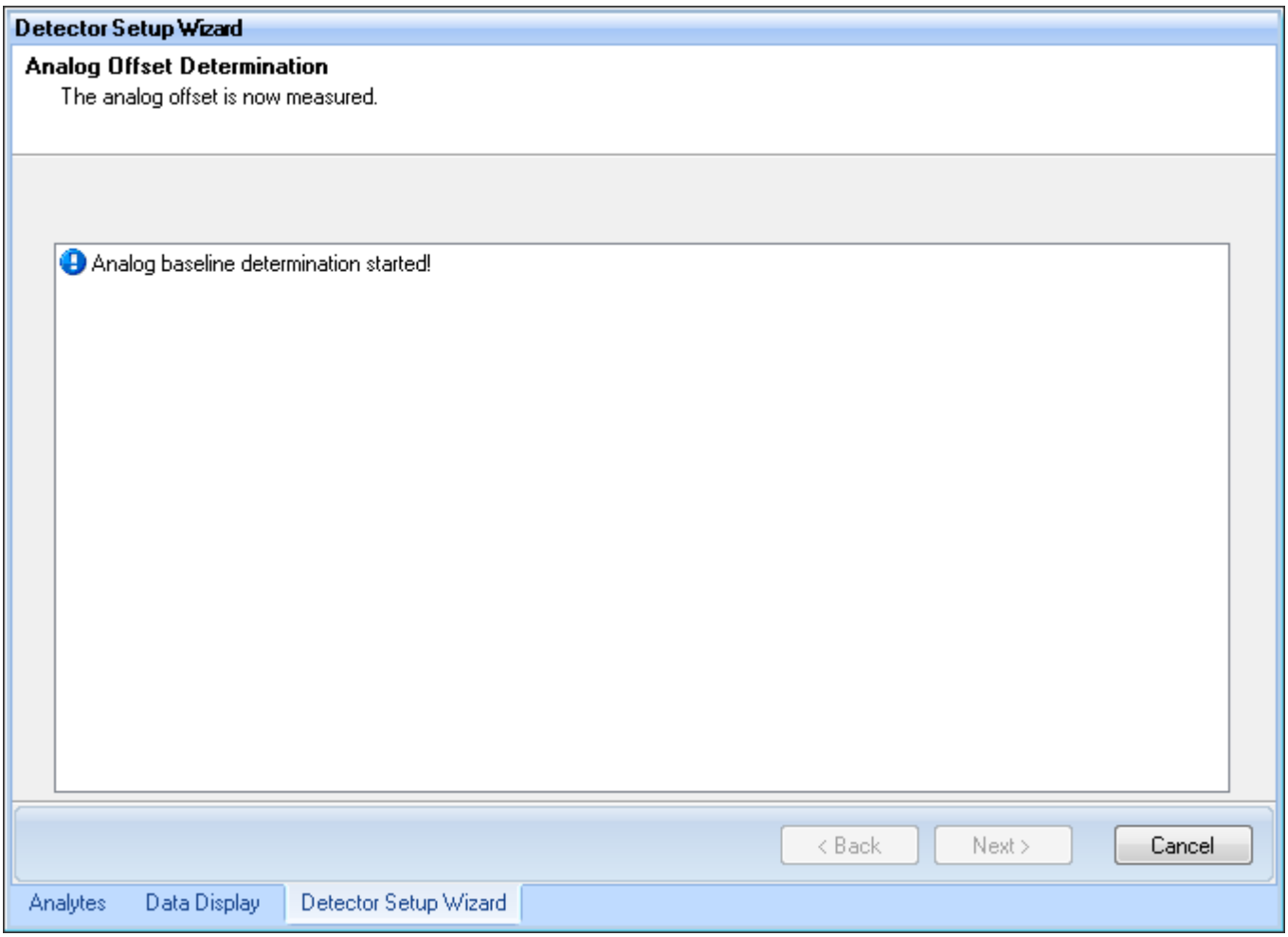


Figure 4-67. Analog Offset Determination in Detector Setup Wizard

The Cross Calibration starts, see Figure 4-68.

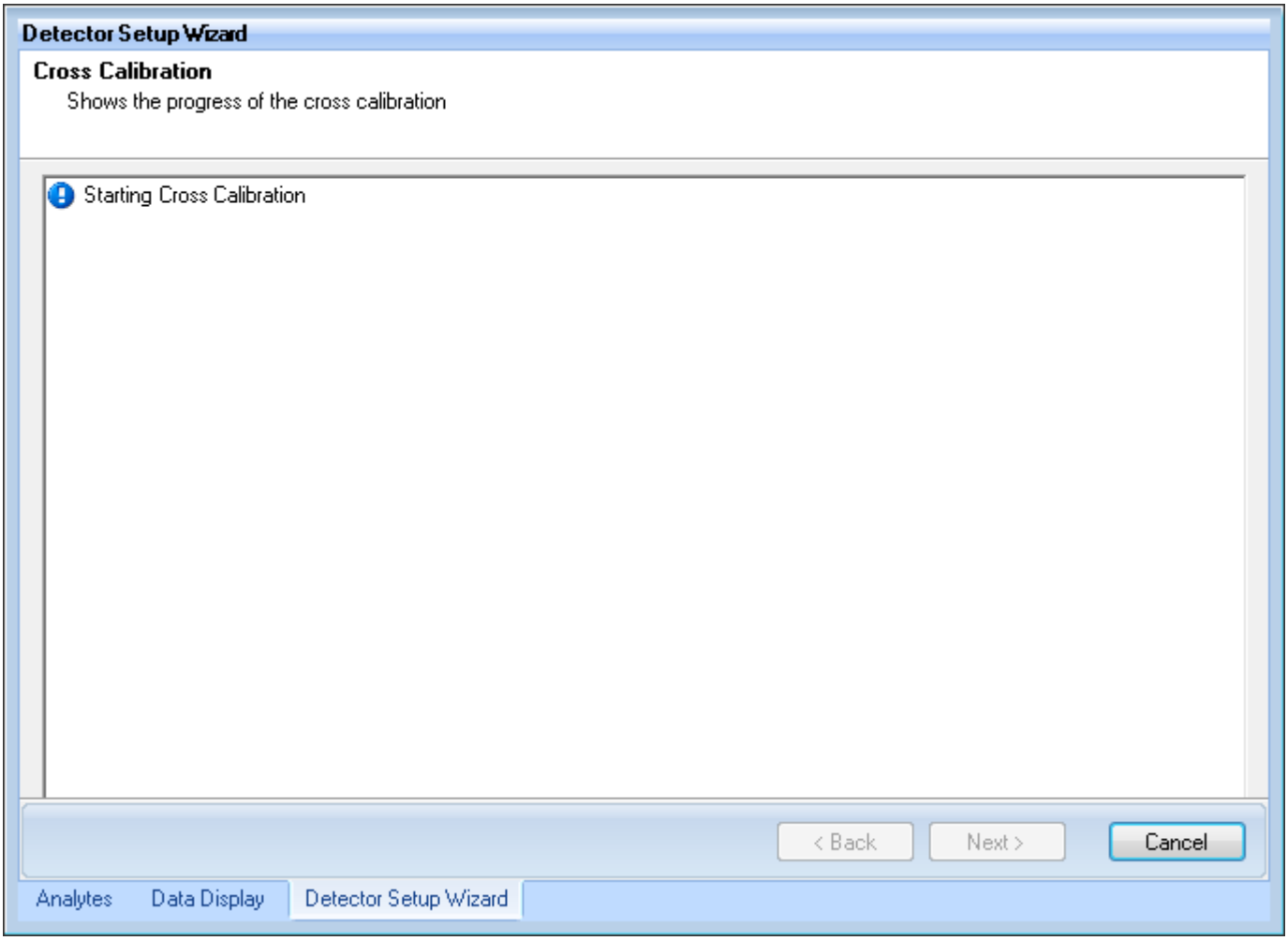


Figure 4-68. Cross Calibration starts in Detector Setup Wizard

The progress of the Cross Calibration is shown, see Figure 4-69.

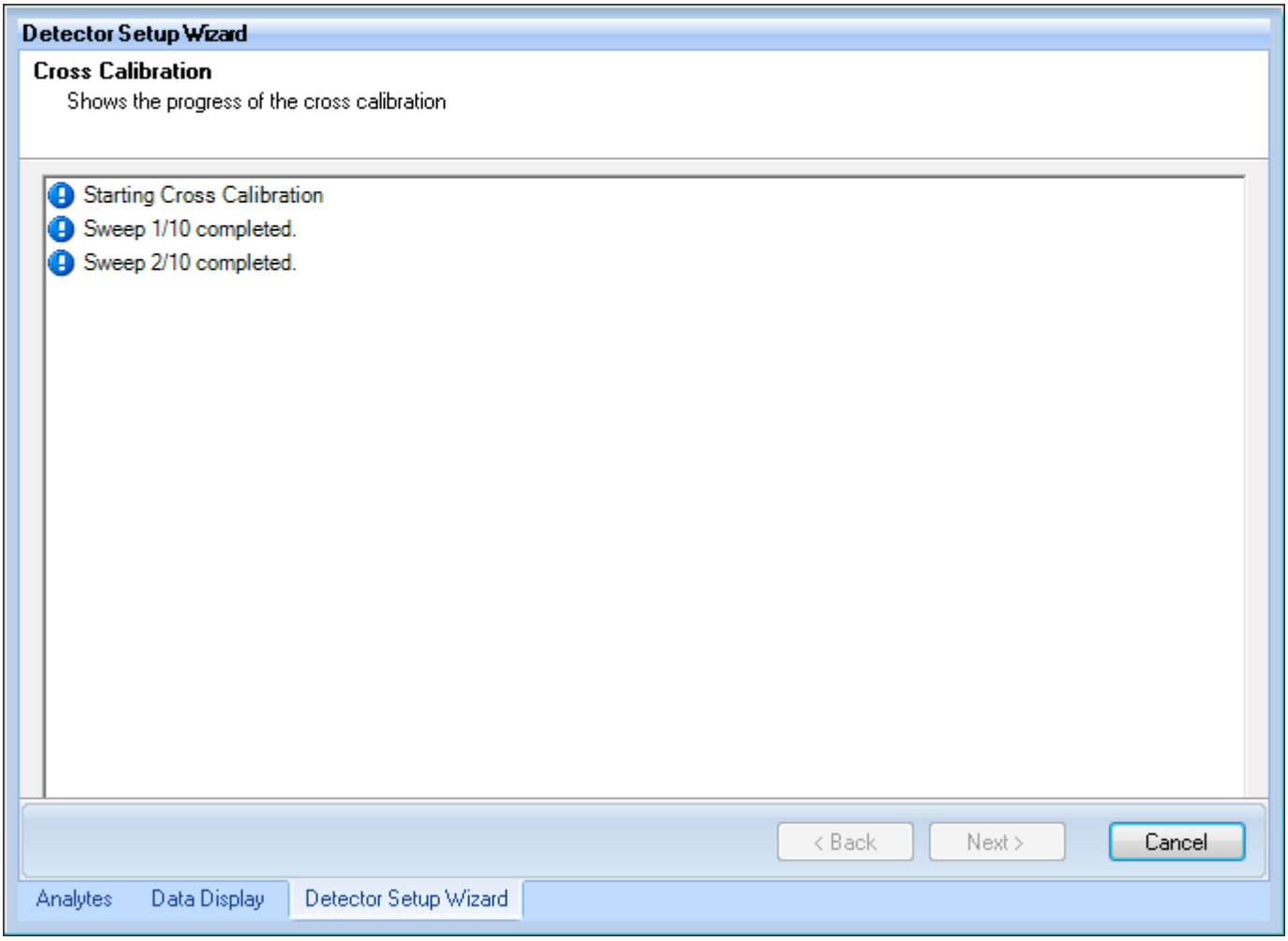


Figure 4-69. Progress of Cross Calibration

13. Click **Next** when the button is activated.
    The summary of the Detector Setup is shown, see Figure 4-70.

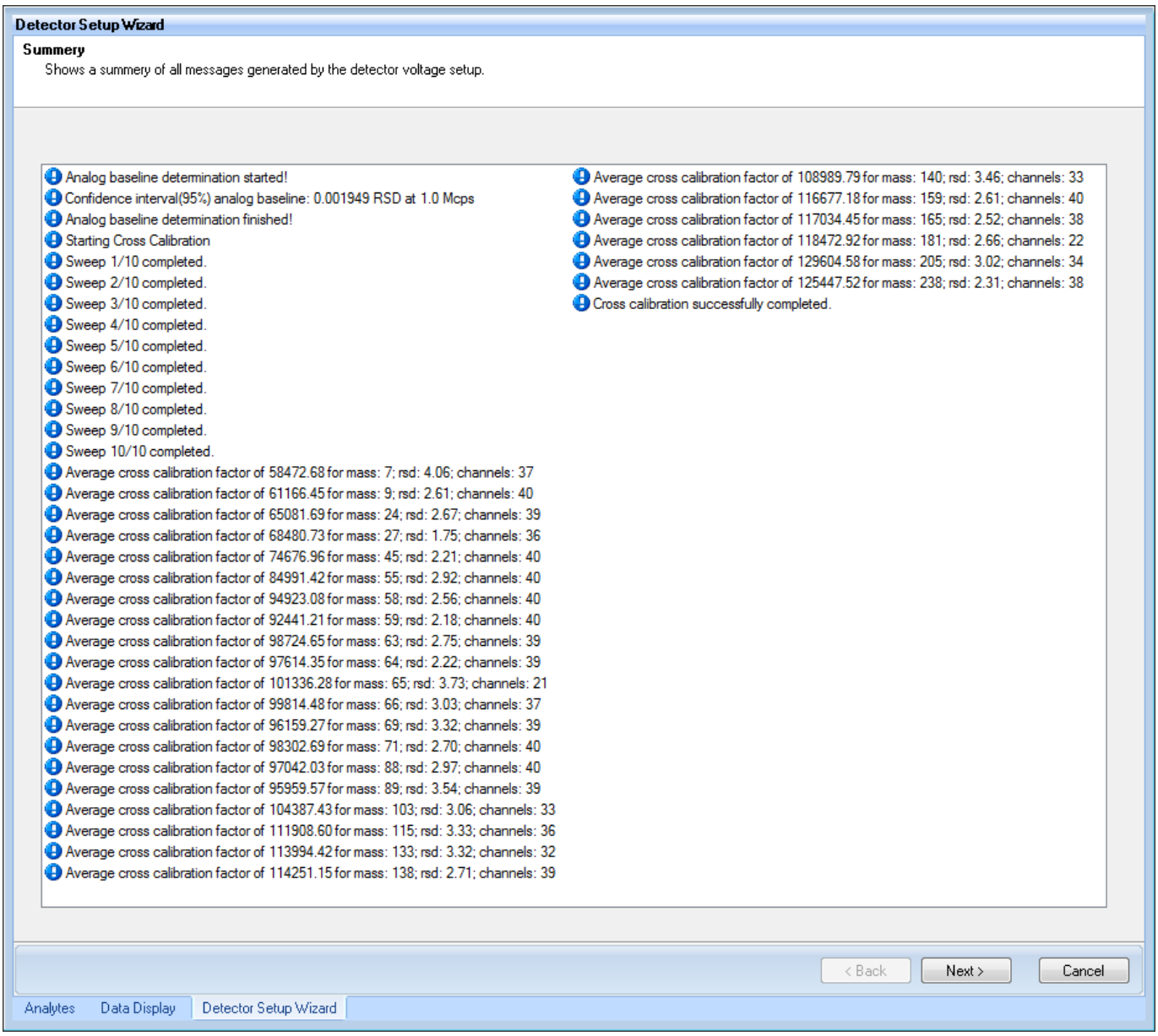


Figure 4-70. Detector Setup summary in wizard

14. Click **Next**, see Figure 4-71.

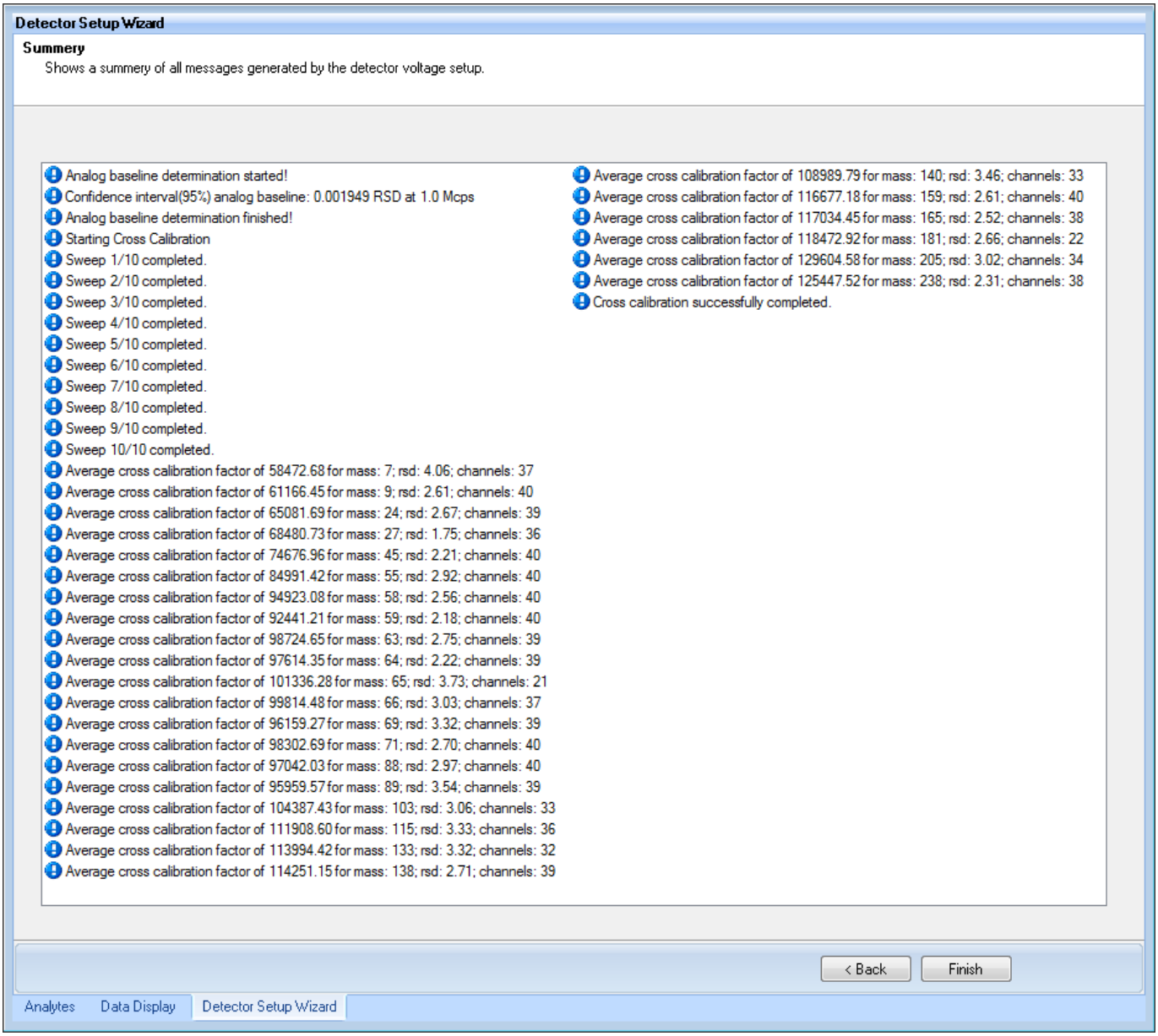


Figure 4-71. Cross calibration completed in wizard

15. Click **Finish** to store the calibration factors and leave the Detector Setup.

❖ **To perform a detector high voltage setup and cross calibration with the Detector Setup Wizard**

1. Click to open **Instrument Control**.
2. Be sure to change to STD/STDS mode before starting the wizard.

3. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

4. In the **Wizard** group, click 

.
   The **Detector Setup Wizard** opens, see Figure 4-72.

Figure 4-72. Welcome to the Detector Setup Wizard

5. Select **Detector HV Setup and Cross Calibration**.

6. Click **Next**.
   The periodic table window opens, see Figure 4-73.

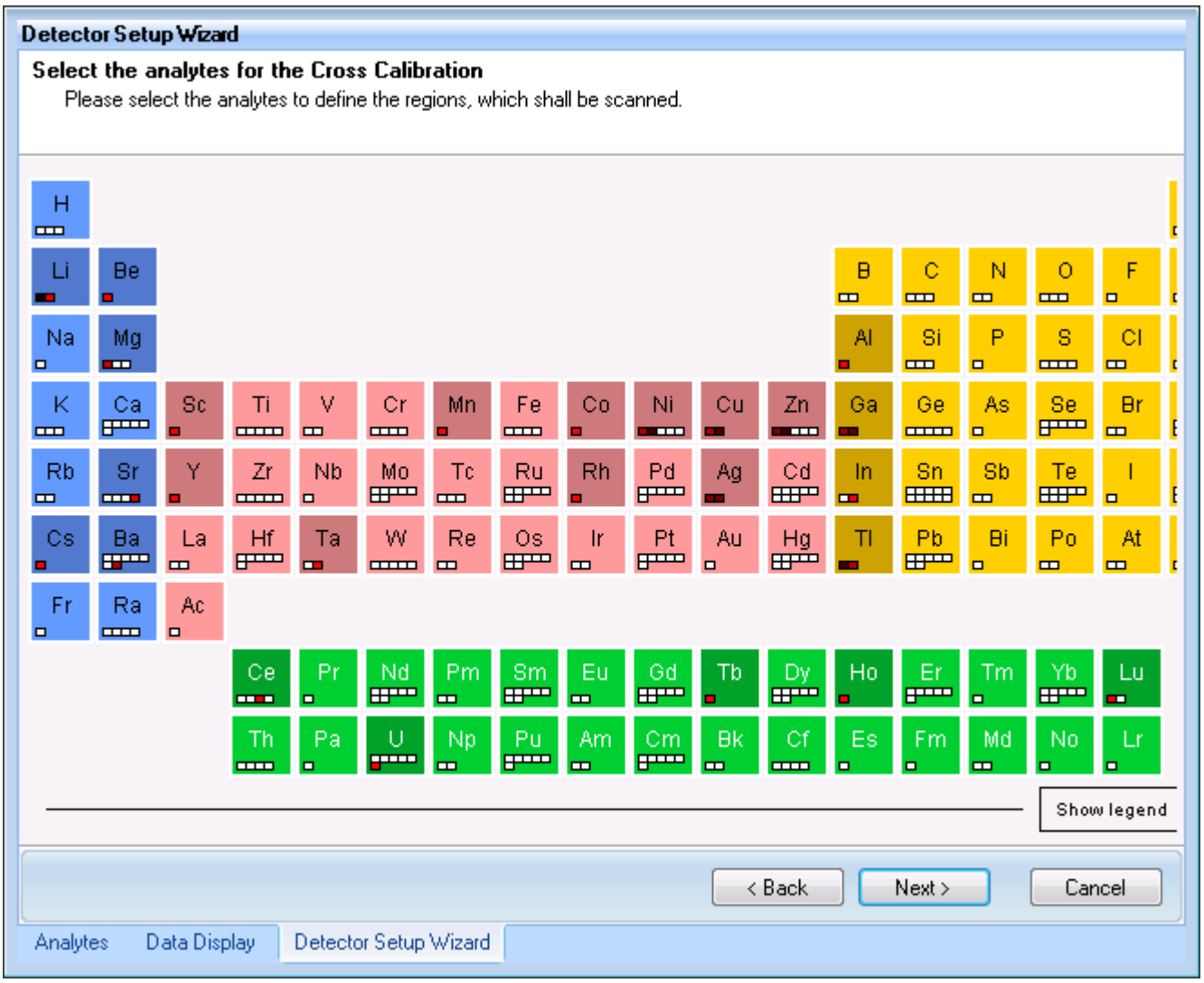


Figure 4-73. Select analytes for Detector Setup Wizard

7. Select your analytes.

8. Click **Next**.
   The Load the Sample window opens, see Figure 4-74.

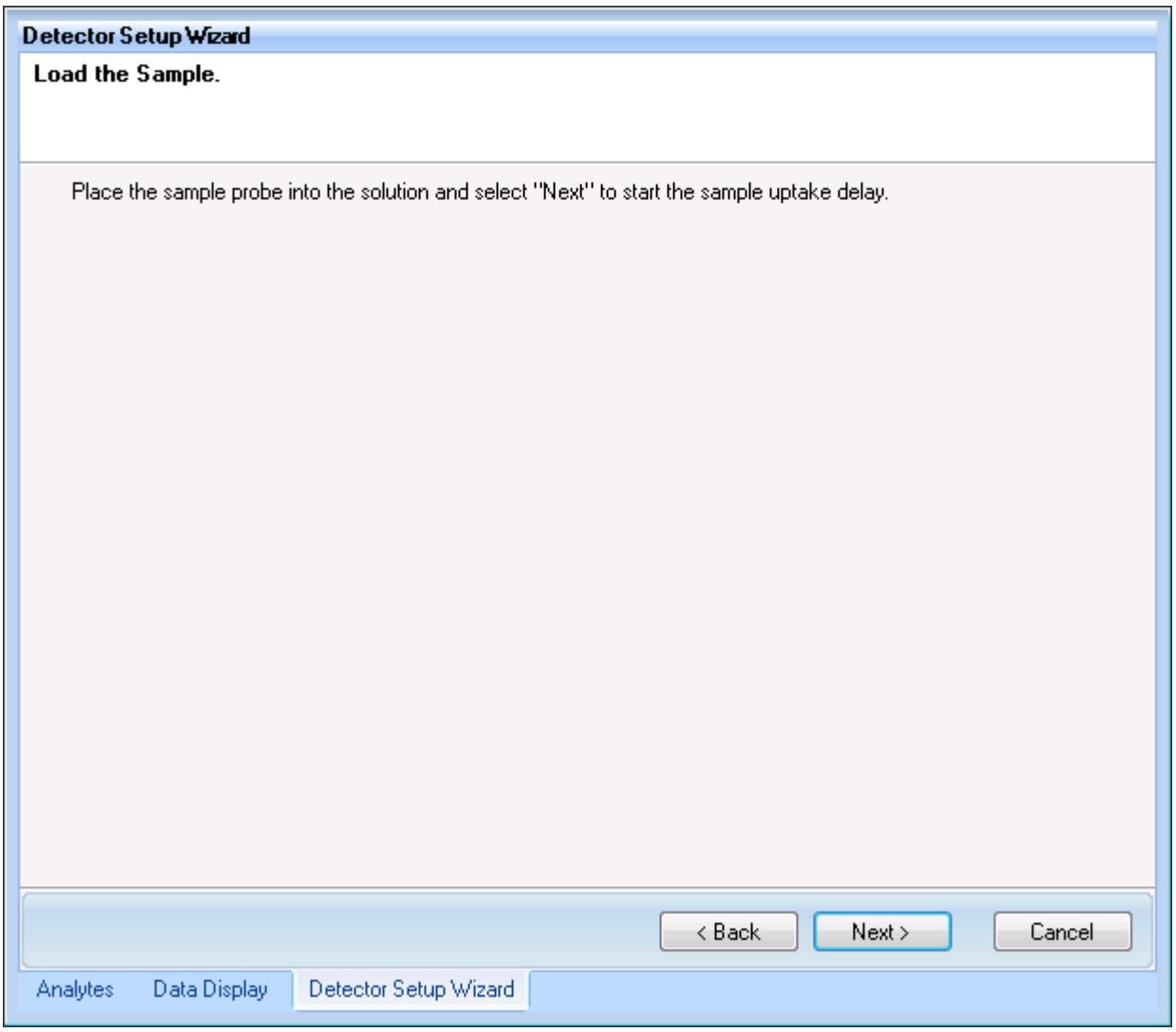


Figure 4-74. Load sample for Detector Setup Wizard

9. Place the probe into the setup solution.

10. Click **Next**.
    The **Waiting for sample uptake** window opens, see Figure 4-75.

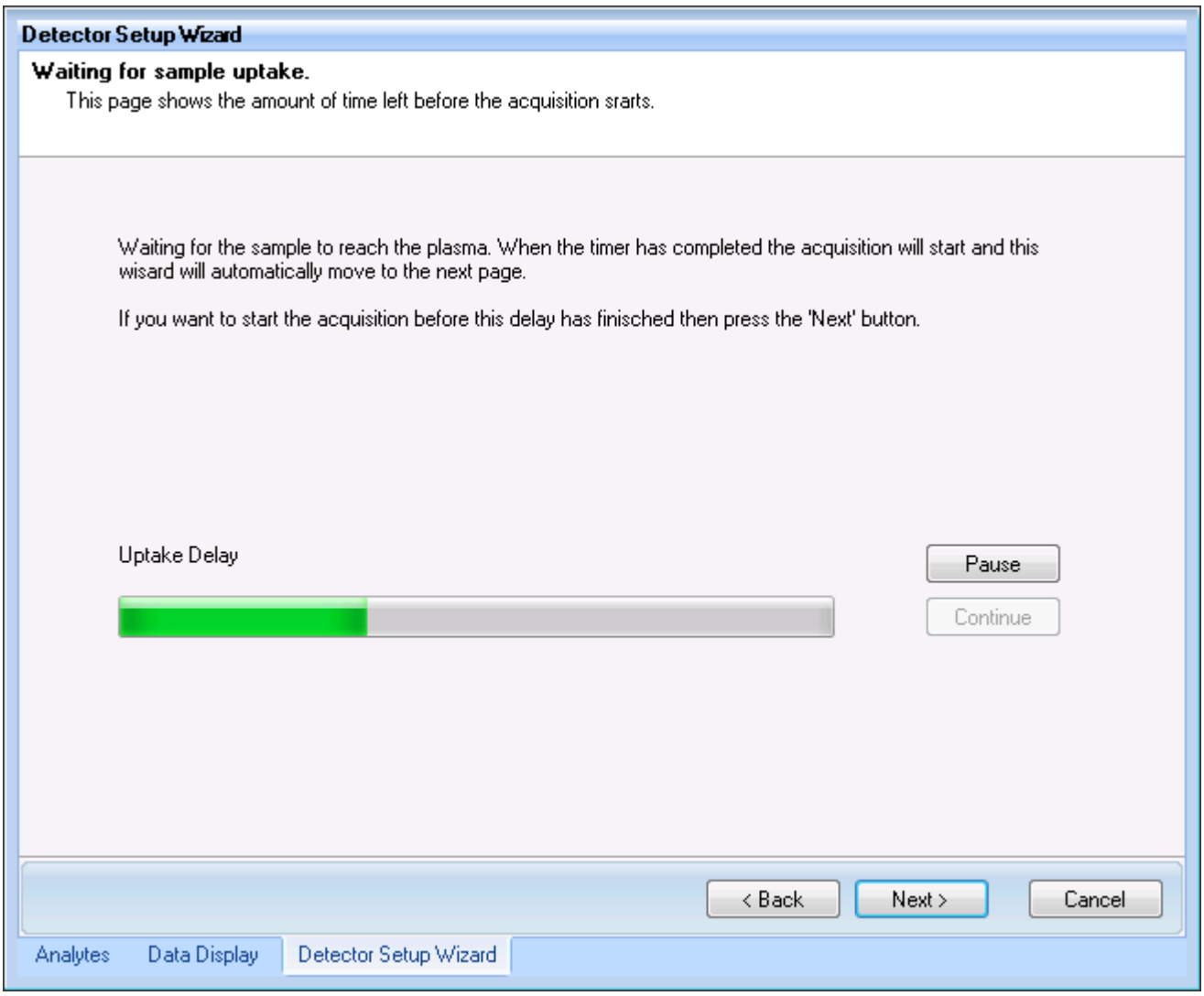


Figure 4-75. Waiting for sample uptake in Detector Setup Wizard

The Detector Setup wizard applies a minimum delay time for sample uptake in order to assure that enough sample has entered the plasma.

11. Click **Pause** to delay further if more time is needed.
    Click **Continue** when ready.

12. To begin the setup before the delay time elapsed, click **Next**.
    The analog baseline determination starts, see Figure 4-76.

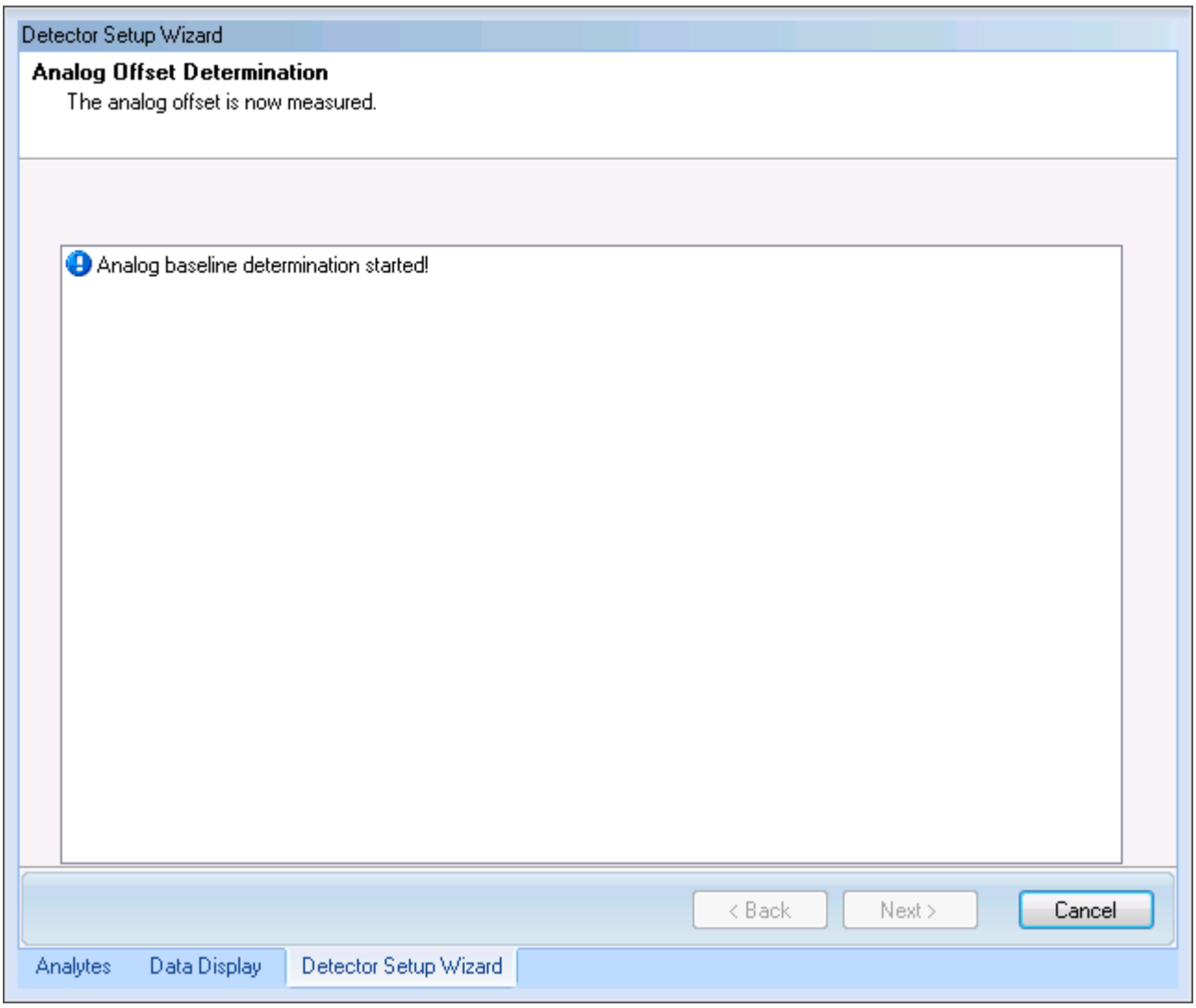


Figure 4-76. Analog baseline determination in Detector Setup Wizard

The Analog baseline determination is followed by a coarse and fine adjustment of the detector voltages, see Figure 4-77.

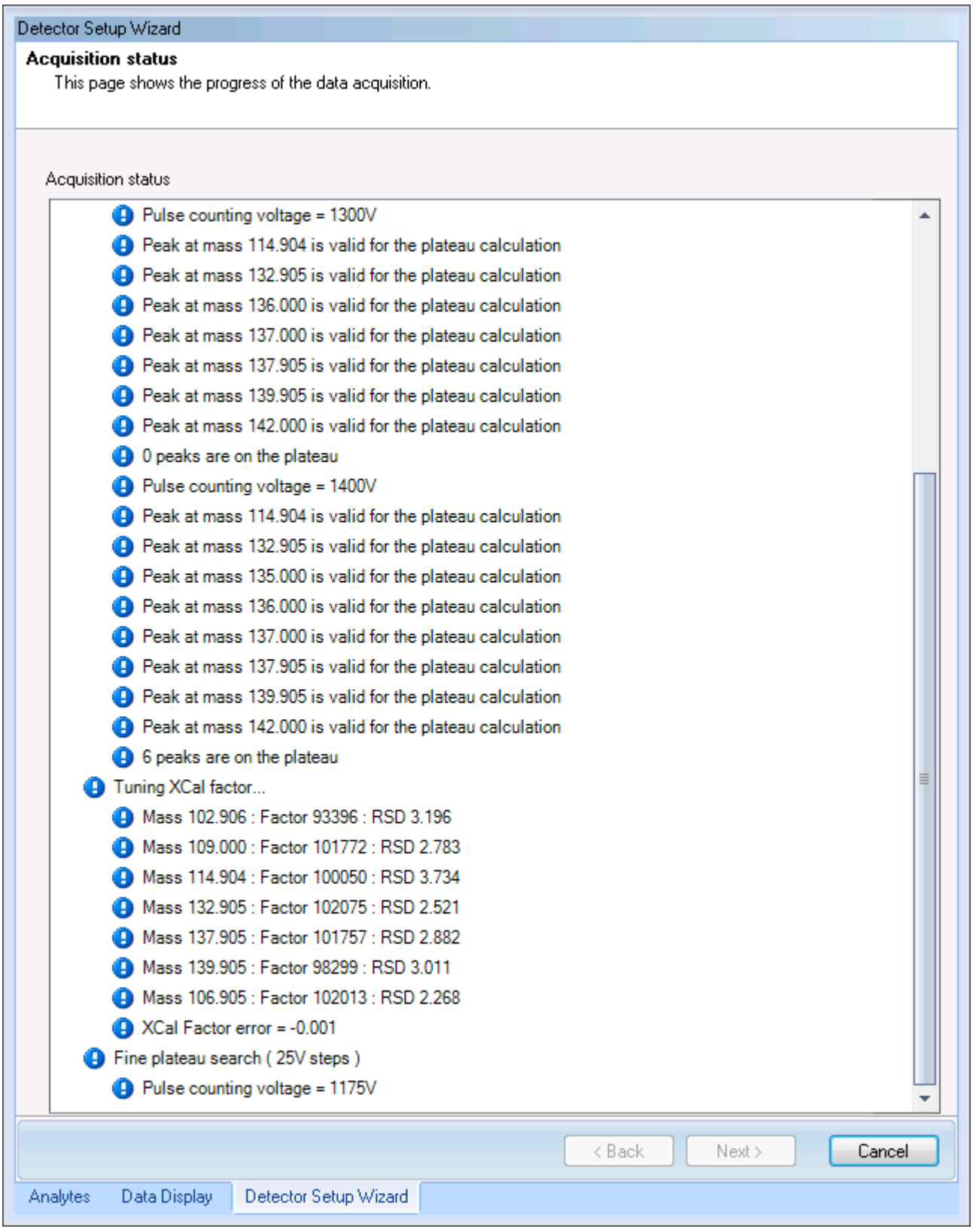


Figure 4-77. Coarse and fine adjustment of detector voltage

Afterwards a cross calibration factor determination is performed. The summary of the detector HV setup and cross calibration is shown, see Figure 4-78.

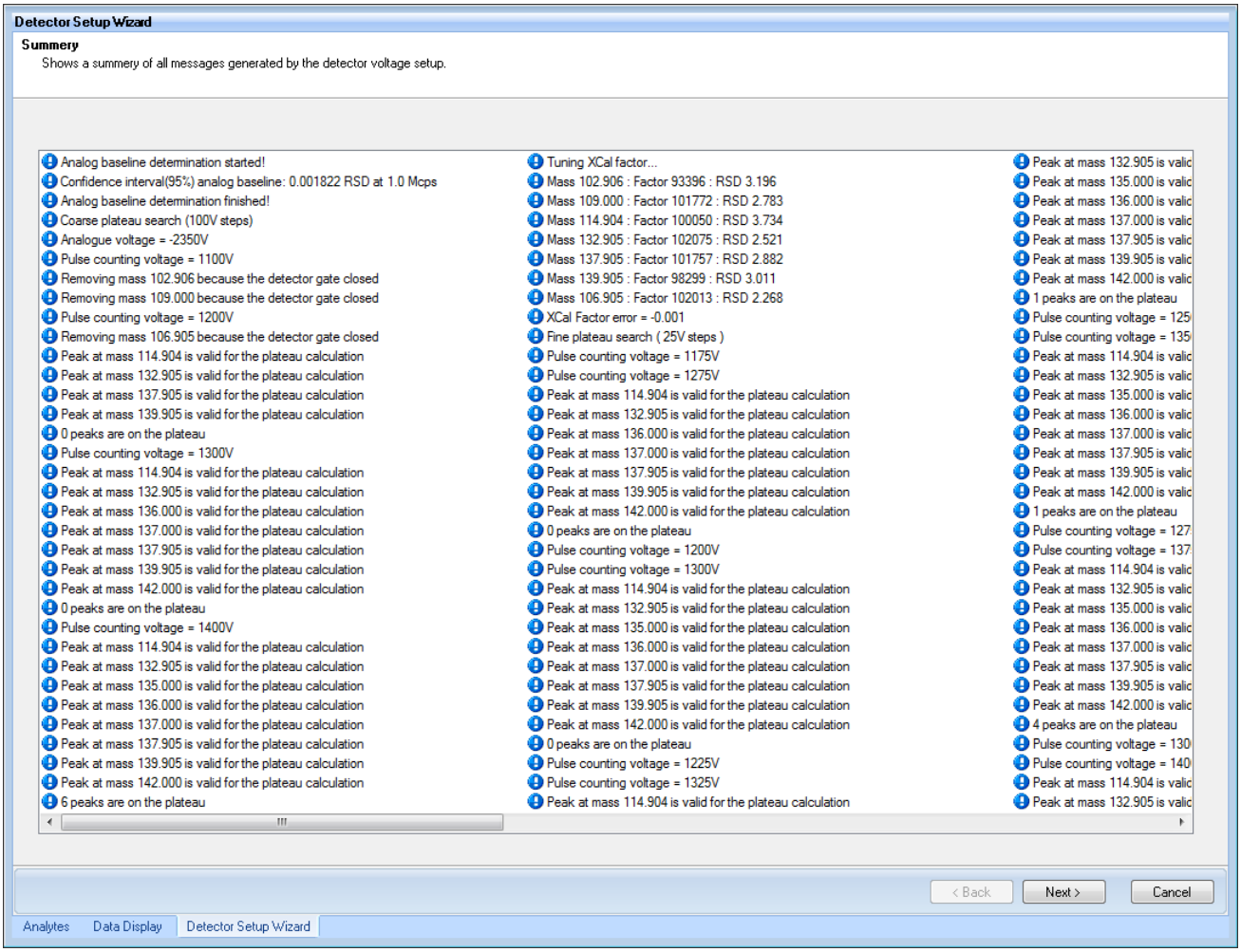


Figure 4-78. Summary of detector HV setup and cross calibration

13. Click **Next**.

The setup is finished, see Figure 4-79.

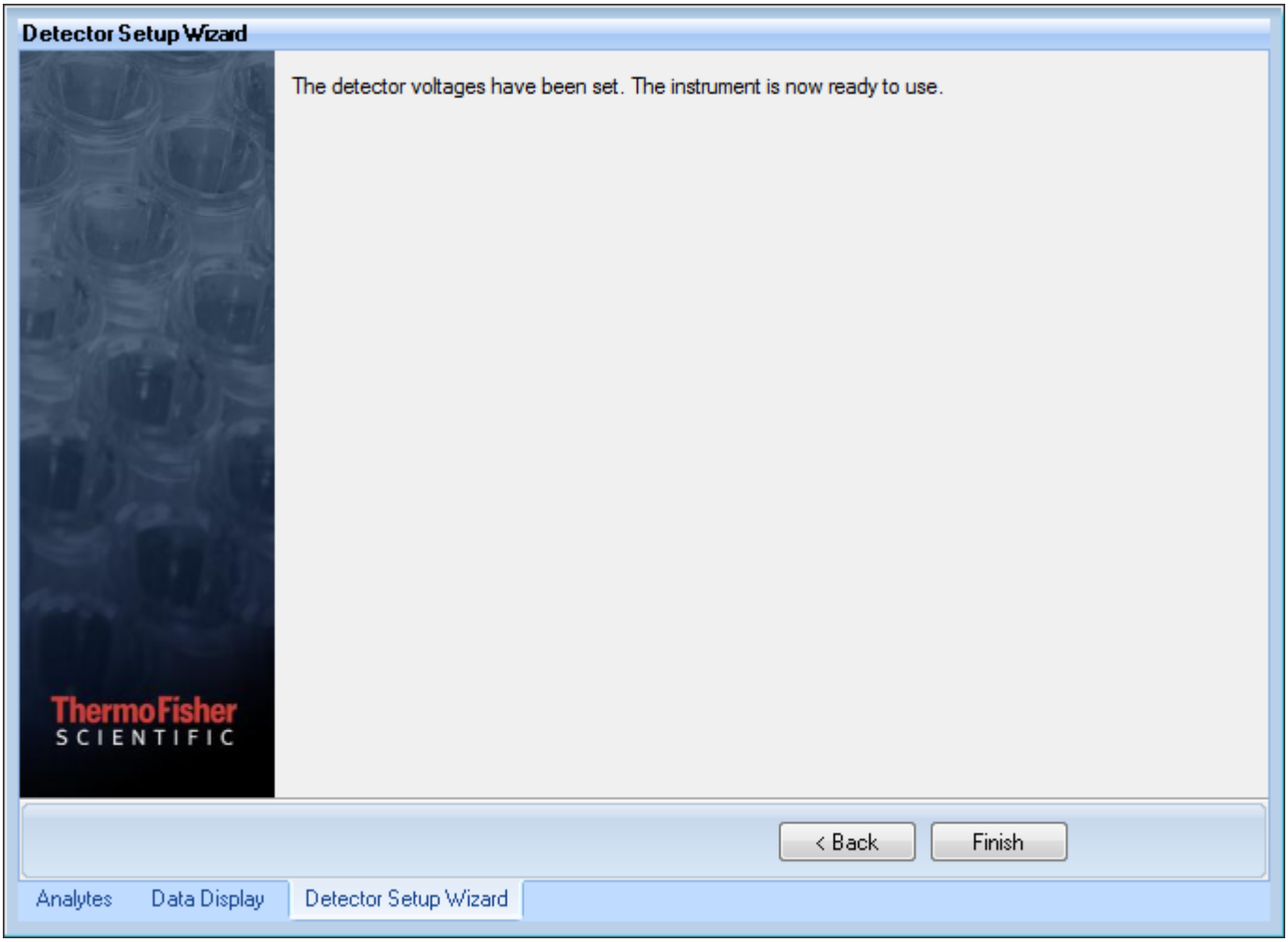


Figure 4-79. Detector HV setup and cross calibration are finished

14. Click **Finish** to store the detector voltages as well as the cross calibration factors and to leave the Detector Setup.

❖ **To perform a detector setup with the wizard Full Detection System Calibration**

1. Click 

to open **Instrument Control**.
2. Be sure to change to STD/STDS mode before starting the wizard.
3. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

4. In the **Wizard** group, click 

.
The **Detector Setup Wizard** opens, see Figure 4-80.

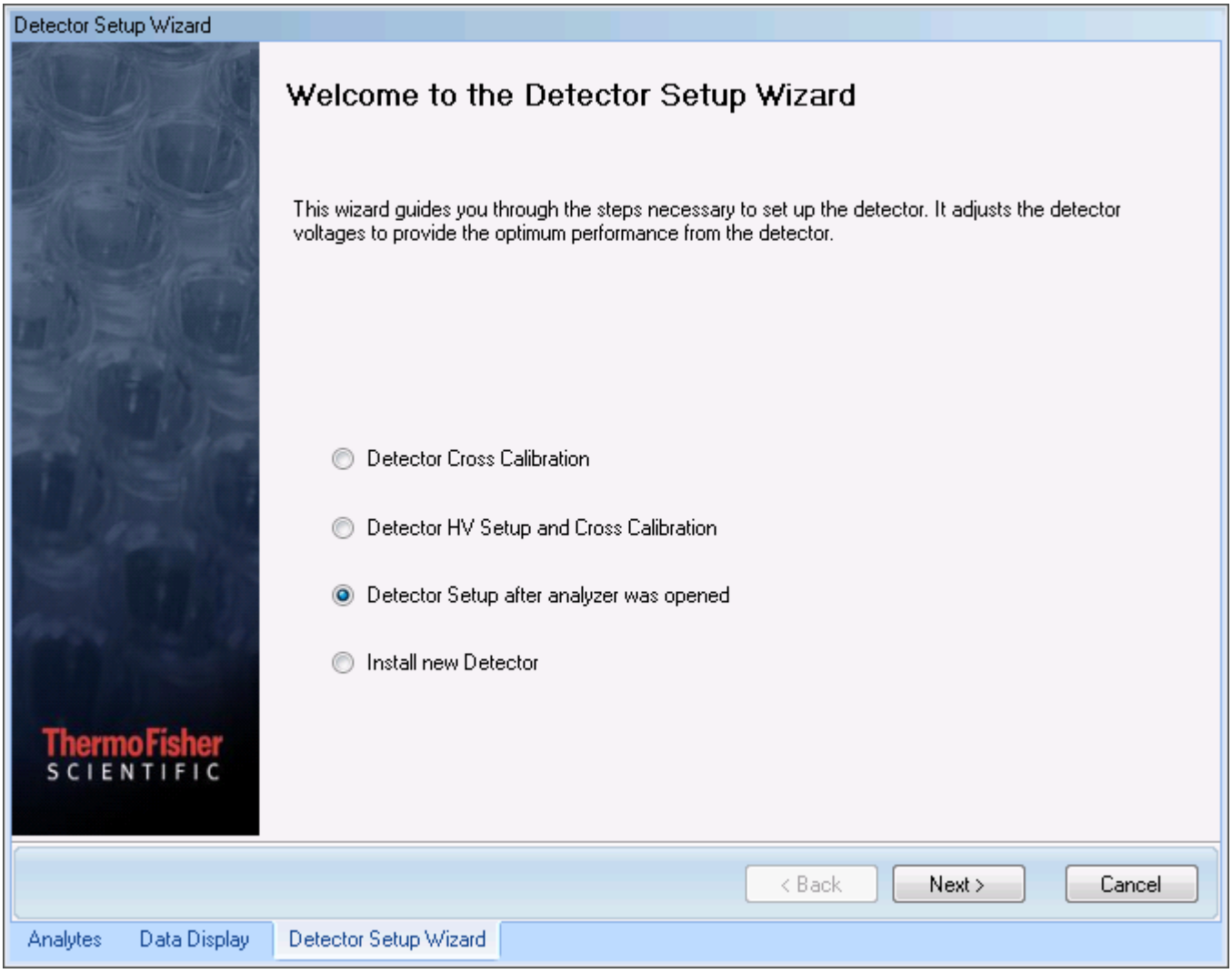


Figure 4-80. Welcome to the Detector Setup Wizard

5. Select **Detector Setup after analyzer was opened**.

6. Click **Next**.
   The periodic table window opens, see Figure 4-81.

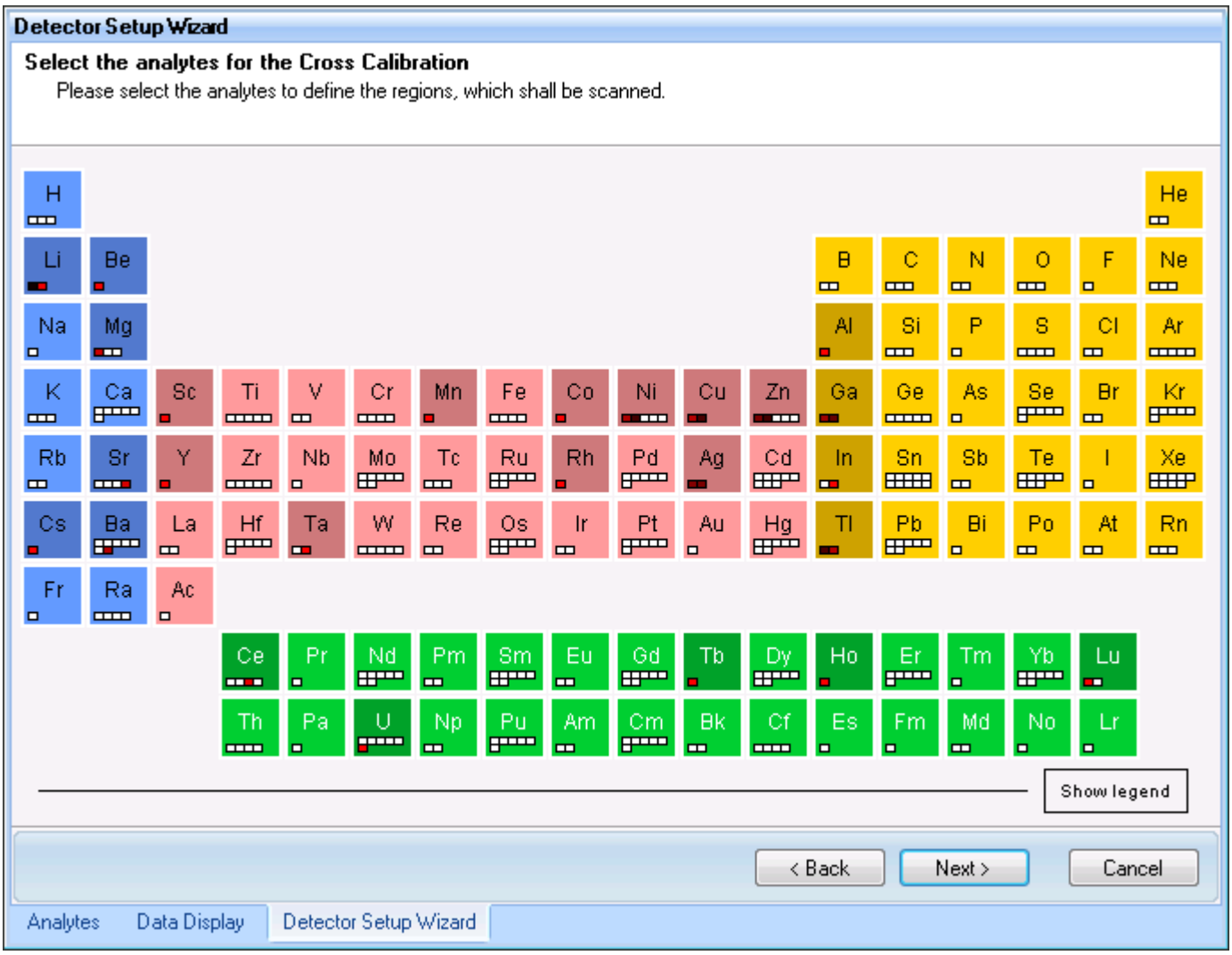


Figure 4-81. Select analytes for Detector Setup Wizard

7. Select your analytes.

8. Click **Next**.
   The Load the Sample window opens, see Figure 4-82.

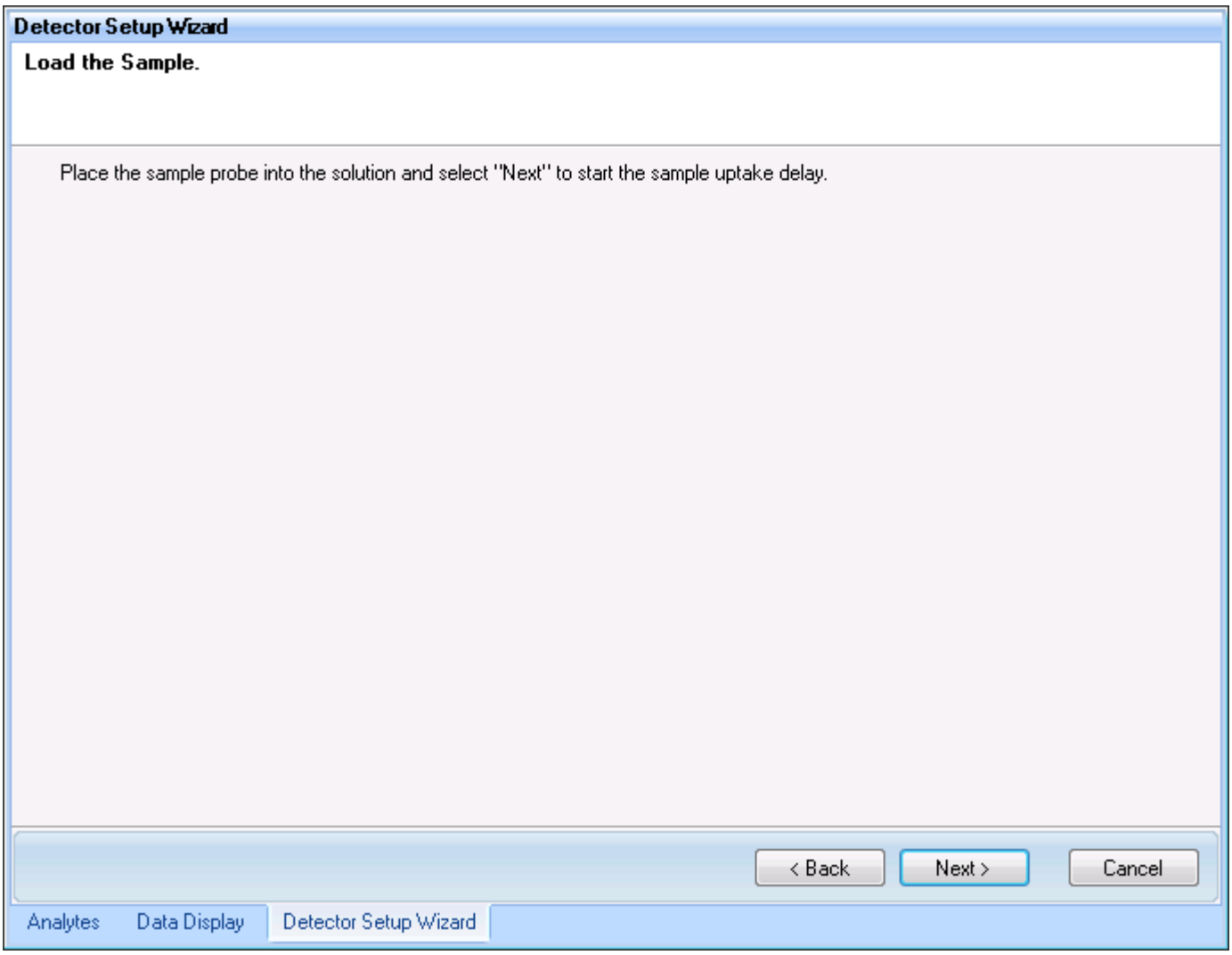


Figure 4-82. Load sample for Detector Setup Wizard

9. Place the probe into the setup solution.

10. Click **Next**.
    The **Waiting for sample uptake** window opens, see Figure 4-83.

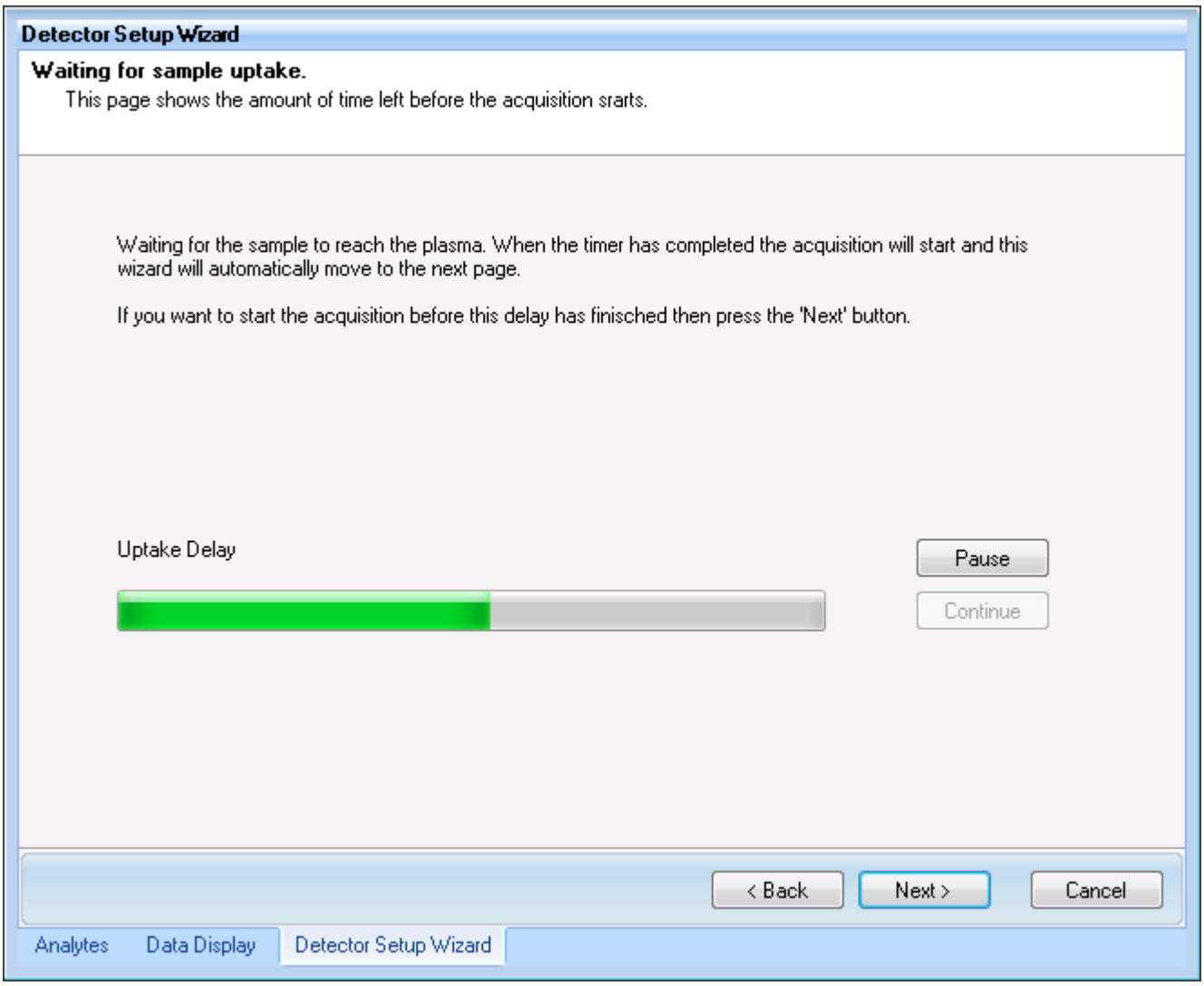


Figure 4-83. Waiting for sample uptake in Detector Setup Wizard

The Detector Setup wizard applies a minimum delay time for sample uptake in order to assure that enough sample has entered the plasma.

11. Click **Pause** to delay further if more time is needed.
    Click **Continue** when ready.

12. To begin the setup before the delay time elapsed, click **Next**. The analog baseline and analog amplifier determination for the analog offset determination starts, see Figure 4-84.

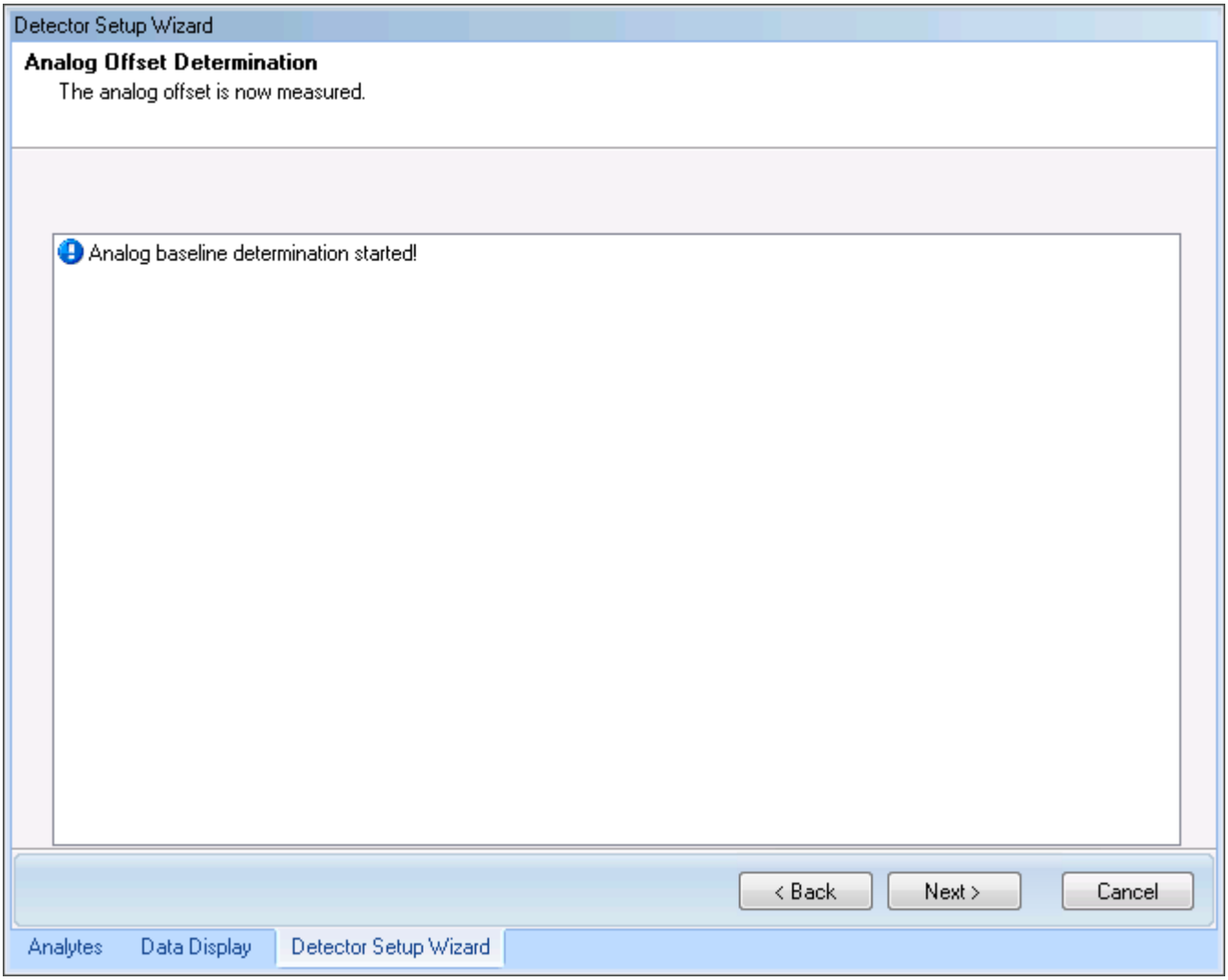


Figure 4-84. Analog offset determination in Detector Setup Wizard

The Analog offset determination is followed by a coarse and fine adjustment of the counting amplifier threshold of the detector voltages, see Figure 4-85.

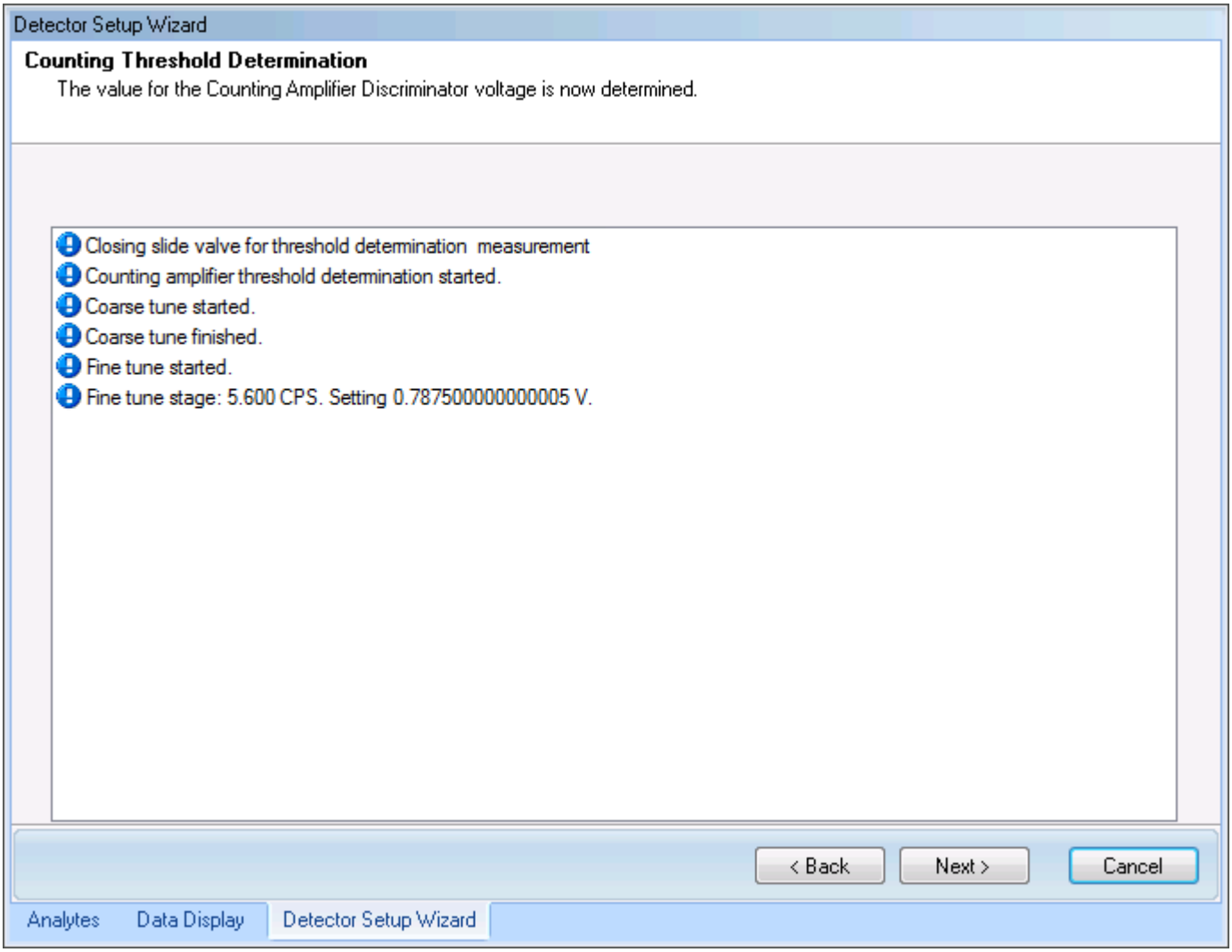


Figure 4-85. Counting threshold determination

Afterwards the detector voltages are adjusted by searching an appropriate plateau of the counting detector voltage and a coarse adjustment of the analog voltage, see Figure 4-86.

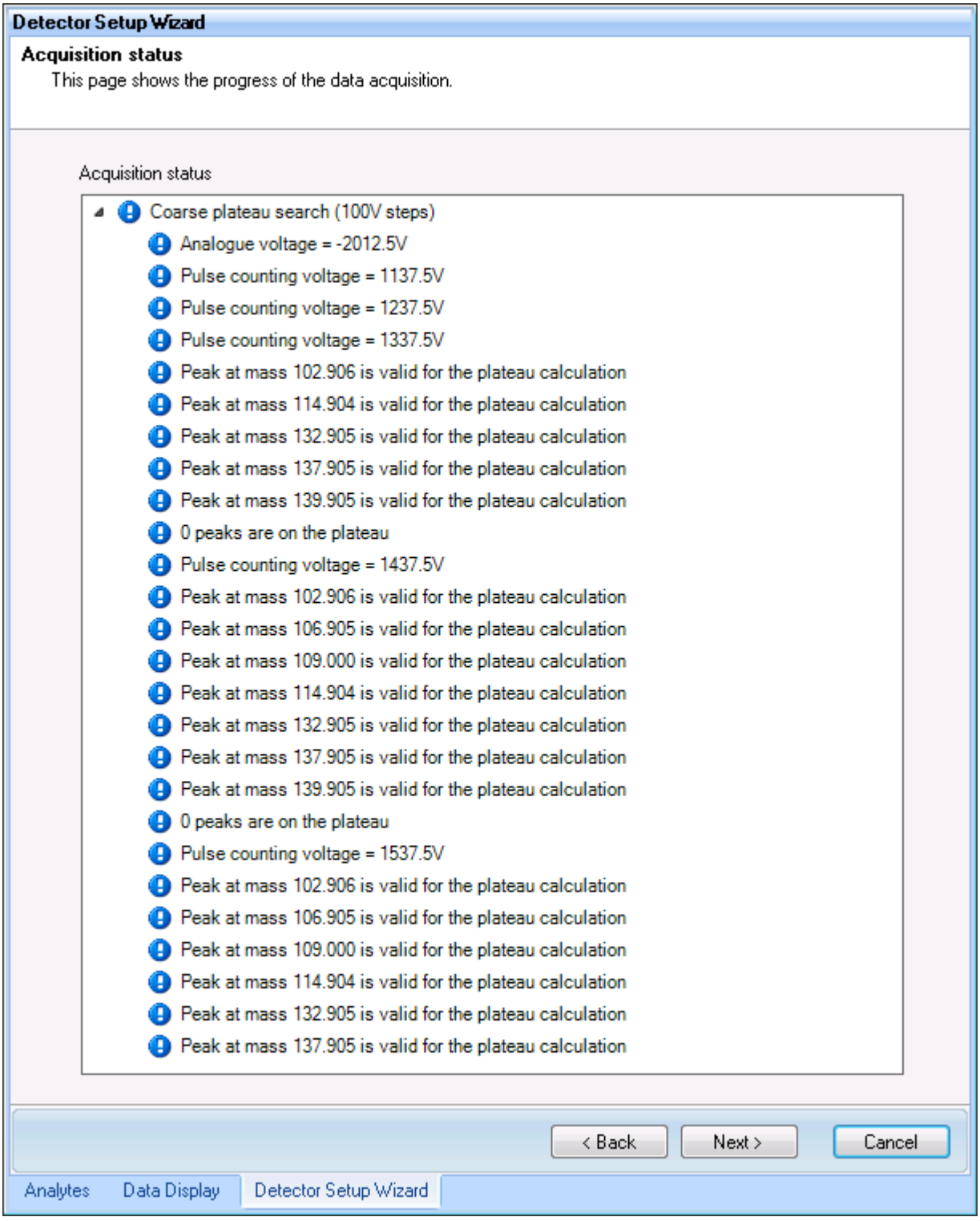


Figure 4-86. Acquisition status of the detector voltage adjustment routine

The determination of the detector voltages is followed by an adjustment of the counting gate level, see Figure 4-87.

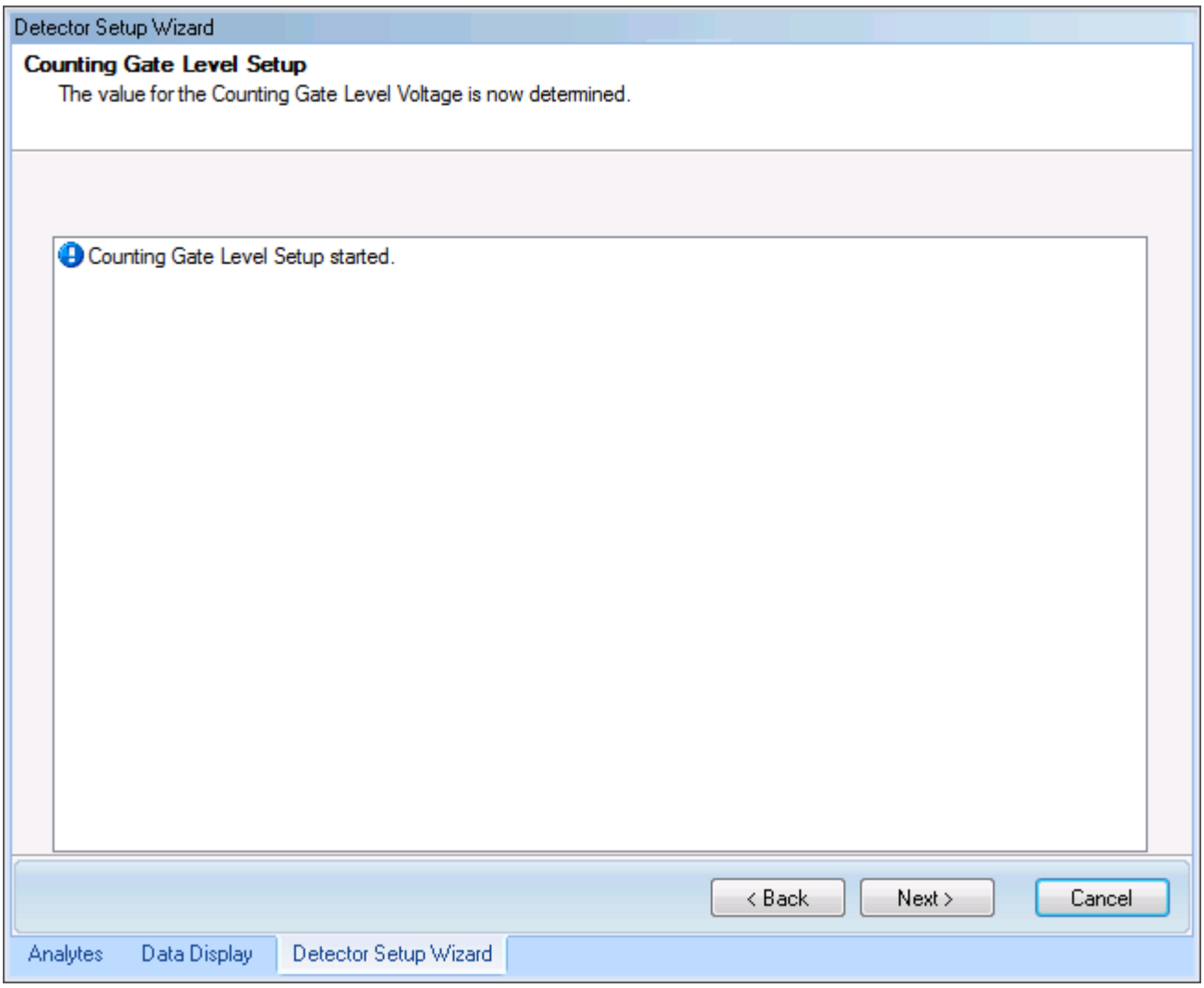


Figure 4-87. Counting gate level setup

The cross calibration progress is shown, see Figure 4-88.

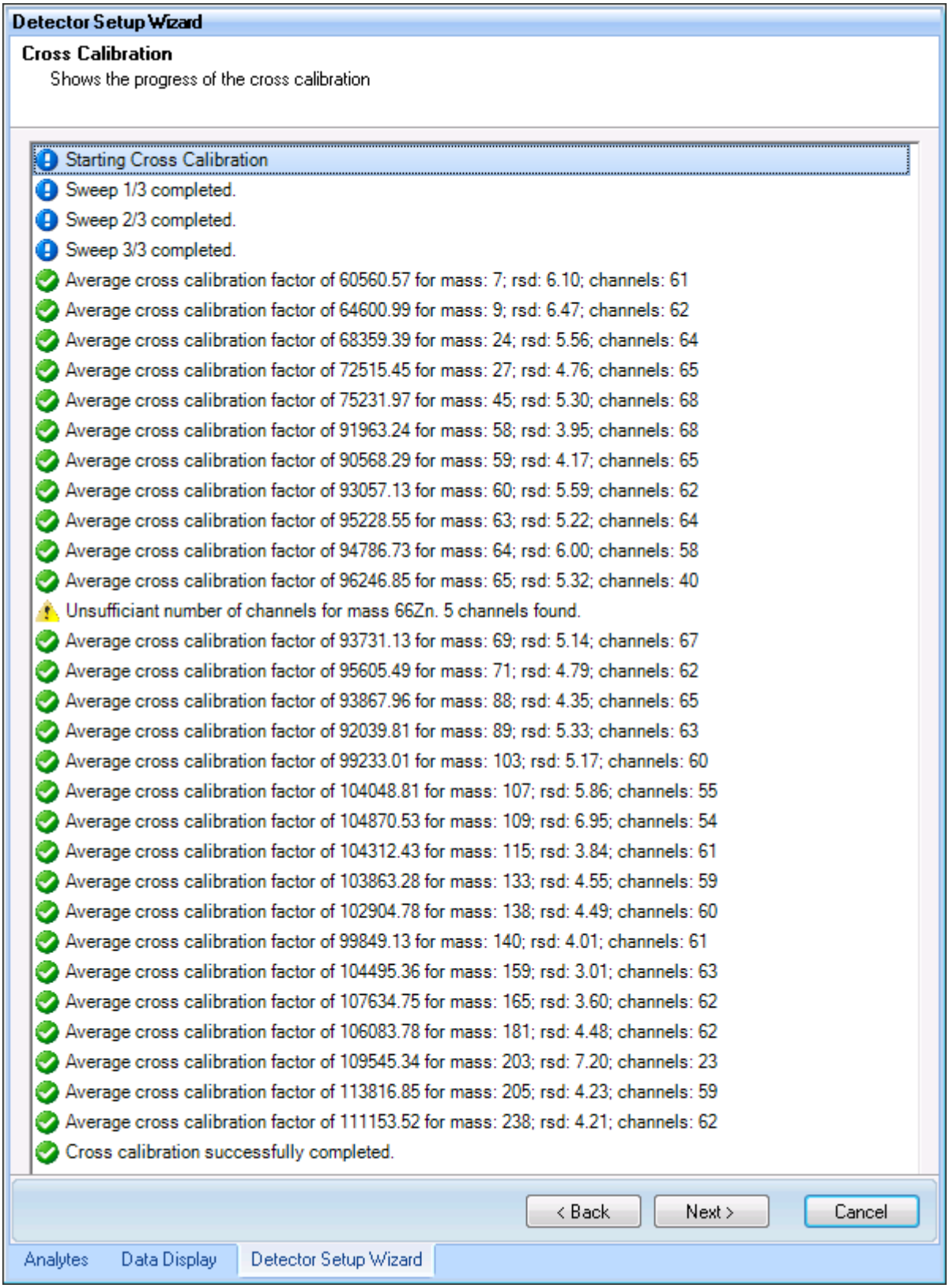


Figure 4-88. Cross calibration progress of detector setup

The summary is shown, see Figure 4-89.

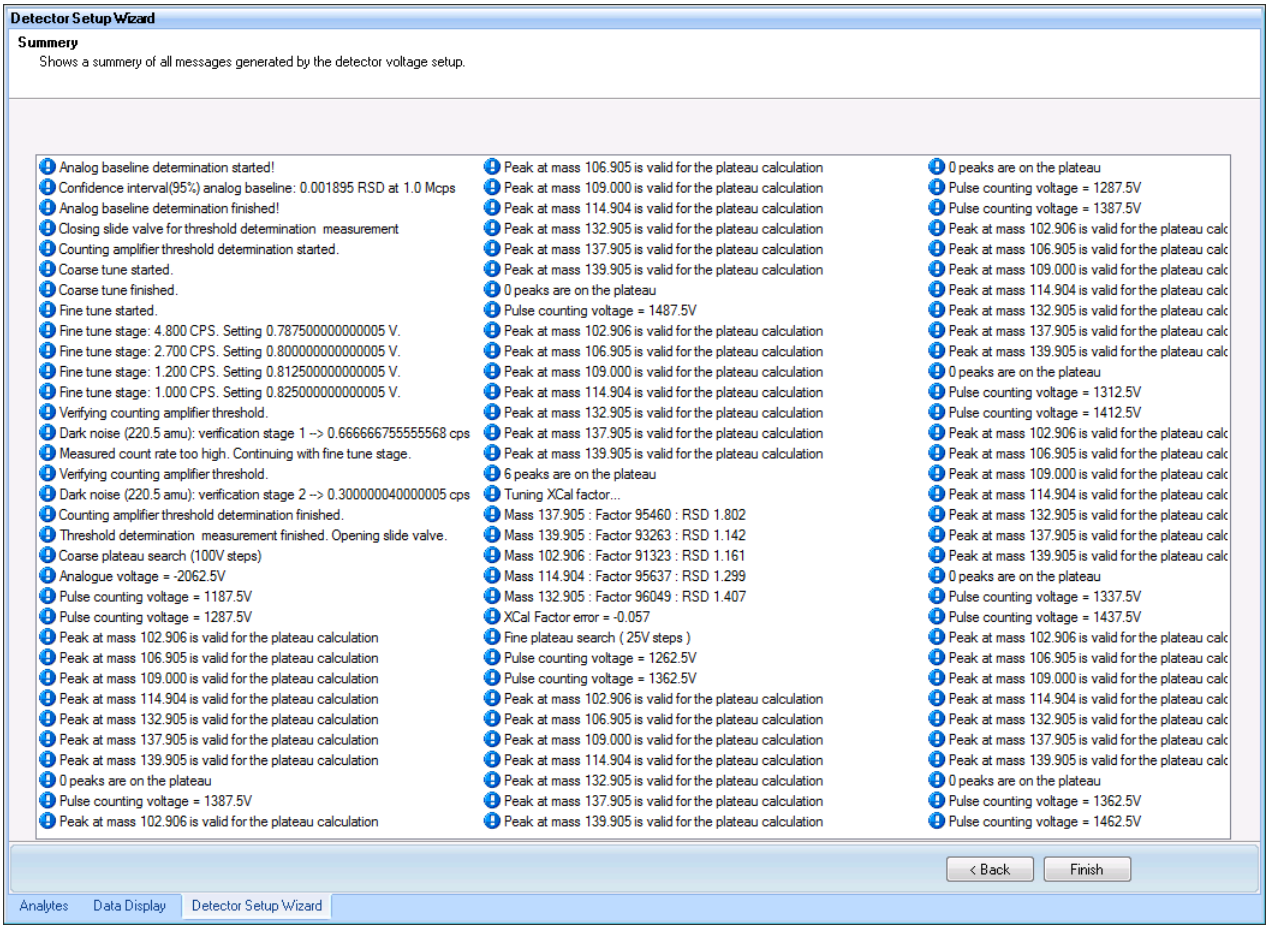


Figure 4-89. Summary of detector setup

The setup is finished, see Figure 4-90.

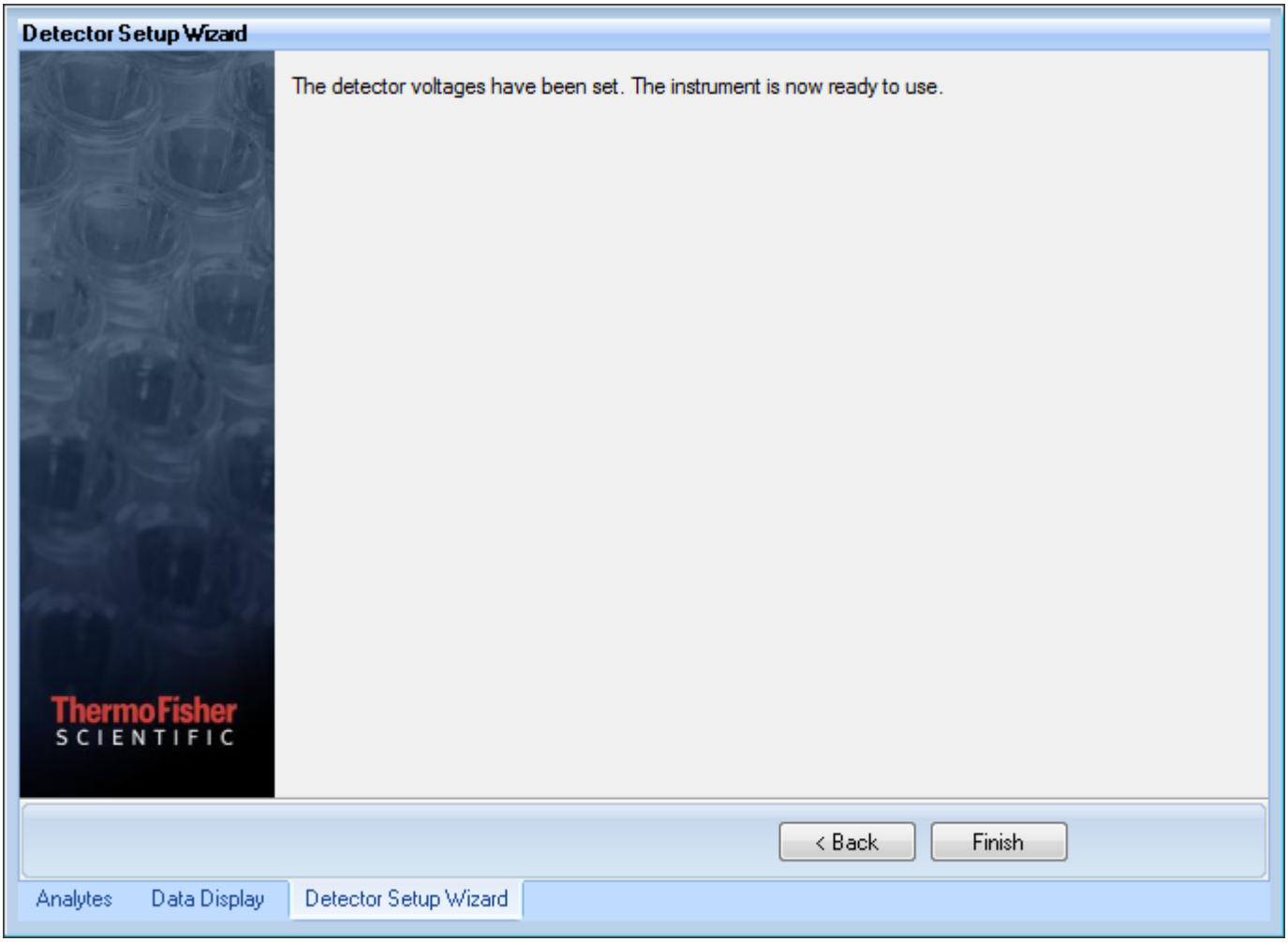


Figure 4-90. Full Detection system calibration is finished

13. Click **Finish** to store the determined offset values, the detector voltages as well as the cross calibration factors and to leave the Detector Setup.

Mass Calibration Wizard

The **Wizards** group of the **iCAP Q** ribbon tab in Instrument Control gives access to the **Mass Calibration** wizard.

It is necessary to perform a mass calibration whenever the peak width determination specified in the performance reports fails or the mass peaks are not aligned correctly. Thermo Fisher Scientific recommends performing the mass calibration after defined time intervals, for example, every month. A mass calibration is also executed every time the Performance Report of the "Getting Ready" on page 5-7 function fails and Autotune did not improve the performance.

The software uses a mass calibration equation so that when a mass is selected for measurement, the control electronics can set the quadrupole to transmit that mass. The mass calibrations are stored such that any experiment can access them when the experiment is being run.

A deviation from the linear mass calibration is due to the nature of the quadrupole. The deviation is calculated with a Fit that divides the entire mass range into four areas (scan regions).

The analytes selected for the measurement and those in the setup solution provide the parameters for the Fits in these scan regions. The calculated parameters and the deviation are then shown in the window "Mass calibration" in the group Views.

If you select **Execute a Coarse Mass Calibration first**, the polyatomics 40Ar.40Ar and 40Ar.16O instead of the analytes are taken for a rough calculation.

The mass calibration wizard executes the mass calibrations for both the normal- and high-resolution quadrupole modes.

❖ **To perform a mass calibration with the wizard**

1. Click 

to open **Instrument Control**.
2. Be sure to change to STD/STDS mode before starting the wizard.
3. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

4. In the **Wizard** group, click 

.
The **Mass Calibration Wizard** opens, see Figure 4-91.

Figure 4-91. Welcome to the Mass Calibration wizard

5. Click **Next**.
   The **Coarse Mass Calibration** window opens, see Figure 4-92.

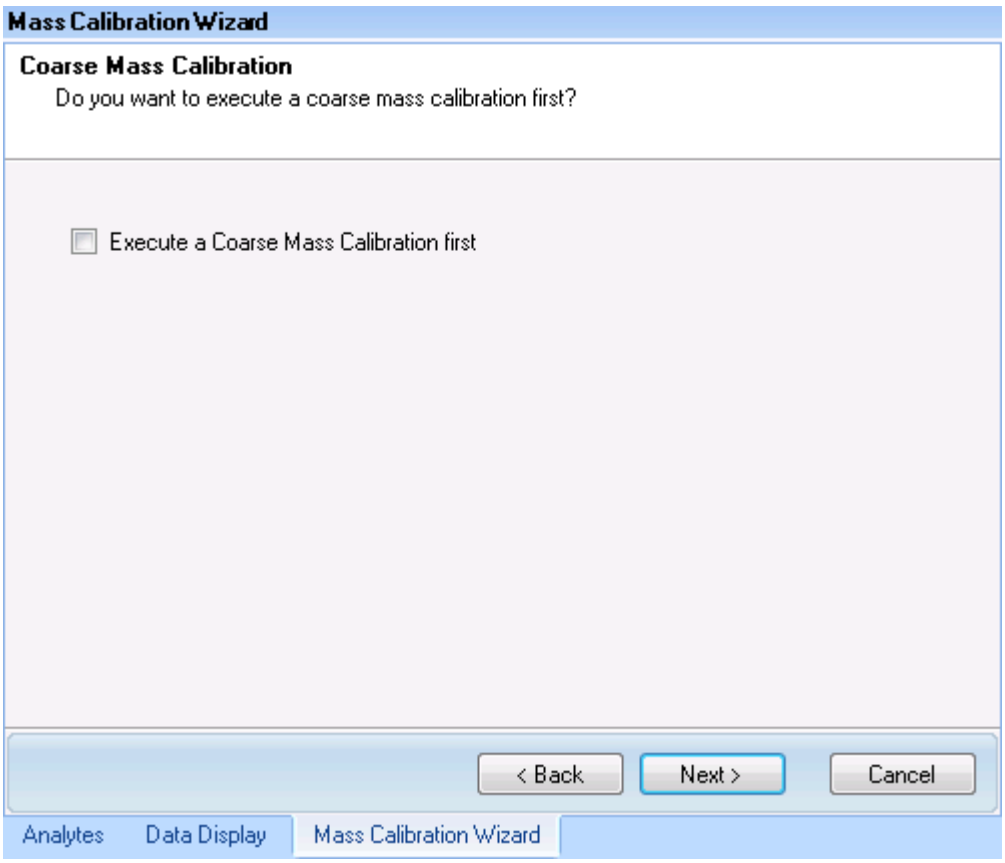


Figure 4-92. Mass Calibration wizard option

6. If you select the check box **Execute a Coarse Mass Calibration first**, the second check box **Load Tune Settings** becomes available. This option only needs to be selected if the mass calibration is expected to be significantly different, for example, due to new

hardware, or if a mass calibration without this option has failed, see Figure 4-93.

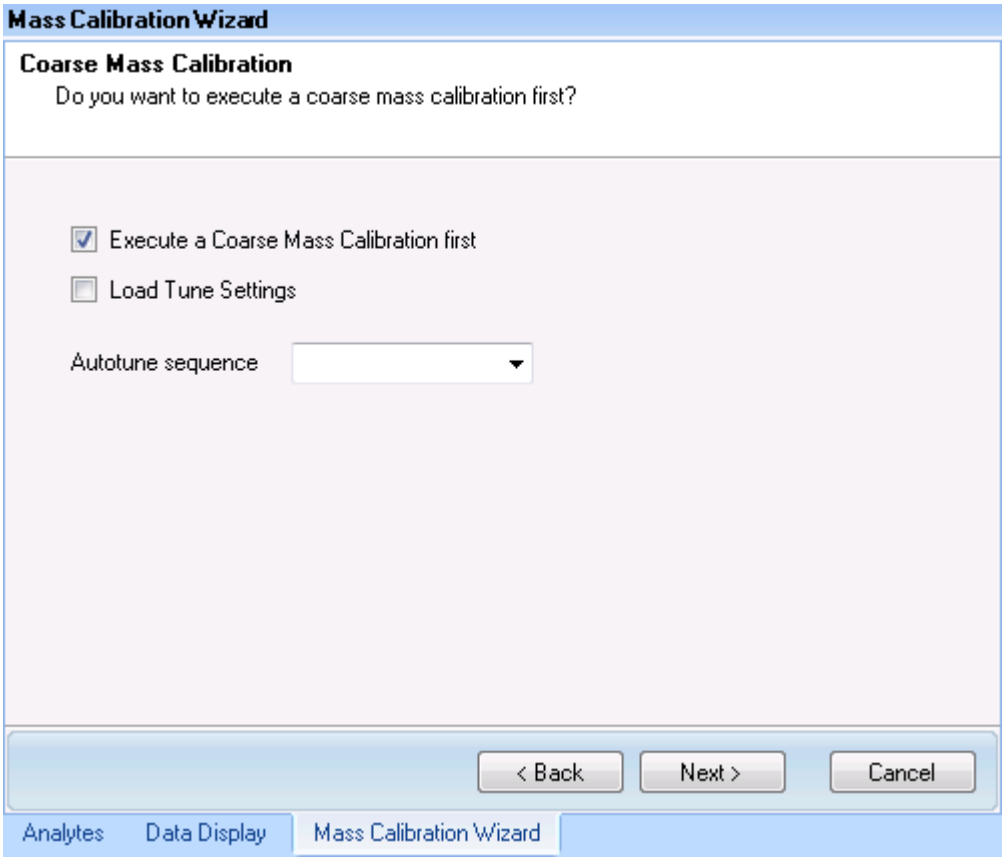


Figure 4-93. Coarse Calibration selected in Mass Calibration wizard

7. If you select **Load Tune Settings**, also select a tune setting from the drop-down list.

If you do not select a setting from the list, see Figure 4-94, the tune settings currently loaded will be used.

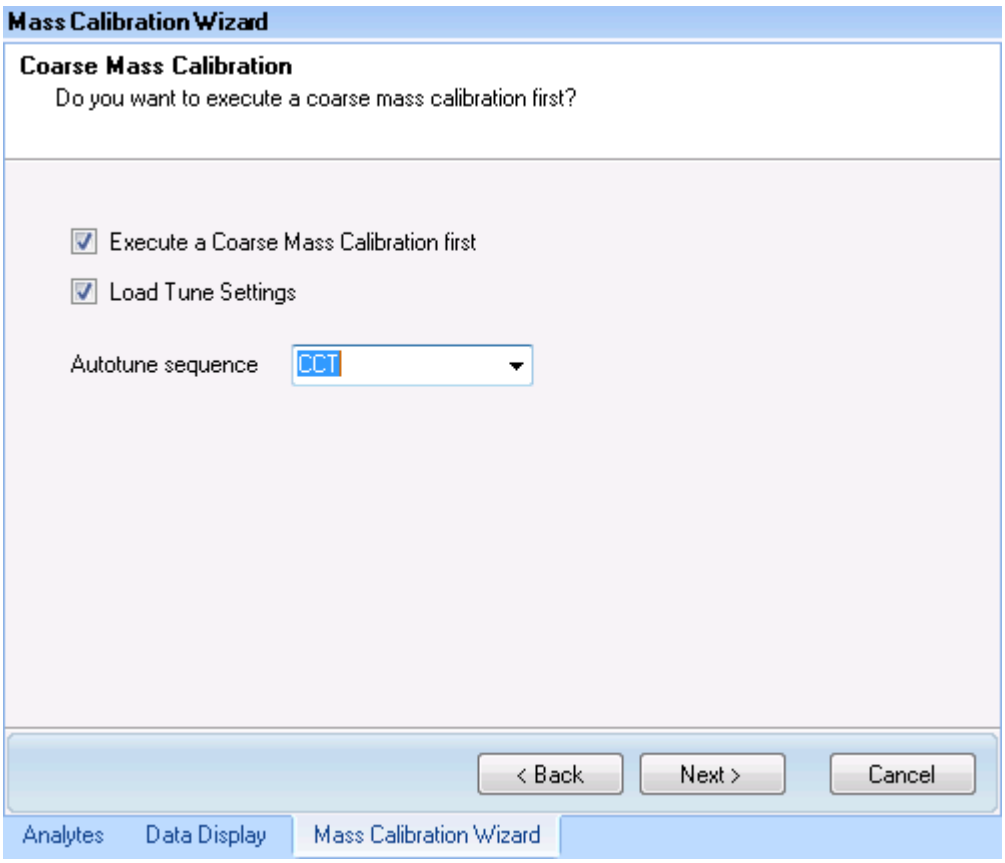


Figure 4-94. Tune setting selected Mass Calibration wizard

8. Click **Next**.
   The Load the Sample window opens, see Figure 4-95.

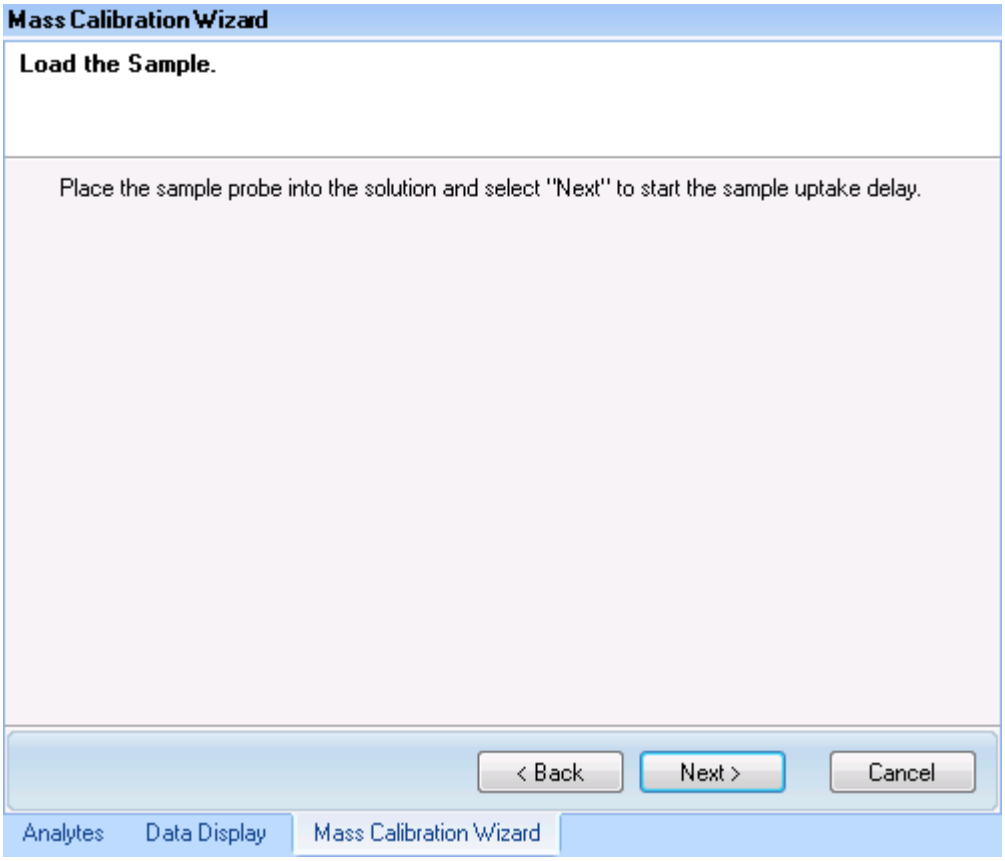


Figure 4-95. Load Sample in Mass Calibration wizard

9. Place your sample probe into the solution and click **Next**, see Figure 4-96.

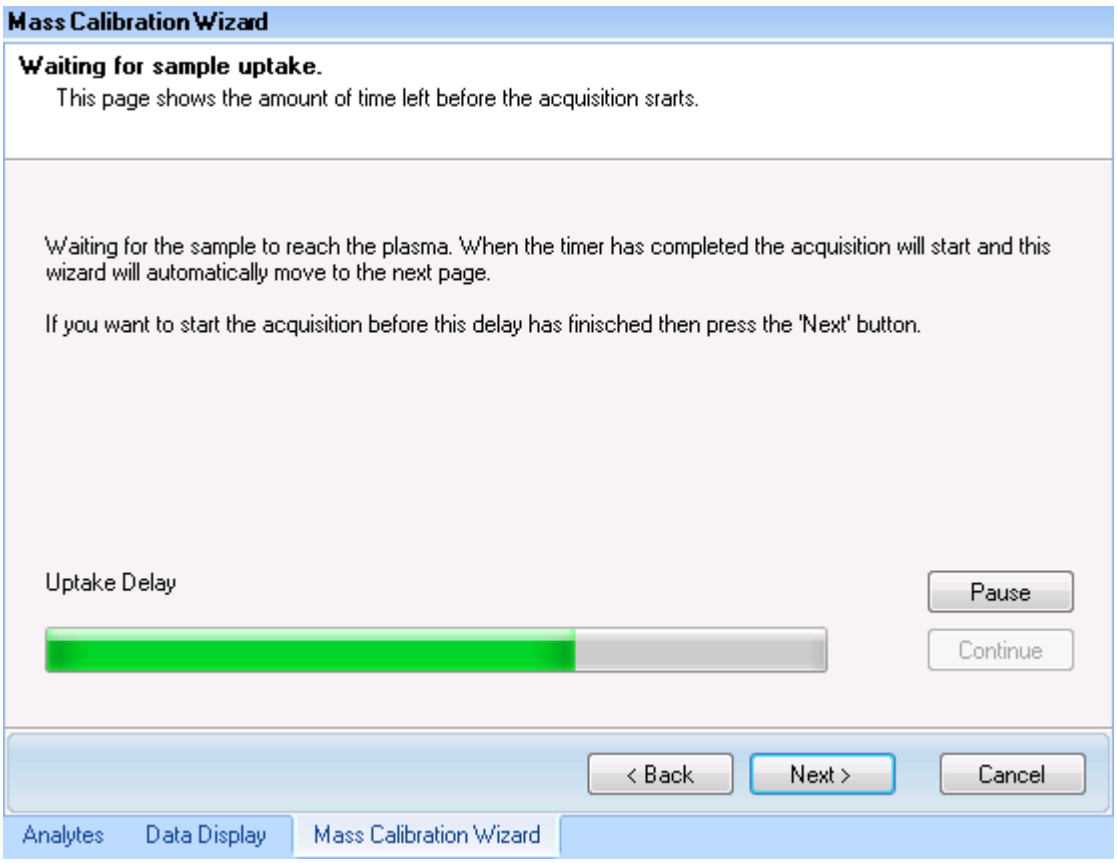


Figure 4-96. Waiting for the sample uptake in Mass Calibration wizard

The Mass Calibration wizards applies a minimum delay time for sample uptake in order to assure that enough sample has entered the plasma.

10. Click **Pause** to delay further if more time is needed.
    Click **Continue** when ready.

11. To begin the calibration before the delay time elapsed, click **Next**.
    The data acquisition for the mass calibration starts.

12. In the data view region, select the **iCAP Q** tab.
    The ribbon **iCAP Q** is activated.

13. Click the lower tab **Data Display**.
    The actual data acquired is shown in the real-time Data Display tab of the data view region, see Figure 4-97.

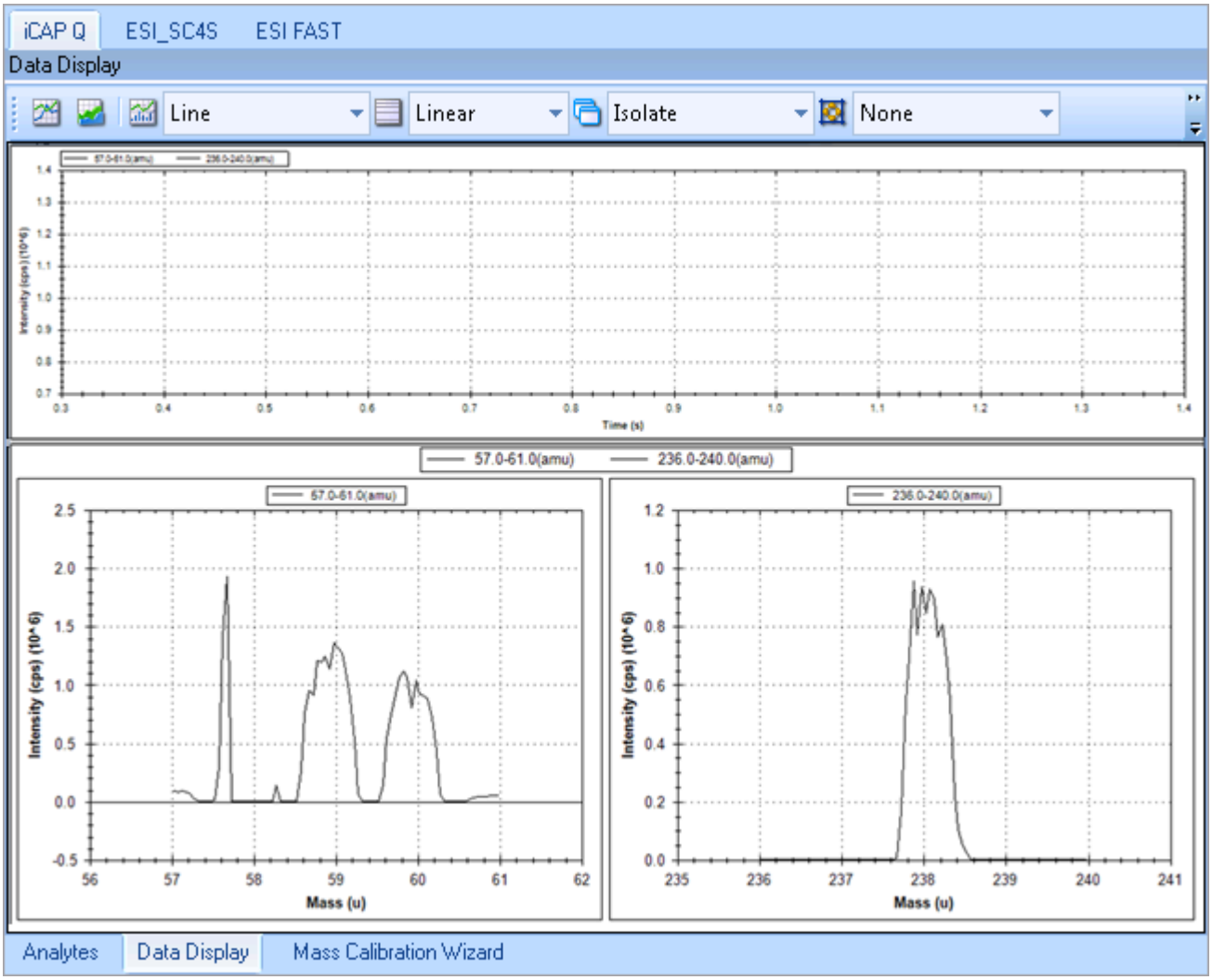


Figure 4-97. Data Display of mass calibration

14. The **Result** window opens automatically when the calibration is finished, see Figure 4-98.

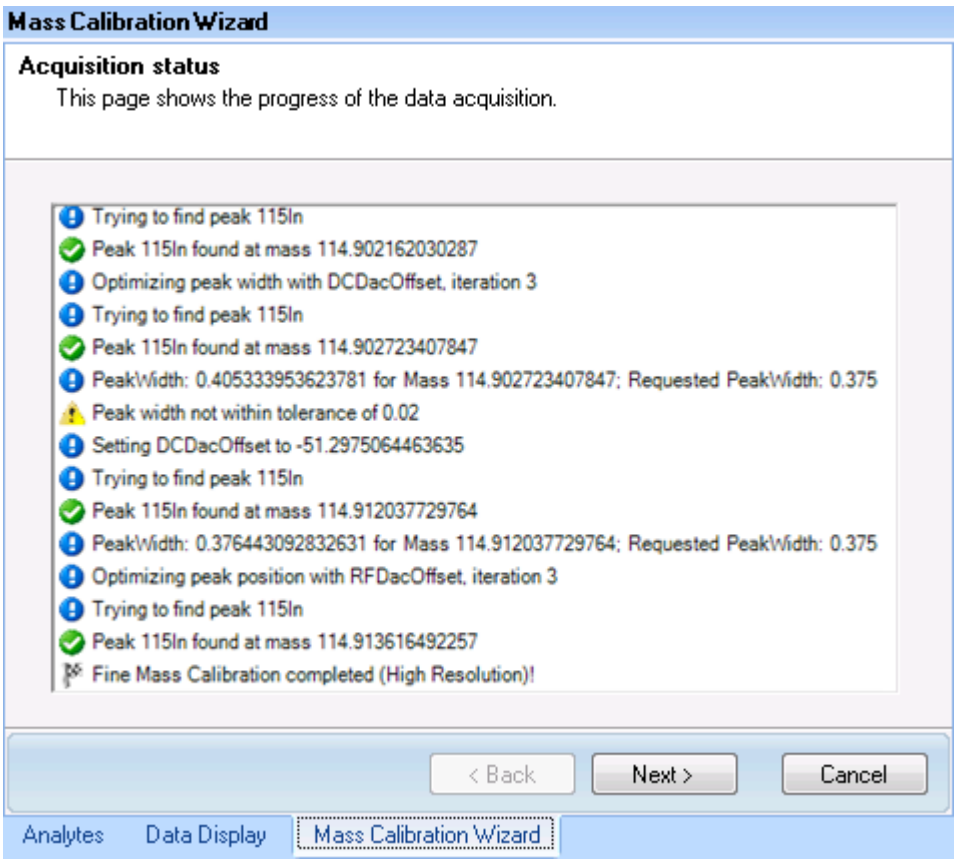


Figure 4-98. Results of Mass Calibration wizard

15. Click **Next**.

16. Click **Finish** to finish the Mass Calibration and store the acquired parameters, see Figure 4-99.

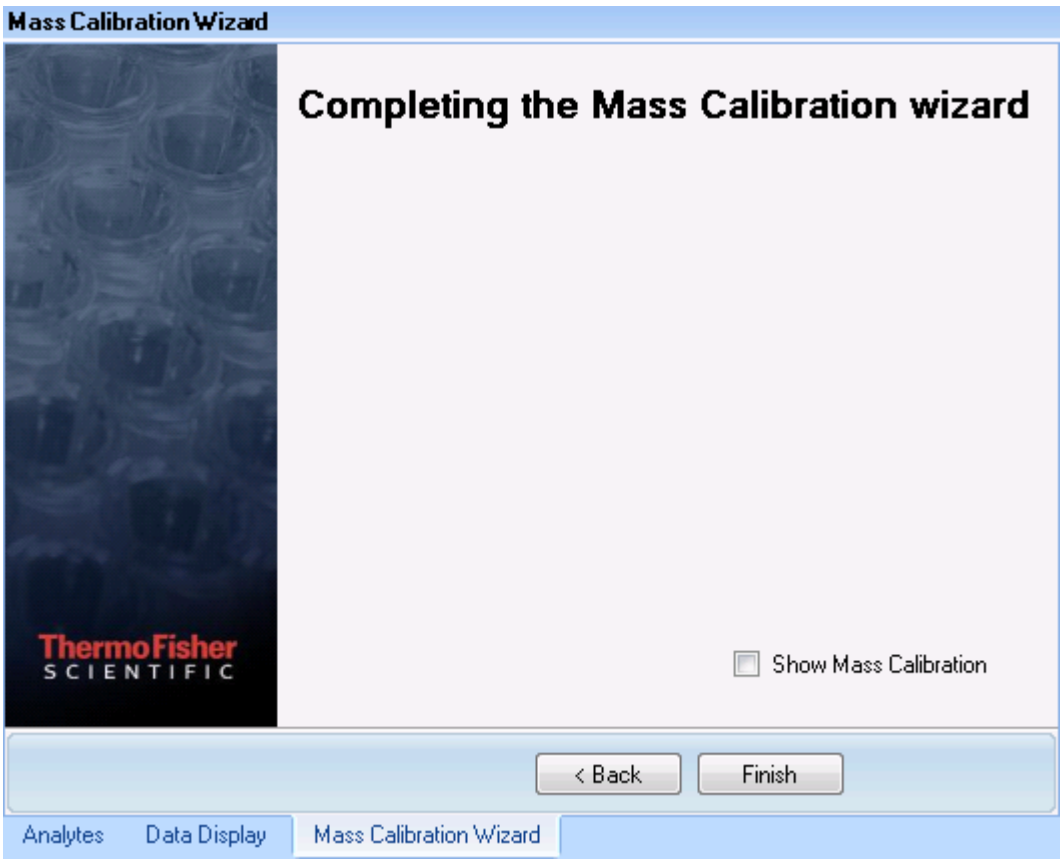


Figure 4-99. Mass Calibration successful in wizard

The Mass Calibration results can be viewed in detail in the "Views Group" on page 4-106.

Views Group

The **Views** group of the **iCAP Q** ribbon tab in Instrument Control, see Figure 4-100, allows you to view instrument calibrations, performance reports and a real-time readback plot of the Control Panel parameters.

Figure 4-100. View group of the iCAP Q ribbon

The buttons of the **Views** group are summarized in Table 4-6.

Table 4-6. Buttons of Views group

Icon	Meaning	Description
	Readback Plot	Opens the Readback Plot tab in the data view region. Specific instrument parameters can be viewed in real time.
	Performance Report	Opens the Performance Report tab in the data view region. Recorded performance reports can be viewed, exported or printed.
	Autotune Report	Opens the Autotune Report tab in the data view region. Recorded Autotune reports can be viewed, exported or printed.
	Detector Setup Report	Opens the Detector Report tab in the data view region. Shows the results of the detector setup.
	Cross Calibration Factors	Opens the Cross Calibration View tab in the data view region. Shows the currently valid and previous cross calibrations.
	Mass Calibration	Opens the Mass Calibration View tab in the data view region. Shows the currently valid and previous mass calibrations.

❖ **To view Readback Plot**

1. Click 

to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
The ribbon **iCAP Q** is activated.

3. In the **Views** group, click  **Readback Plot**.
   The **Readback Plot** tab opens in the data view region, see Figure 4-101.

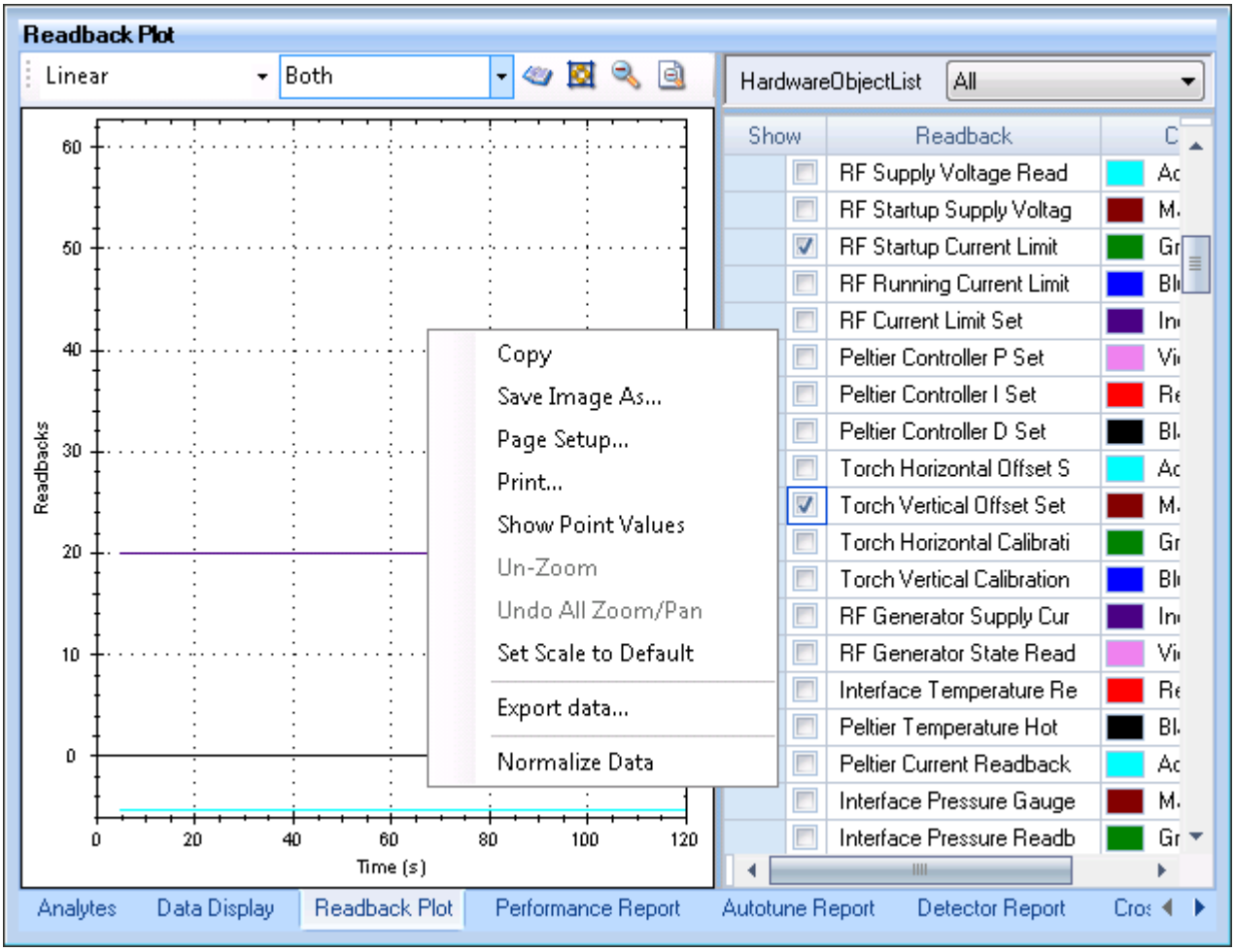


Figure 4-101. Readback Plot in data view region

The toolbar and the context menu of the report offer options, for example, to scale the y-axis, change the grid display, show the legend or to print or export data.

❖ **To view Performance Report**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. In the **Views** group, click  **Performance Report**.
   The **Performance Report** tab opens in the data view region, see

Figure 4-102.

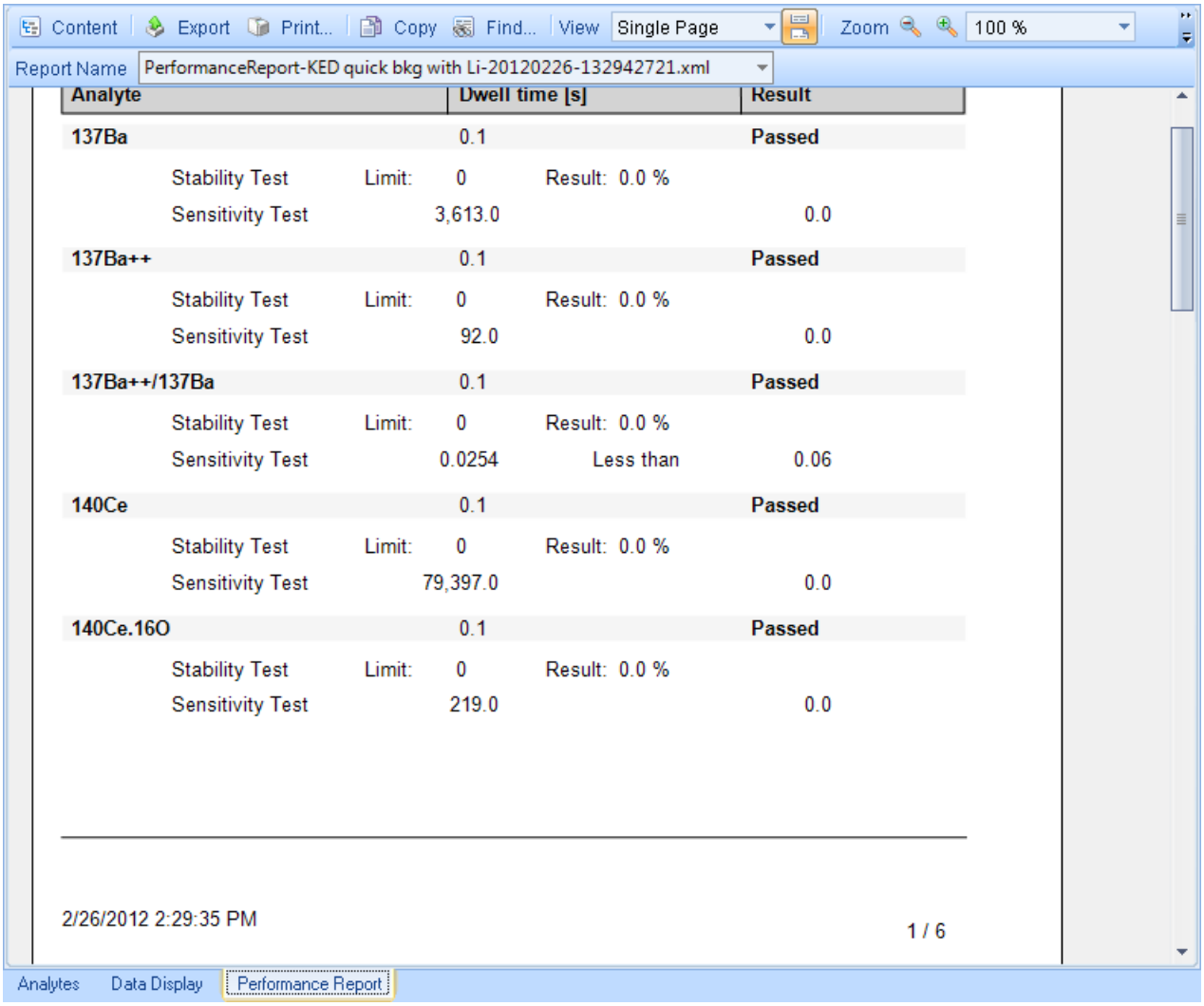


Figure 4-102. Performance Report in data view region

The toolbar of the report offers options, for example, to view the report, or print or export data.

❖ **To view Autotune Report**

1. Click to open **Instrument Control**.
2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. In the **Views** group, click  **Autotune Report**.
   The **Autotune Report** tab opens in the data view region, see Figure 4-103.

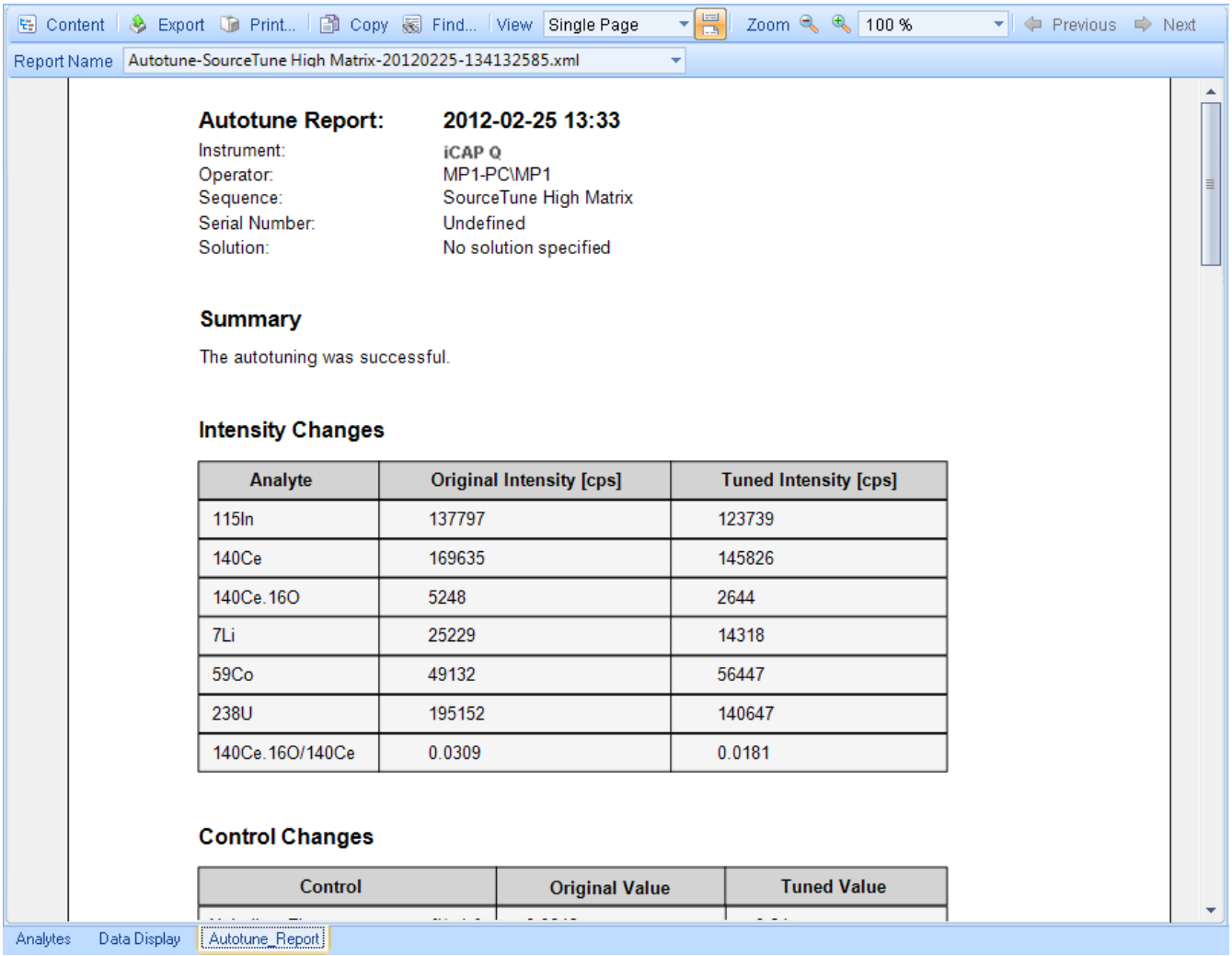


Figure 4-103. Autotune Report in data view region

The toolbar of the report offers options, for example, to view the report, or print or export data.

❖ **To view Detector Setup Report**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. In the **Views** group, click  **Detector Setup Report**.
   The **Detector Setup Report** tab opens in the data view region, see Figure 4-104.

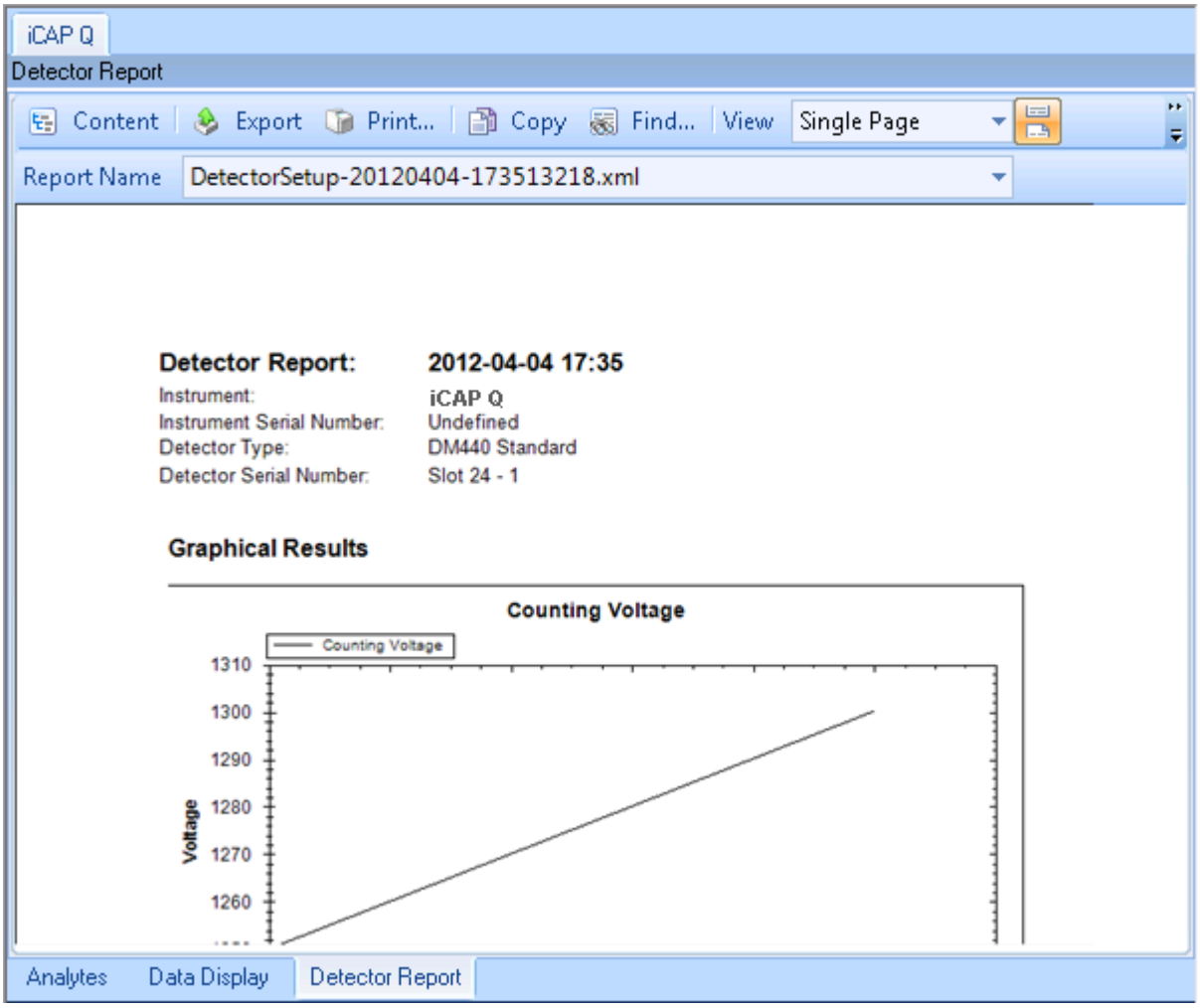


Figure 4-104. Detector Setup Report in data view region

The toolbar of the report offers options, for example, to view the report, or print or export data.

❖ **To view Cross Calibration result**

1. Click 

to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. In the **Views** group, click  **Cross Calibration Factors**.
   The **Cross Calibration View** tab opens in the data view region, see

Figure 4-105.

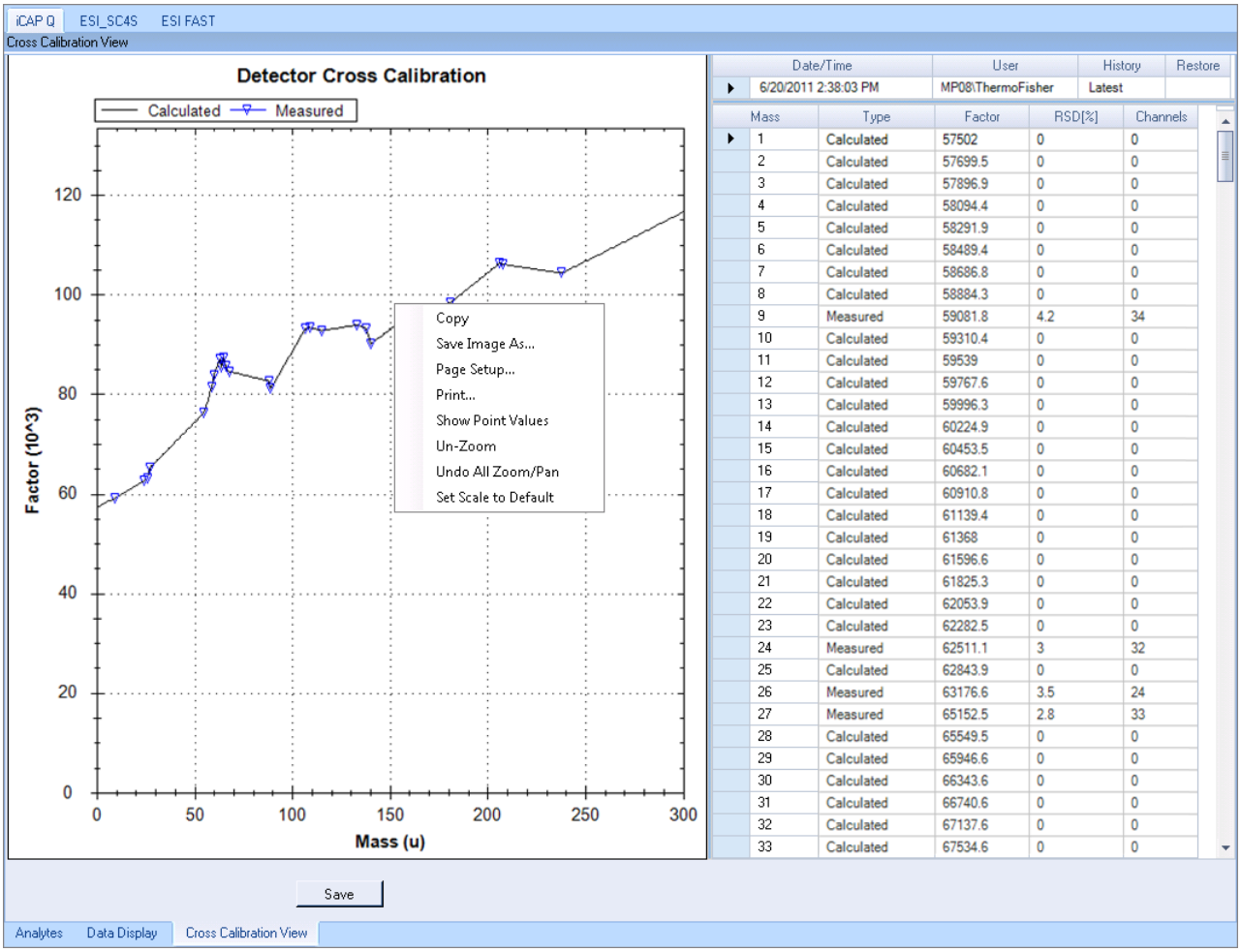


Figure 4-105. Cross Calibration Factors in data view region

The context menu offers options, for example, to save the graph as image, show point values, or copy or print the graph.

❖ **To view Mass Calibration result**

1. Click to open **Instrument Control**.

2. In the data view region, select the **iCAP Q** tab.
   The ribbon **iCAP Q** is activated.

3. In the **Views** group, click  **Mass Calibration**.
   The **Mass Calibration View** tab opens in the data view region, see Figure 4-106.

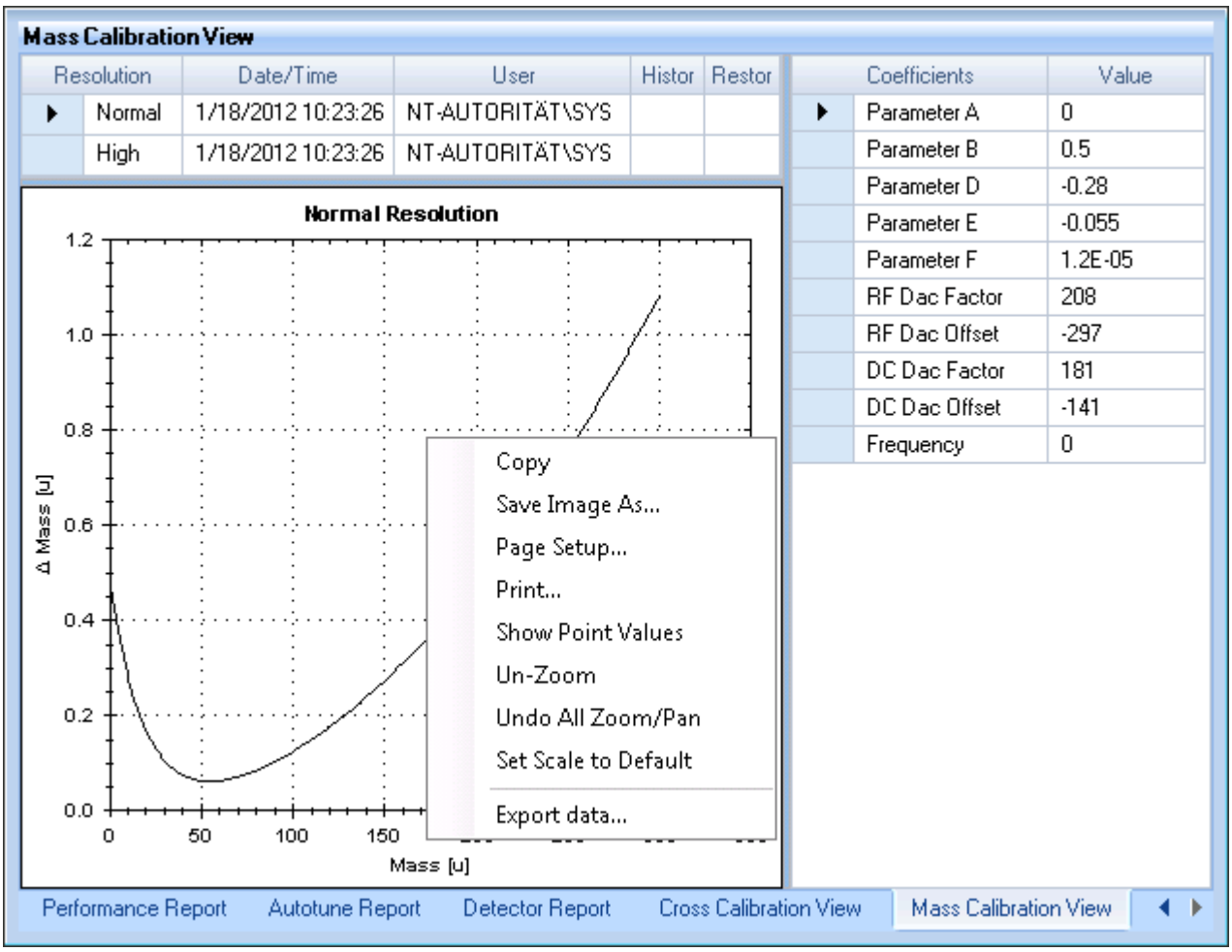


Figure 4-106. Mass Calibration View tab in data view region

The context menu offers options, for example, to save the graph as image, show point values, or copy or print the graph.

Window Ribbon Tab

The **Window** ribbon tab (Figure 4-107) allows you to change the appearance of the Instrument Control tool, store favorite display settings and Layouts and access the Qtegra software version information.

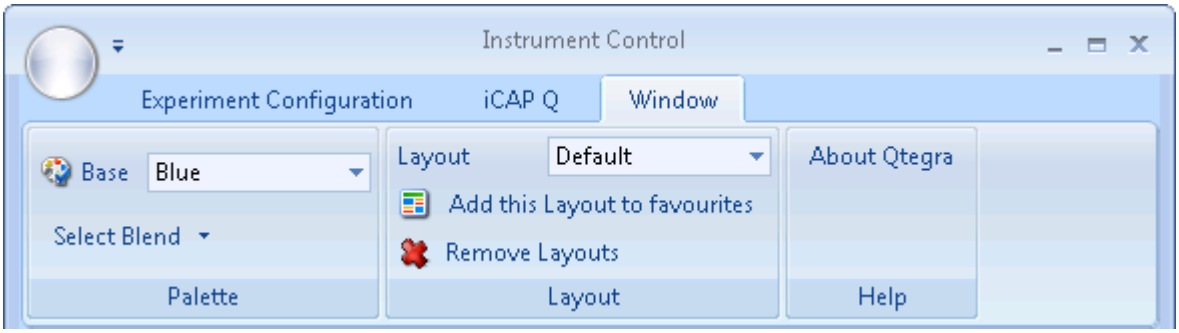


Figure 4-107. Window tab

❖ **To select the layout**

1. Click 

to open **Instrument Control**.
2. Click the **Window** ribbon tab.
3. In the group **Layout**, click  to display the list of available layout and select a layout.
The layout is changed accordingly.

❖ **To add a layout**

1. Click 

to open **Instrument Control**.
2. Click the **Window** ribbon tab.

3. In the group **Layout**, click  to add this to the list of **Layouts**.
   A dialog window opens, see Figure 4-108.

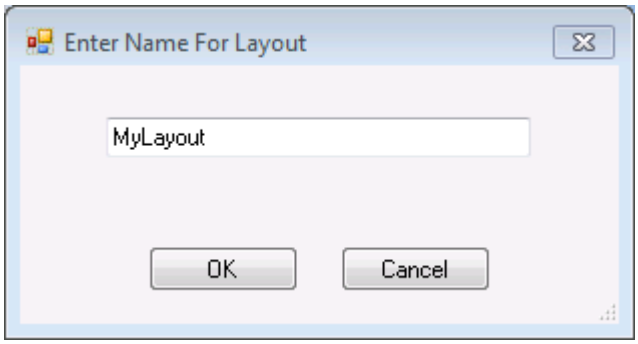


Figure 4-108. Enter Name For Layout dialog

4. Enter a name for your layout.
5. Click **OK**.
   Your layout is saved under this name.

❖ **To delete a layout**

1. Click 

to open **Instrument Control**.
2. Click the **Window** ribbon tab.
3. Click  .
   A dialog window opens, see Figure 4-109.

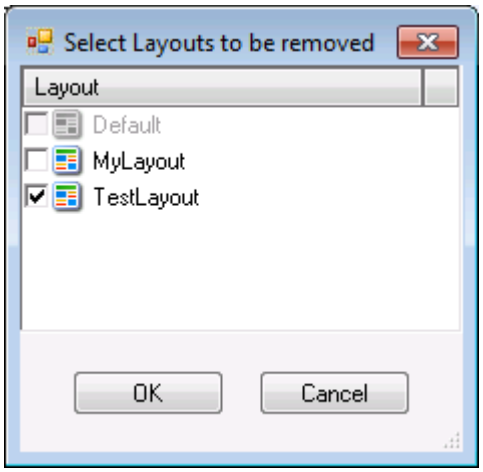


Figure 4-109. Select Layouts to be removed dialog

4. Select the check box of the layout to be deleted.
5. Click **OK**.

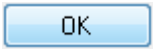
❖ **To change the appearance of the Instrument Control tool**

1. Click 

to open **Instrument Control**.
2. Click the **Window** ribbon tab.
3. In the **Palette** group, click  to open the **Base** drop-down list and select the base color from the list of preset colors.
The base color changes.
4. In the **Palette** group, click  to open the **Select Blend** drop-down menu and select a blend of color from the palette.
The color blend of the window changes.

❖ **To display the Qtegra information**

1. Click 

to open **Instrument Control**.
2. Click the **Window** ribbon tab.
3. In the **Help** group, click **About Qtegra** to display the software details.
A window opens which display copyright and version information.
4. Click 

to close the window.

Control Panel

The **Control Panel** tab (Figure 4-110) of Instrument Control contains several pages for interactive tuning and instrument monitoring.

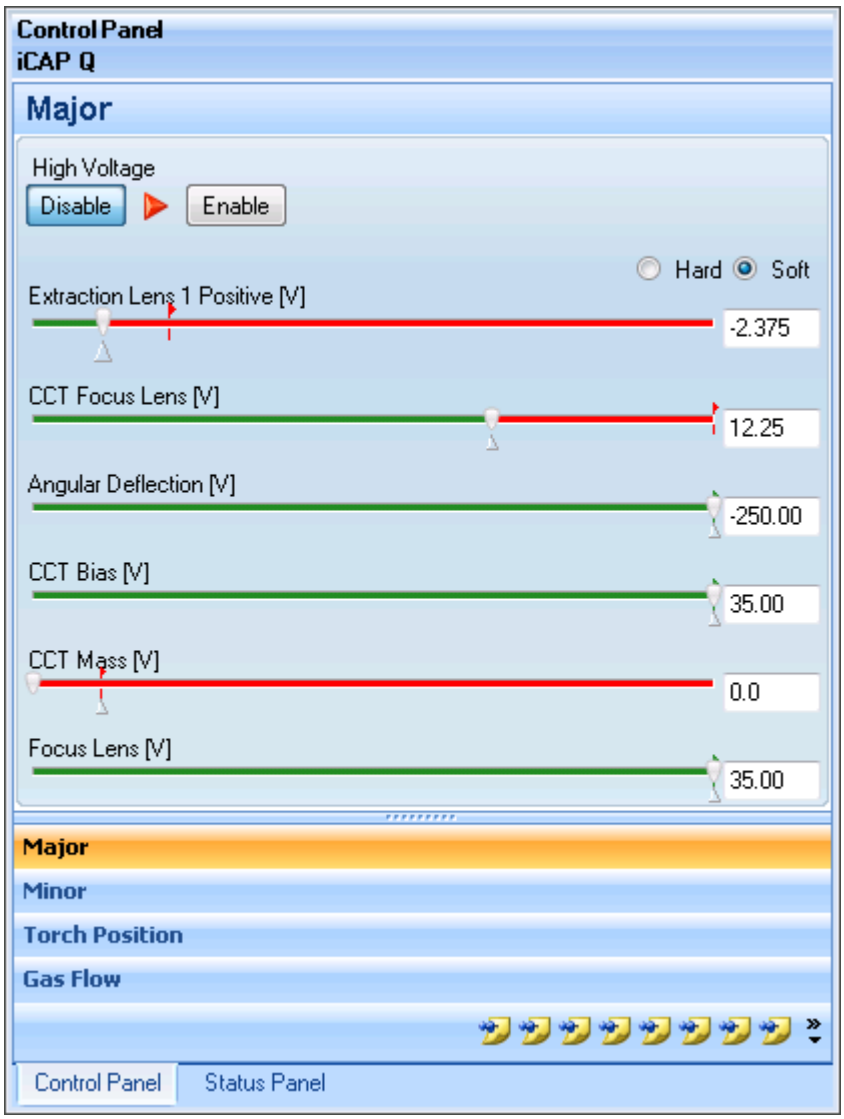


Figure 4-110. Control Panel

As with all Qtegra tools, the number and type of tuning pages depend on the configuration of the instrument the software controls and the selected application. The following lists all tuning pages available for the use with the iCAP Q instrument.

The sliders and buttons will differ according to the settings for the controls. Typical slider ranges which are the normally expected running ranges are set as default values.

The indicators between the buttons show the readback values. If the indicator is green, the readback value has reached the preset value, if red, the preset value has not been reached.

The grey pointers below the bars indicate the values set in the tune settings, while the flags above indicate the current value. See also "Change Tune Settings of a Measurement Mode" on page 4-17.

❖ **To open Control Panel**

1. Click 

to open **Instrument Control**.
2. Click the **Control Panel** tab on the lower left side of the Instrument Control window.

❖ **To define the order and display of Control Panel pages**

1. Click 

to open **Instrument Control**.
2. Click the **Control Panel** tab on the lower left side of the Instrument Control window.
3. Click  at the bottom of the **Control Panel** tab.
The **Configure buttons** menu opens, see Figure 4-111.

Figure 4-111. Selecting Navigation Pane Options

4. Click **Navigation Pane Options**.
The **Navigation Pane Options** dialog opens, see Figure 4-112.

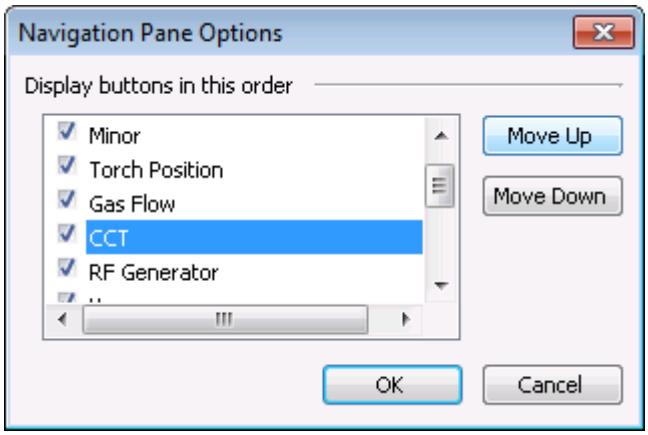


Figure 4-112. Navigation Pane Options dialog

5. Select the check boxes of the pages you wish to show.
6. Deselect the check boxes of the pages you do not wish to show.
7. Select the page you wish to move and click Move Up to move it up.
8. Select the page you wish to move and click Move Down to move it down.
9. Click OK to confirm your selection and close the window.

❖ **To add or remove pages**

1. Click 

to open **Instrument Control**.
2. Click the **Control Panel** tab on the lower left side of the Instrument Control window.
3. Click  at the bottom of the **Control Panel** tab.
The **Configure buttons** menu opens, see Figure 4-113.

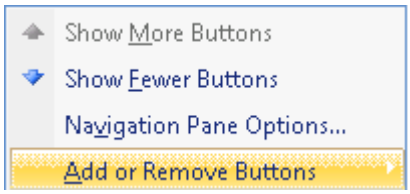


Figure 4-113. Selecting Add or Remove Buttons

4. Select **Add or Remove Buttons** to open the selection menu, see Figure 4-113.

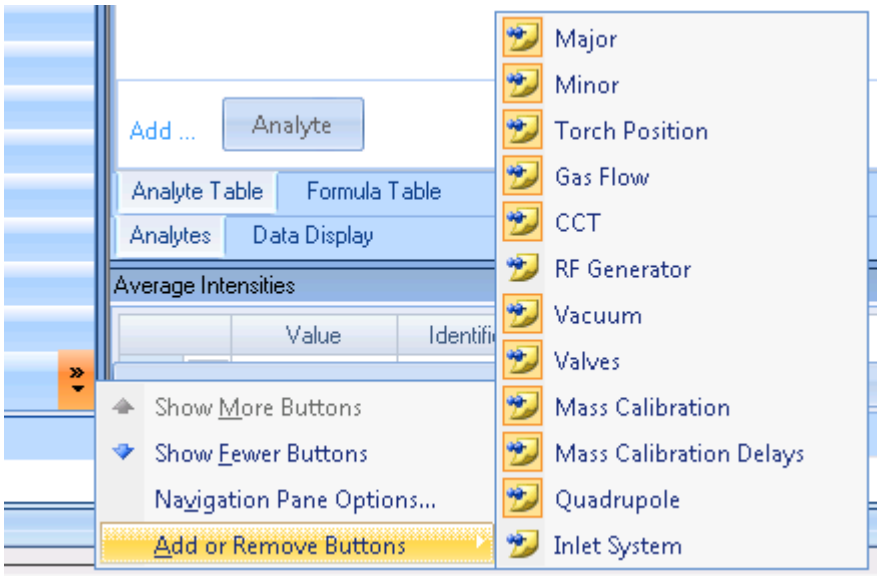


Figure 4-114. Selecting the Control Panel pages to be displayed

5. Click a deactivated page to activate the display.
   The selection menu closes and the page is added to the display.

6. Click an activated page to deactivate the display.
   The selection menu closes and the page is removed from the display.

Major

The **Major** page (see Figure 4-115) of the Control Panel tab in Instrument Control contains the iCAP Q parameters that are most commonly used and typically have the most effect on the performance of the instrument.

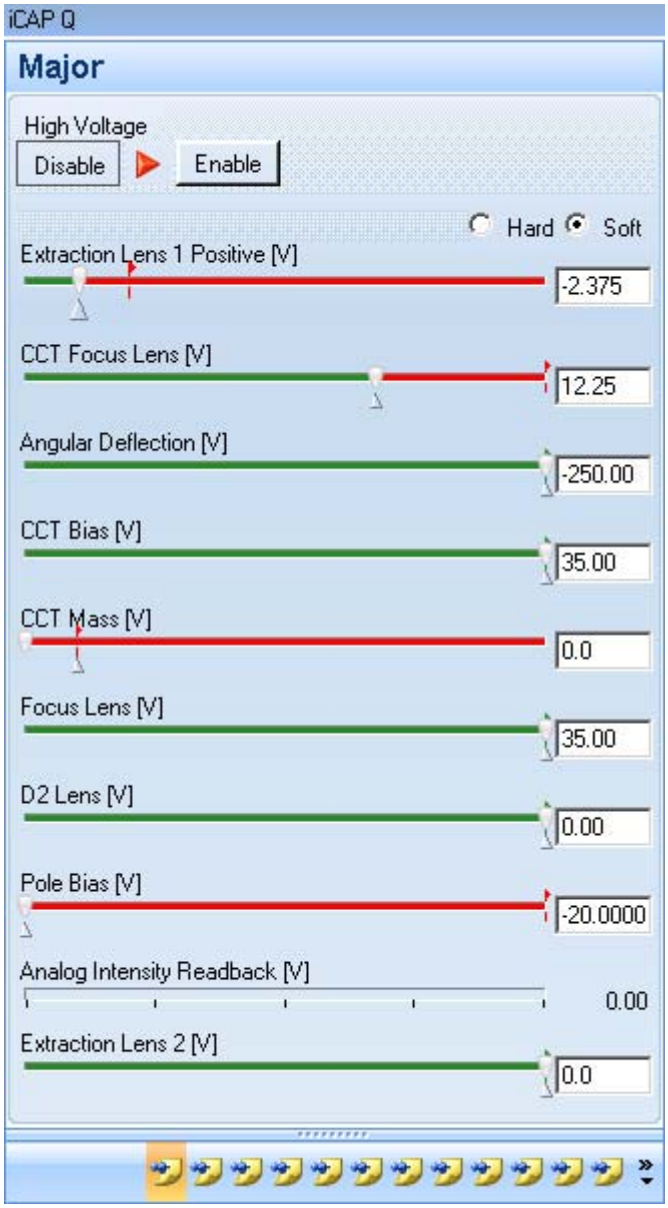


Figure 4-115. Tuning page Major

The tuning parameters of the Major page are described in Table 4-7.

Table 4-7. Tuning parameters of the Major page

Parameter	Description
High Voltage	Buttons switch high voltage for all ion-optical lenses. After the plasma is started, the high voltage is switched on, the button **Enable** is activated. When the plasma goes out, the high voltage is switched off, button **Disable** is activated. Buttons can also be switched manually if all safety locks are closed on door and torch and the vacuum is reached. With the radio buttons **Hard** and **Soft** it is possible to apply different voltages to extraction lens 1. Positive voltage (-5 to 20 V) for Soft, negative voltage (0 to 1000 V) for Hard.
Extraction Lens 1 Positive [V]	Voltage applied to extraction lens 1.
CCT Focus Lens [V]	Voltage of focus lens in front of the flatapole.
Angular Deflection [V]	Voltage of RAPID lens.
CCT Bias [V]	Ground voltage applied to the flatapole.
CCT Mass [V]	Readback of amplitude applied to the flatapole.
Focus Lens [V]	Voltage of focus lens in front of the DA stack.
D2 Lens [V]	Voltage of D2 lens (part of the DA stack).
Pole Bias [V]	Ground voltage applied on the quadrupole.
Analog Intensity Readback [V]	Readback of the measured intensities in the analog mode of the detector.
Extraction Lens 2 [V]	Voltage applied to extraction lens 2.

Minor

The **Minor** page (Figure 4-116) of the Control Panel tab in Instrument Control contains iCAP Q parameters that have a minor effect on the performance of the instrument and are less commonly used.

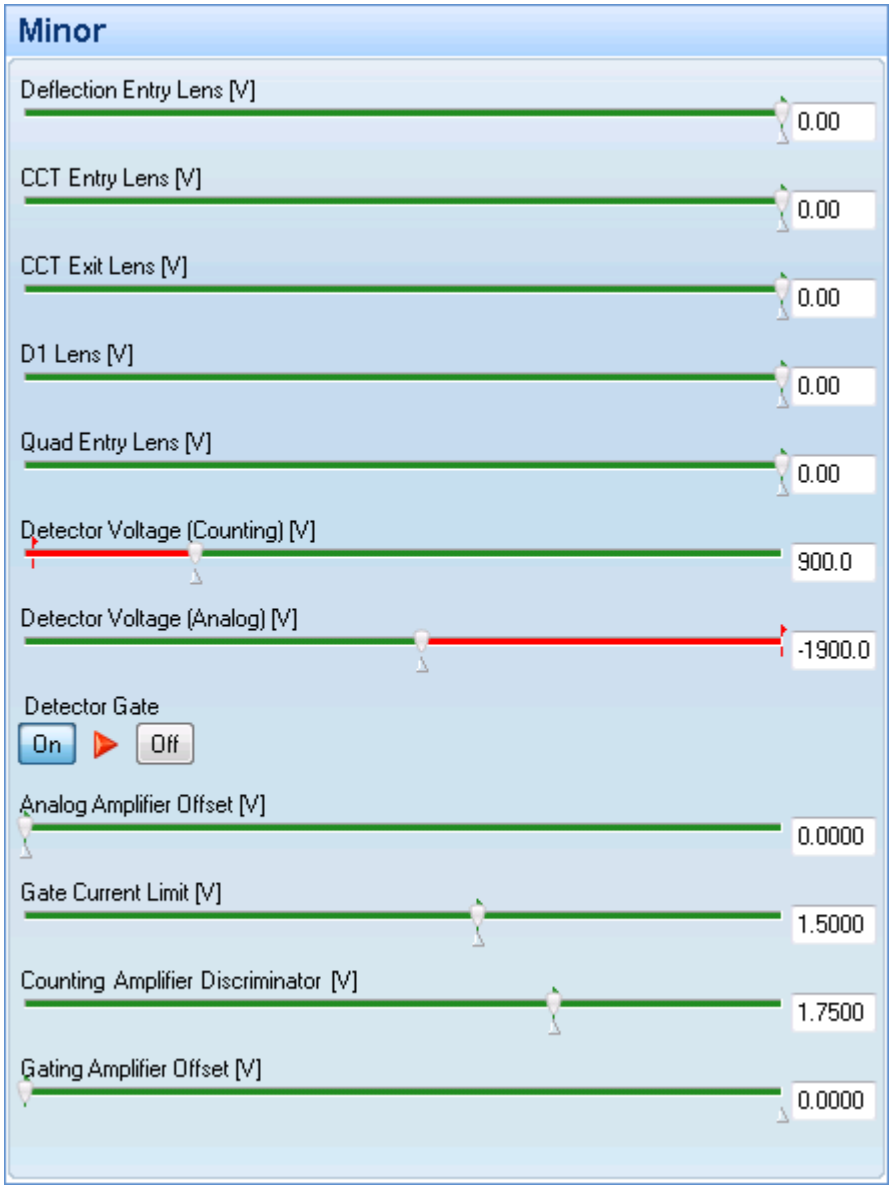


Figure 4-116. Tuning page Minor

The tuning parameters of the Minor page are described in Table 4-8.

Table 4-8. Tuning parameters of the Minor page

Parameter	Description
Deflection Entry Lens [V]	Voltage of lens before the RAPID lens.
CCT Entry Lens [V]	Voltage of CCT entry lens.
CCT Exit Lens [V]	Voltage of CCT exit lens.

Table 4-8. Tuning parameters of the Minor page

Parameter	Description
D1 Lens [V]	Voltage of D1 lens (part of DA stack).
Quad Entry Lens [V]	Voltage of lens in front of the quadrupole mass analyzer.
Detector Voltage (Counting) [V]	Voltage applied to the detector in pulse mode.
Detector Voltage (Analog) [V]	Voltage applied to the detector in analog mode.
Detector Gate	Amplifier and offset values of the ion detection unit.
Analog Amplifier Offset [V]	
Gate Current Limit [V]	
Counting Amplifier Discriminator [V]	
Gating Amplifier Offset [V]	Voltage of amplifier offset.

Torch Position

The **Torch Position** page (Figure 4-117) of the Control Panel tab in Instrument Control shows the position and state of the torch.

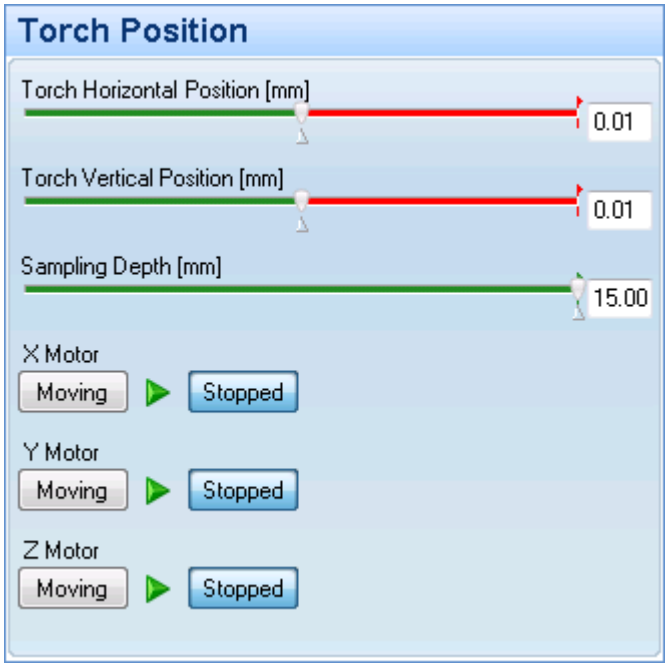


Figure 4-117. Tuning page Torch Position

The tuning parameters of the Torch Position page are described in Table 4-9.

Table 4-9. Tuning parameters of the Torch Position page

Parameter	Description
Torch Horizontal Position [mm]	Horizontal torch position.
Torch Vertical Position [mm]	Vertical torch position.
Sampling Depth [mm]	Sampling depth (z-position of torch). Distance of torch to sample cone.
X Motor	Button **Moving** is activated when the step motor is running to move the torch in x-direction. Button **Stopped** is activated when motor is stopped.
Y Motor	Button **Moving** is activated when the step motor is running to move the torch in y-direction. Button **Stopped** is activated when motor is stopped.
Z Motor	Button **Moving** is activated when the step motor is running to move the torch in z-direction. Button **Stopped** is activated when motor is stopped.

Gas Flow

The **Gas Flow** page (Figure 4-118) of the Control Panel tab in Instrument Control shows the current gas flow of cool, auxiliary and nebulizer gas, as well as the additional gas parameters.

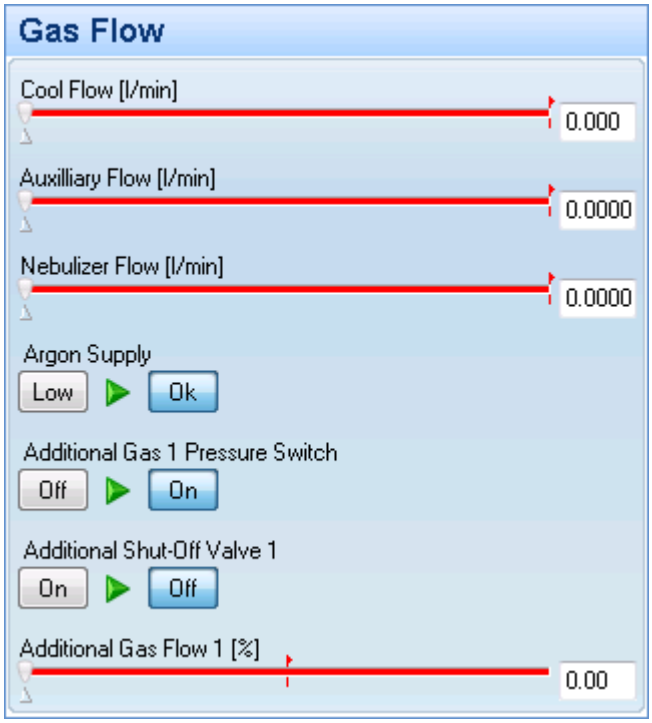


Figure 4-118. Tuning page Gas Flow

The tuning parameters of the Gas Flow page are described in Table 4-10.

Table 4-10. Tuning parameters of the Gas Flow page

Parameter	Description
Cool Flow [l/min]	Gas flow of the cooling gas argon in L/min.
Auxiliary Flow [l/min]	Gas flow of the auxiliary gas argon in L/min.
Nebulizer Flow [l/min]	Gas flow of the nebulizer gas argon in L/min.
Argon Supply	Button **Low** is activated when the readback pressure value of the gas supply is too low to actuate the valves or run the plasma. The plasma goes out and the instrument shuts down. Button **OK** is activated when the readback pressure is sufficiently high to operate the plasma.

Table 4-10. Tuning parameters of the Gas Flow page

Parameter	Description
Additional Gas 1 Pressure Switch	Button **On** is activated when the readback pressure value for additional gas is sufficient. Button **Off** is activated when the readback pressure value for additional gas is not sufficient.
Additional Shut-Off Valve 1	Readback value for shut-off valve. Valve is switched automatically. Button **On** is activated when the additional gas flow is turned on. Button **Off** is activated when the additional gas flow is turned off.
Additional Gas Flow 1 [%]	Additional gas flow in percent.

CCT

The **CCT** page (Figure 4-119) of the Control Panel tab in Instrument Control shows the parameters and state of the CCT gas flow.

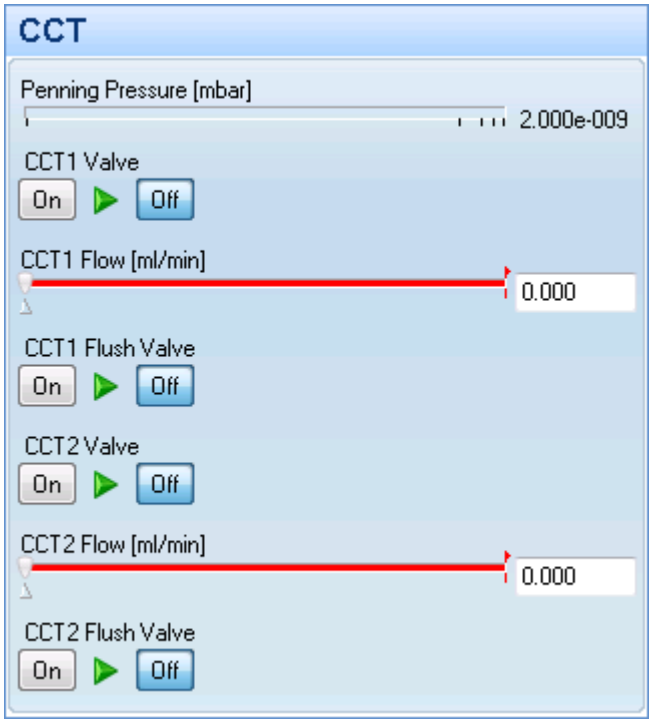


Figure 4-119. Tuning page CCT

The tuning parameters of the CCT page are described in Table 4-11.

Table 4-11. Tuning parameters of the CCT page

Parameter	Description
Penning Pressure [mbar]	Readback value for pressure of Penning gauge (vacuum of interface).
CCT1 Valve	Button **On** is activated when the CCT1 gas valve is open. Button **Off** is activated when the valve is closed.
CCT1 Flow [ml/min]	CCT1 gas flow in mL/min.
CCT1 Flush Valve	Button **On** is activated when the CCT1 gas flush valve is open. Button **Off** is activated when the valve is closed.
CCT2 Valve	Button **On** is activated when the CCT2 gas valve is open. Button **Off** is activated when the valve is closed.
CCT2 Flow [ml/min]	CCT2 gas flow in mL/min.
CCT2 Flush Valve	Button **On** is activated when the CCT2 gas flush valve is open. Button **Off** is activated when the valve is closed.

RF Generator

The **RF Generator** page (Figure 4-120) of the Control Panel tab in Instrument Control shows the parameters and state of the plasma generator.

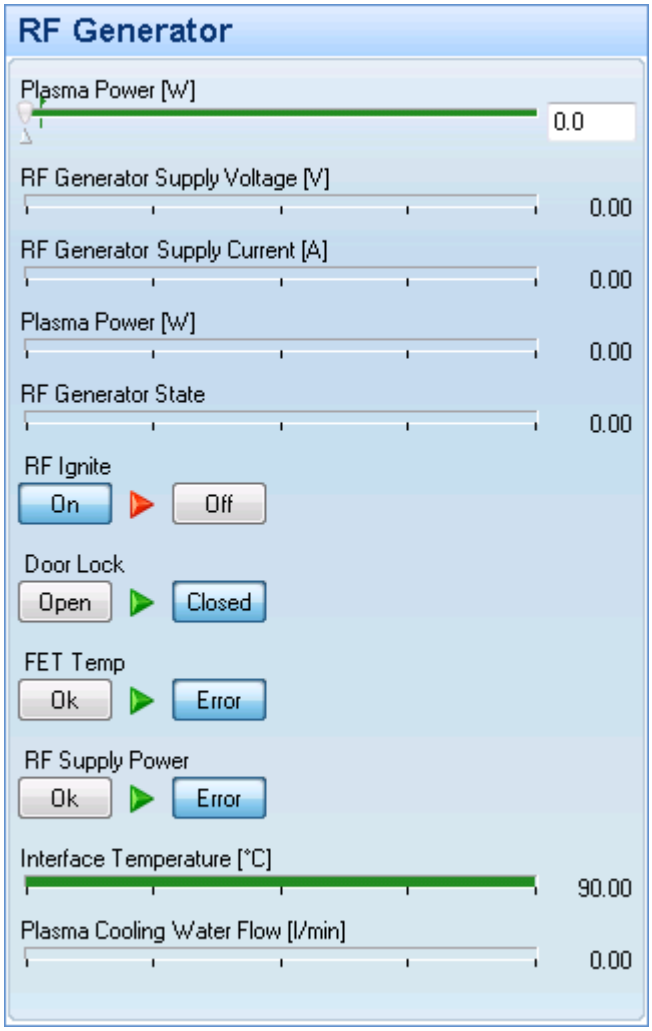


Figure 4-120. Tuning page RF Generator

The tuning parameters of the RF Generator page are described in Table 4-12.

Table 4-12. Tuning parameters of the RF Generator page

Parameter	Description
Plasma Power [W]	Preset plasma power in watt.
RF Generator Supply Voltage [V]	Indicates readback value for RF generator supply voltage.
RF Generator Supply Current [A]	Indicates readback value for RF generator supply current.
Plasma Power [W]	Indicates readback value for plasma power in watt.

Table 4-12. Tuning parameters of the RF Generator page

Parameter	Description
RF Generator State	Indicates readback value for RF generator state.
RF Ignite	**For service or maintenance operation only**. Button **On** to start radio frequency (RF) for ignition of plasma. Button **Off** to switch off RF. **NOTICE** Operates without interlocks. ▲
Door Look	Button **Open** is activated when the plasma door is open (readback). Button **Closed** is activated when plasma door is closed (readback).
FET Temp (temperature of field effect transistor)	Button **Ok** and **Error** to indicate status.
RF Supply Power	Button **Ok** and **Error** to indicate status of RF power supply.
Interface Temperature [°C]	Indicates readback value for interface temperature.
Plasma Cooling Water Flow [l/min}	Indicates readback value of cooling water flow for plasma and interface cooling.

Vacuum

The **Vacuum** page (Figure 4-121) of the Control Panel tab in Instrument Control shows the parameters and state of the vacuum system.

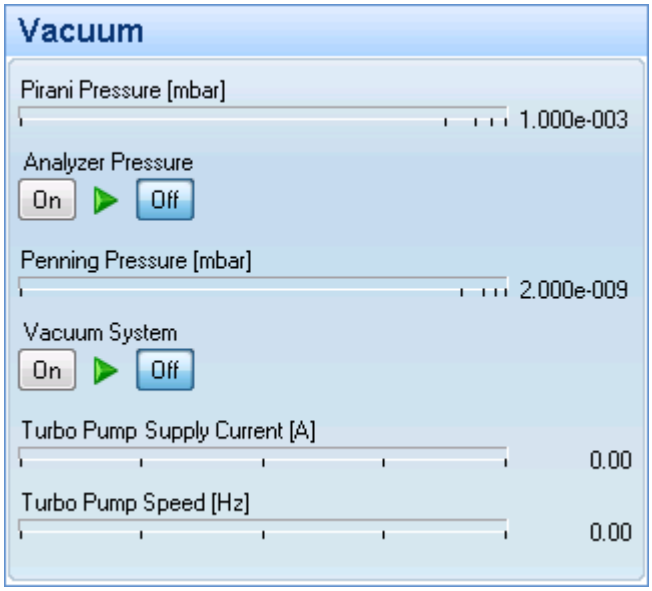


Figure 4-121. Tuning page Vacuum

The tuning parameters of the Vacuum page are described in Table 4-13.

Table 4-13. Tuning parameters of the Vacuum page

Parameter	Description
Pirani Pressure [mbar]	Indicates readback value for pressure of Pirani gauge (fore vacuum stage).
Analyzer Pressure	Shows status of analyzer pressure sensor. Button automatically switches to **On** if vacuum falls below preset values. Button **Off** to indicate sensor is off.
Penning Pressure [mbar]	Indicates readback value for pressure of Penning gauge (high vacuum stage).
Vacuum System	Button **On** to switch on the vacuum system. Button **Off** to switch off the vacuum system. Used, for example, when the system is vented.

Table 4-13. Tuning parameters of the Vacuum page

Parameter	Description
Turbo Pump Supply Current [A]	Indicates readback value for power supply current of turbo molecular pump.
Turbo Pump Speed [Hz]	Indicates readback value for speed of turbo molecular pump.

Valves

The **Valves** page (Figure 4-122) of the Control Panel tab in Instrument Control shows the parameters and state of the valves.

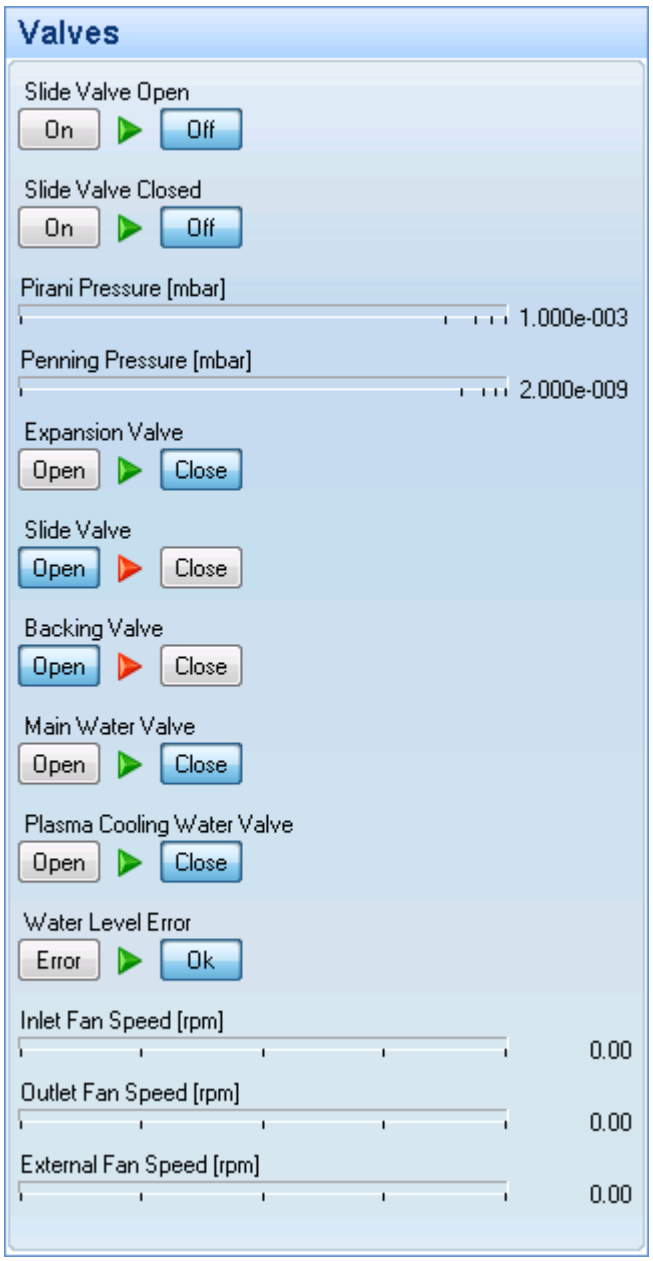


Figure 4-122. Tuning page Valves

The tuning parameters of the Valves page are described in Table 4-14.

Table 4-14. Tuning parameters of the Valves page

Parameter	Description
Slide Valve Open	Indicates readback value for **Slide Valve Open**.
Slide Valve Closed	Indicates readback value for **Slide Valve Closed**.
Pirani Pressure [mbar]	Indicates readback value for pressure of Pirani gauge.
Penning Pressure [mbar]	Indicates readback value for pressure of Penning gauge.
Expansion Valve	Button **Open** to open the Expansion valve. Button **Close** to close the Expansion valve.
Slide Valve	Button **Open** to open the Slide valve. Button **Close** to close the Slide valve.
Backing Valve	Button **Open** to open the Backing valve. Button **Close** to close the Backing valve.
Main Water Valve	Button **Open** to open the Main Water valve. Button **Close** to close the Main Water valve.
Plasma Cooling Water Valve	Button **Open** to open the Plasma Cooling Water valve. Button **Close** to close the Plasma Cooling Water valve.
Water Level Error	Button **Error** to indicate the water level inside the instrument is too high. Water might also leak from the instrument. Button **Ok** to indicate the correct water level inside the instrument.
Inlet Fan Speed [rpm]	Indicates readback value for speed of inlet fan.
Outlet Fan Speed [rpm]	Indicates readback value for speed of outlet fan.
External Fan Speed [rpm]	Indicates readback value for speed of external fan if available.

Mass Calibration

The **Mass Calibration** page (Figure 4-123) of the Control Panel tab in Instrument Control shows the parameters relevant for mass calibration.

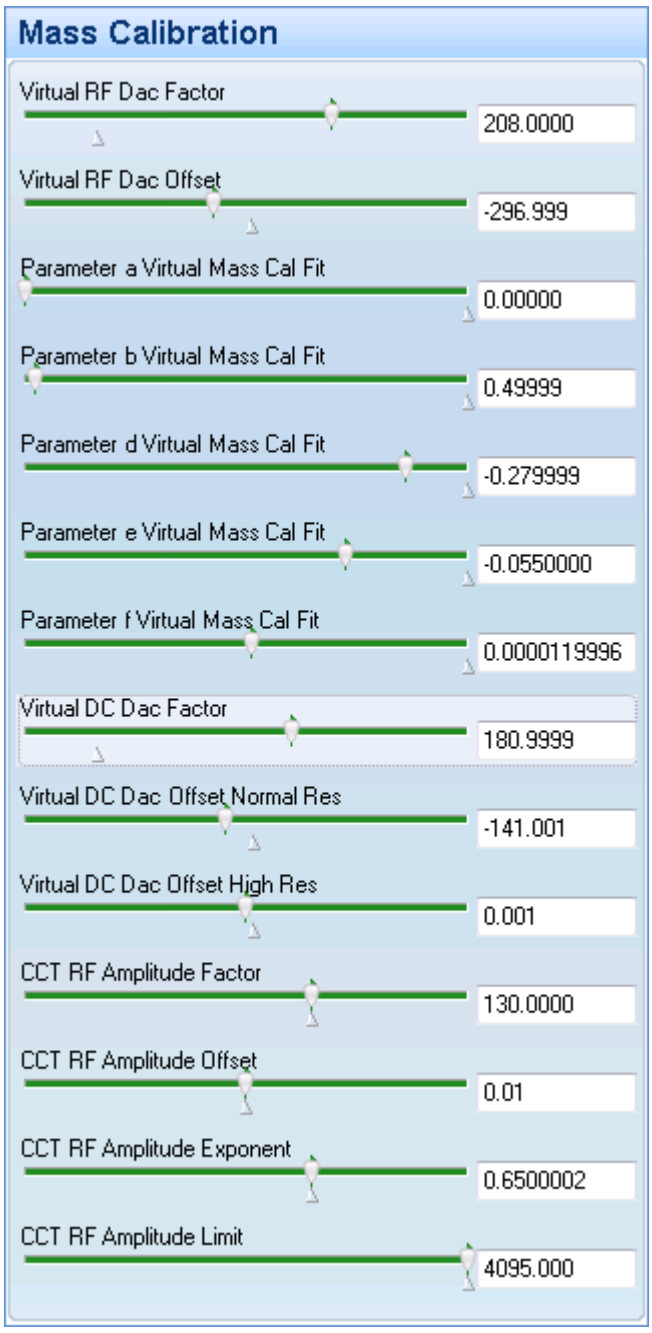


Figure 4-123. Tuning page Mass Calibration

The tuning parameters of the Mass Calibration page are described in Table 4-15.

Table 4-15. Tuning parameters of the Mass Calibration page

Parameter	Description
Virtual RF Dac Factor	Virtual radio frequency Dac factor.
Virtual RF Dac Offset	Virtual radio frequency Dac offset.
Parameter a Virtual Mass Cal Fit	Parameter *a* of virtual mass calibration fit.
Parameter b Virtual Mass Cal Fit	Parameter *b* of virtual mass calibration fit.
Parameter c Virtual Mass Cal Fit	Parameter *c* of virtual mass calibration fit.
Parameter d Virtual Mass Cal Fit	Parameter *d* of virtual mass calibration fit.
Parameter e Virtual Mass Cal Fit	Parameter *e* of virtual mass calibration fit.
Parameter f Virtual Mass Cal Fit	Parameter *f* of virtual mass calibration fit.
Virtual DC Dac Factor	Virtual DC Dac factor.
Virtual DC Dac Offset Normal Res	Virtual DC Dac offset normal resolution.
Virtual DC Dac Offset High Res	Virtual DC Dac offset high resolution.
CCT RF Amplitude Factor	Radio frequency amplitude factor for QCell.
CCT RF Amplitude Offset	Radio frequency amplitude offset for QCell.
CCT RF Amplitude Exponent	Radio frequency amplitude exponent for QCell.
CCT RF Amplitude Limit	Radio frequency amplitude limit for QCell.

Mass Calibration Delays

The **Mass Calibration Delays** page (Figure 4-124) of the Control Panel tab in Instrument Control shows the delays relevant for mass calibration.

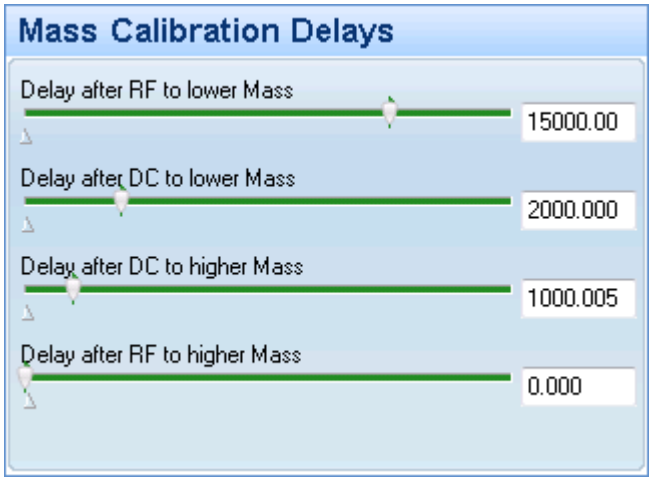


Figure 4-124. Tuning page Mass Calibration Delays

The tuning parameters of the Mass Calibration Delays page are described in Table 4-16.

Table 4-16. Tuning parameters of the Mass Calibration Delays page

Parameter	Description
Delay after RF to lower Mass	Delay after radio frequency to lower mass.
Delay after DC to lower Mass	Delay after DC to lower mass.
Delay after DC to higher Mass	Delay after DC to higher mass.
Delay after RF to higher Mass	Delay after radio frequency to higher mass.

Quadrupole

The **Quadrupole** page (Figure 4-125) of the Control Panel tab in Instrument Control shows the values for and state of the quadrupole.

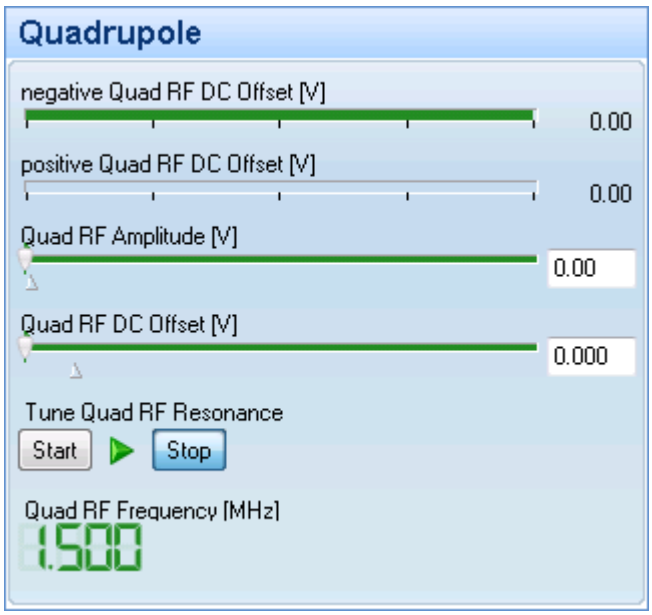


Figure 4-125. Tuning page Quadrupole

The tuning parameters of the Quadrupole page are described in Table 4-17.

Table 4-17. Tuning parameters of the Quadrupole page

Parameter	Description
negative Quad RF DC Offset [V]	Indicates readback value of negative quadrupole RF DC offset voltage.
positive Quad RF DC Offset [V]	Indicates readback value of positive quadrupole RF DC offset voltage.
Quad RF Amplitude [V]	Quadrupole RF amplitude voltage.
Quad RF DC Offset [V]	Quadrupole RF DC offset voltage.
Tune Quad RF Resonance	**For service or maintenance operation only.** Button **Start** to determine RF resonance frequency of the quadrupole. Button **Stop** is activated when the measurement of the resonance frequency is completed.
Quad RF Frequency [MHz]	Shows quadrupole RF frequency.

Inlet System

The **Inlet System** page (Figure 4-126) of the Control Panel tab in Instrument Control shows the values for and state of the inlet system.

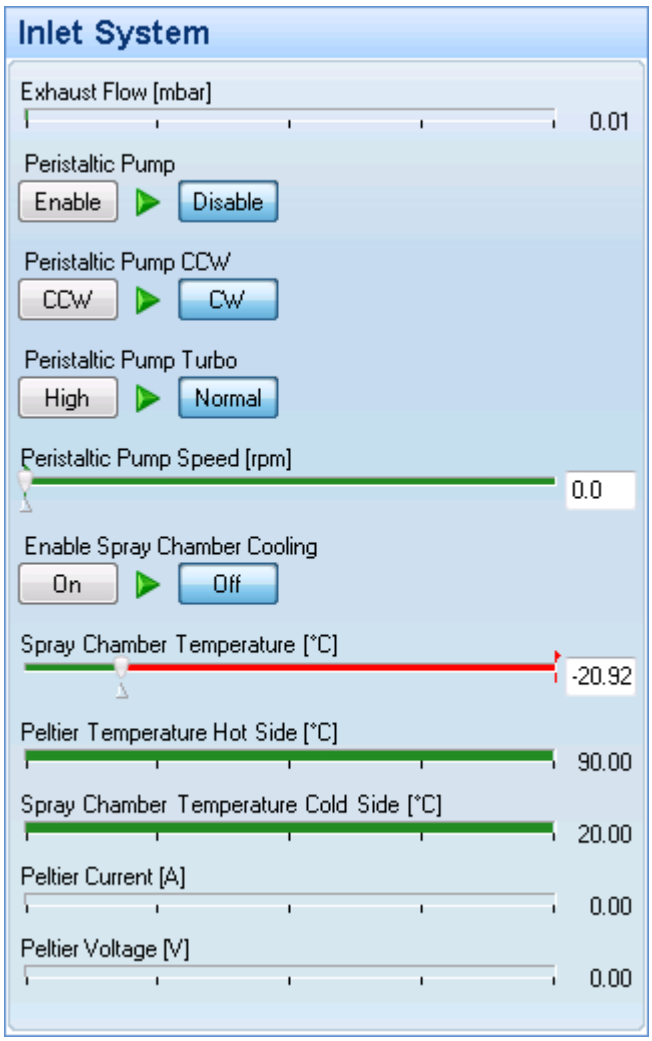


Figure 4-126. Tuning page Inlet System

The tuning parameters of the Inlet System page are described in Table 4-18.

Table 4-18. Tuning parameters of the Inlet System page

Parameter	Description
Exhaust Flow [mbar]	Indicates readback value of exhaust flow pressure difference.
Peristaltic Pump	Button **Enable** to activate the peristaltic pump. Button **Disable** to deactivate the peristaltic pump.
Peristaltic Pump CCW	Button **CCW** to activate the peristaltic pump counter clockwise. Button **CW** to switch to clockwise.

Table 4-18. Tuning parameters of the Inlet System page

Parameter	Description
Peristaltic Pump Turbo	Button **High** to activate the peristaltic turbo pump maximum speed (100 rpm). Button **Normal** to switch to normal speed (preset speed typically 40 rpm).
Peristaltic Pump Speed [rpm]	Speed of the peristaltic turbo pump in rpm.
Enable Spray Chamber Cooling	Button **On** is activated when the spray chamber cooling is enabled. Button **Off** when disabled.
Spray Chamber Temperature [°C]	Sets spray chamber temperature in °C.
Peltier Temperature Hot Side [°C]	Indicates Peltier temperature on hot side in °C.
Spray Chamber Temperature Cold Side [°C]	Indicates spray chamber temperature on cold side in °C.
Peltier Current [A]	Indicates readback value of Peltier current in ampere.
Peltier Voltage [V]	Indicates readback value of Peltier voltage.

Status Panel

In the **Status Panel** tab (Figure 4-127) of the Instrument Control tool you manage your scripts.

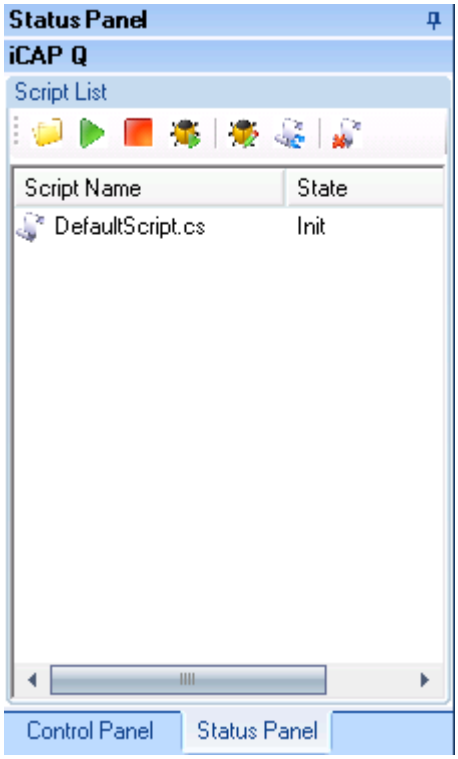


Figure 4-127. Control Panel

❖ **To open Status Panel**

1. Click Instrument Control to open **Instrument Control**.
2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.

❖ **To load a script to the Status Panel**

1. Click Instrument Control to open **Instrument Control**.
2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.

3. Click  in the toolbar of **Script List**.
   The **Open** dialog opens, see Figure 4-128.

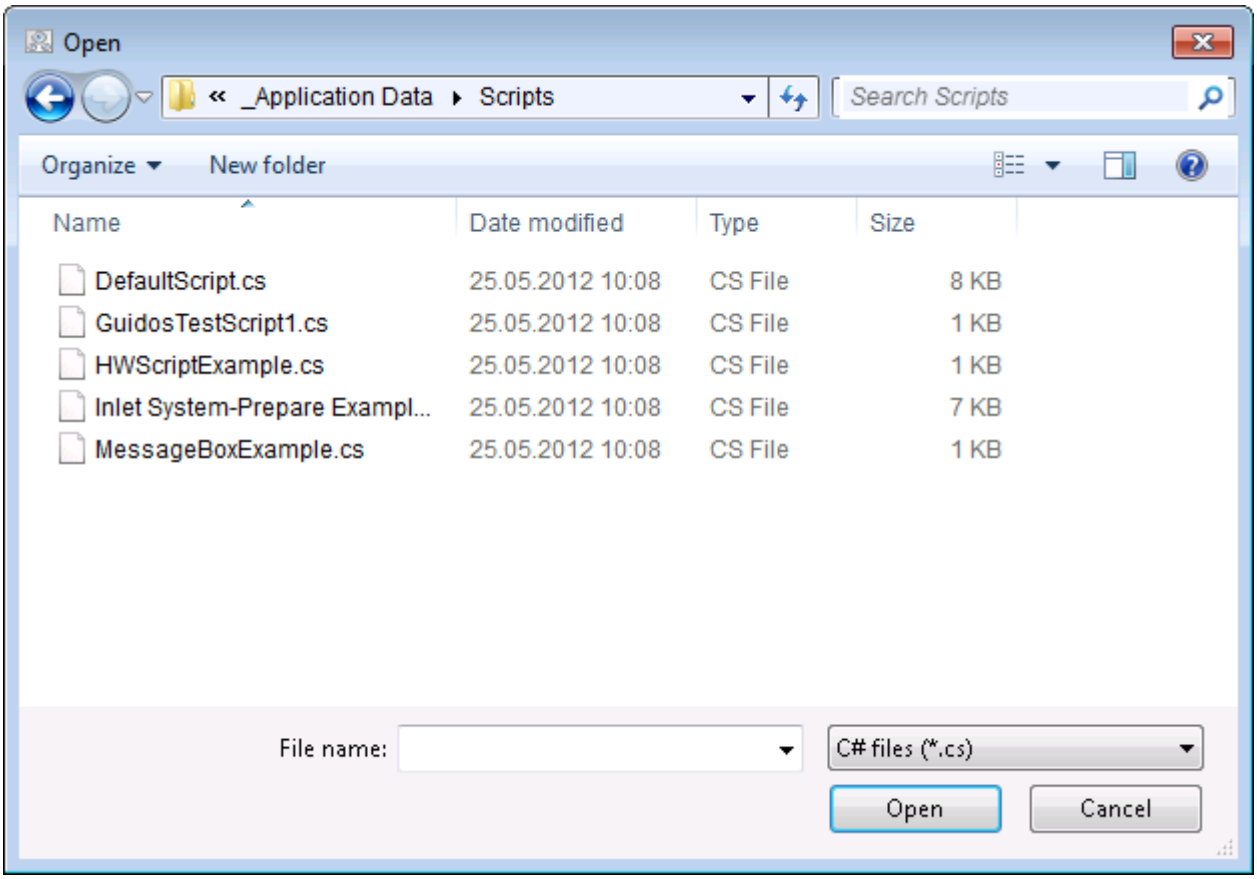


Figure 4-128. Dialog to open scripts

4. Select the script you wish to open.

5. Click Open.
   The script is loaded into the **Status Panel**, see Figure 4-129.

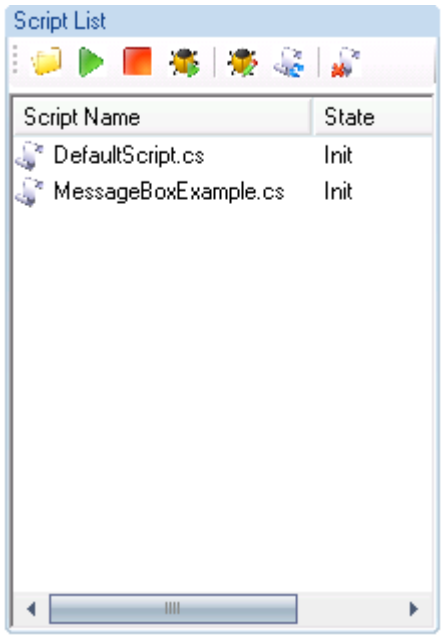


Figure 4-129. Scripts loaded into Script List of Status Panel

❖ **To run a script**

1. Click Instrument Control to open **Instrument Control**.
2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.
3. Select the script you wish to execute in the **Script List** of the **Status Panel**.
4. Click in the toolbar of **Script List**.
   The selected script is executed.

❖ **To stop a script**

1. Click Instrument Control to open **Instrument Control**.
2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.
3. Select the script you wish to execute in the **Script List** of the **Status Panel**.

4. Click  in the toolbar of **Script List**.
   The selected script is executed.

5. Click  in the toolbar of **Script List**.
   The script execution is stopped.

❖ **To debug a script**

1. Click  to open **Instrument Control**.

2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.

3. Select the script you wish to debug in the **Script List** of the **Status Panel**.

4. Click  in the toolbar of **Script List**.
   The selected script is debugged if debugging has been activated.

❖ **To reset a script**

1. Click  to open **Instrument Control**.

2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.

3. Select the script you wish to reset in the **Script List** of the **Status Panel**.

4. Click  in the toolbar of **Script List**.
   The selected script is reset.

❖ **To edit a script**

1. Click  to open **Instrument Control**.

2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.

3. In the **Script List**, select the script you wish to edit.

4. Click  in the toolbar of **Script List**.
   The script editor opens, see Figure 4-130.

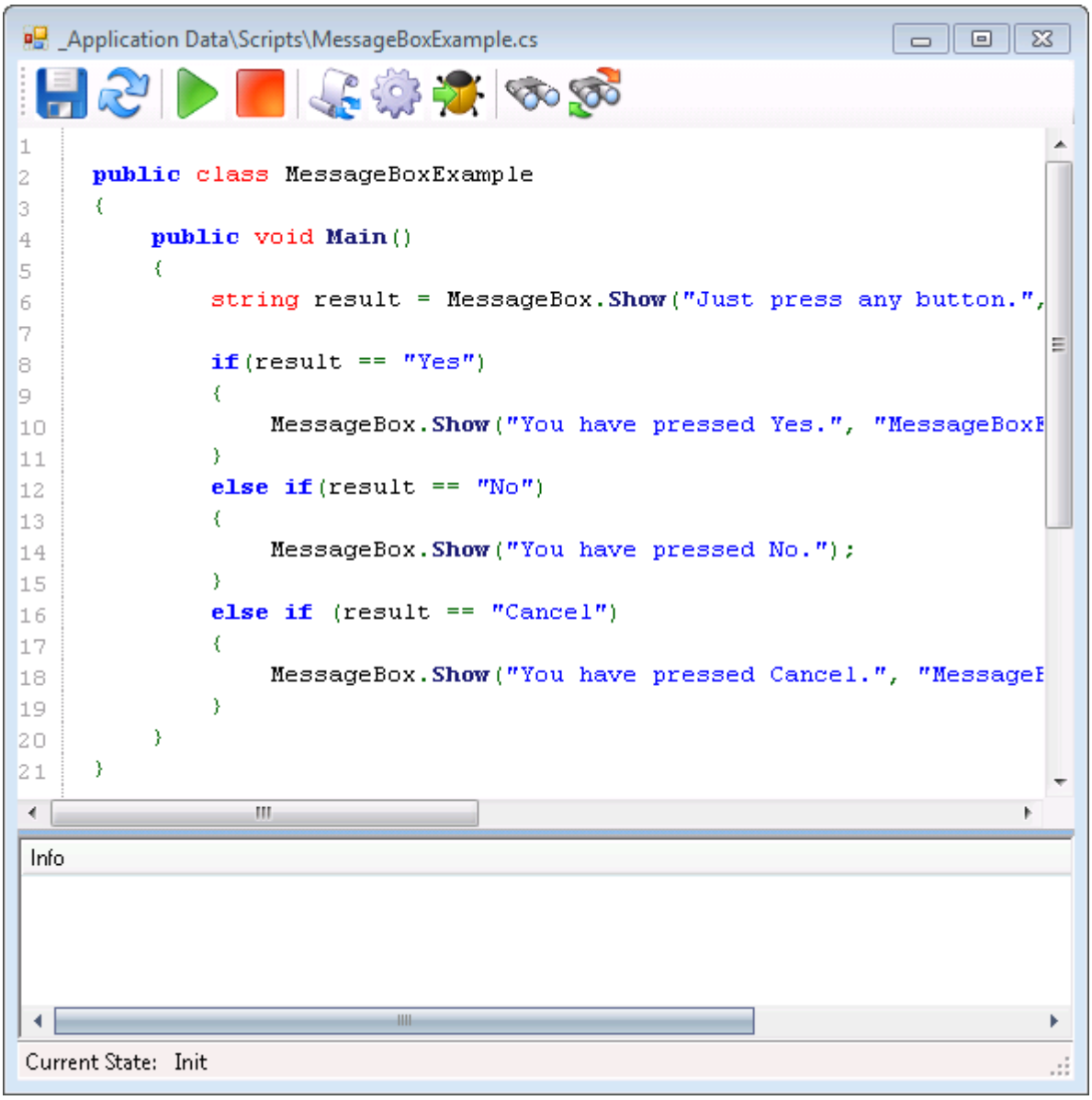


Figure 4-130. Script Editor

5. Edit your script.

6. Click  to save the script.

7. Click  .
   The script editor closes.

❖ To remove a script from the Script List

1. Click 

to open **Instrument Control**.
2. Click the **Status Panel** tab on the lower left side of the Instrument Control window.
3. Select the script you wish to delete from the **Script List** in the **Status Panel**.
4. Click  in the toolbar of **Script List**.
The selected script is removed from the **Script List** in the **Status Panel**.

Log View Region

The **Log View** region of Instrument Control (Figure 4-131) displays a list of messages, such as errors and warnings. By default, different types of messages are displayed.

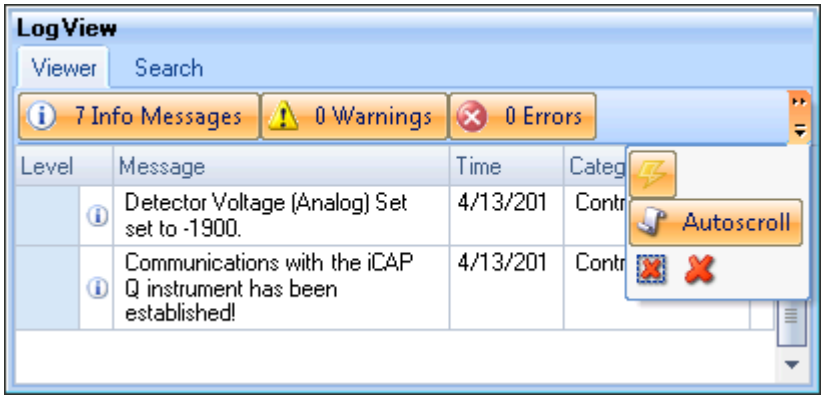


Figure 4-131. Log View Instrument Control

NOTICE The Viewer tab is also shown in "Experiment Editor" on page 5-1 and "Configurator" on page 3-1. ▲

❖ To change the location of the Log View region

1. Click to open **Instrument Control**.

2. Right-click the **Log View** title bar.
   The context menu opens, see Figure 4-132.

Figure 4-132. Log View context menu

3. Select an item from the menu.

   If **Dockable** is selected, the Log view region is shown below the data region. If you deselect it, the Log view region is added as new tab above. **Floating** shows the Log View region in a separate window that can be moved as needed. **Auto Hide** minimizes the Log View region as soon as you click anywhere outside the data region. Simply click the remaining tab below the Control Panel tab to show the Log View region again.

Chapter 5 Experiment Editor

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

Contents

- User Interface of the Experiment Editor Tool
- Dashboard Page of Experiment Editor
- Analysis Page
- Templates Page
- Results Page
- Manage Files Page
- Help Page
- Scheduler
- Completed LabBooks
- Log View Region

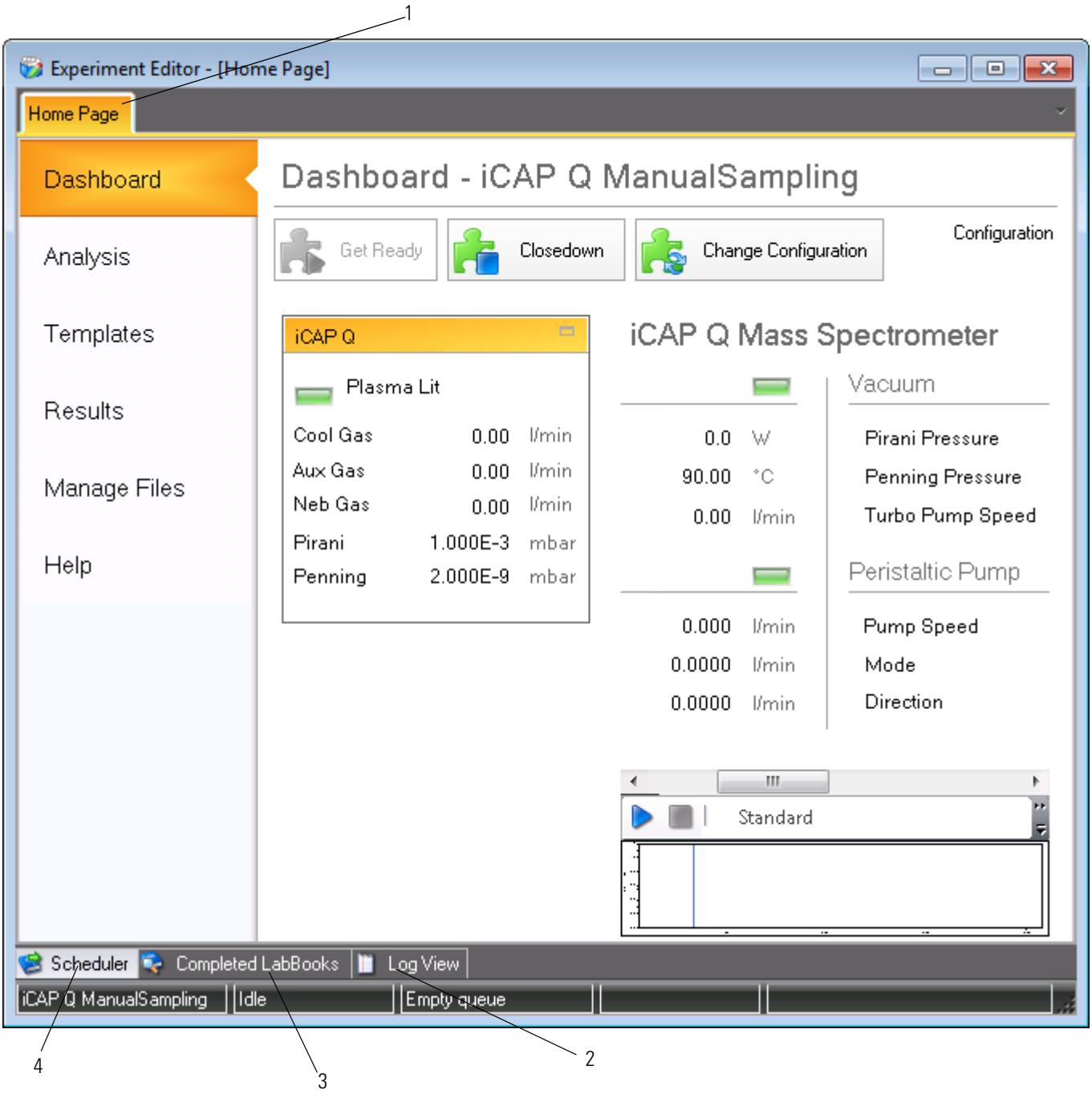
❖ **To open the Experiment Editor tool**

1. Click 

to open **Experiment Editor**.

User Interface of the Experiment Editor Tool

The Experiment Editor tool is shown in Figure 5-1:



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

Figure 5-1. Home Page of Experiment Editor

The **Home Page** (**1** in Figure 5-1) of the Experiment Editor tool by default shows the Dashboard page. The pages for measurement, result analysis, the management of files and helpful links are also accessed via the Home Page.

The **Log View** tab (**2** in Figure 5-1) of the Experiment Editor tool shows system messages, warnings and errors of the iCAP Q system.

The **Completed LabBooks** tab (**3** in Figure 5-1) of the Experiment Editor tool lists the LabBooks previously run.

In the **Scheduler** tab (**4** in Figure 5-1) of the Experiment Editor tool all LabBooks assigned to be run are listed.

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

1. Click 

to open **Experiment Editor**.

2. Right-click the **Scheduler, Log View** or **Completed LabBooks** title bar or tab.
   The context menu opens, see Figure 5-2.

Figure 5-2. Context menu of title bar

3. Select **Floating** to show the selected tab in a separate window. Move the window or resize as required.

4. Select **Auto Hide** to hide the selected tab when the cursor leaves the tab area.

   You can also 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.

5. Deselect the items from the context menu to undo the selection.

6. Click and drag the **Scheduler, Log View** or **Completed LabBooks** title bar or tab, see Figure 5-2.

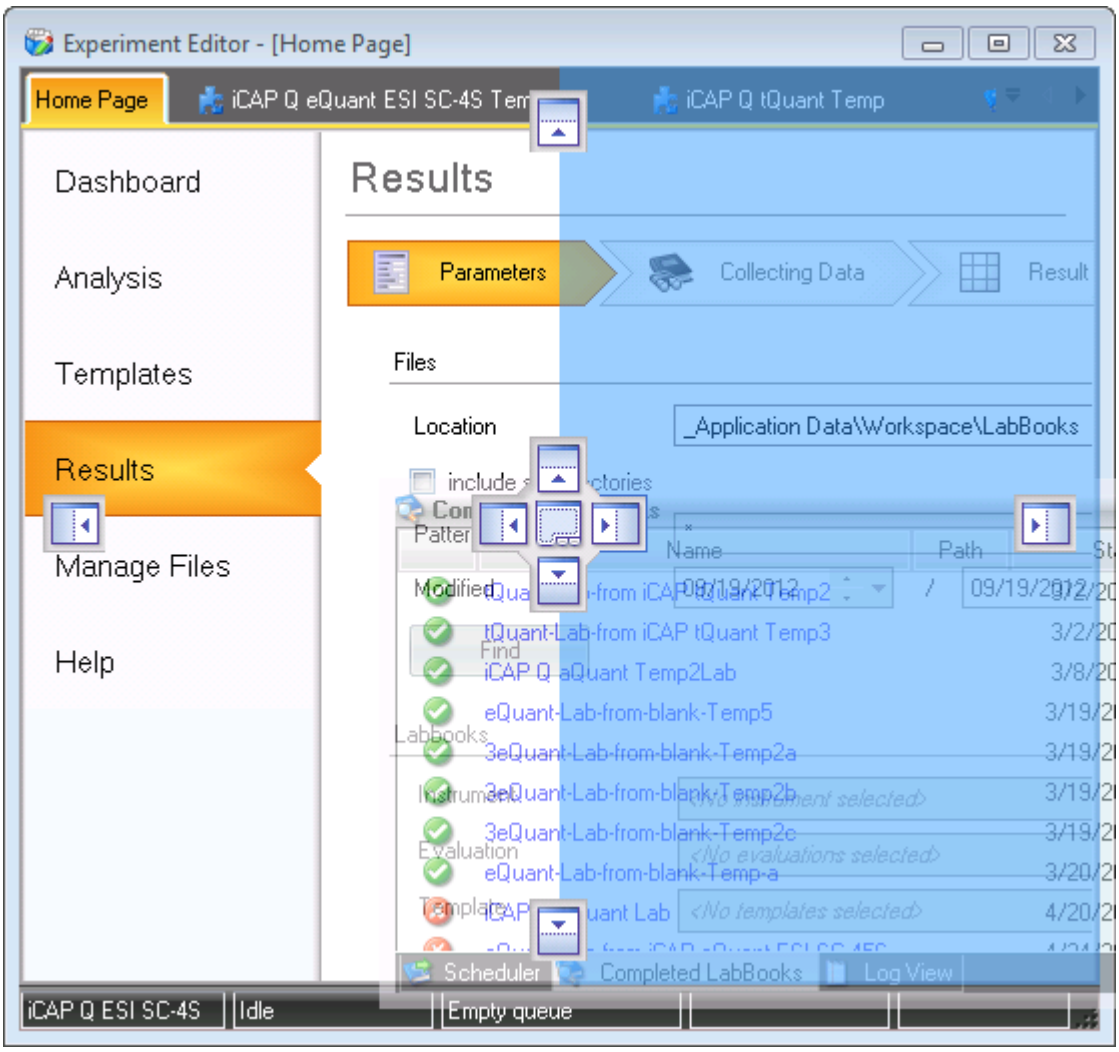


Figure 5-3. Moving Completed LabBooks

The selected tab is shown transparent and the new position colored and transparent.

7. Move the cursor over the position indicators, see Figure 5-4.

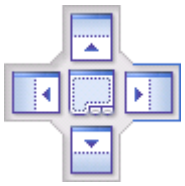


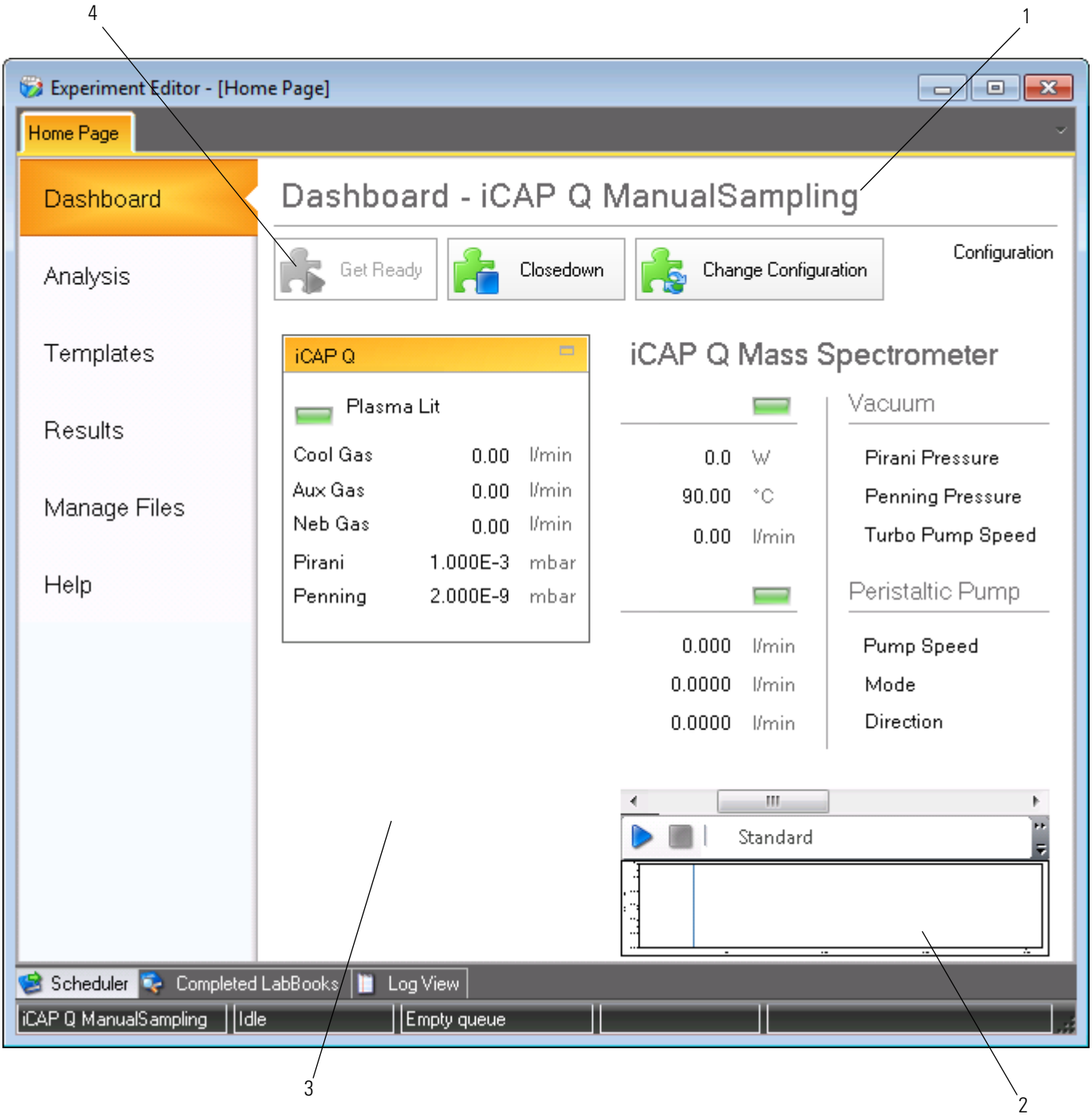
Figure 5-4. Position indicator to move tab

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

Dashboard Page of Experiment Editor

The Home Page opens on the **Dashboard** page by default when you start Experiment Editor. The Dashboard Page contains all functions offered by the Experiment Editor tool and gives access to all existing Templates and LabBooks.

The **Dashboard** page of Experiment Editor shows on one page the instrument controls and main settings of the iCAP Q instrument, see Figure 5-5.



Labeled Components: 1=current Configuration, 2=real-time display, 3=important parameters of the iCAP Q system, 4=functions of Dashboard

Figure 5-5. Dashboard Page of Experiment Editor

On top of the Dashboard page the currently loaded Configuration (**1** in Figure 5-5) is displayed.

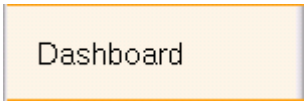
In the graphical display at the lower right side (**2** in Figure 5-5) you can check whether the intensity of the iCAP Q system is sufficient for the elements to be measured.

The main part (**3** in Figure 5-5) of the Dashboard page presents an overview of all main settings of the iCAP Q system.

The Dashboard page offers several functions (**4** in Figure 5-5) to prepare the iCAP Q system for measurement, close down the system or change the Configuration.

❖ **To open the Dashboard page of Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
The **Dashboard** page of Experiment Editor opens.

Getting Ready

The **Get Ready** function on the **Dashboard** page of Experiment Editor helps to start the instrument. It switches on the plasma and waits for the instrument to warm up. Then the performance report is started with modes defined by the operator. Once the performance report is passed, the instrument is ready for operation.

If the performance report fails, autotune or mass calibration are started automatically, followed by the performance report, again as specified by the operator.

❖ **To check the iCAP Q system before measurement**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Dashboard**.
The **Dashboard** page of Experiment Editor opens.

3. Click 

.
The **Get Ready** window opens, see Figure 5-6.

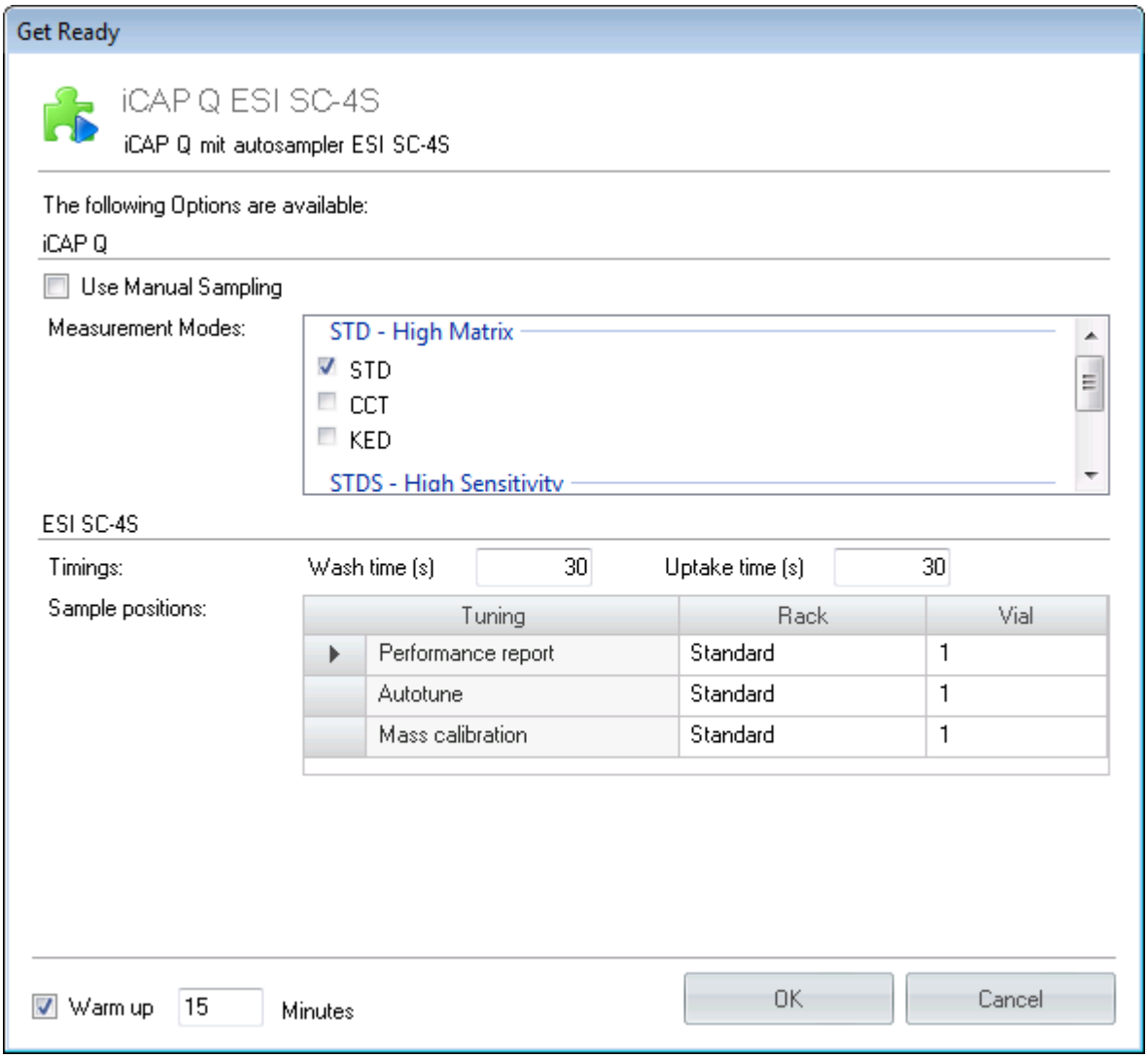


Figure 5-6. Get Ready window

4. Select a **Measurement Mode**.

5. Click 

.
The plasma is switched on. During warm-up the Dashboard shows the remaining warm-up time, see Figure 5-7.

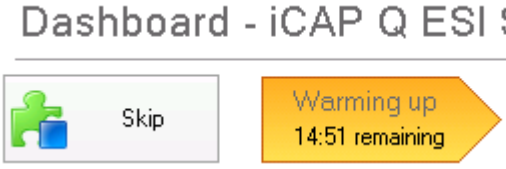


Figure 5-7. Dashboard window during warm-up

After warm-up, the performance report is started.

You can click 

to skip the warm-up.

6. If you wish to stop the procedure, click 

.

Closing Down the System

The iCAP Q system can be shut down with the **Closedown** function on the **Dashboard** page of Experiment Editor.

❖ **To close the iCAP Q system down**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Dashboard**.
The **Dashboard** page of Experiment Editor opens.

3. Click 

.
The iCAP Q system closes down.

Changing the Configuration

It is frequently necessary to change the Configuration of the iCAP Q instrument. For example, you might check for sensitivity with a water-based solution using the appropriate Configuration, then change the Configuration to start a measurement with laser ablation.

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

❖ **To change the Configuration**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Dashboard**.
The **Dashboard** page of Experiment Editor opens.

3. Click 

Change Configuration.
The **Select Configuration** window opens.

4. Select the Configuration you wish to load, see Figure 5-8.

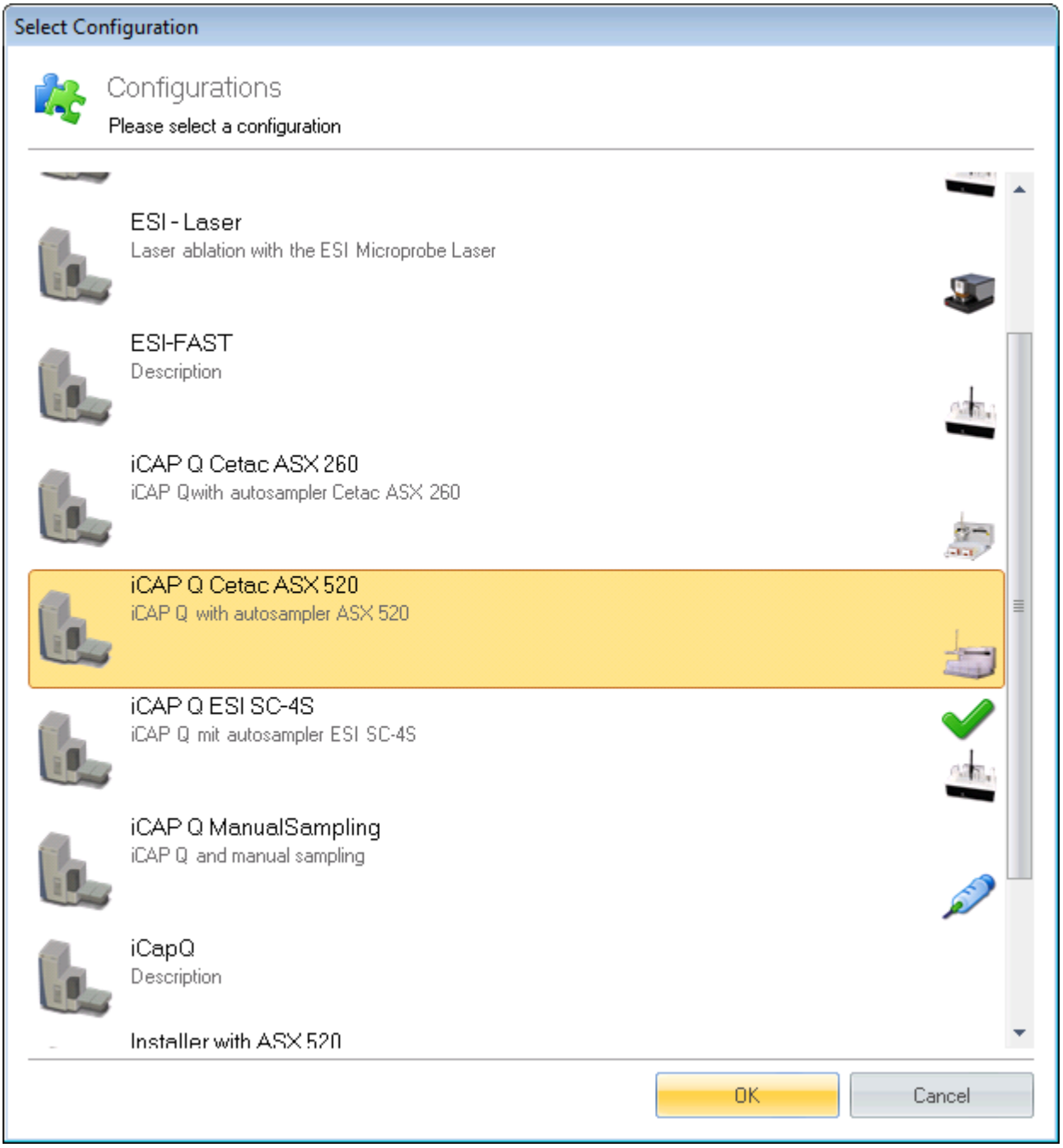


Figure 5-8. Select Configuration window

5. Click **OK**.
The selected Configuration is loaded.

Checking the System Status

Before starting measurement, the system status should be checked on the **Dashboard** of Experiment Editor.

❖ **To check the system status**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Dashboard**.
The **Dashboard** page of Experiment Editor opens.
3. Check the values and indicators of each subsystem, see Figure 5-9.

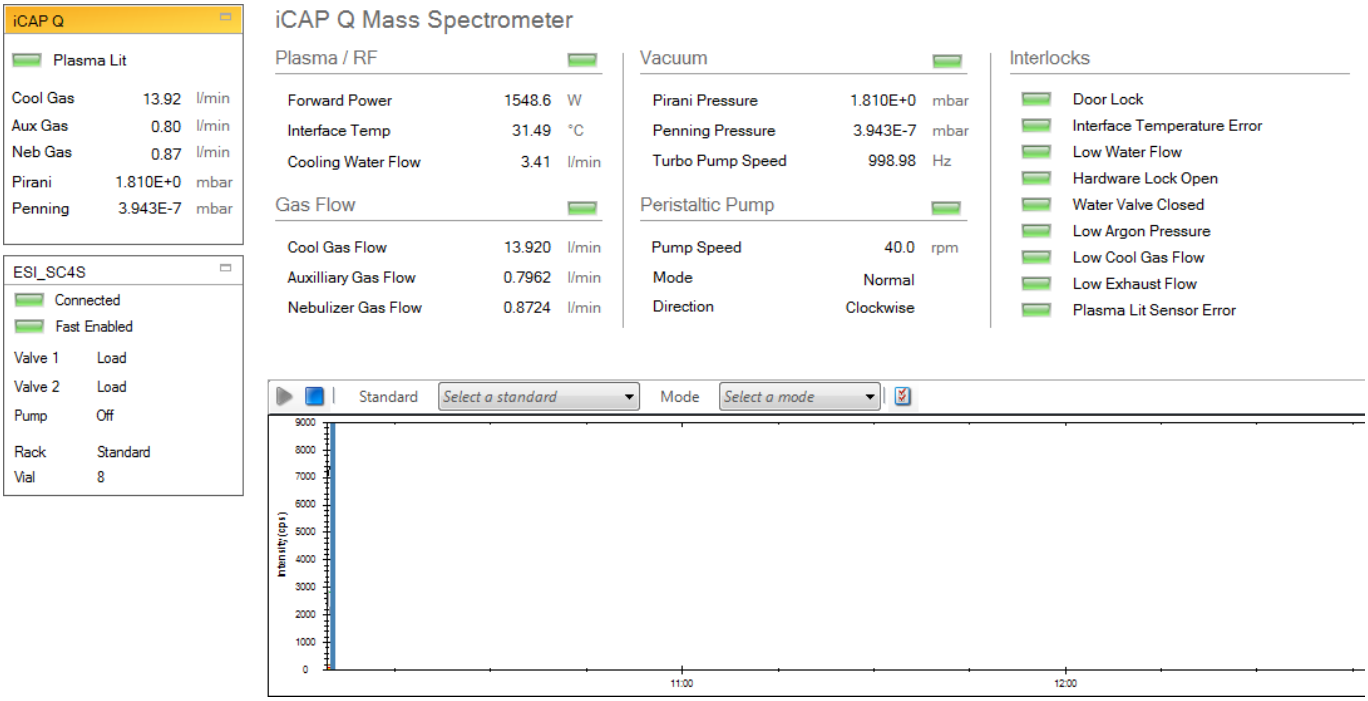


Figure 5-9. System Statuses on Dashboard

A green indicator signals the system is ready for operation.

Reviewing the Instrument Performance in Real-Time Display

The real-time display on the **Dashboard** page of Experiment Editor shows the count rate for your defined analytes vs. time. It is the same as the real-time display in "Data Display Tab" on page 4-7 of Instrument Control.

❖ **To check the intensity of the iCAP Q instrument**

1. Click to open **Experiment Editor**.
2. On the **Home Page**, click **Dashboard**.
   The **Dashboard** page of Experiment Editor opens.
3. For the real-time display, select a **Standard** from the drop-down list.
4. Select a **Mode** from the drop-down list.
5. Click to start the real-time display, see Figure 5-10.

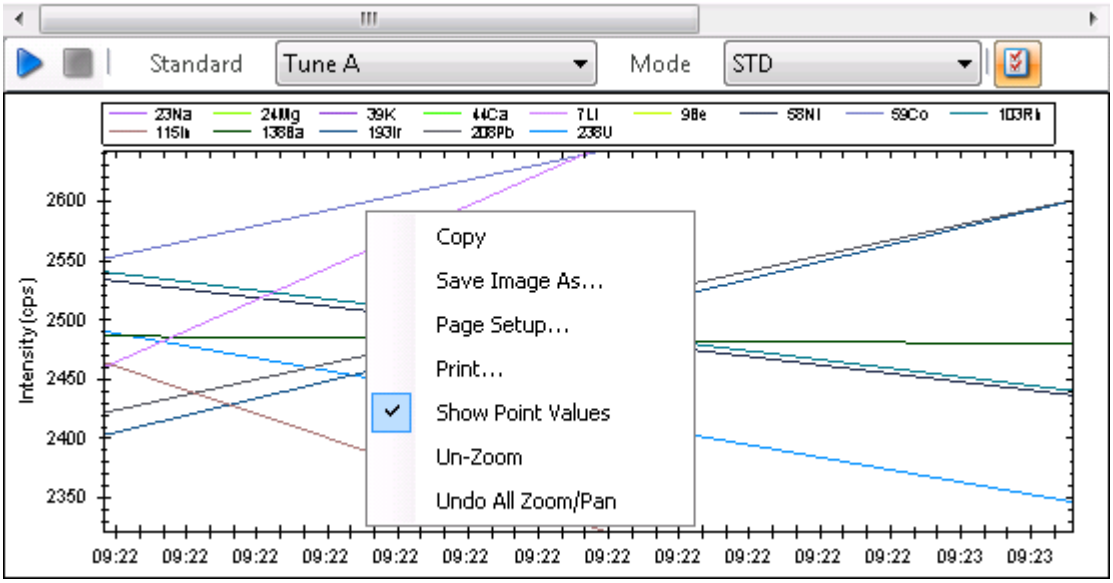


Figure 5-10. Real-time display on Dashboard

6. Click to stop the real-time display.
7. Right-click in the diagram to open the context menu.
   The context menu offers functions to change the appearance of the diagram and to copy or save the image.
8. Click to show the legend of the diagram.

Analysis Page

On the **Analysis** page of Experiment Editor, see Figure 5-11, LabBooks are created and opened.

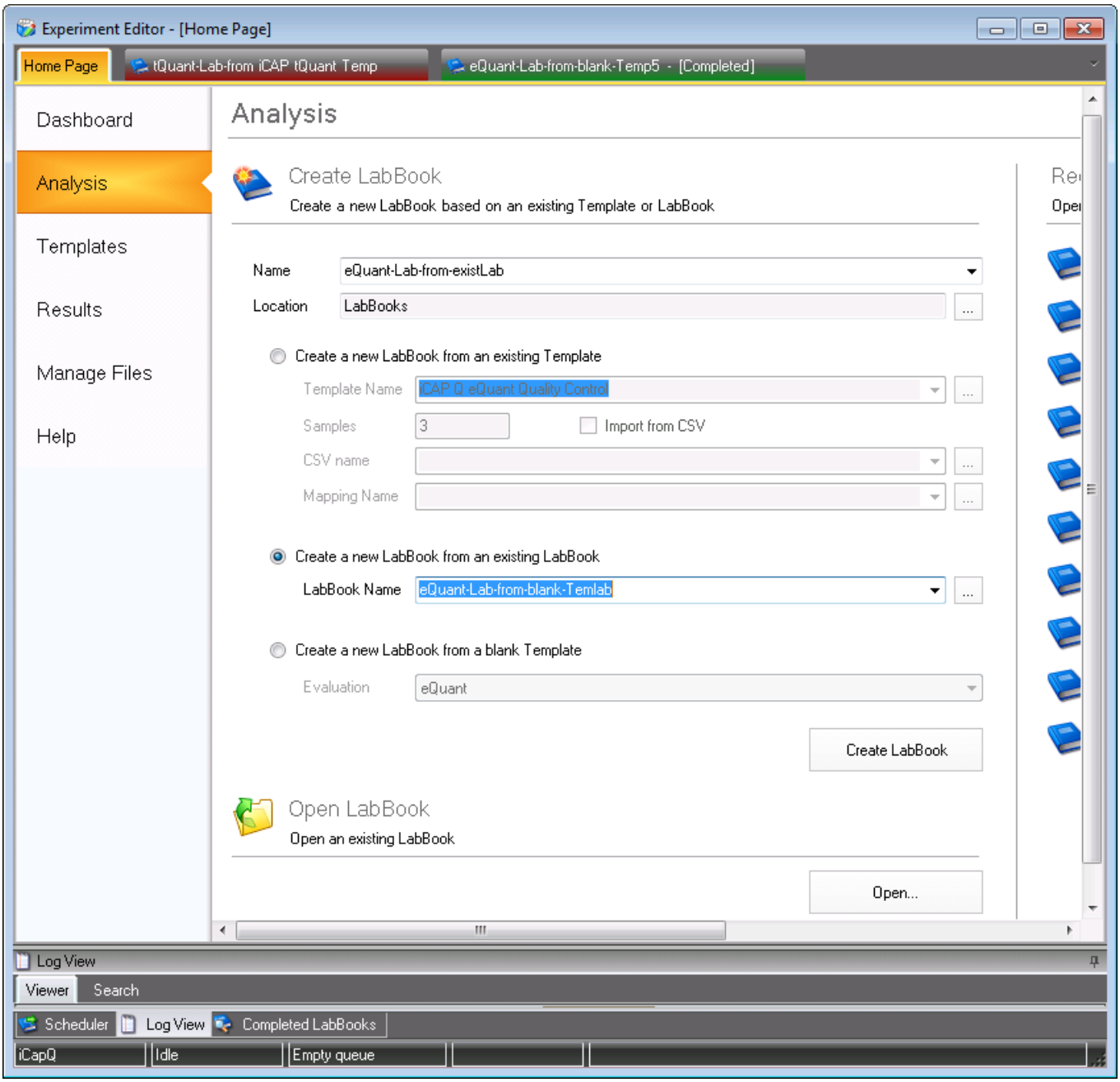


Figure 5-11. Analysis Page of Experiment Editor

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.

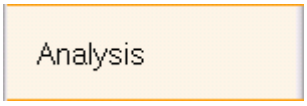
Data of analytical concentrations, raw intensities and other data formats can be defined to be automatically exported from a LabBook, either to an associated LIMS system or as report documentation.

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, concentrations and spectra are stored within the LabBook.

Additionally, for LabBooks that have finished acquiring data and have exited the Scheduler there are Status Report, Reports, Log Messages and Query views. See "LabBooks" on page 7-1 for details on LabBooks.

❖ **To open the Analysis page of Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
The **Analysis** page of Experiment Editor opens.

Opening a LabBook

LabBooks are opened either from the **Analysis** page of Experiment Editor which is described here, or from the **Manage Files** page, see "Manage Files Page" on page 5-38.

❖ **To open a LabBook in Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Analysis**.
The **Analysis** page of Experiment Editor opens.

3. Below  , click Open....
   The **Browse for LabBook** window opens, see Figure 5-12.

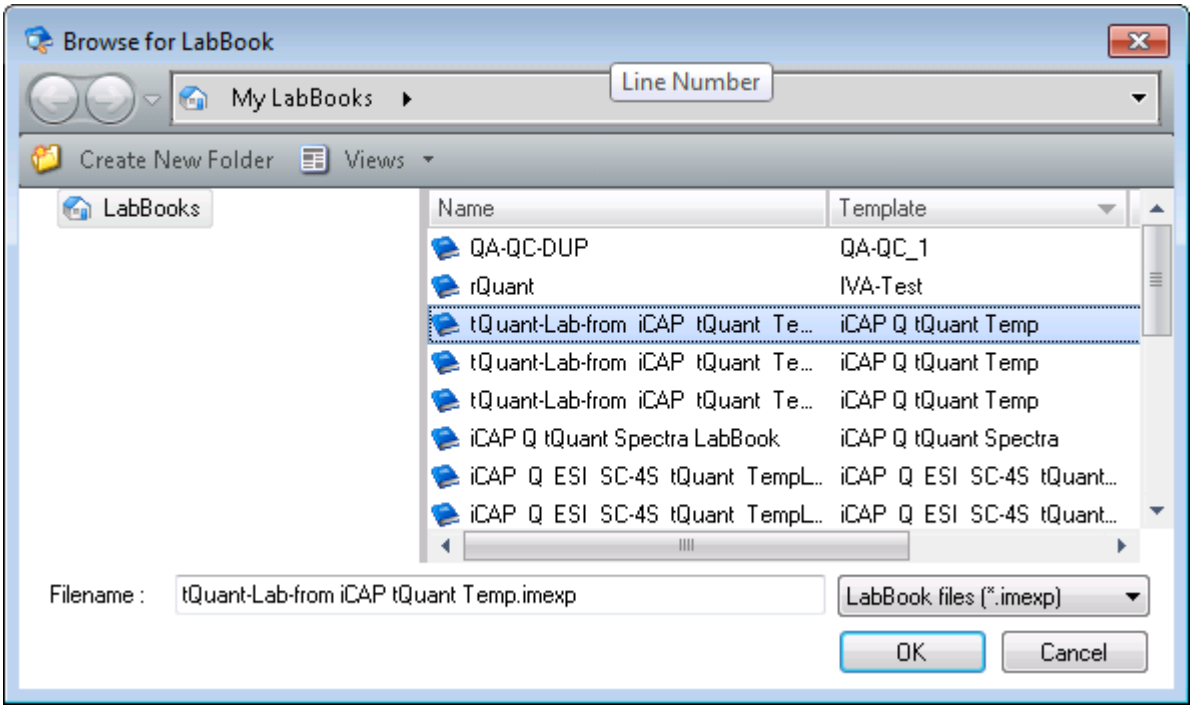


Figure 5-12. Browse for LabBook window

4. Select a LabBook.

5. Click OK to open the LabBook.
   The LabBook opens in a new tab of the Experiment Editor tool.

❖ **To open a Recent LabBook**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Analysis**.
   The **Analysis** page of Experiment Editor opens.

3. Click on a LabBook in the **Recent LabBooks** section, see Figure 5-13.

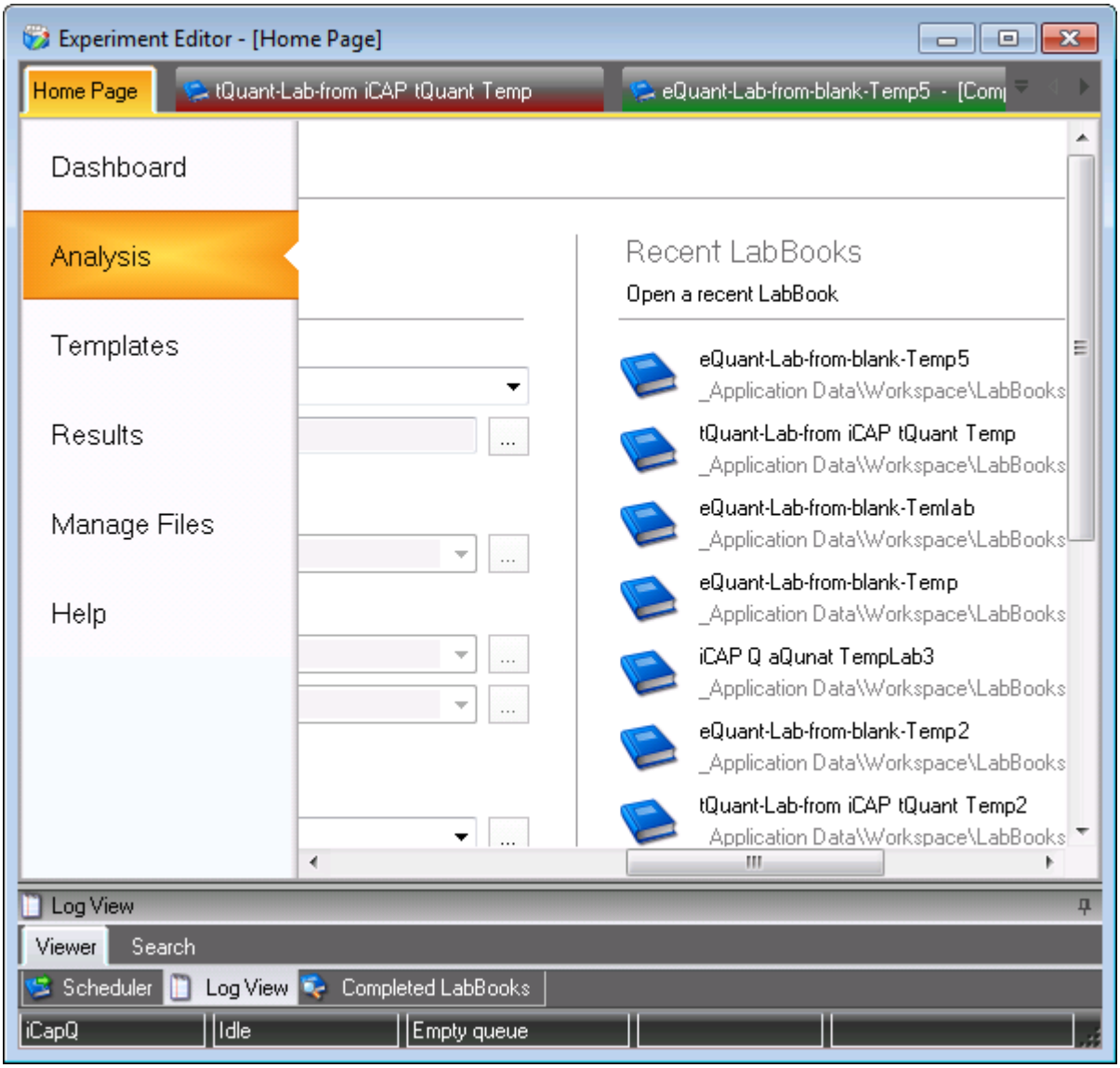


Figure 5-13. Recent LabBooks

The selected LabBook opens in a separate tab.

Creating a LabBook

LabBooks are created from blank Templates, existing Templates or from existing LabBooks on the **Analysis** page of Experiment Editor.

❖ **To create a LabBook in Experiment Editor**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Analysis**.
   The **Analysis** page of Experiment Editor opens.

3. Enter a **Name** for the LabBook and select a **Location**, see Figure 5-14.

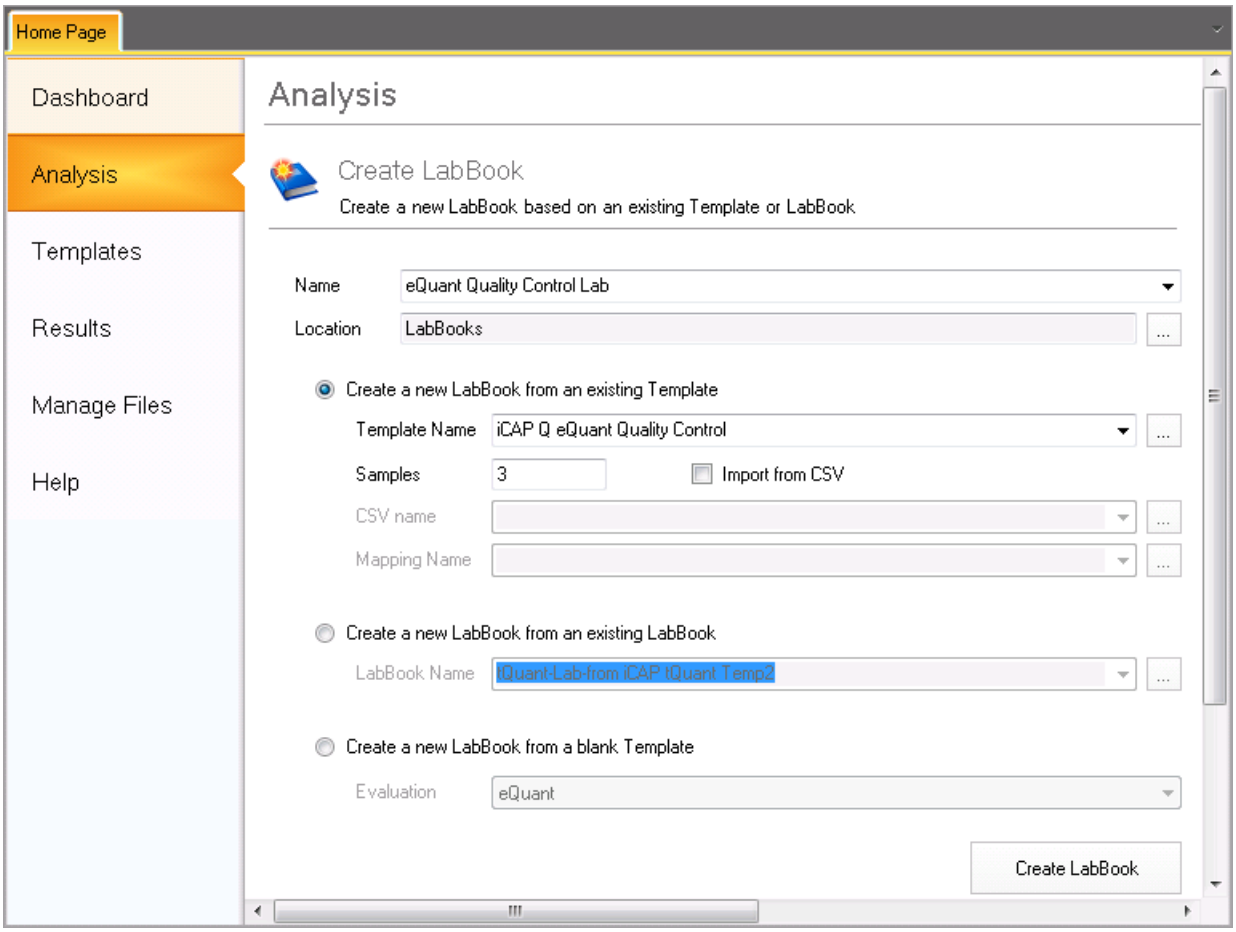


Figure 5-14. Enter Name for new LabBook

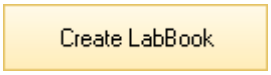
4. Click the first radio button if you wish to **Create a new LabBook from an existing Template** and select a **Template Name** from the drop-down list. Enter a number for **Samples**.
   To import a sample list, click **Import from CSV**, and select a **CSV name** and a **Mapping Name** from the drop-down list.

   You can also enter a name or browse ... for it.

5. Click the second radio button if you wish to **Create a new LabBook from an existing LabBook** and select a **LabBook Name** from the drop-down list.

   You can also enter a name or browse ... for it.

6. Click the third radio button if you wish to **Create a LabBook from a blank Template**, and select an **Evaluation** from the drop-down list.

7. Click 

to create the new LabBook.
A new tab opens for the new LabBook.

8. If you created the LabBook from a blank Template, define the **Method Parameters**.
See "Method Parameters" on page 6-15 for details.

9. 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 6-117.

10. Click **Automated Export** to define the data for export.
See "Automatic Export - Template" on page 6-125 for details.

11. In the toolbar of your **LabBook** page, click 

to save your LabBook.

Editing a LabBook

LabBooks are edited in Experiment Editor. Editing a LabBook involves a number of parameters, see "LabBooks" on page 7-1 for a complete description of LabBooks.

❖ **To edit a LabBook**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Analysis**.
The **Analysis** page of Experiment Editor opens.

3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

4. Edit your LabBook.
See also "Method Parameters" on page 6-15 and "Sample List - LabBook" on page 7-14.

5. On the toolbar of your **LabBook** page, click 

to save your LabBook.

Deleting a LabBook

LabBooks are deleted in the **Manage Files** page of Experiment Editor.

❖ **To delete a LabBook**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Manage Files**.
The **Manage Files** page of Experiment Editor opens.
3. Click the **LabBooks** folder (or the subfolder for the LabBook you wish to delete), see Figure 5-15.

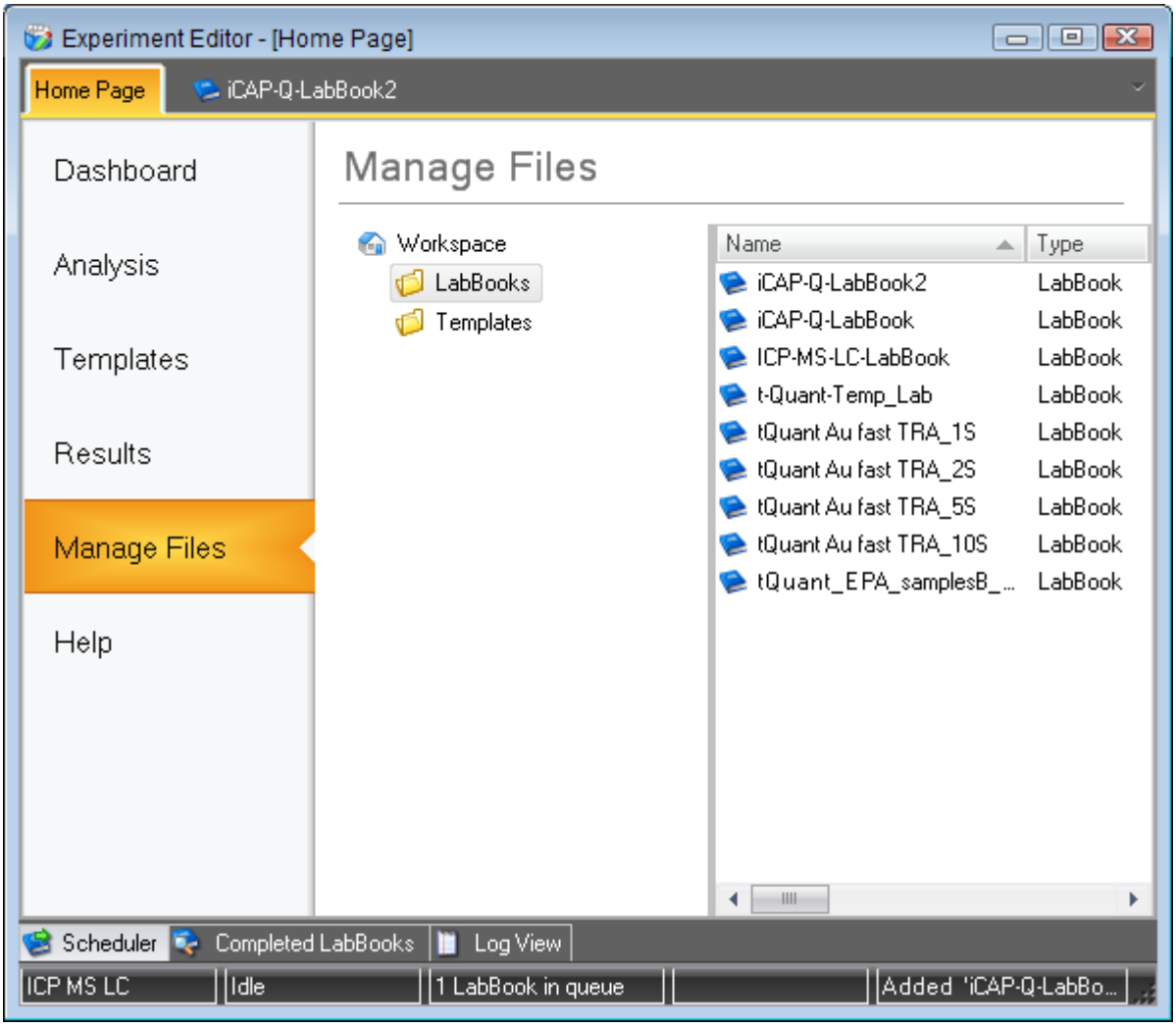


Figure 5-15. Manage Files - LabBooks

4. Right-click the LabBook you wish to delete in the list on the right.
   A context menu opens, see Figure 5-16.

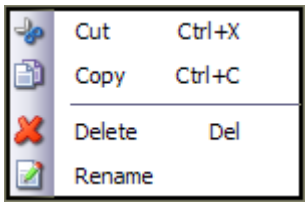


Figure 5-16. Context menu Manage Files

5. Click **Delete**.
   The LabBook is deleted.

Closing a LabBook

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

❖ **To close a LabBook**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Analysis**.
   The **Analysis** page of Experiment Editor opens.

3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

4. On the toolbar of your **LabBook** page, click 

to close your LabBook.

   You can also click  in the tab of the LabBook.

Templates Page

On the **Templates** page of Experiment Editor, see Figure 5-17, Templates for your methods are created and opened.

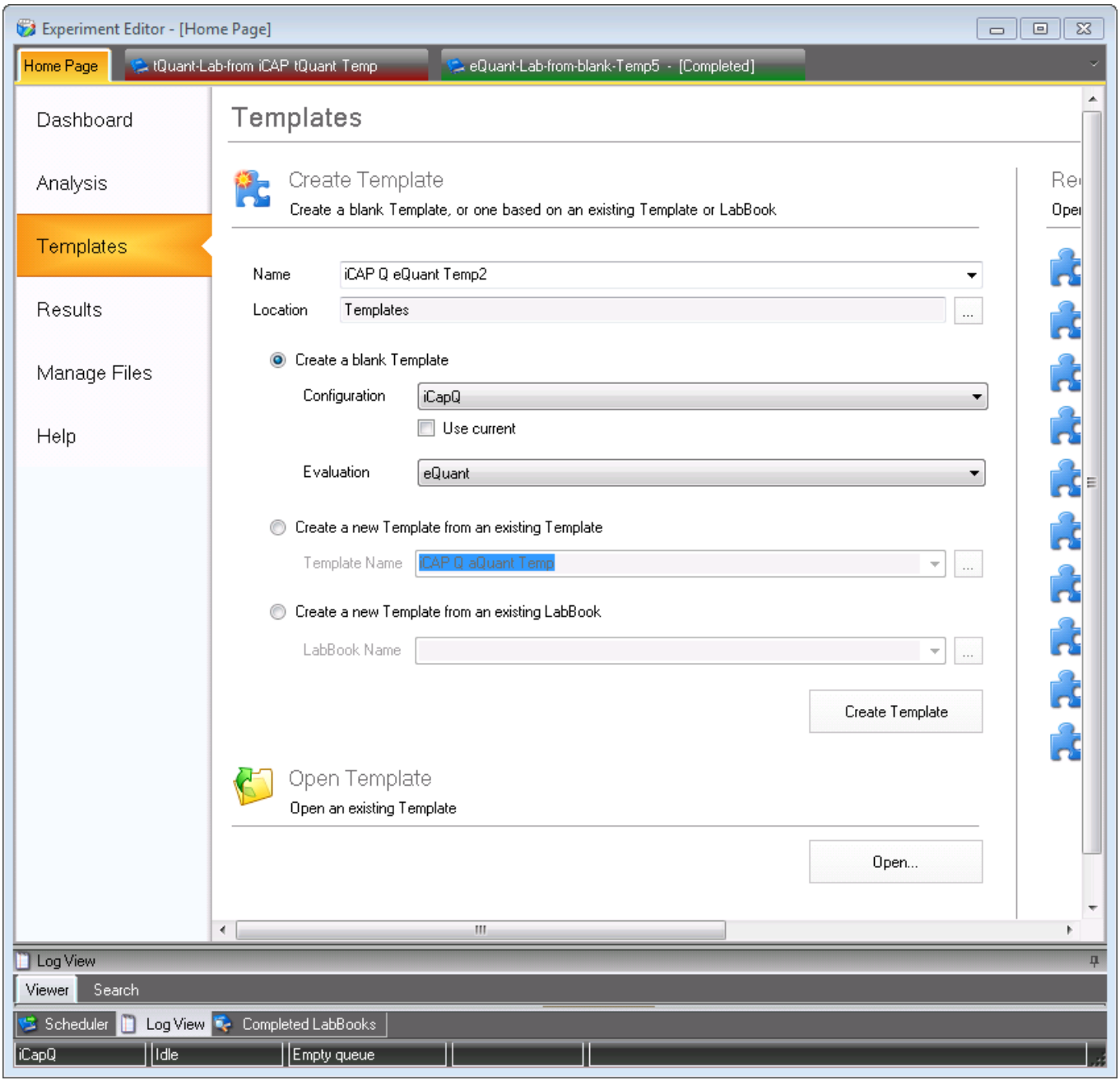


Figure 5-17. Templates Page of Experiment Editor

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 Manager for different types of applications. Once a Template is created and saved, it can serve as the basis for different analytical measurements (LabBooks).

❖ **To open the Templates page of Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
The **Templates** page of Experiment Editor opens.

Opening a Template

Templates are opened either from the Templates page of Experiment Editor which is described here, or from the Manage Files page, see "Manage Files Page" on page 5-38.

❖ **To open a Template in Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Templates**.
The **Templates** page of Experiment Editor opens.

3. Below , click Open....
   The Browse for Template window opens, see Figure 5-18.

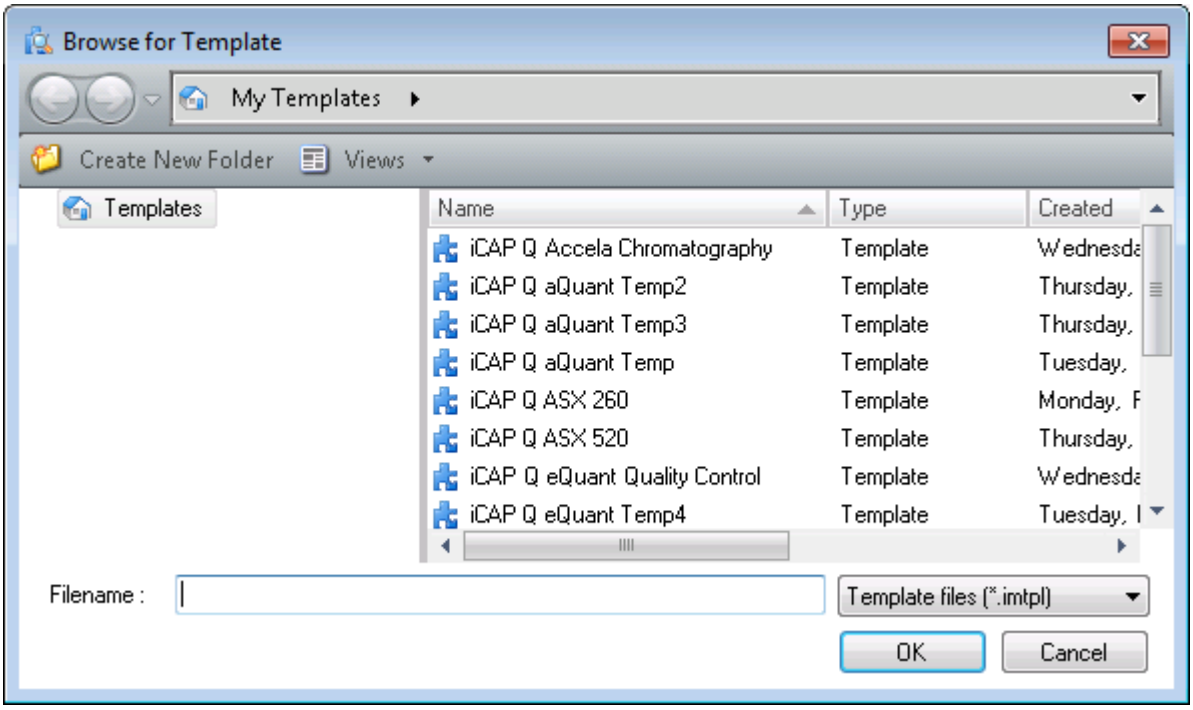


Figure 5-18. Browse for Template window

4. Select a Template.

5. Click OK to open the new Template.
   The Template opens in a new tab of the Experiment Editor tool.

❖ **To open a Recent Template**

1. Click Experiment Editor to open **Experiment Editor**.

2. On the **Home Page**, click **Templates**.
   The **Templates** page of Experiment Editor opens.

3. Click on a Template in the **Recent Templates** section, see Figure 5-19.

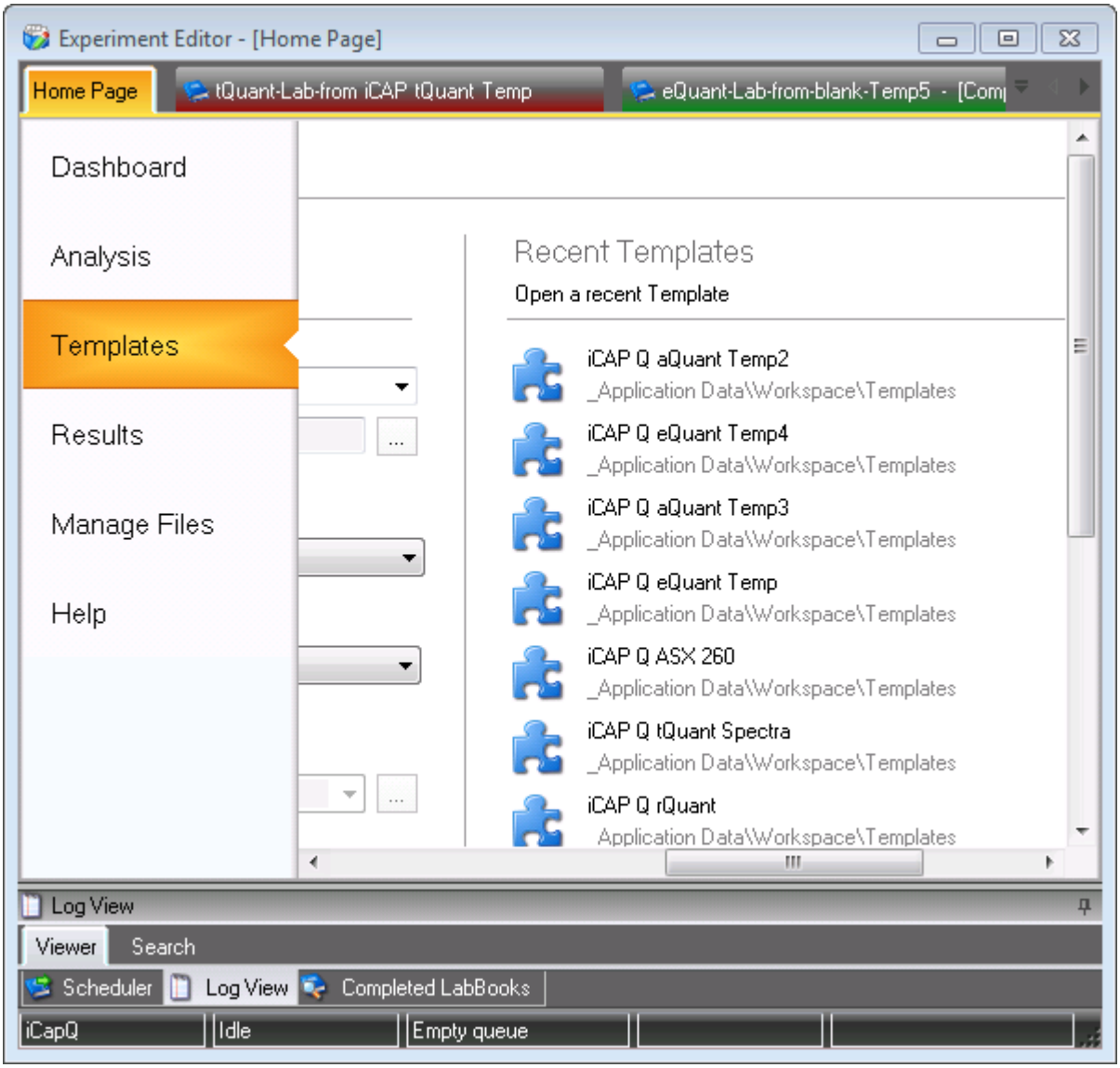


Figure 5-19. Recent Templates

The selected Template opens in a separate tab.

Creating a Template

Templates are created from blank Templates, existing Templates or existing LabBooks in Experiment Editor. For blank Templates, you need to select a system **Configuration**. Configurations, including peripherals (**Instruments**), are defined by your Administrator in the applet **Experiment Configurator** of the Configurator tool (see "Experiment Configurator" on page 3-13).

❖ **To create a new Template in Experiment Editor**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Templates**.
The **Templates** page of Experiment Editor opens.

3. Enter a **Name** for the Template and select a **Location**, see Figure 5-20.

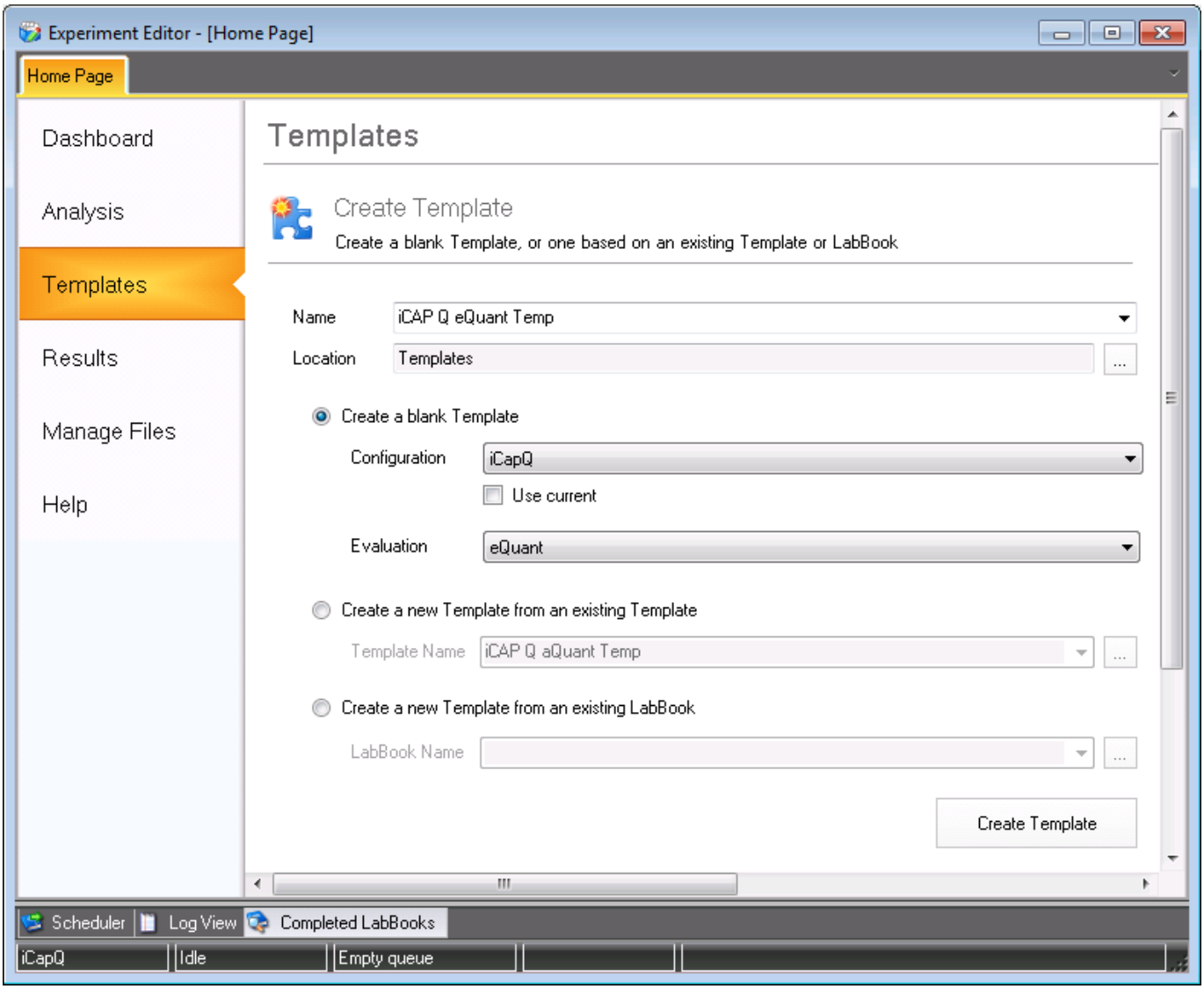


Figure 5-20. Enter Name for Template

4. Click the first radio button 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

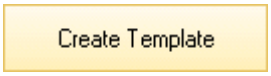
peripheral settings, are automatically loaded.
Only Configurations that have previously been configured in the Experiment configurator applet of the Configurator may be selected (see "Experiment Configurator" on page 3-13).

5. Click the second radio button if you wish to **Create a new Template from an existing Template** and select a **Template Name** from the drop-down list.

   You can also enter the name or browse  for it.

6. Click the third radio button if you wish to **Create a new Template from an existing LabBook** and select a **LabBook Name** from the drop-down list.

   You can also enter the name or browse  for it.

7. Click 

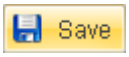
to create the new Template.
A new tab opens for the new Template.

8. In the tab of your template, define the **Method Parameters**.
   See "Method Parameters" on page 6-15 for details.

9. Click **Sample Definition** to set up the sample list parameters.
   See "Sample Definition for a Template" on page 6-117 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.

10. Click **Automated Export** to define the data for export. See "Automatic Export - Template" on page 6-125 for details.

11. In the toolbar of your **Template** page, click 

to save your Template.

Editing a Template

Templates are edited in Experiment Editor. See "Templates" on page 6-1 for a complete description of the parameters involved.

❖ **To edit a Template in Experiment Editor**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Templates**.
   The **Templates** page of Experiment Editor opens.

3. Open a Template as described in "Opening a Template" on page 5-22.
4. Edit the **Method Parameter** settings.
   See "Method Parameters" on page 6-15 for details.
5. Edit the **Sample Definition** settings.
   See "Sample Definition for a Template" on page 6-117 for details.
6. On the toolbar of your **Template** page, click 

to save your Template.

Deleting a Template

Templates are deleted in the **Manage Files** page of Experiment Editor.

❖ **To delete a Template**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Manage Files**.
   The **Manage Files** page of Experiment Editor opens.

3. Click the **Templates** folder, see Figure 5-21.

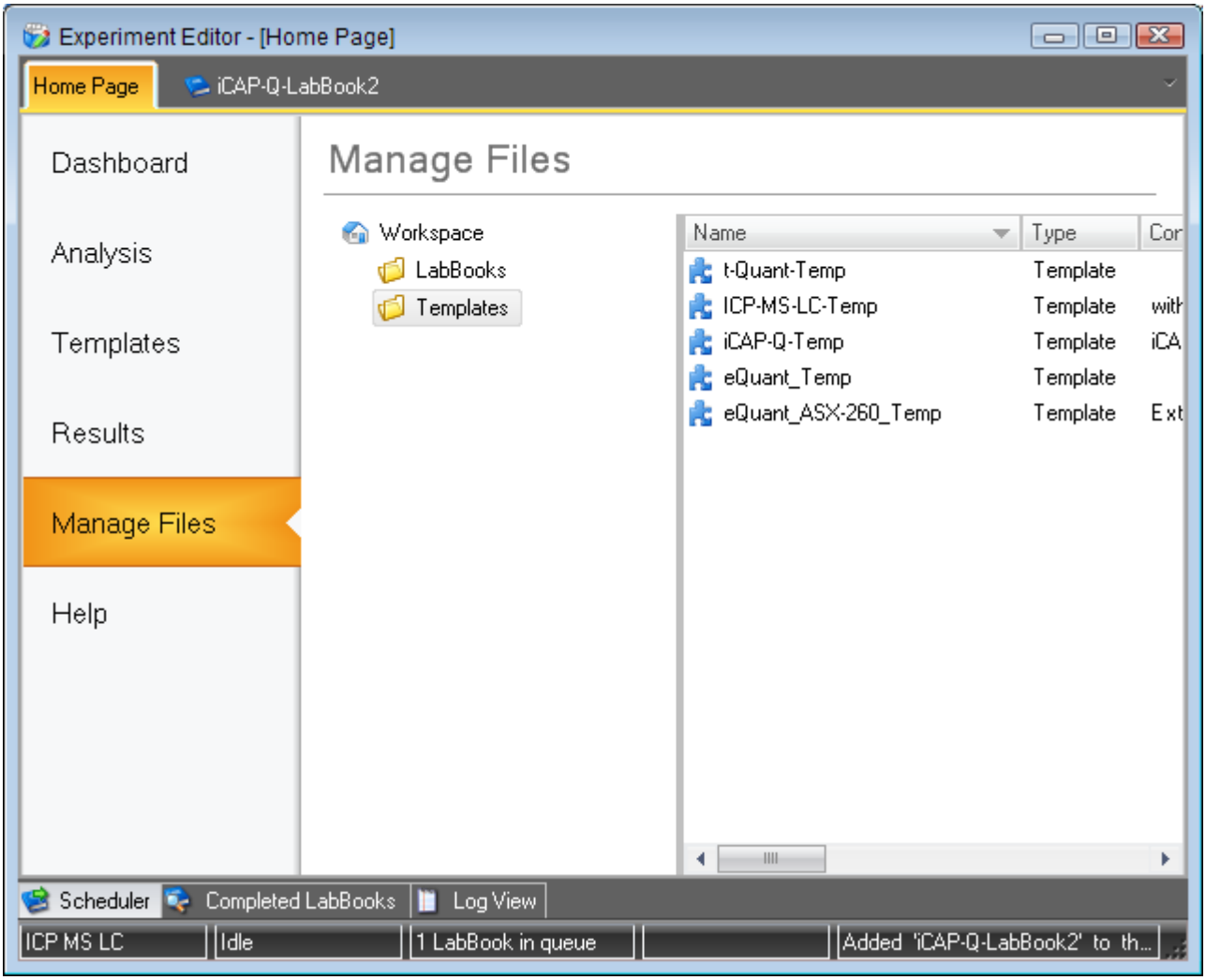


Figure 5-21. Manage Files - Templates

4. On the right, right-click the Template you wish to delete.
A context menu opens, see Figure 5-22.

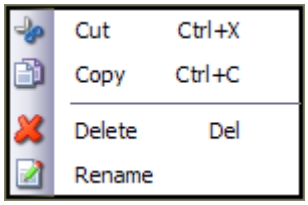


Figure 5-22. Context menu Manage Files

5. Click **Delete**.
The Template is deleted.

Closing a Template

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

❖ **To close a Template**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Templates**.
The **Templates** page of Experiment Editor opens.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. On the toolbar of your Template page, click 

to close your Template.

   You can also click  in the tab of the Template.

Results Page

On the **Results** page of Experiment Editor, see Figure 5-23, results of a measurement can be viewed.

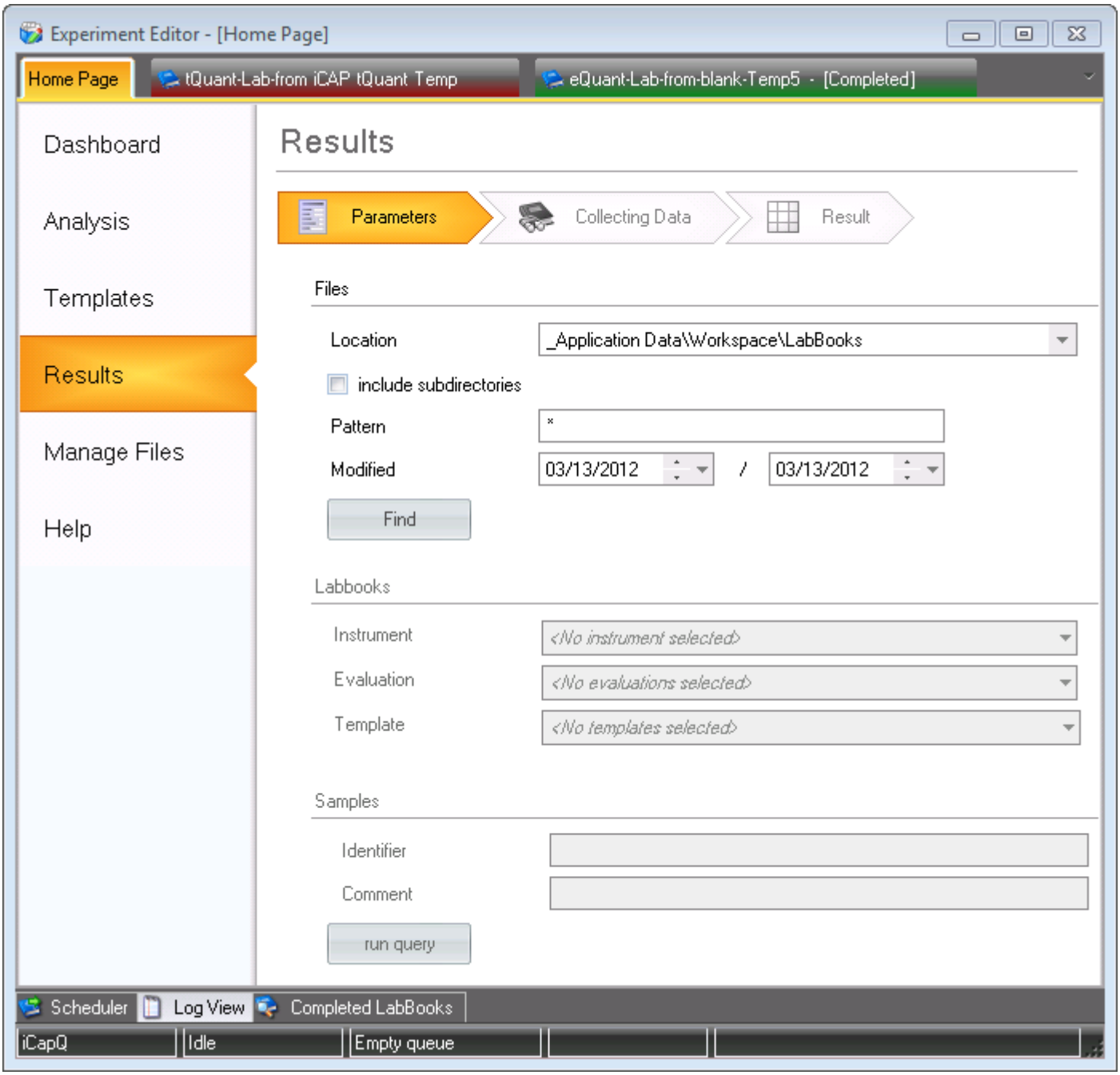
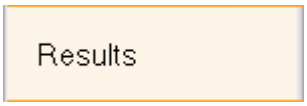


Figure 5-23. Results Page of Experiment Editor

❖ **To open the Result page of Experiment Editor**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Click 

.
The **Results** page of Experiment Editor opens.

Displaying Result Data

The parameters of a measurement are set to be displayed on the **Results** page of Experiment Editor.

❖ **To display result data on the Result page of Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Results**.
The **Results** page of Experiment Editor opens.
3. In the **Parameters** view of the **Results** page, select the **Location** from the drop-down list.
4. Enter the **Pattern** and select the date for **Modified** when the LabBooks were acquired, see Figure 5-24.

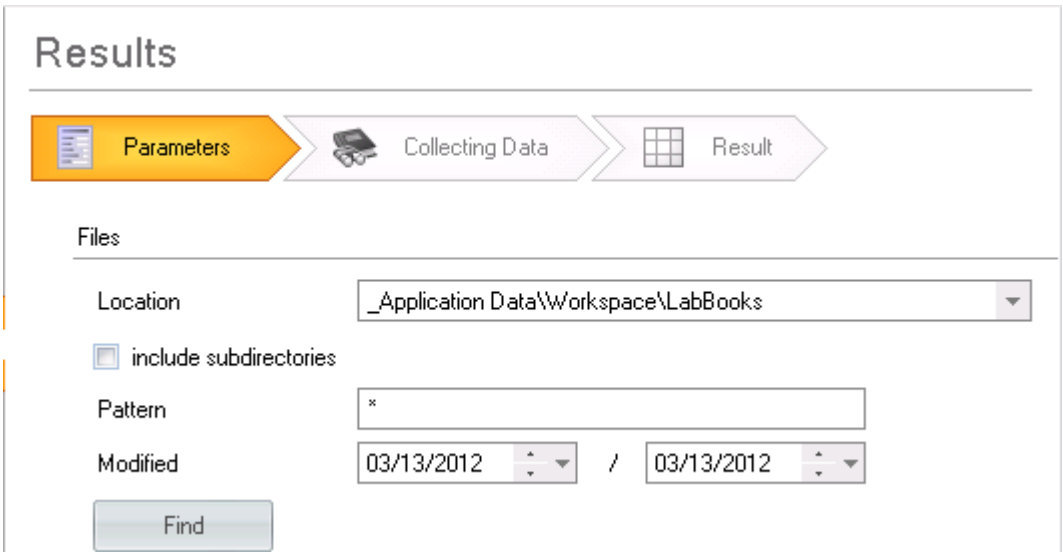


Figure 5-24. Files section in Results page

If you enter <*> in the field **Pattern**, all LabBooks in the folder are searched.

5. Click Find to start the search for LabBooks that match the defined values.
   The field **LabBooks** displays the first entries in the list of results, see Figure 5-25.

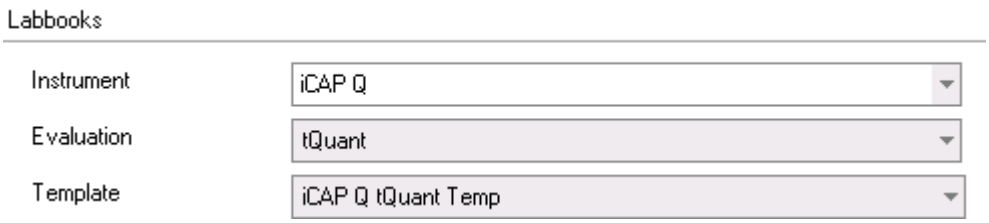


Figure 5-25. LabBooks found in Results page

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

7. For **Samples**, enter the **Identifier** as in the sample list, for example, **Standard 1 ppb**.

8. Click run query to start the query.
   Qtegra collects the data, see Figure 5-26.

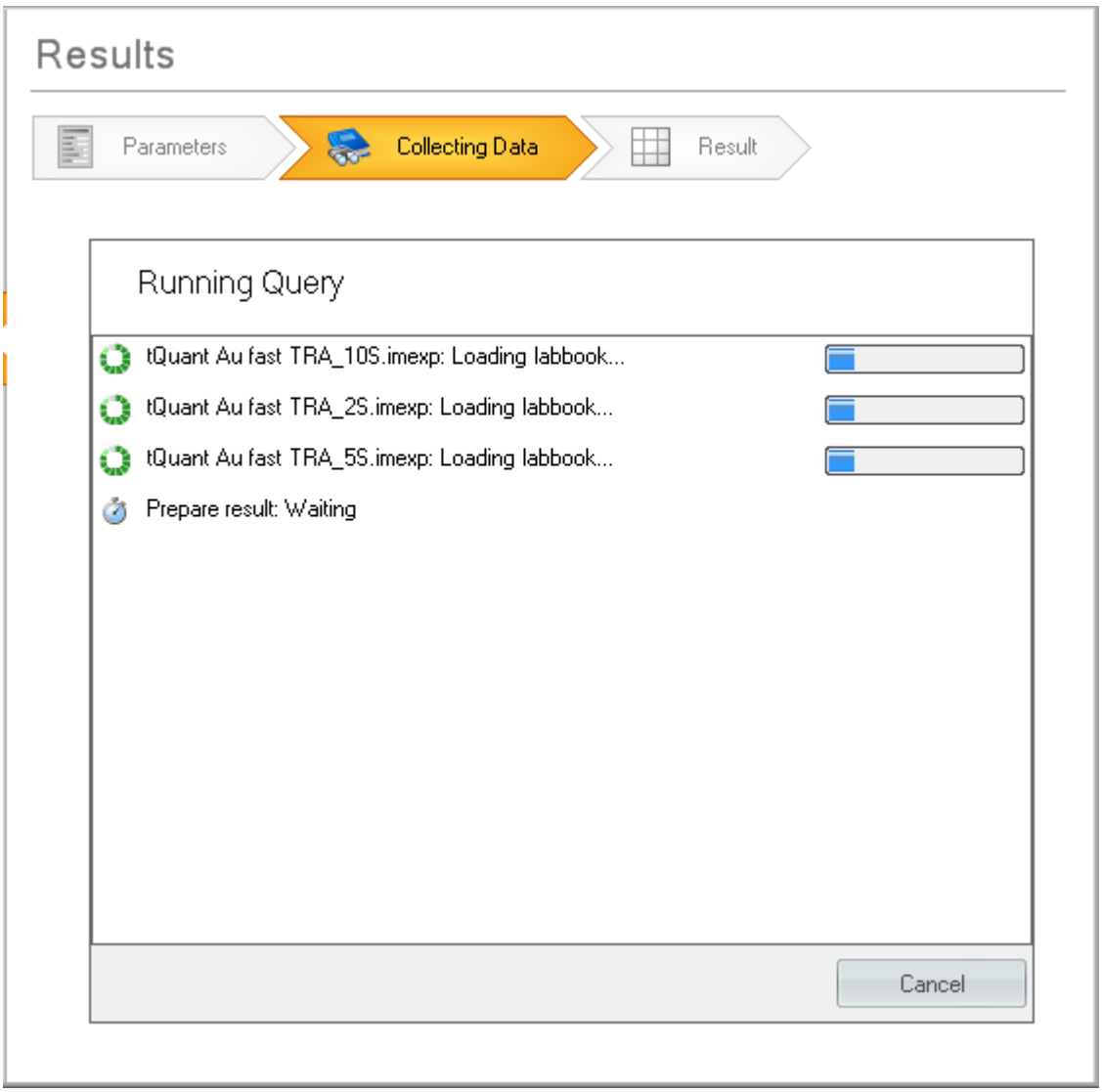


Figure 5-26. Results page collecting data in Experiment Editor

The results are displayed when the query has been executed, see Figure 5-27.

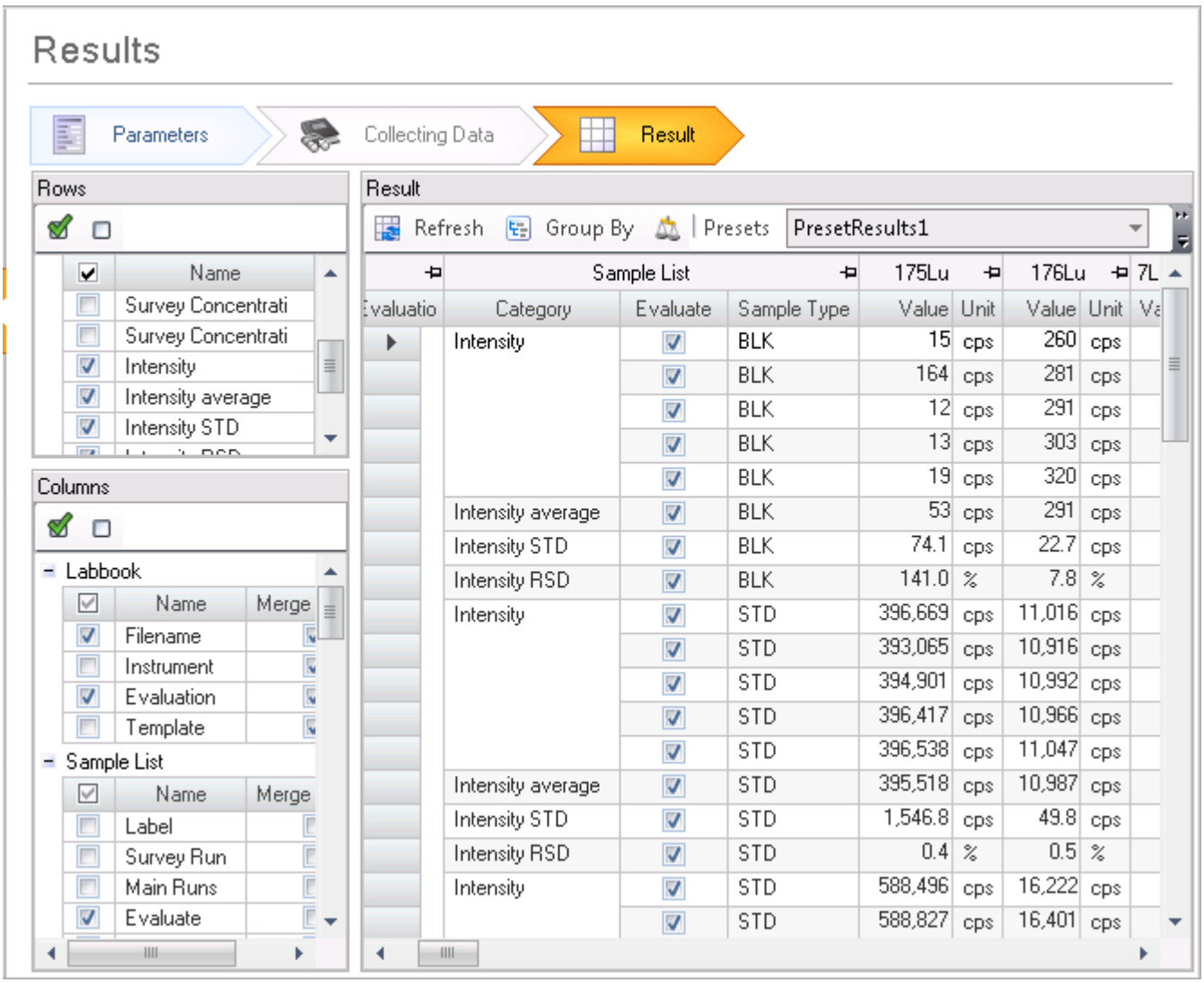


Figure 5-27. Results page displaying results in Experiment Editor

9. Select the check boxes for the data you wish to display.

10. Click  to refresh the view region.
    The data are displayed.

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

12. Click Group By if you wish to group the results.
    The **Group By** button is activated, see Figure 5-28.

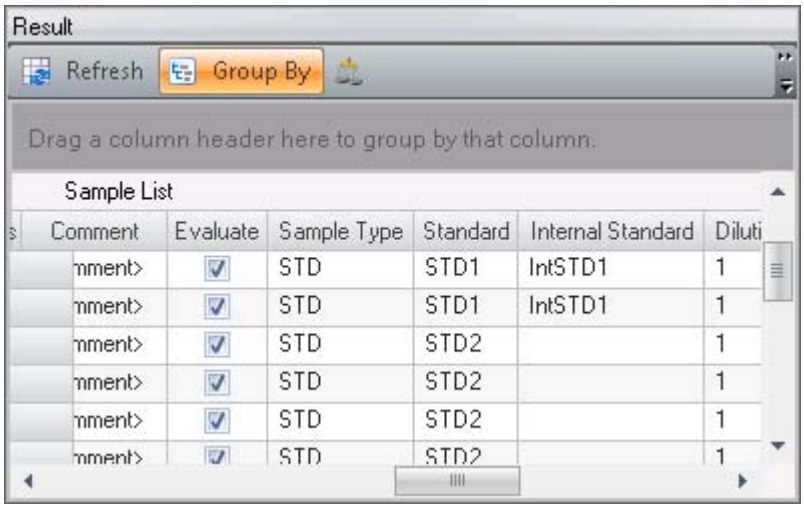


Figure 5-28. Results page asking to drag column in Experiment Editor

13. Drag and drop a column header onto the assigned area.
    The results are grouped by that column, see Figure 5-29.

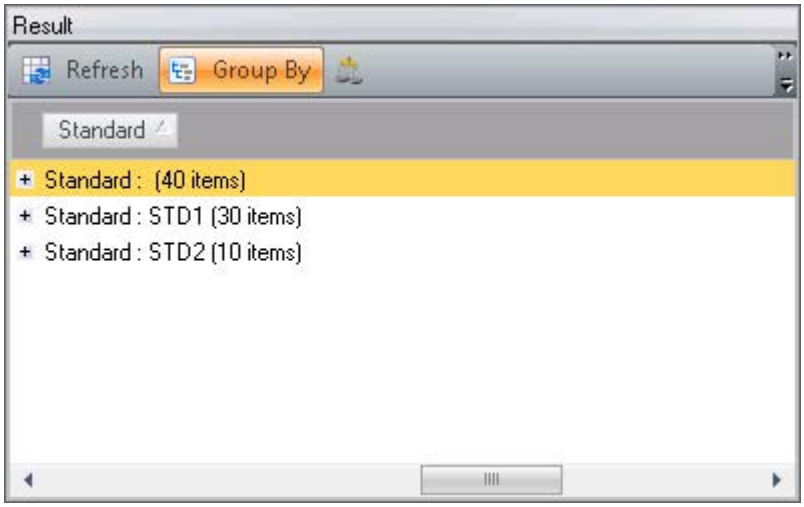


Figure 5-29. Results grouped by column in Experiment Editor

14. Drag and drop the column header back to redo the grouping, see Figure 5-30.

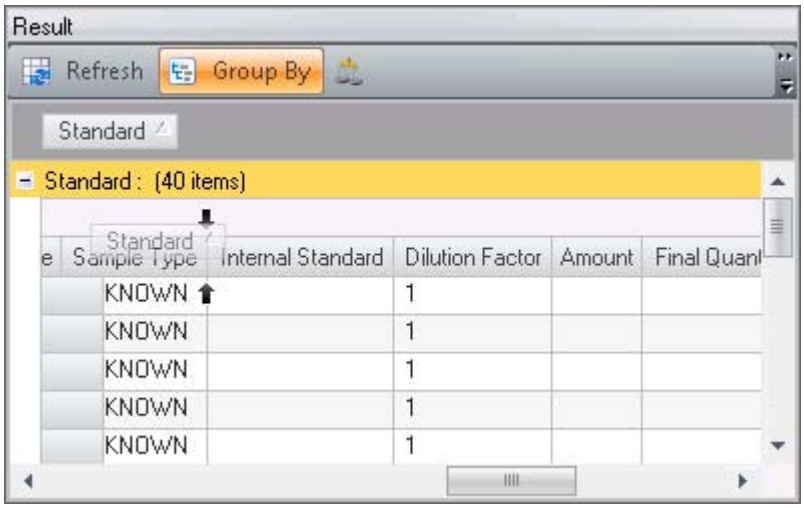


Figure 5-30. Redo results grouping by column in Experiment Editor

Saving Results

In Experiment Editor, the displayed result data of a measurement can be saved or saved as preset, see Figure 5-31.

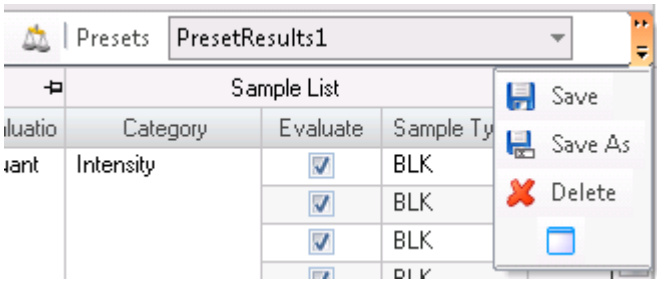


Figure 5-31. Drop-down on Results Page of Experiment Editor

❖ **To save result data**

1. Click Experiment Editor to open **Experiment Editor**.
2. On the **Home Page**, click **Results**.
   The **Results** page of Experiment Editor opens.
3. Select the results you wish to display as described in "Displaying Result Data" on page 5-31.
4. Click Save to save the result data.

❖ **To save result data as preset**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Results**.
The **Results** page of Experiment Editor opens.
3. Select the results you wish to display as described in "Displaying Result Data" on page 5-31.
4. Click  **Save as** to save the results data as new preset.
The **Save New Preset** dialog is displayed, see Figure 5-27.

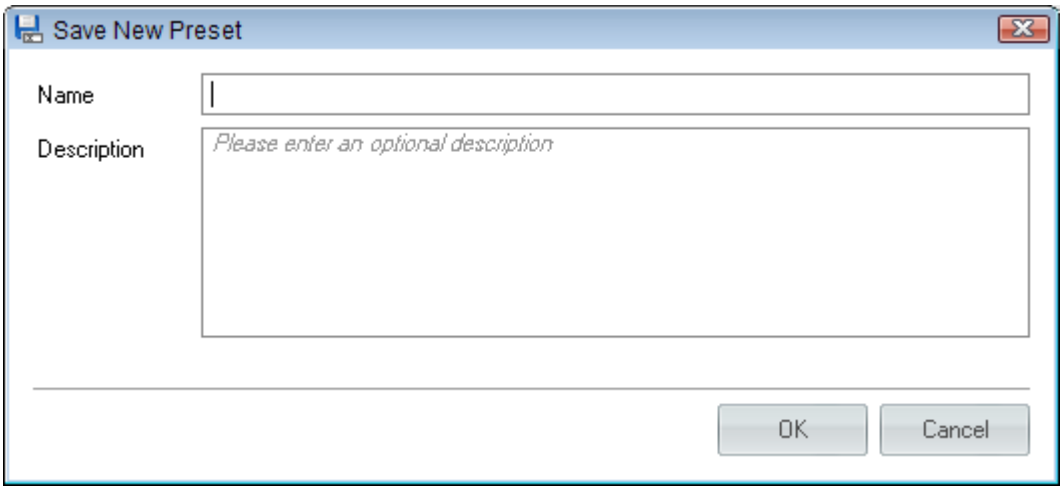


Figure 5-32. Save New Preset dialog in Experiment Editor

5. Enter a **Name** for the preset.
6. Enter a **Description**.
7. Click **OK**.

Manage Files Page

On the **Manage Files** page of Experiment Editor, see Figure 5-33, you organize your Template and LabBook files.

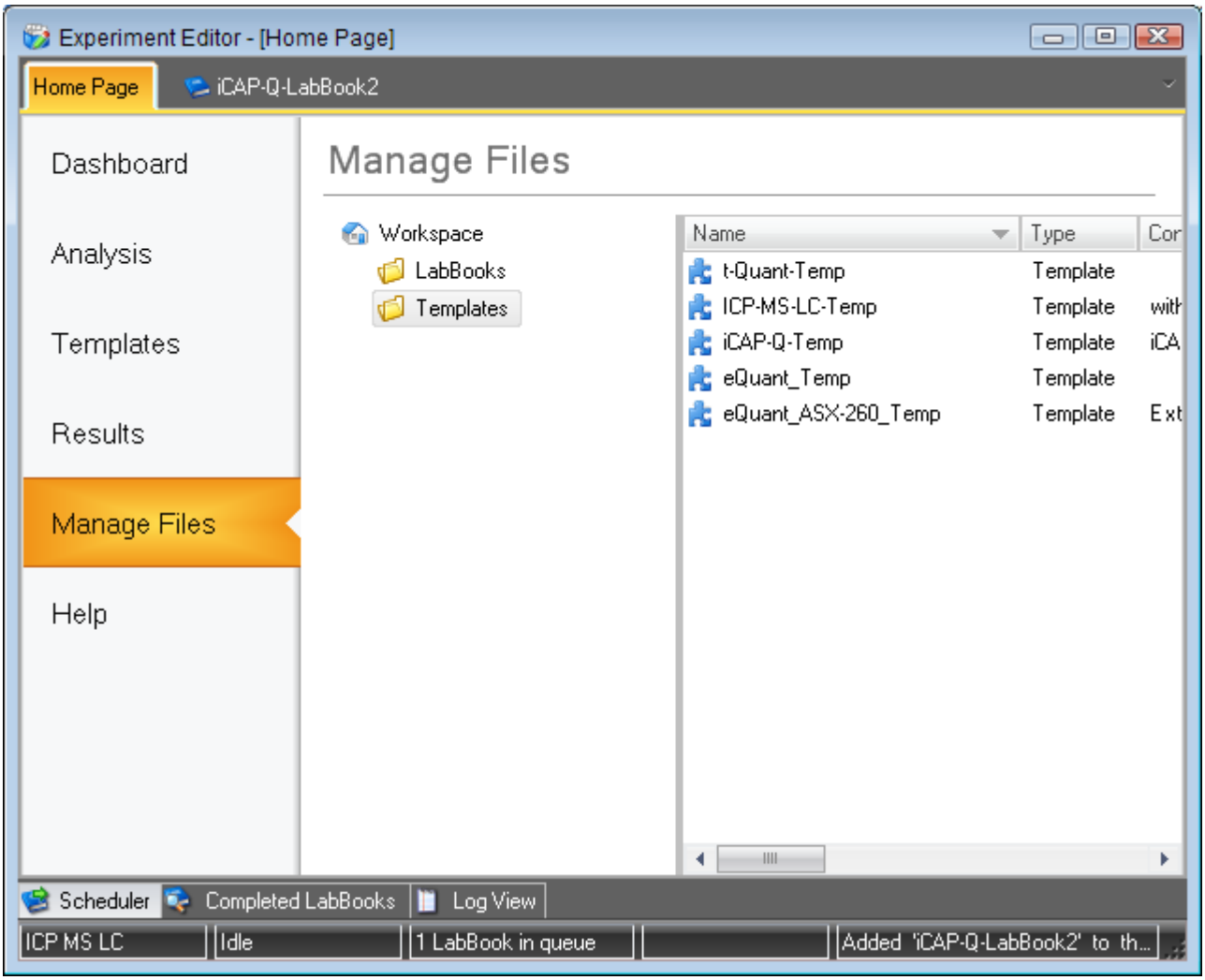


Figure 5-33. Manage Files Page of Experiment Editor

❖ **To open the Manage Files page of Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
The **Manage Files** page of Experiment Editor opens.

❖ **To open a Template from the Manage Files page of Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
The **Manage Files** page of Experiment Editor opens.
4. Select the directory **Templates**.
5. Double-click the Template you wish to open.
The Template is opened in a new tab.

❖ **To open a LabBook from the Manage Files page of Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
The **Manage Files** page of Experiment Editor opens.
4. Select the directory **LabBooks**.
5. 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. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Manage Files**.
The **Manage Files** page of Experiment Editor opens.

3. Right-click **Workspace** to create a new folder, see Figure 5-34.

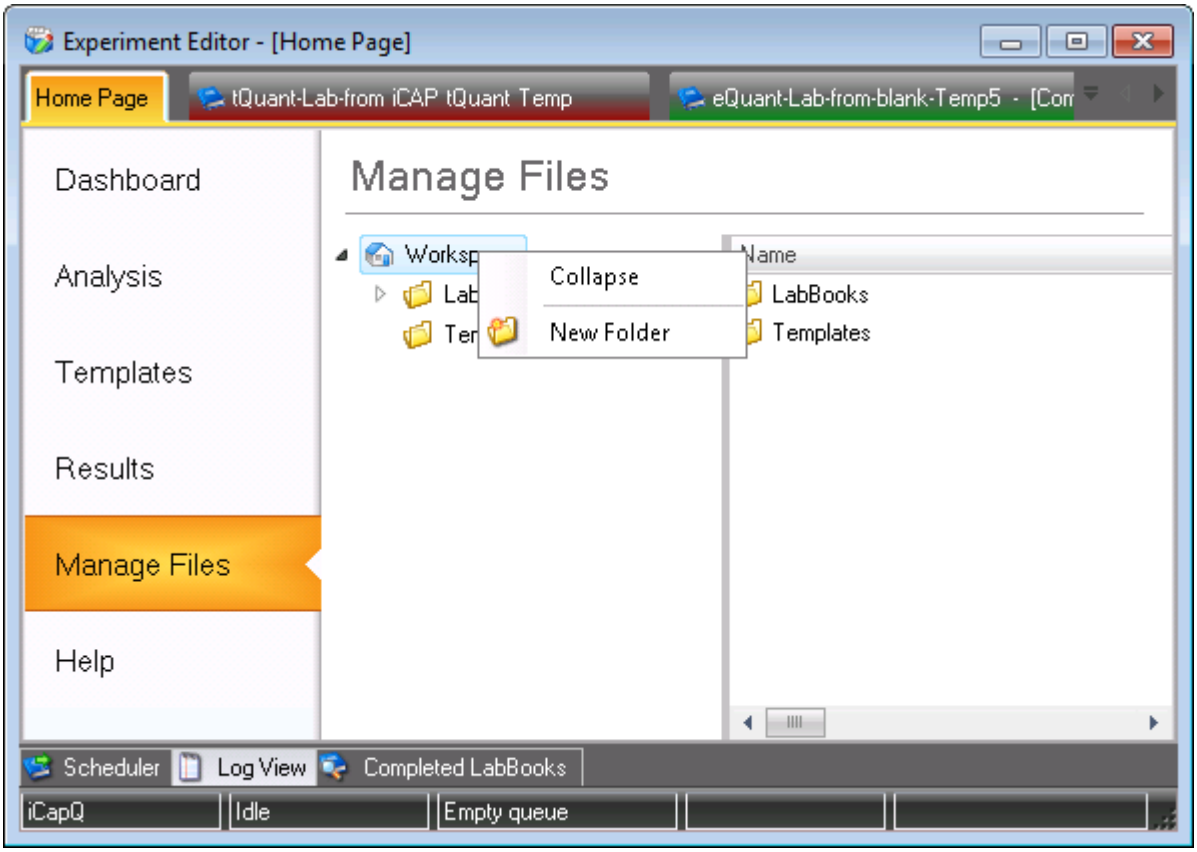


Figure 5-34. Context menu Manage Files Workspace

4. Select **New Folder** from the context menu.
5. Enter a name for the new folder.
6. Click anywhere in the folder.
   The new name is accepted.

❖ **To create a new folder in LabBooks or Templates**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Manage Files**.
   The **Manage Files** page of Experiment Editor opens.

3. Right-click the **LabBooks** or **Templates** folder to create a new folder, see Figure 5-35.

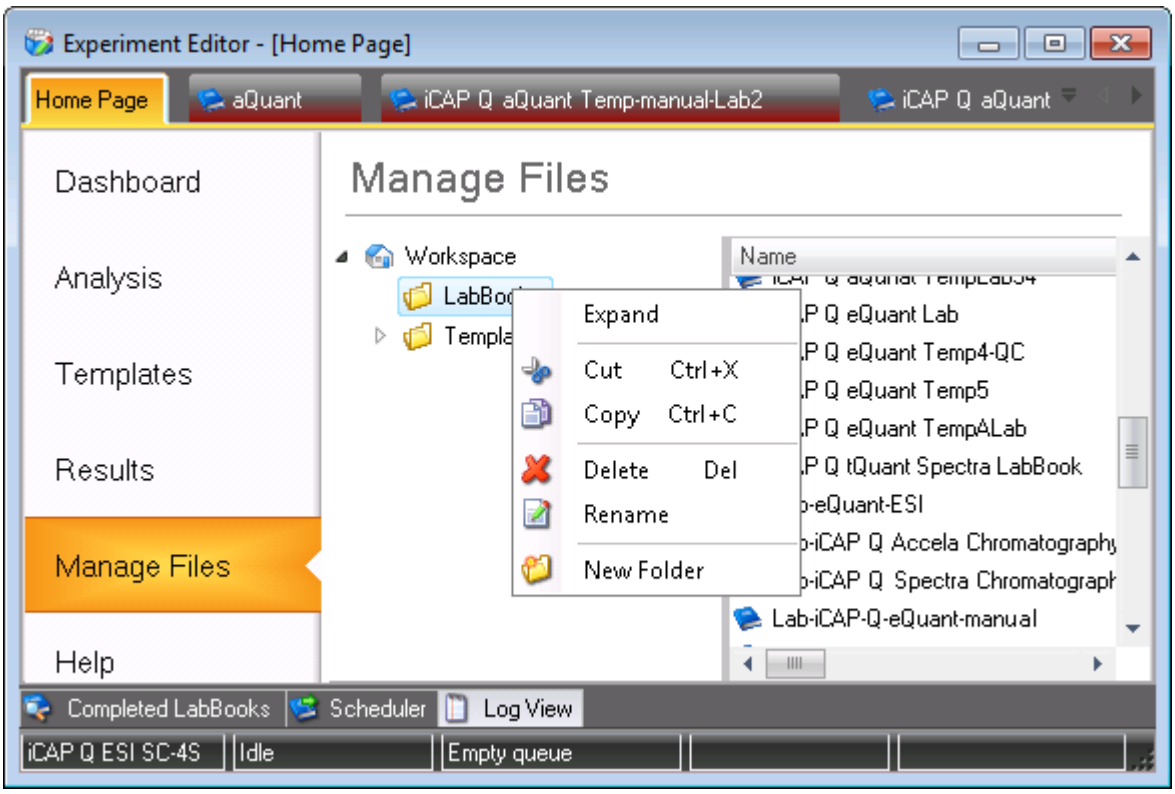


Figure 5-35. Context menu Manage Files subfolder

4. Select **New Folder** from the context menu.

NOTICE It is also possible to **Expand**, **Cut**, **Copy**, **Delete**, or **Rename** the folders via the context menu. ▲

5. Enter a name for the new folder.
   The first subfolder is shown on the right.

6. Click anywhere in the folder.
   The new name is accepted.

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

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Manage Files**.
   The **Manage Files** page of Experiment Editor opens.

3. Select the directory for the file you wish to cut, for example, **LabBooks**.

4. Right-click on the file you wish to cut, see Figure 5-36.

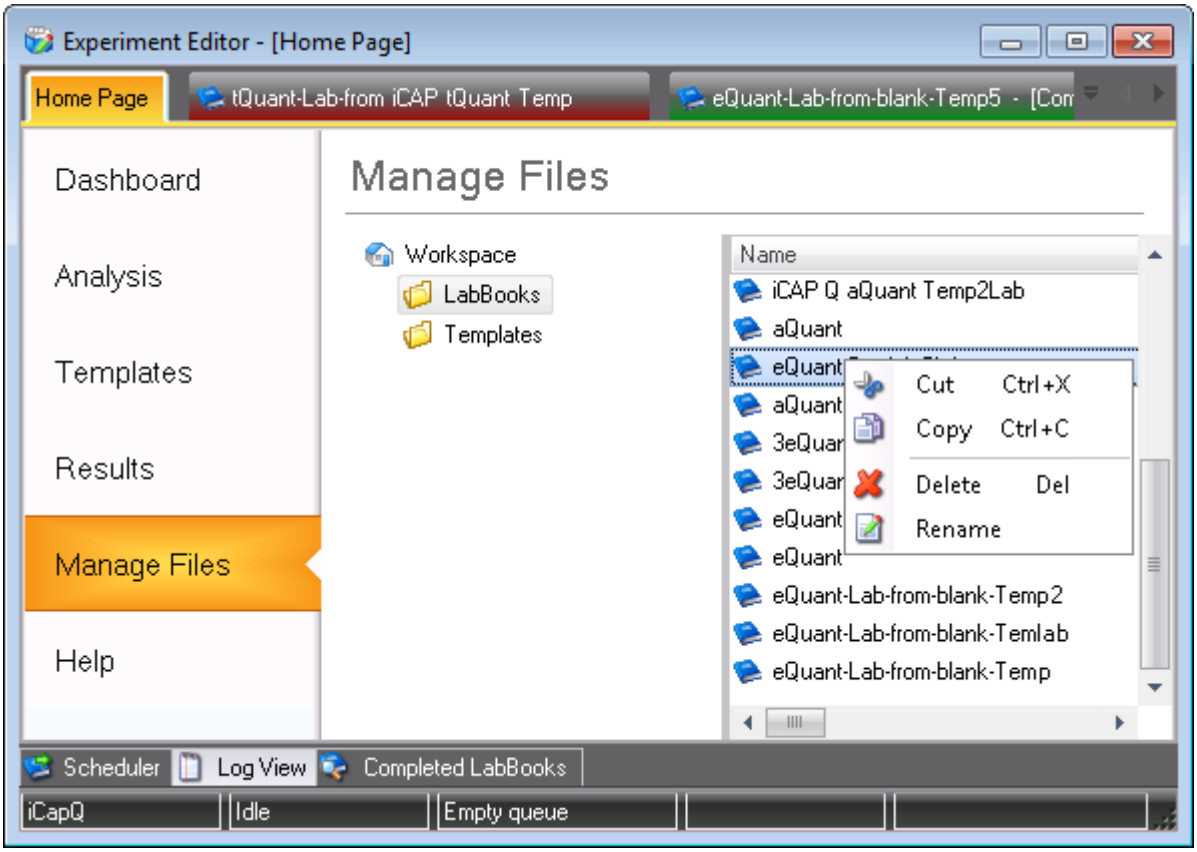


Figure 5-36. Context menu of file

5. Select **Cut** from the context menu.

6. Right-click in the new location for the file, see Figure 5-37.

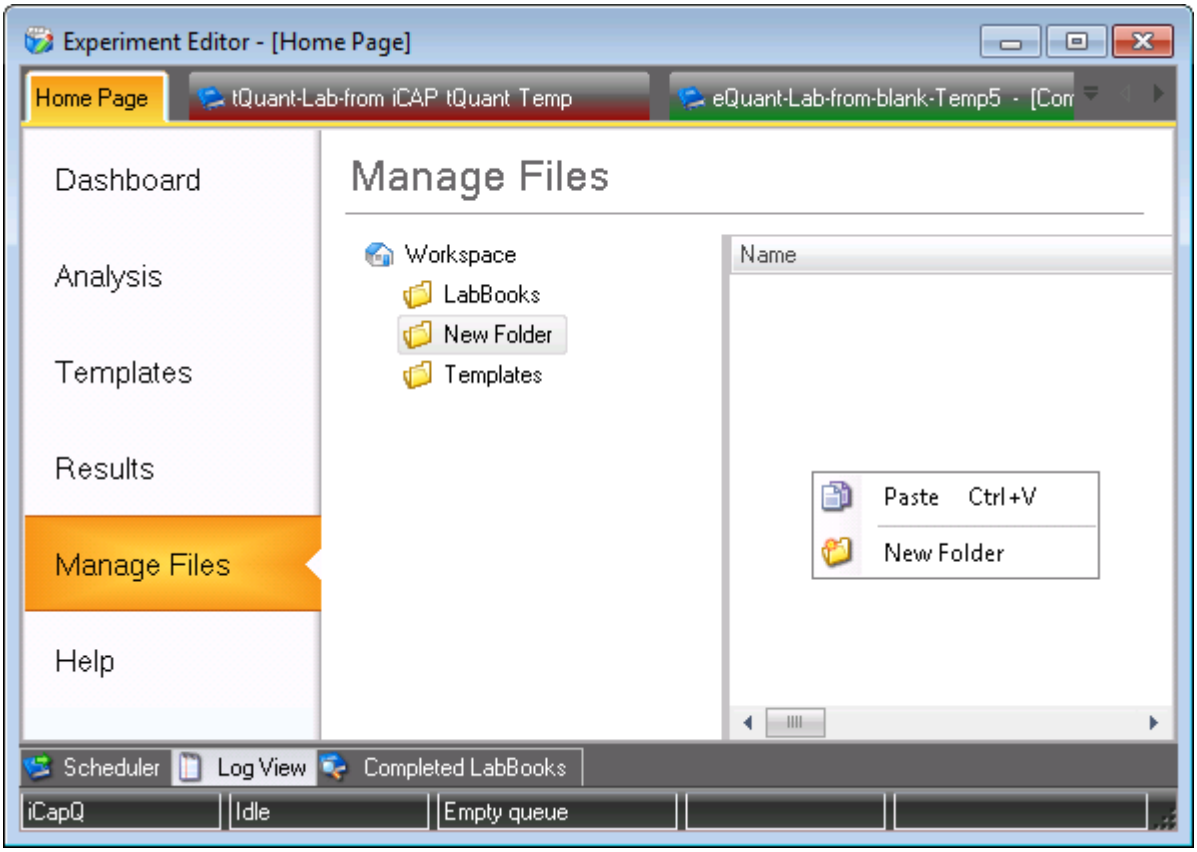


Figure 5-37. Context menu Paste

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

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

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Manage Files**.
   The **Manage Files** page of Experiment Editor opens.

3. Select the directory for the file you wish to copy, for example, **LabBooks**.

4. Right-click on the file you wish to copy, see Figure 5-38.

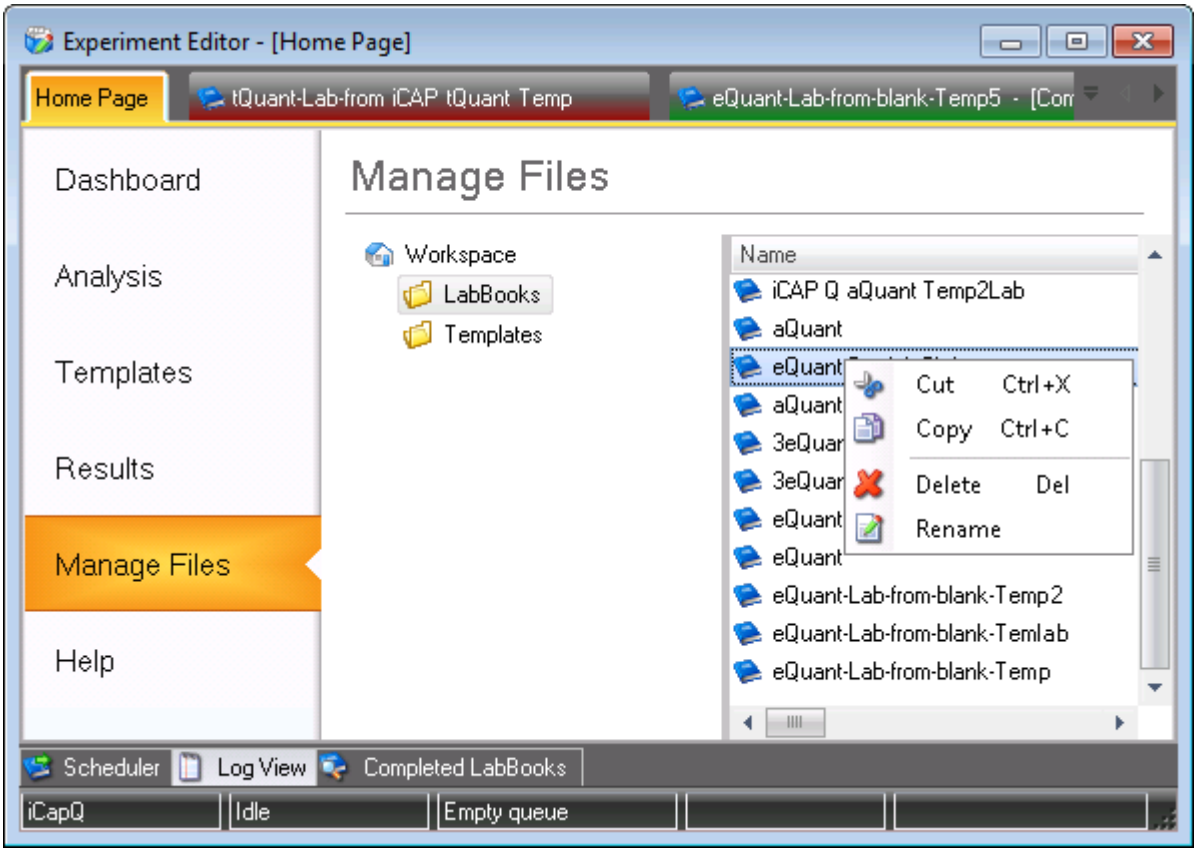


Figure 5-38. Context menu of file

5. Select **Copy** from the context menu.
6. Select the location for the file.
7. Right-click and select **Paste** from the context menu.
   The file is copied to the selected location.

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

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Manage Files**.
   The **Manage Files** page of Experiment Editor opens.
3. Select the directory of the file you wish to delete.
4. Right-click on the file you wish to delete.

5. Select **Delete** from the context menu.
   A confirmation dialog opens, see Figure 5-39.

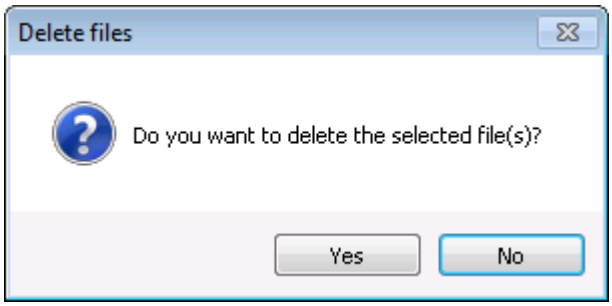


Figure 5-39. Confirmation window to delete file

6. Click Yes.
   The file is deleted.

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

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Manage Files**.
   The **Manage Files** page of Experiment Editor opens.

3. Select the directory of the file you wish to rename.

4. Right-click on the file you wish to rename, see Figure 5-40.

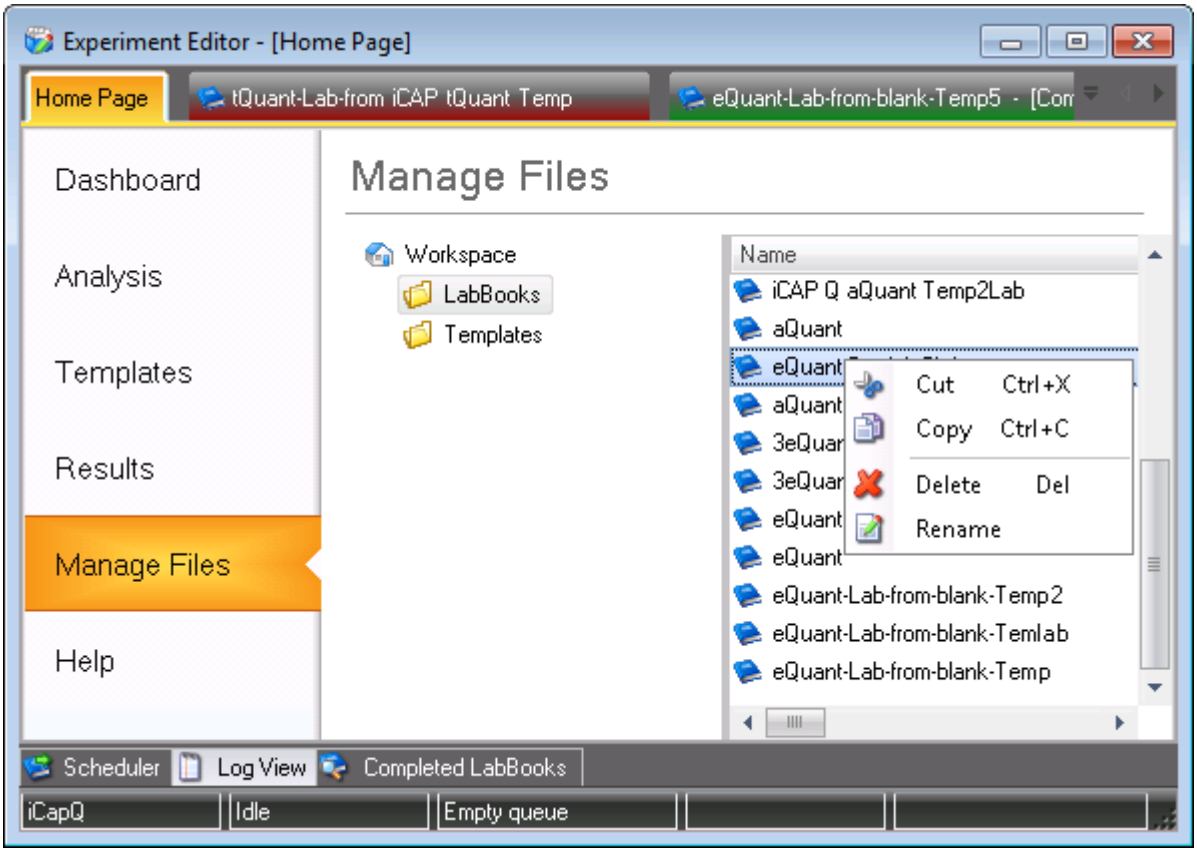


Figure 5-40. Context menu of file

5. Select **Rename** from the context menu.
6. Enter the new name for the file.
7. Click anywhere in the folder.
   The new name is accepted.

Help Page

The **Help** page of Experiment Editor, see Figure 5-41, provides information about Qtegra, support and tools.

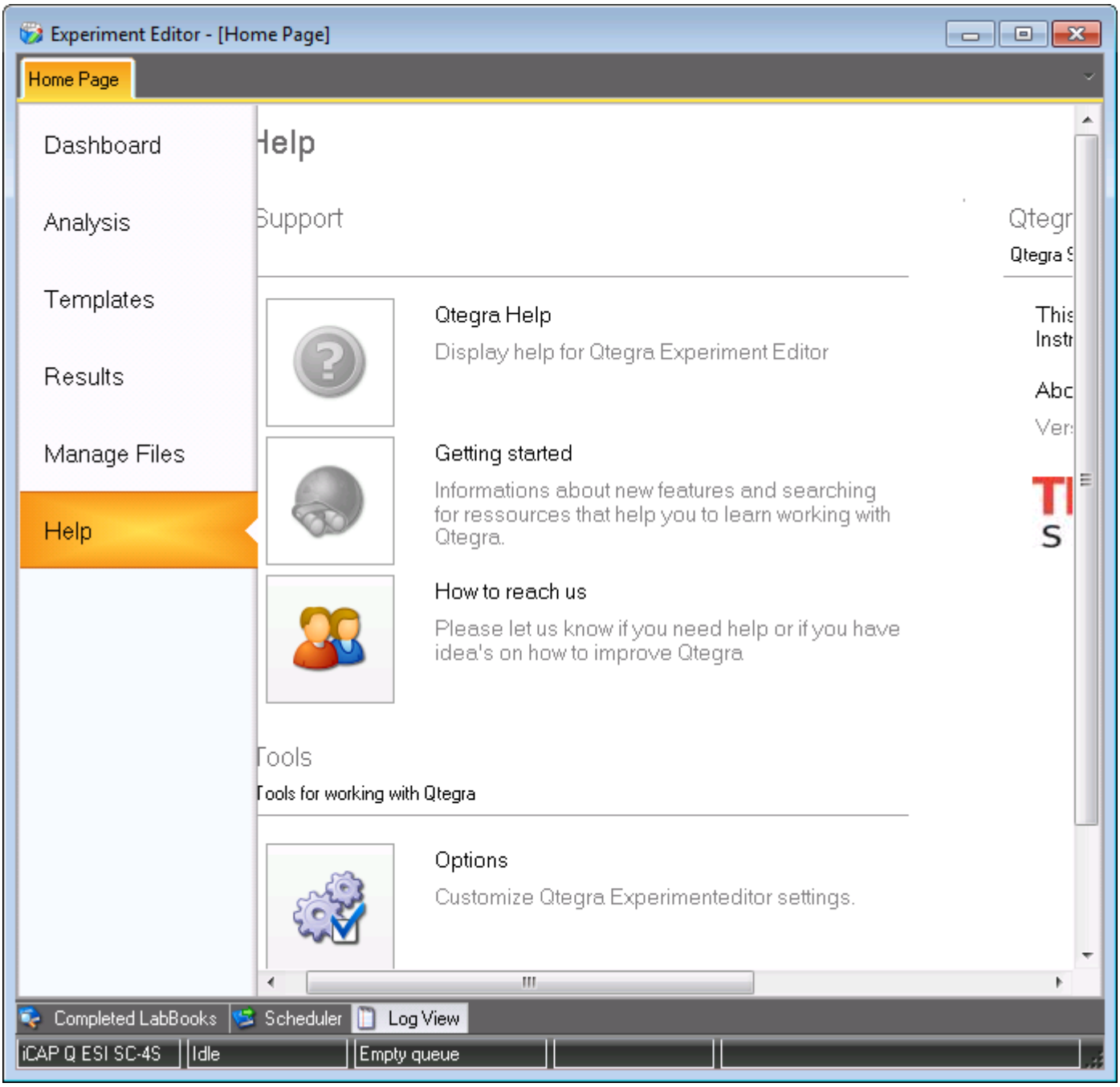
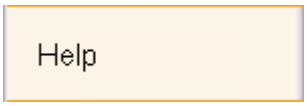


Figure 5-41. Help Page of Experiment Editor

❖ **To open the Help page of Experiment Editor**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Click 

.
The **Help** page of Experiment Editor opens.

Support on the Help Page

The **Support** section on the **Help** page of Experiment Editor offers a useful link how to contact Thermo Fisher Scientific.

❖ **To contact Thermo Fisher Scientific**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Help**.
The **Help** page of Experiment Editor opens.
3. Click  **How to reach us**.
The web page of Thermo Fisher Scientific opens.

Customizing Home Page Settings

In the **Tools** section on the **Help** page of Experiment Editor, you can customize your **Home Page** settings.

❖ **To customize the Home Page settings**

1. Click 

to open **Experiment Editor**.
2. On the **Home Page**, click **Help**.
The **Help** page of Experiment Editor opens.
3. Click  **Options**.

4. In the field **Available** on the left, select **Home Page**, see Figure 5-42.

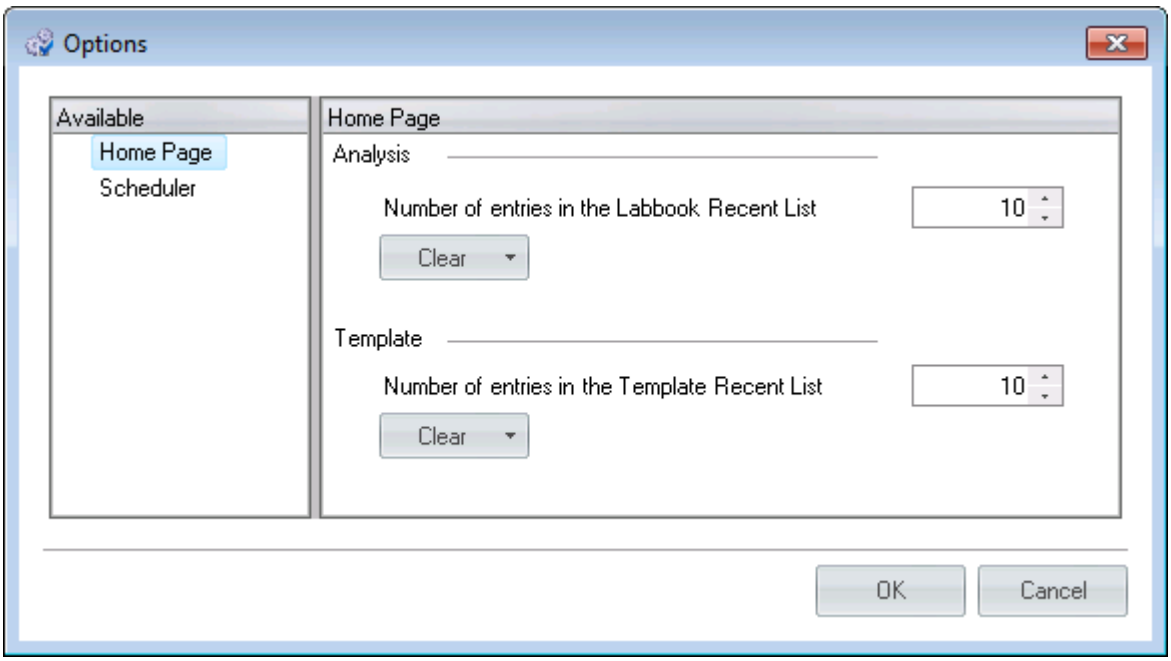


Figure 5-42. Home Page settings in Options dialog of Help page

5. For **Analysis** on the right, select the number of entries for **LabBook Recent List**.
6. From the drop-down list **Clear**, select **All entries** or **Unpinned entries** if you wish to clear the list.
7. For **Template** on the right, select the number of entries for **Template Recent List**.
8. From the drop-down list **Clear**, select **All entries** or **Unpinned entries** if you wish to clear the list.
9. Click 

.

Customizing Scheduler Settings

In the **Tools** section on the **Help** page of Experiment Editor, you can define your **Scheduler** settings.

❖ **To customize Scheduler settings**

1. Click 

to open **Experiment Editor**.

2. On the **Home Page**, click **Help**.
   The **Help** page of Experiment Editor opens.

3. Click  **Options**.

4. In the field **Available** on the left, select **Scheduler** to define the settings, see Figure 5-43.

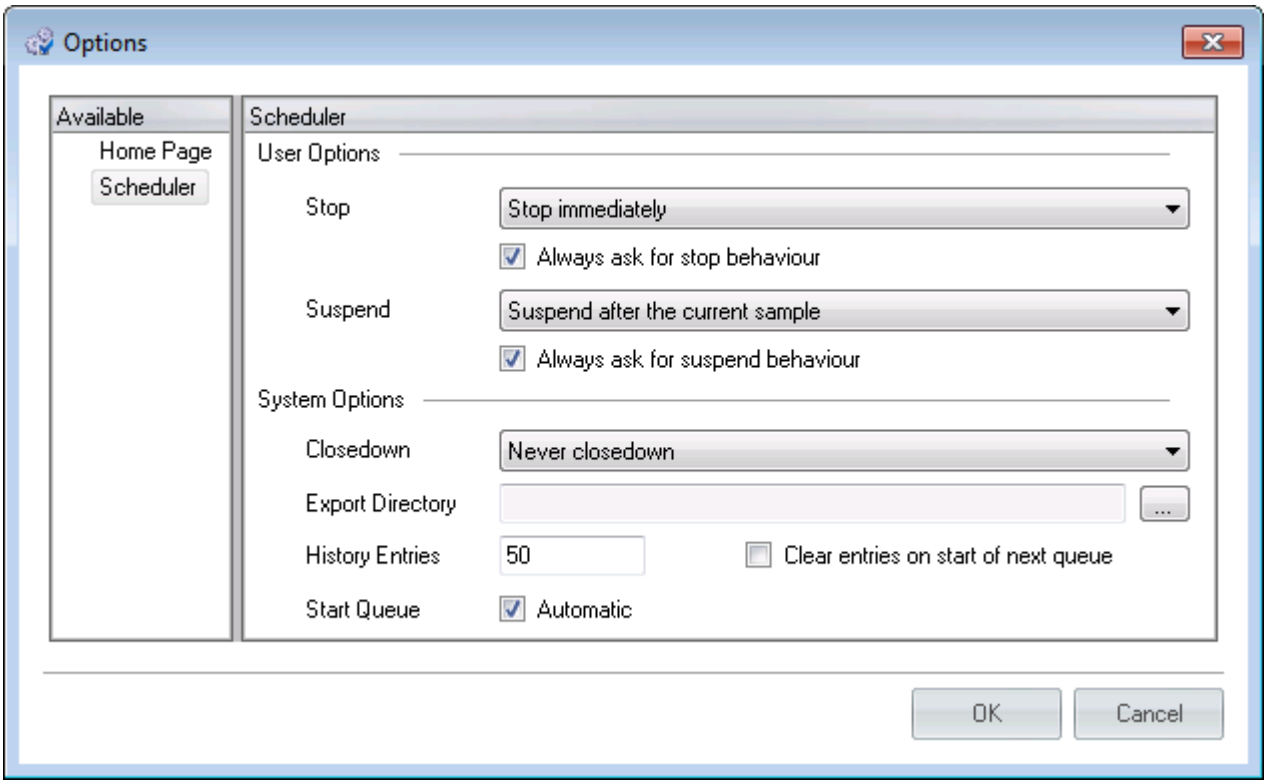


Figure 5-43. Scheduler settings in Options dialog of Help page

5. For **User Options** on the right, select the stop behavior of the Scheduler from the drop-down list **Stop**.

6. Select the check box **Always ask for stop behavior** if you wish to be asked every time.

7. Select the suspend behavior from the drop-down list **Suspend**.

8. Select the check box **Always ask for suspend behavior** if you wish to be asked every time.

9. For **System Options**, select the close-down options from the **Closedown** drop-down list.

10. Click  to select the **Export Directory**.

11. Enter a number for **History Entries**.

12. Select the check box **Clear entries on start of next queue** if you wish to activate this feature.

13. Select the check box **Automatic** next to **Start Queue** if you wish to activate this feature.
    The measurement of a LabBooks is started immediately when the LabBook is added to the Scheduler.

14. Click 

.

Scheduler

In the **Scheduler** tool of Experiment Editor, the measurement for a scheduled LabBook is executed. The completed LabBook is automatically deleted from the Scheduler and added to "Completed LabBooks" on page 5-54.

The Scheduler settings can be customized via the Options button in the Scheduler toolbar, or in the **Tools** section on the **Help** page of Experiment Editor, see "Customizing Scheduler Settings" on page 5-49.

NOTICE To move the Scheduler region in Experiment Editor, see "User Interface of the Experiment Editor Tool" on page 5-2. ▲

❖ **To open the Scheduler of Experiment Editor**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click Scheduler to open the **Scheduler** tab, see Figure 5-44.

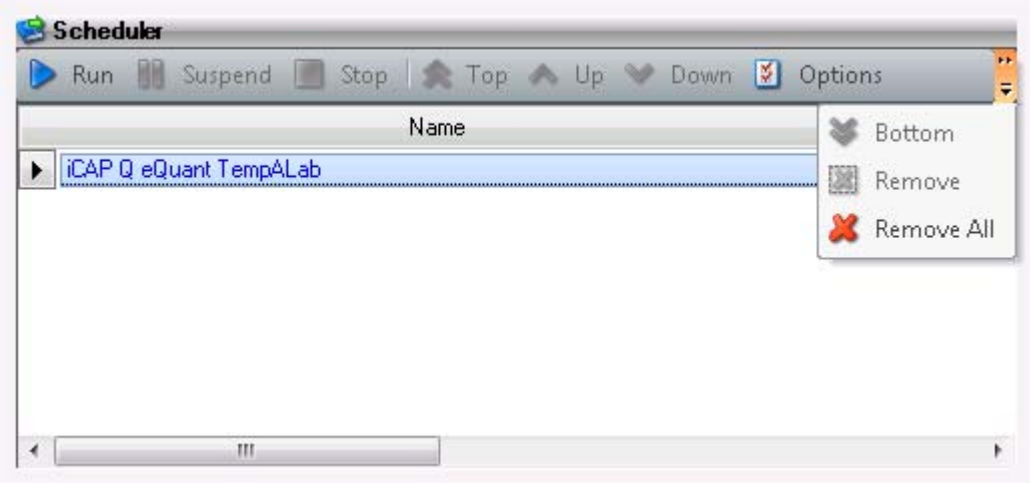


Figure 5-44. Scheduler tool

❖ **To add a LabBook to the Scheduler**

1. Click Experiment Editor to open **Experiment Editor**.
2. Open a LabBook as described in "Opening a LabBook" on page 5-14.

3. In the toolbar of the LabBook, click Run to schedule the LabBook.
   The LabBook is added to the Scheduler and the execution is started immediately if so configured, see Figure 5-45.

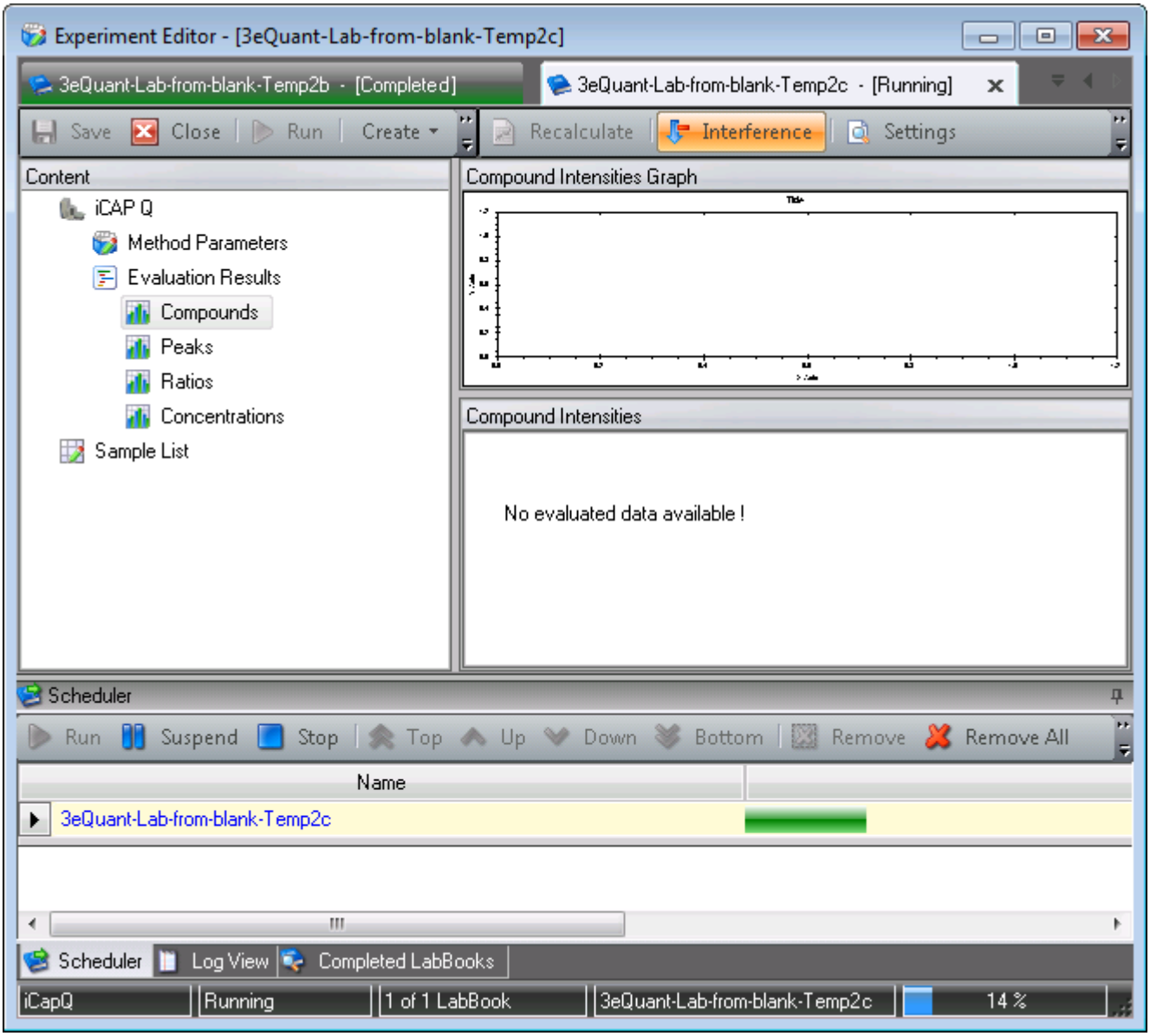


Figure 5-45. Scheduler tool

The green bar shows the progress of the execution.

Completed LabBooks

Upon completion of a LabBook, the LabBook is automatically deleted from Scheduler and added to the **Completed LabBooks** tab in Experiment Editor, see Figure 5-46.

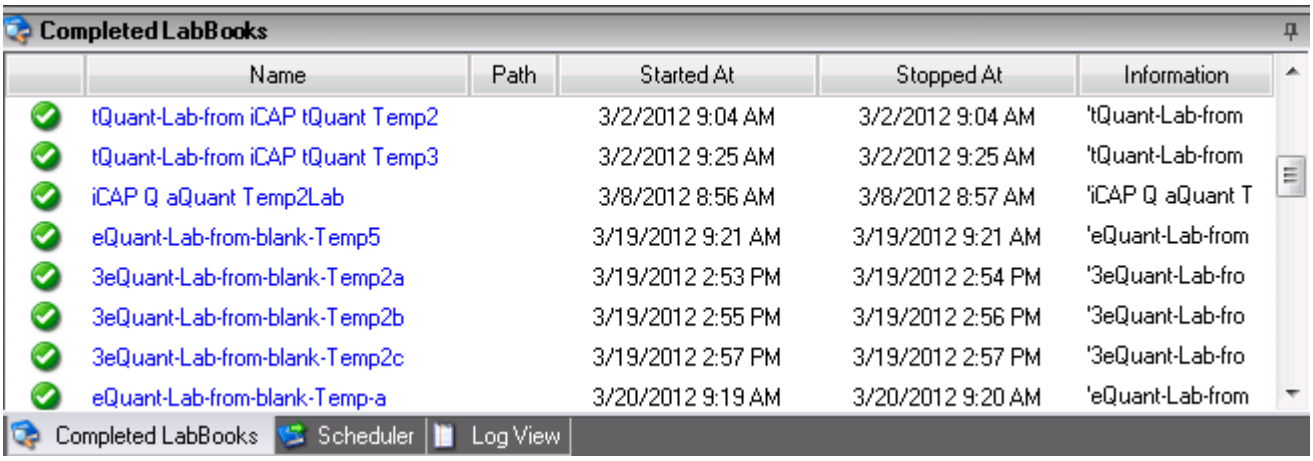


Figure 5-46. Completed LabBooks

NOTICE To move the Completed LabBooks region in Experiment Editor, see "User Interface of the Experiment Editor Tool" on page 5-2. ▲

❖ **To open the Completed LabBooks**

1. Click 

to open **Experiment Editor**.

2. Click 

to open the **Completed LabBooks** tab. All LabBooks that have already been executed are listed.

Log View Region

The **Log View** region of Experiment Editor displays a list of messages, such as errors and warnings. By default, different types of messages are displayed. The Viewer tab is also shown in "Configurator" on page 3-1 and "Instrument Control" on page 4-1.

NOTICE To move the Log View region in Experiment Editor, see "User Interface of the Experiment Editor Tool" on page 5-2. ▲

❖ **To open the Log View of Experiment Editor**

1. Click 

to open **Experiment Editor**.

2. Click 

to open the **Log View** tab, see Figure 5-47.

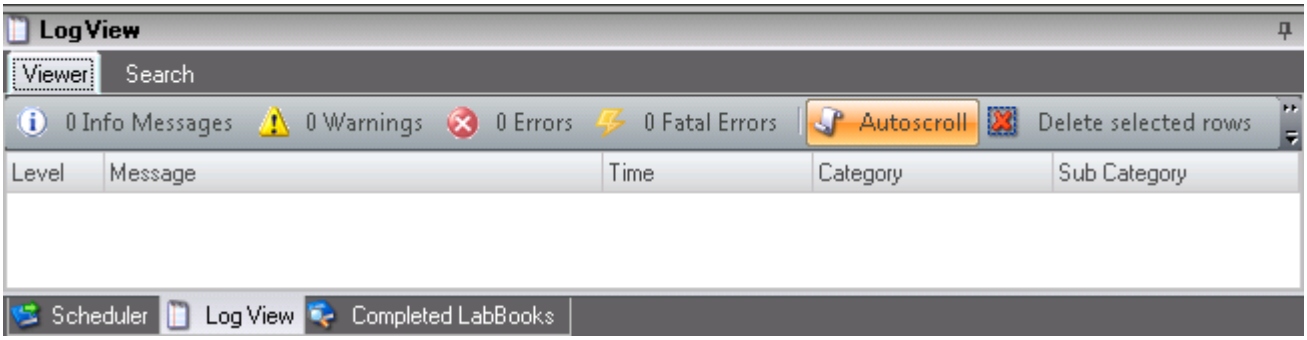


Figure 5-47. Log View in Experiment Editor

Chapter 6 Templates

The analytical workflow for sample measurement is defined in a Template. Templates are created in the "Experiment Editor" on page 5-1.

Templates are based on a particular Configuration which is usually defined by the Manager (see "Experiment Configurator" on page 3-13) 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 6-10). For every application an appropriate Template can be created.

Contents

- Template Toolbar
- Evaluation Methods
- Color Scheme of the Periodic Table
- Method Parameters
- Peripherals
- Manual Sample Control
- Sample Definition for a Template
- Automatic Export - Template

❖ **To open a Template in the Experiment Editor tool**

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click **Templates**.
4. Open a Template as described in "Opening a Template" on page 5-22.

Template Toolbar

In the Template tab of Experiment Editor, Qtegra offers buttons to save, close or run a Template, see Figure 6-1.

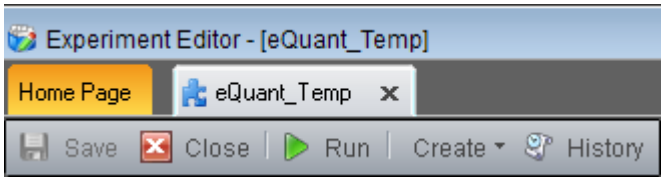


Figure 6-1. Template toolbar

Additionally, you can create a new LabBook or Template from the existing current Template, view the history of the current Template or hide the Content pane.

❖ **To save a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Change the settings as appropriate.
5. Click  to save your Template.

❖ **To close a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  in the toolbar to close the Template.

   You can also click  in the tab of the Template.

❖ **To run a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to create a LabBook to schedule for execution.
The **Create LabBook** window opens, see Figure 6-2.

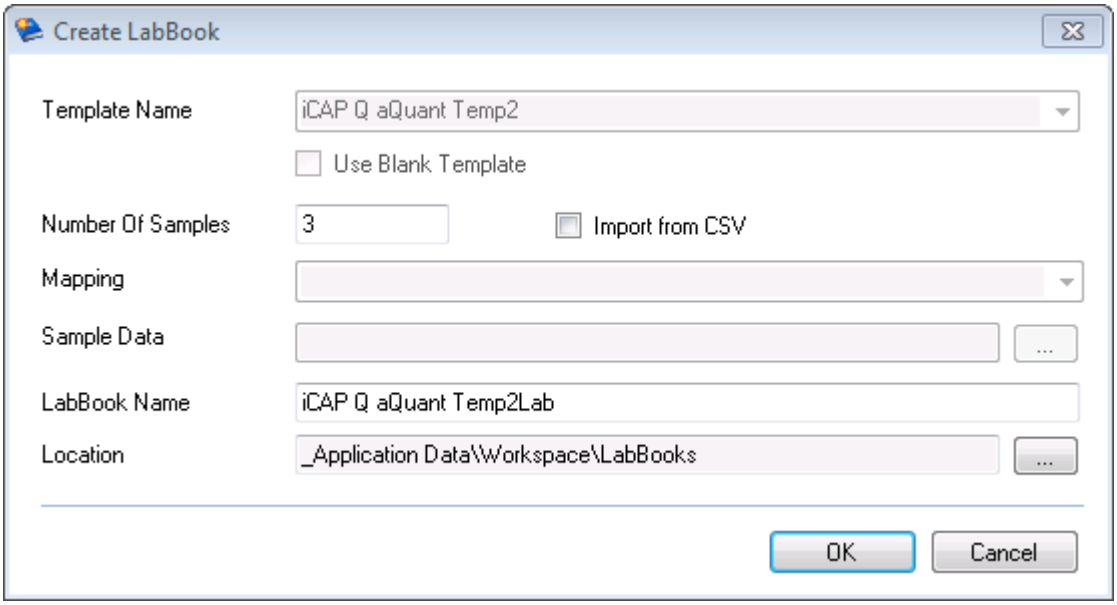
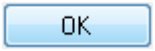


Figure 6-2. Create LabBook window from Run in Templates toolbar

5. Enter **Number Of Samples**.
6. Enter **LabBook Name**.
7. Click 

.
The LabBook is created and executed.

❖ **To create a LabBook or Template from an existing Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click **Create**.
   The **Create** drop-down menu opens, see Figure 6-3.

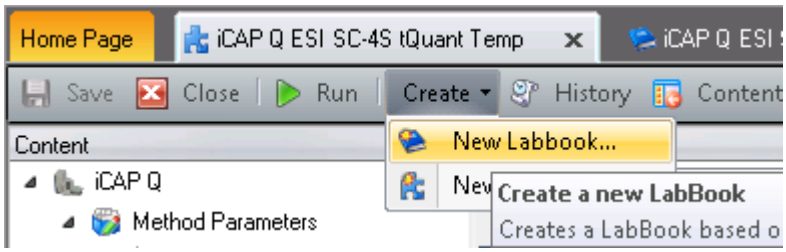


Figure 6-3. Create drop-down in Templates toolbar

5. Click **New LabBook** if you wish to create a new LabBook from the existing current Template.
   The **Analysis** view of the **Home Page** opens. See "Creating a LabBook" on page 5-16 for further details.

6. If you wish to create a new Template from the existing current Template, click **New Template**.
   The **Template** view of the **Home Page** opens. See "Creating a Template" on page 5-24 for further details.

❖ **To view the history of a Template**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click History.
   The **History** window for this Templates opens, see Figure 6-4.

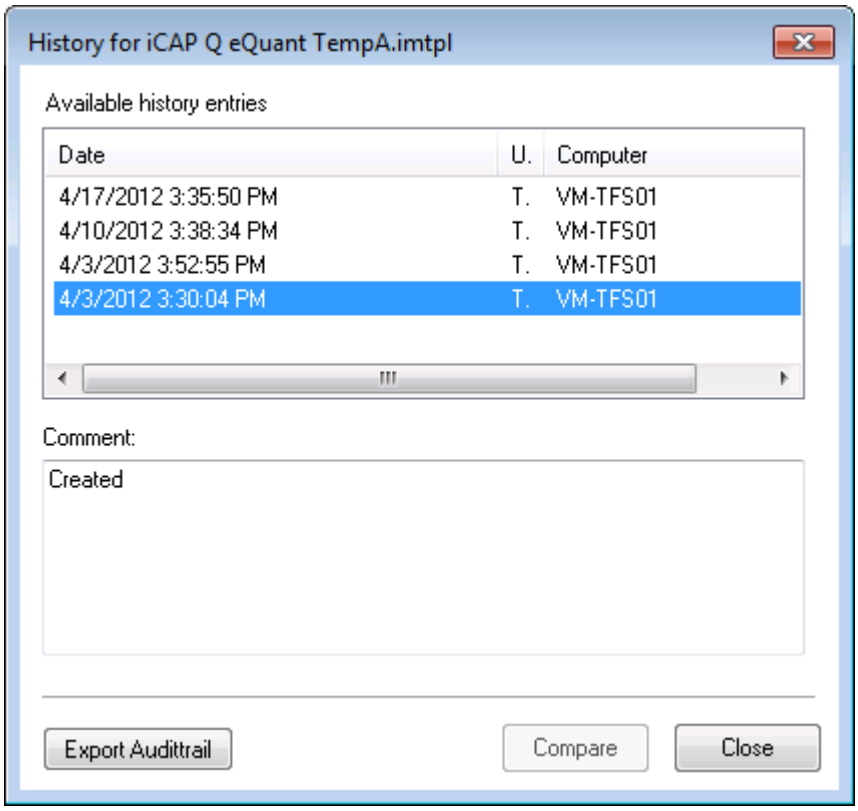


Figure 6-4. History dialog of Template

5. Click Close to close the **History** dialog for this Template.

❖ **To compare the history entries of a Template**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click History.
   The **History** dialog for this Templates opens, see Figure 6-4.

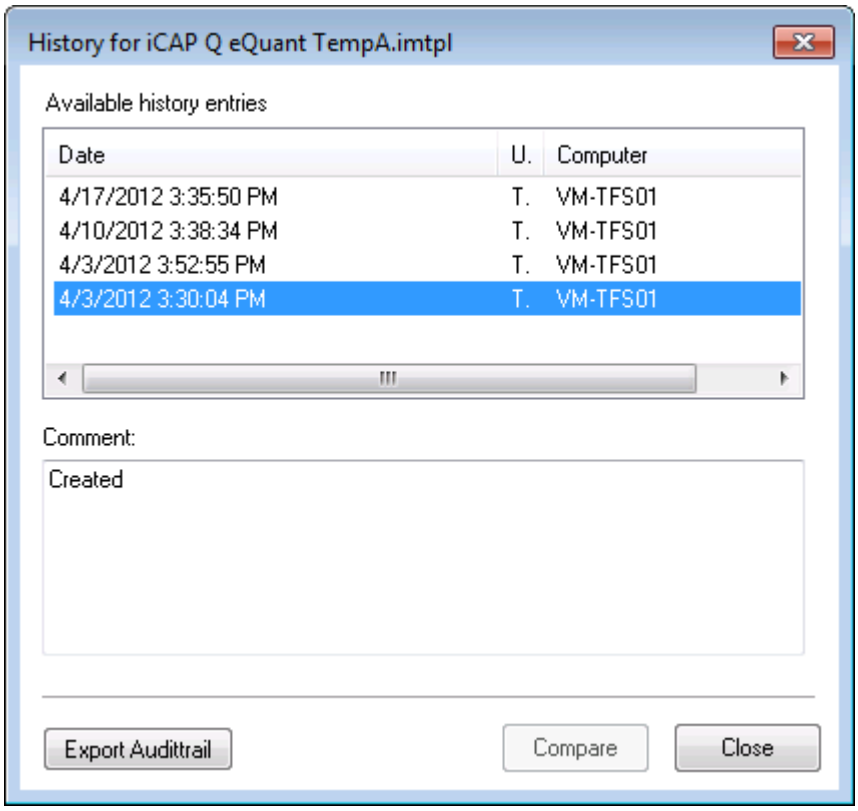


Figure 6-5. History dialog of Template

5. Press <**Ctrl**> and select the entries you wish to compare.

6. Click Compare to compare the selected entries. The **Comparison** dialog opens, see Figure 6-6.

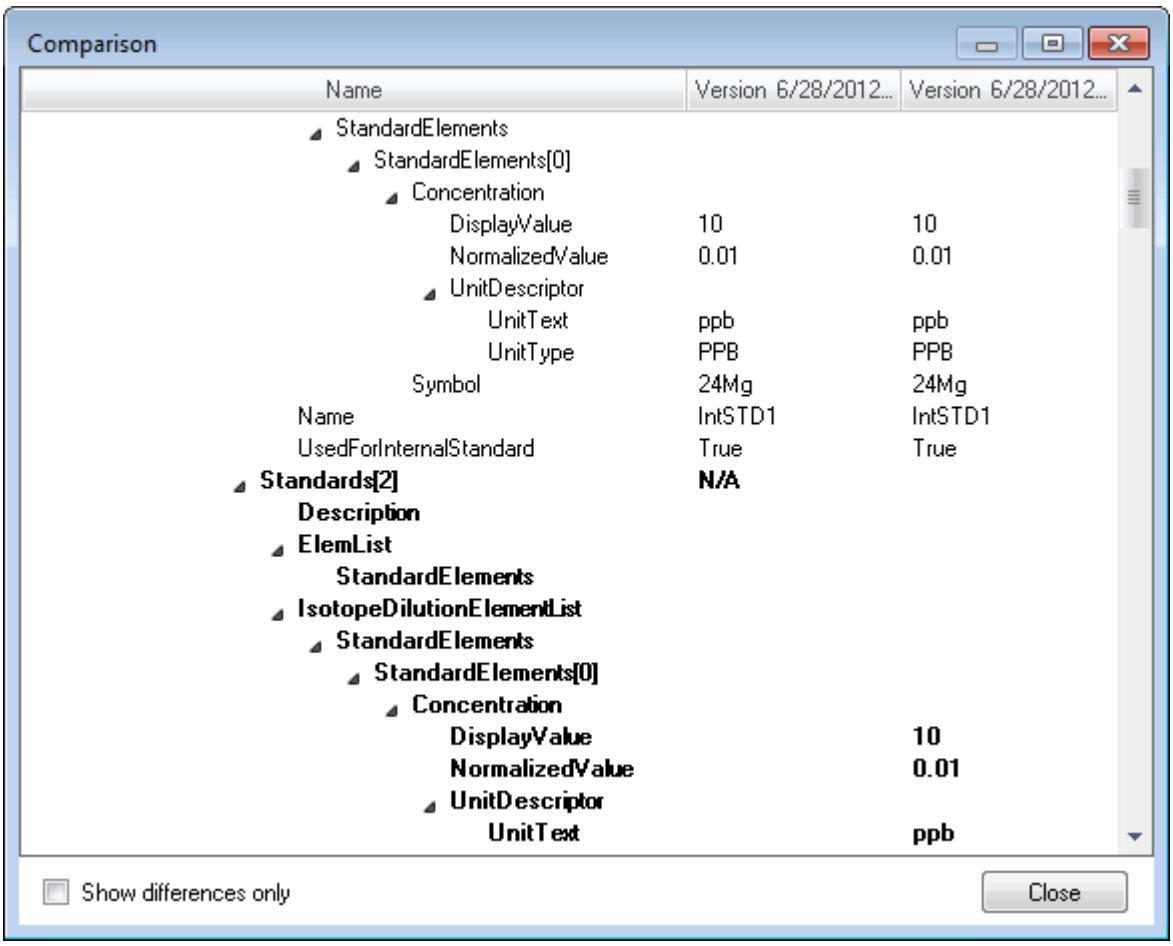


Figure 6-6. History Compare Template dialog

7. Select the check box **Show differences only** if you wish to view only the differences.

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

9. Click Close to close the **History** dialog for this Template.

❖ **To export the audit trail of a Template**

1. Click Experiment Editor to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click History.
   The **History** dialog for this Templates opens, see Figure 6-7.

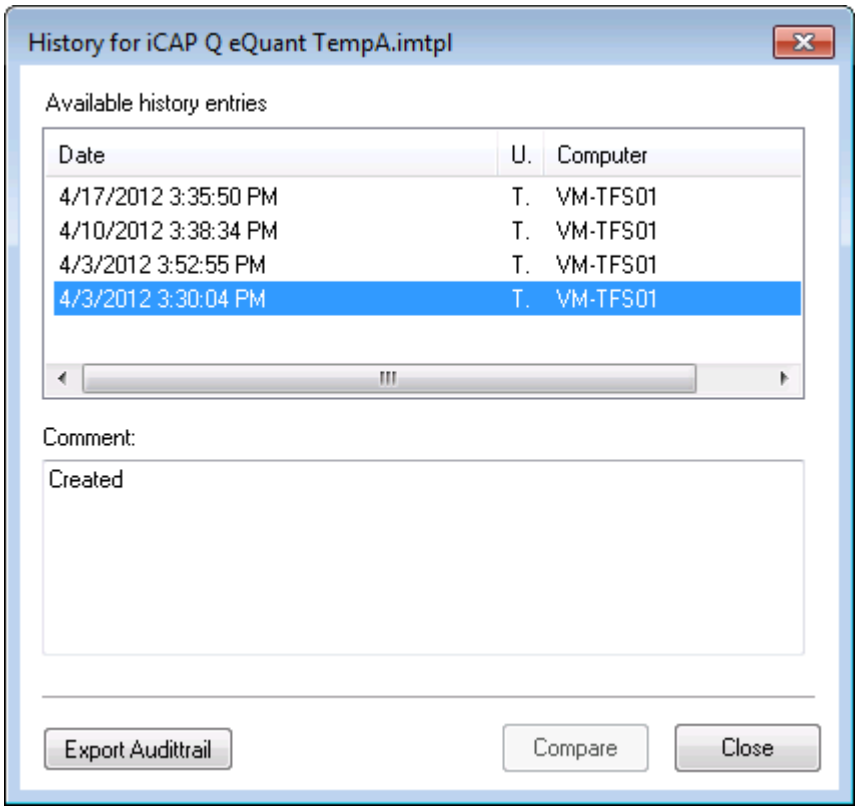


Figure 6-7. History dialog of Template

5. Select the Template for which you wish to export the audit trail.

6. Click Export Audittrail.
   The **Export Audittrail** dialog opens, see Figure 6-8.

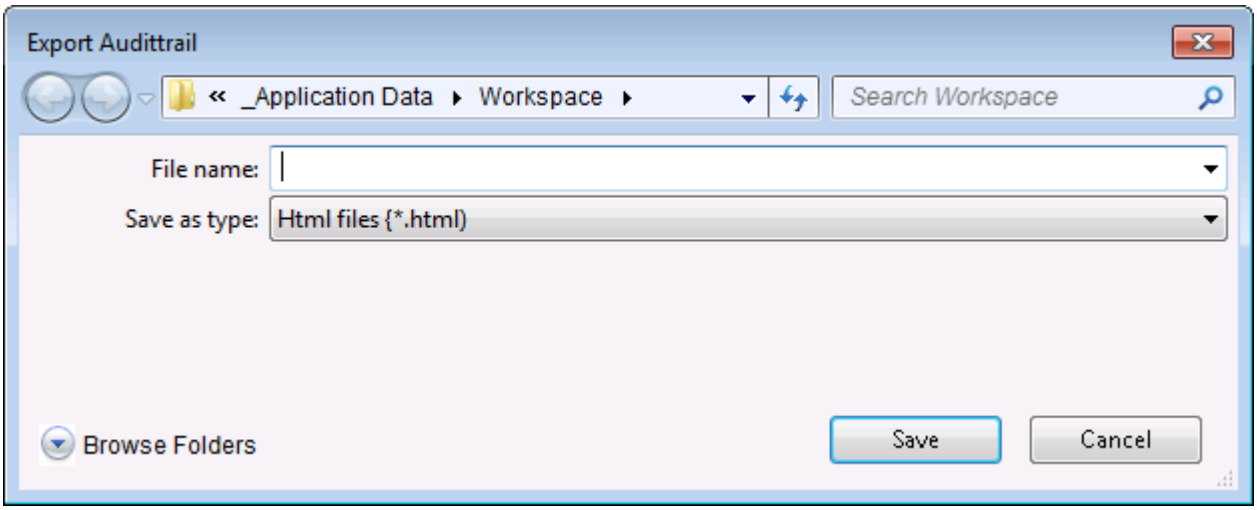


Figure 6-8. History Export Audittrail dialog

7. Click **Browse Folder** if you wish to change the pre-configured location of the file and select the directory.

8. Enter a **File name** for the HTML file, and click Save. Your standard web browser opens displaying the audit trail information.

9. Click Close to close the **History** dialog for this Template.

❖ **To hide Content pane**

1. Click Experiment Editor to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
The **Content** pane of the Template is shown on the left, see Figure 6-9.

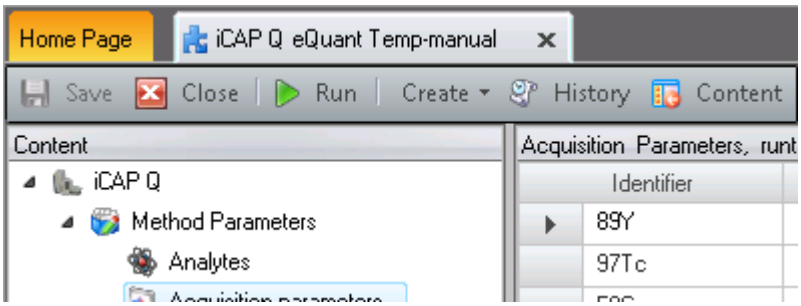


Figure 6-9. Content pane of Template visible

4. Click Content.
The **Content** pane is hidden, see Figure 6-10.

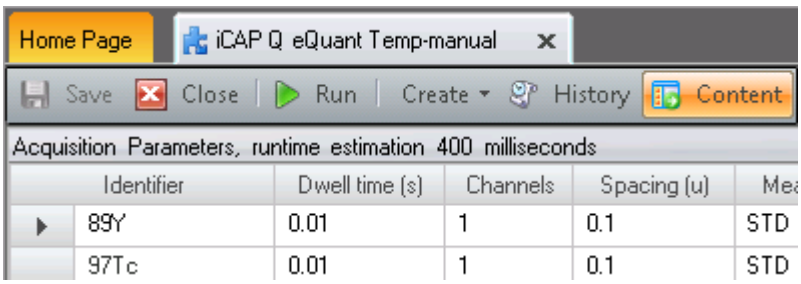


Figure 6-10. Content pane of Template hidden

5. Click Content to show the **Content** pane again.

Evaluation Methods

Qtegra offers a range of **Evaluation** methods (see Figure 6-11) to be selected when creating a Template in Experiment Editor to accommodate any type of analysis required.

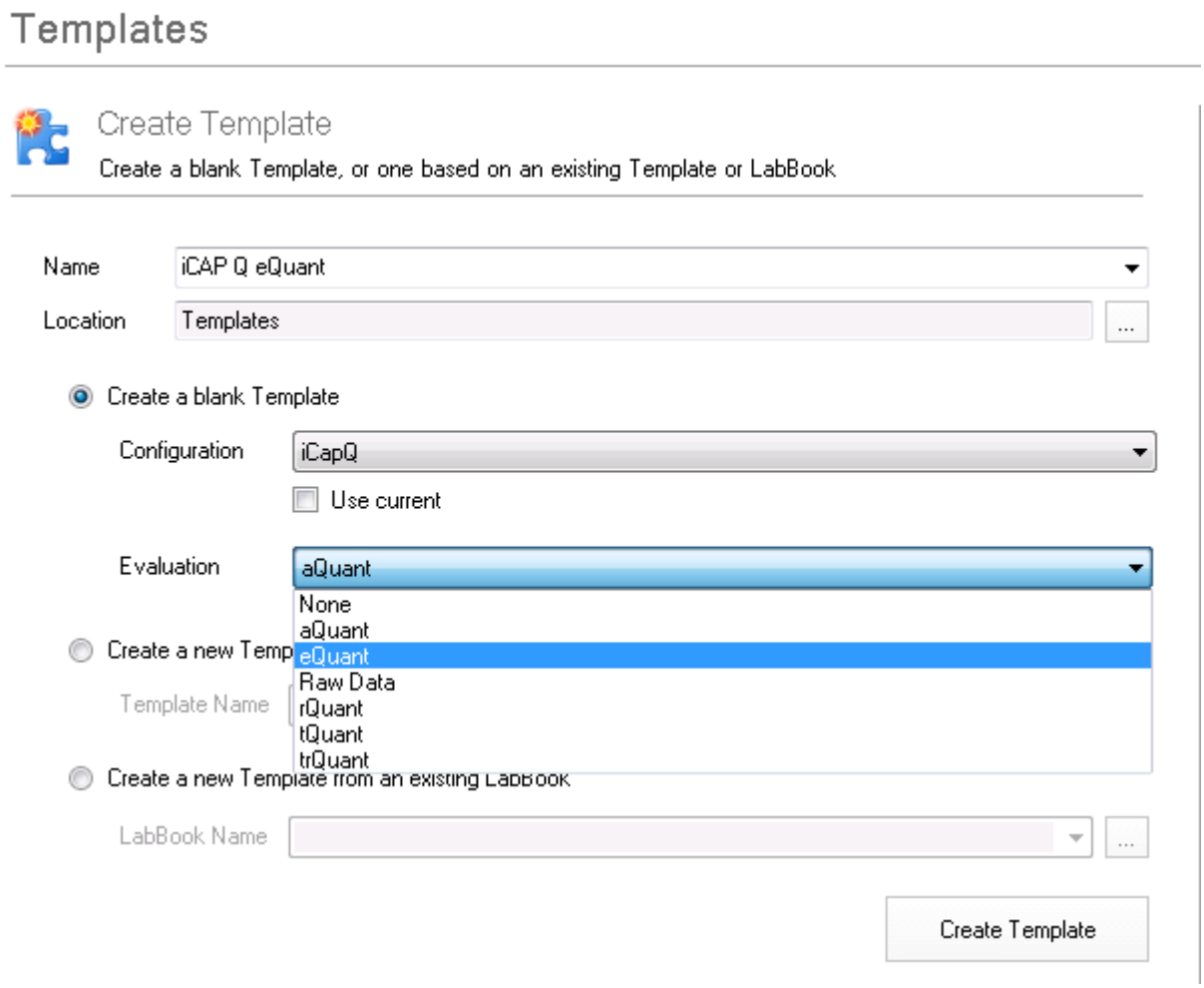


Figure 6-11. Evaluation types drop-down menu

The main applications for the Evaluations are summarized in Table 6-1.

Table 6-1. Evaluation methods

Evaluation	Description
aQuant	Created for Standard Addition analysis. In Standard Addition analysis, a known amount of analyte is added to the sample to determine the relative response of the detector to an analyte within the sample matrix. The difference in analytical response between the spiked and unspiked samples is due to the amount of analyte in the spike. This provides one or more calibration points to determine the analyte concentration in the original sample. The Standard Addition technique is generally used when matrix effects occur and cannot be circumvented through either further dilution or matrix elimination.
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. A different evaluation strategy can be chosen for each analyte and also for each isotope of an analyte.
Raw Data	Displays the acquired raw intensities which are then used by the different evaluations.
rQuant	Uses the isotope dilution equation to give fully quantitative results. Measures the isotopic ratio changes of an element in a sample. The isotopic ratio change is measured between an isotopically enriched standard spike and the analyte with known isotopic abundance.
tQuant	Used for chromatographic evaluations or for applications which require the recording and subsequent integration of transient signals. This evaluation method should be used, for example, if all components in a sample have been previously separated to be detected and quantified individually using an appropriate separation technique.
trQuant	For solid samples, laser ablation systems. In contrast to tQuant evaluation the transient signals in trQuant are defined as regions in which the signal is constant over time and the average value of the defined region is used for quantification.

Color Scheme of the Periodic Table

The periodic table, see Figure 6-12, is part of the Analytes section of the Method Parameters in Experiment Editor, independent of 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.

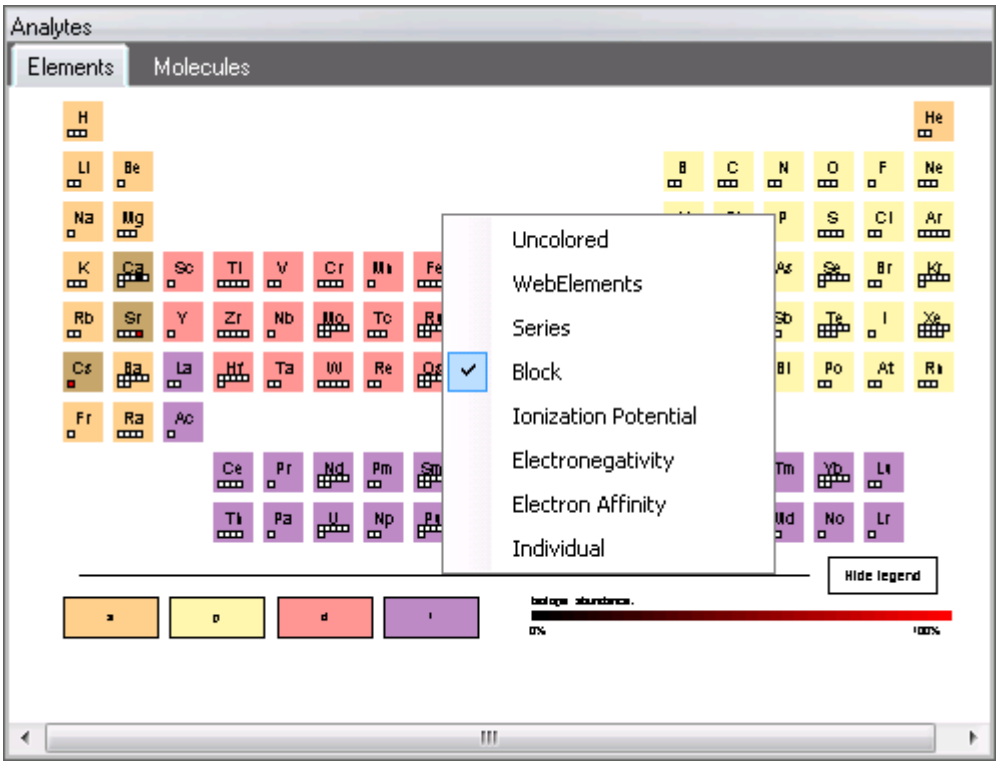


Figure 6-12. Periodic table with drop-down menu

A context menu offers several color schemes for the periodic table, see Table 6-2.

Table 6-2. Color scheme of periodic table

Item	Description
Uncolored	All elements in the periodic table are displayed as grey boxes.
WebElement™	The elements are colored according to www.webelements.com.
Series	The elements are color-coded in groups according to their chemical properties or series.
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.

Table 6-2. Color scheme of periodic table

Item	Description
Ionization Potential	The elements are color-coded in groups according to their ionization potential, that is, the work required to remove an outermost electron in the atom.
Electronegativity	The elements are marked according to their electronegativity, that is, their ability to attract electrons.
Electron Affinity	The elements are marked according to their electron affinity, that is, the work required to remove an electron from the corresponding anion.
Individual	All elements are marked individually, for example, each showing a different color based on the color scheme selected in the Configurator module "Element Editor" on page 3-9.

❖ **To change the color scheme of the periodic table**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Analytes** view.
5. Select the **Elements** page in the **Analytes** view.

6. Right-click next to the periodic table (but not on the table itself) to open the context menu, see Figure 6-13.

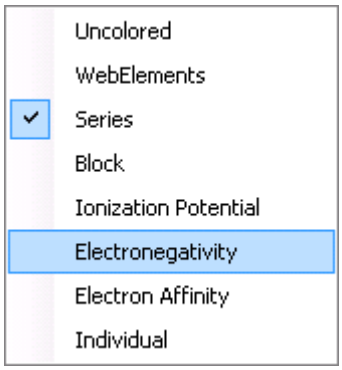


Figure 6-13. Context menu color schemes

7. Select an item from the context menu.
   The colors in the periodic table changes accordingly.

Method Parameters

Method Parameters differ for each Template, depending on the **Evaluation** selected for the Template in Experiment Editor. All Method Parameters are listed in Table 6-3. The availability of each parameter is controlled by the type of Evaluation defined for the Template.

Table 6-3. Method Parameters of Qtegra

Method Parameter	Evaluation
Analytes	eQuant, aQuant, tQuant, rQuant, trQuant, Raw Data
Acquisition Parameters	eQuant, aQuant, tQuant, rQuant, trQuant, Raw Data
Monitor Analytes	eQuant, aQuant, rQuant, Raw Data
Survey Scan Settings	eQuant, aQuant, rQuant, Raw Data
Interference Correction	eQuant, aQuant, tQuant, rQuant, trQuant, Raw Data
Standards	eQuant, aQuant, tQuant, rQuant, trQuant
Compounds	tQuant
Peak Detection	tQuant
Parameters	rQuant, trQuant
Regions	trQuant
Quantification	eQuant, aQuant
Ratios	eQuant, aQuant, tQuant
Quality Control	eQuant

Analytes

For all Template types, the analytes to be acquired during the measurement are selected in the Method Parameter view **Analytes** of Experiment Editor.

Analytes can be selected from the periodic table display in the **Elements** page, see Figure 6-14.

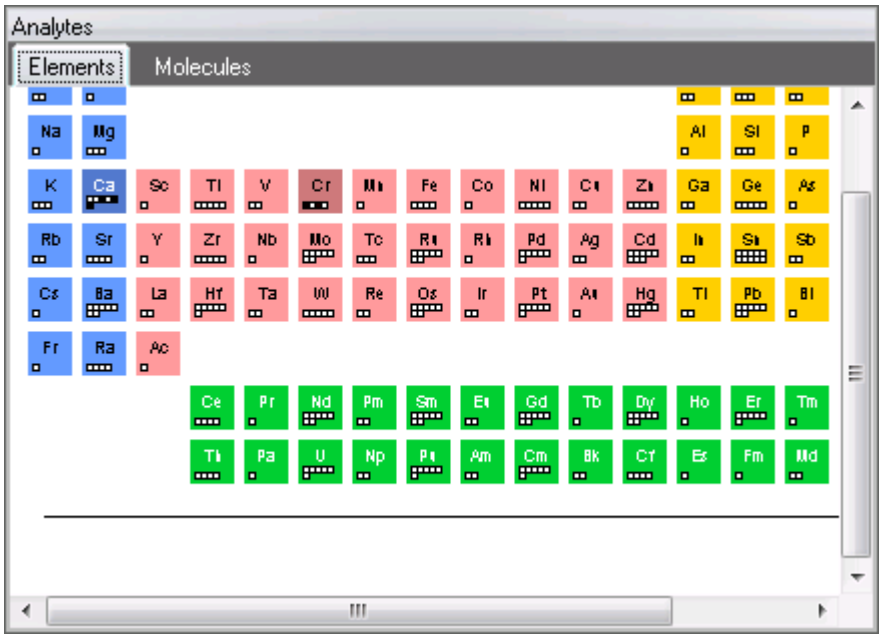


Figure 6-14. Elements page of Analytes

Default element properties defined in the database are automatically selected for dwell time, channels, spacing, resolution, and possible interferences of the selected isotope. These element properties can be redefined by the operator in "Acquisition Parameters" on page 6-19.

NOTICE If any isotopes or interferences need to be added to an experiment, the Manager can edit the element database in the **Configurator** with the "Element Editor" on page 3-9. ▲

On the **Molecules** page, see Figure 6-15, analytes can be selected from a tabulated list of the analyte isotopes, and matrix components can be defined.

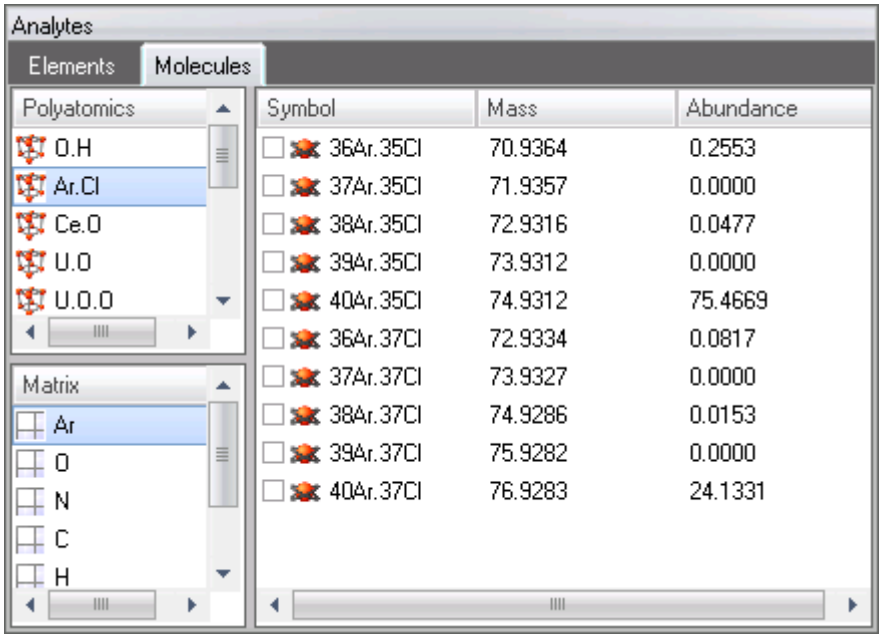


Figure 6-15. Molecules page of Analytes

In the **Polyatomics** table, polyatomic ions and background ions can be selected. The column Symbol displays the combinations of the different isotopes of the participating elements of the polyatomic ion (or the background). The column Mass displays the mass of the polyatomic ion. The column Abundance displays the value of the calculated natural abundance of the polyatomic ion.

Matrix ions are the analytes at a high concentration in the samples to be analyzed. Upon selecting a **Matrix** analyte in the **Molecules** page, polyatomic ions arising from combination of the analyte with another ion can be defined.

❖ **To open the Analytes view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Analytes** view.

Selecting Elements/Analytes

In the **Elements** page of the Analytes view in Experiment Editor, isotopes of an element are displayed as white squares in the element field of the periodic table. As soon as one or more isotopes are selected, the square corresponding to the selected isotope will become colored, according to the **Isotope abundance** legend shown below the periodic table. Clicking on **Show legend** or **Hide legend** respectively shows or hides the **Isotope Abundance** legend.

❖ **To select the default isotope of an element (left mouse click)**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Analytes** view.
5. Select the **Elements** page in the **Analytes** view.
6. Left-click the element in the periodic table to select the default isotope for this element.
   The isotope and its default information stored in the database are added to the Acquisition Parameters view ("Acquisition Parameters" on page 6-19).
7. To deselect an isotope, click the element again.

❖ **To select different isotopes of an element (right mouse click)**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Analytes** view.
5. Select the **Elements** page in the **Analytes** view.

6. Right-click the element in the periodic table to display the list of isotopes for this element.

   A list of the isotopes if this element is displayed (see Figure 6-16) with symbol, mass, abundance and known interference as stored in the element database.

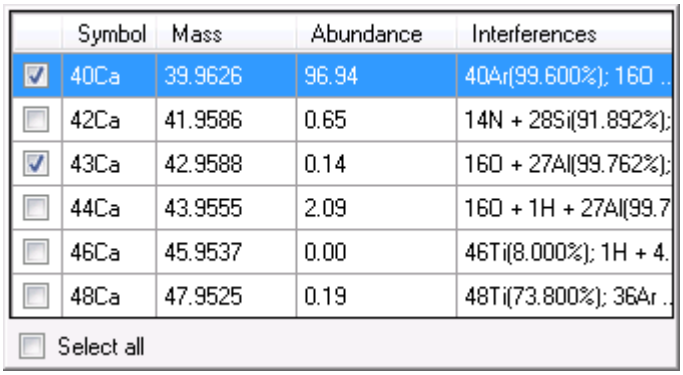


Figure 6-16. List of isotopes for selected element Ca

7. Select the check boxes of the isotopes of interest.
8. To select all isotopes for the element, select the check box **Select all**. The check boxes for all isotopes are selected.
9. Click outside the list to confirm the selection.

   The isotope(s) and default information stored in the database are added to the Acquisition Parameters view ("Acquisition Parameters" on page 6-19).

Acquisition Parameters

For all Template types, the list of analytes selected for the Template is displayed in the **Acquisition Parameters** view of the Experiment Editor tool. Acquisition details such as dwell time and number of channels can be defined.

In the lower part of the Acquisition Parameters view the Advanced Parameters are displayed, see Figure 6-17.

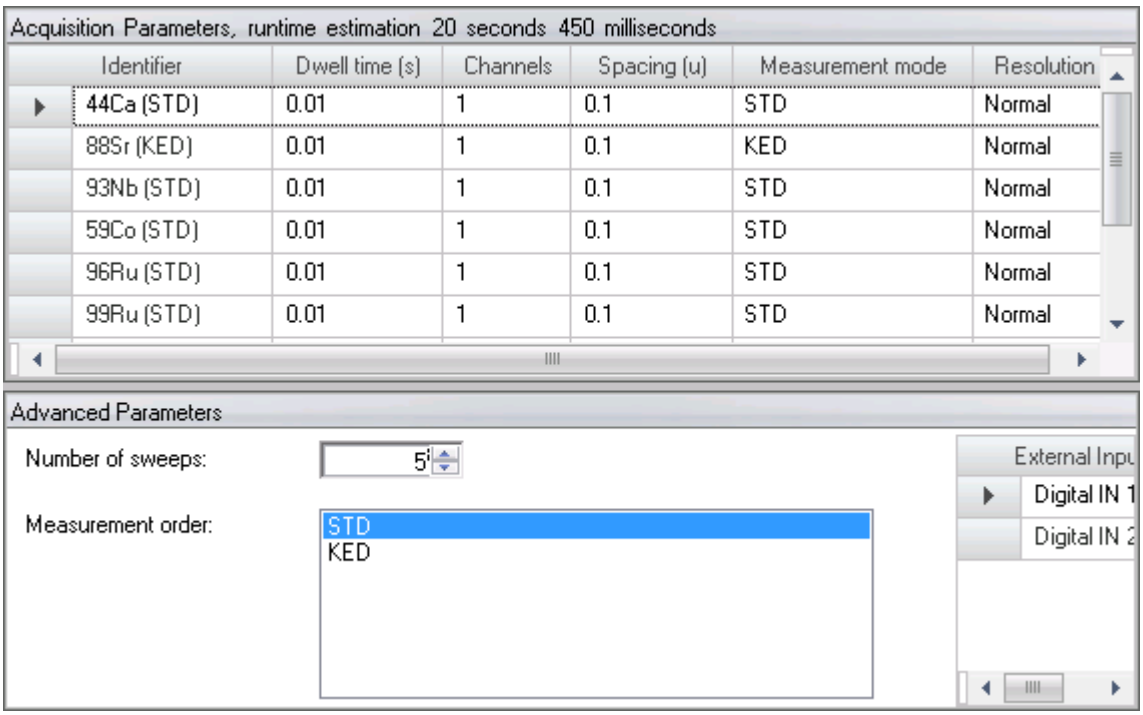


Figure 6-17. Acquisition Parameters and Advanced Parameters (eQuant)

The **Acquisition Parameters** are explained in Table 6-4.

Table 6-4. Acquisition Parameters

Column	Description
Identifier	Displays the symbol for the chemical element/isotope/molecule.
Dwell Time	Displays the dwell time for the selected isotope, for example, the time spent measuring this analyte on a single channel. By default, this value is set to 0.01 seconds. **Recommended Settings:** Typically, dwell times are related to the expected concentration of the analyte in the samples and the tune setting. Major analytes (ppm level) require shorter dwell times. Minor analytes (ppt, ppb level) require longer dwell times.
Channels	Displays the number of channels used for each peak. The default number is 1. When entering an even number, the system will automatically enter the higher odd number.
Spacing	Displays the distance in atomic mass units [amu] between the channels. **Recommended Settings:** Defining the distance between the channels is closely related to the number of channels selected. For example, spacing of 0.1 with 9 channels covers a mass width of ± 0.4 amu either side of the central channel of the peak (total peak width of 0.8 amu).

Table 6-4. Acquisition Parameters

Column	Description
Measurement mode	Measurement mode defined for the analyte.
Resolution	Displays the resolution (**Normal** or **High**) for the selected isotope. By default, the resolution setting is **Normal**. **Recommended Settings:** Typically most analytes are acquired using normal resolution (NR). High resolution (HR) can be selected for analytes which are at high concentration in the samples (HR results in small intensity).

In the section **Advanced Parameters** the **Number of sweeps** to be performed during one main run can be defined for all Templates types except for t- and trQuant. The **Measurement order** and **Trigger** can be defined for all Template types.

❖ **To open the Acquisition Parameters view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Acquisition Parameters** view.

❖ **To display the list of interferences**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  below the Method Parameters to open the **Acquisition Parameters** view in the Template.
5. Click 

in the Toolbar of the Template.
The list of interferences and the abundance of the interference on

the isotope opens, see Figure 6-18.

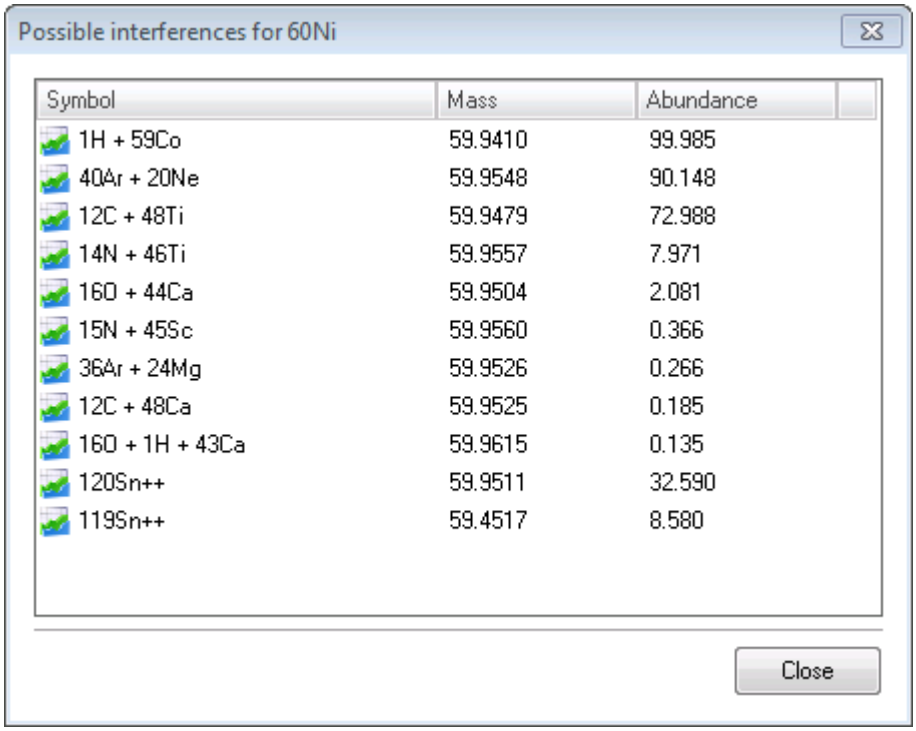
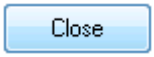


Figure 6-18. List of interferences

6. Click another **Identifier** in the Acquisition Parameters table.
   The list displays the interferences for the newly selected isotope.

7. Click 

.

❖ **To duplicate rows**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click  below the Method Parameters to open the **Acquisition Parameters** view in the Template.

5. Click the gray field in front of the row or rows you wish to duplicate to select the row or rows.
   This way, isotopes in one sample can be defined to be measured with different settings.

6. Right-click on the selected rows.
   A context menu opens, see Figure 6-19.

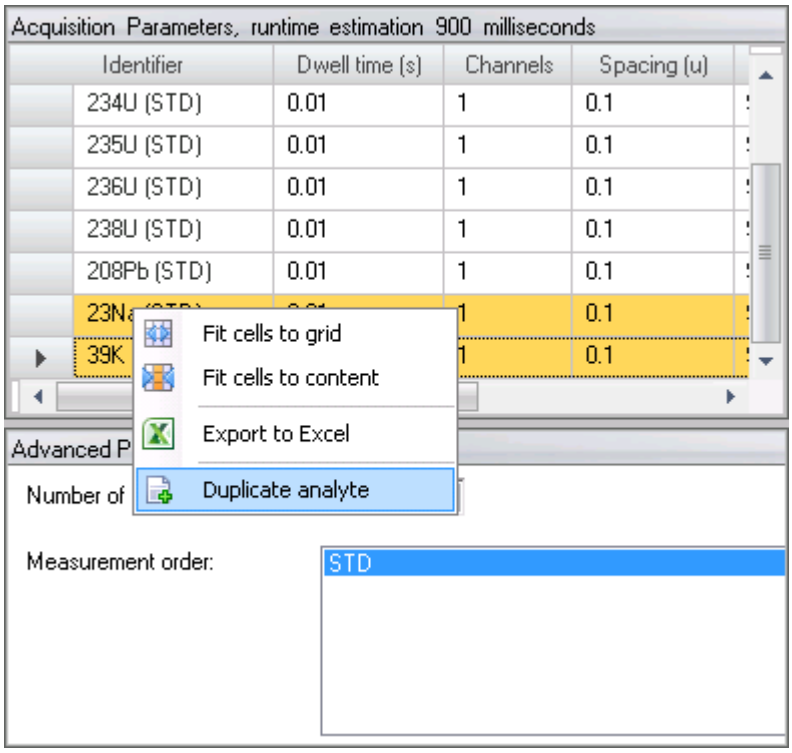


Figure 6-19. Duplicate rows of Acquisition Parameters

❖ **To define Acquisition Parameters**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click  below the Method Parameters to open the **Acquisition Parameters** view in the Template.
   The column Identifier lists all analytes selected.

5. Enter **Dwell time (s)**, **Channels** and **Spacing (u)** for each analyte, as appropriate.
   With a right-click on a cell you open the context menu. You can select, for example, **Fill down** or **Fill up**, as appropriate. Then the entries from the first selected cell are copied down or up to all cells selected.

6. In the section **Advanced Parameters**, enter the **Number of sweeps**.
   This option is not available for tQuant or trQuant Templates.

7. Select a **Measurement mode** for each analyte.
   The Measurement mode is displayed in brackets after the analyte in the column **Identifier**.
8. Select a **Resolution** from the drop-down list for each analyte.
9. Define the **Measurement order** if several modes were defined.
10. If appropriate, define the Trigger settings.
11. Click  to save the changes to your Template.

Exporting Analytes List

The list of analytes defined in the **Acquisition Parameters** view of a Template in Experiment Editor can be exported as .xls file to be opened in Microsoft™ Excel™.

❖ **To export the analytes list in Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  in the list of Method Parameters to open the **Acquisition Parameters** view in the Template.
5. In the **Acquisition Parameters** table, right-click inside a cell.
6. Select  **Export To Excel** in the context menu.
7. Browse for the correct file destination.
8. Type in a name for the .xls file.
9. Click **Save** to save the .xls file.

Monitor Analytes

For all Template types except tQuant and trQuant, the **Monitor Analytes** view of the Experiment Editor tool is available.

Delays for Uptake and Wash can be defined for the analytes added to the table, see Figure 6-20.

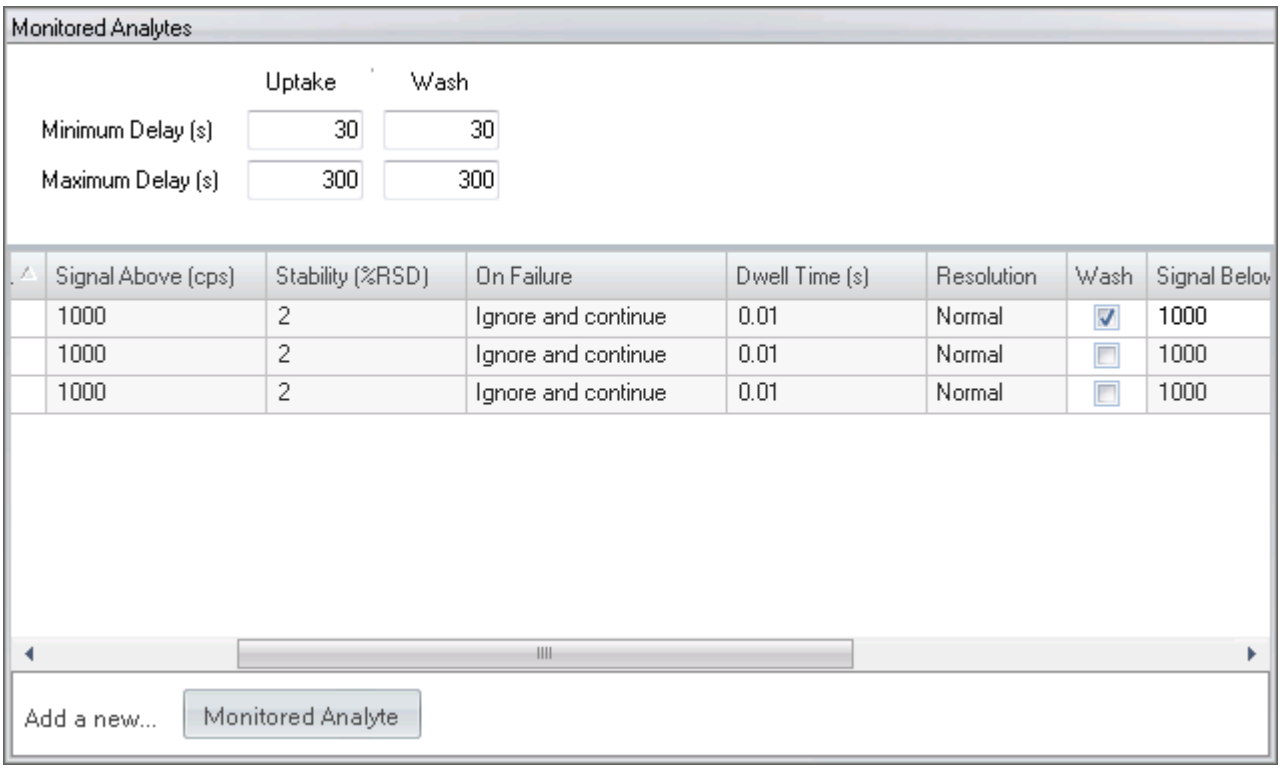


Figure 6-20. Monitored Analytes

The Monitor Analytes 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** procedure starts.

❖ **To open the Monitor Analytes view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Monitor Analytes** view.

❖ **To add an analyte to be monitored**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  in the list of Method Parameters to open the **Monitor Analytes** view in the Template.
5. Define the **Minimum Delay [s]** and **Maximum Delay [s]** for **Uptake** and **Wash**.
6. Click 

to add a row to the table.
7. Enter the analyte, for example, 43Ca.

NOTICE Analytes must be entered as shown in column Symbol of the isotope table (right-click) in the Analytes view. ▲

8. Define the parameters for this analyte.
9. Select the check boxes for **Uptake** and **Wash** to activate monitoring for the analyte.
10. For **Signal Above**, select **Ignore and continue** or **Skip this sample** from the drop-down menu **On Failure**.
11. For **Signal Below**, select **Ignore and continue** or **Abort LabBook** or **Abort queue** from the drop-down menu **On Failure**.
12. Click  to save the changes to your Template.

Survey Scan Settings

For all Template types except tQuant and trQuant, the **Survey scan settings** view in Experiment Editor shows the details of the scan region. A table lists the individual survey scan regions.

Above the table, the settings are displayed as **Scan Regions Graph** which is editable, see Figure 6-21.

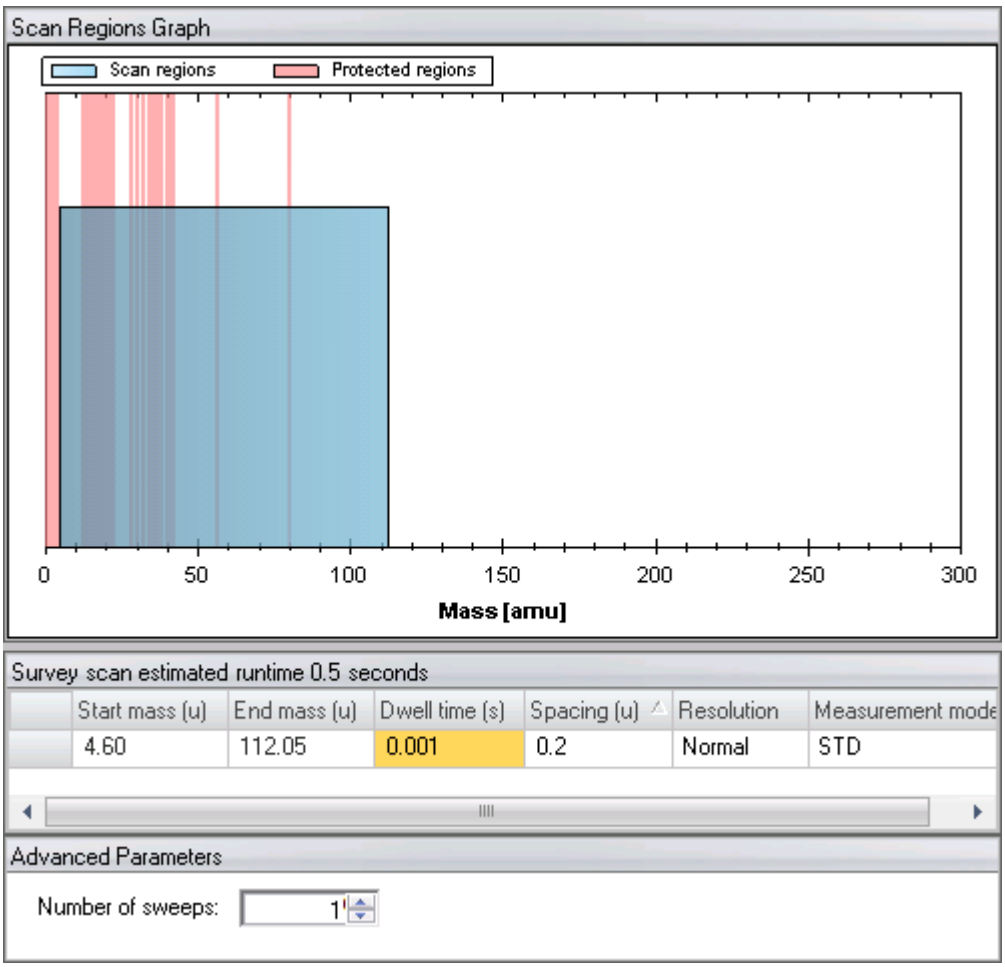


Figure 6-21. Survey Scan Settings view

Existing scan regions can be changed and defined, and new scan regions can be added. The parameters are summarized in Table 6-5.

Table 6-5. Survey can settings

Column	Description
Start mass	Start mass of a scanned region.
End mass	End mass of a scanned region.
Dwell time	Dwell time (in s) for each channel scanned.
Spacing	Spacing (in mass units) of the channels.
Resolution	Resolution setting of the quadrupole.
Measurement mode	Measurement mode to be used for the scanned region.
Advanced Parameters	Number of sweeps.

In the **Advanced Parameters** field at the bottom of the Acquisition Parameters view, the number of sweeps to be performed during one survey scan can be defined.

❖ **To open the Survey scan settings view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Survey scan settings** view.

❖ **To define scan regions**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  in the list of Method Parameters to open the **Survey scan settings** view in the Template.
5. Drag the scan region borders in the graphic above the table to define the **Start mass** and **End mass** of the scan region.
   The new values are immediately displayed in the table below.
6. Enter the desired values for **Dwell time** and **Spacing**.
7. Select **Normal** or **High** from the drop-down menu **Resolution**.
8. Select a **Measurement mode** from the drop-down menu.
9. Click  to save the changes to your Template.

❖ **To add a scan region**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  in the list of Method Parameters to open the **Survey scan settings** view in the Template.
5. Right-click in the graphic outside the scan region.
   A context menu opens, see Figure 6-22.

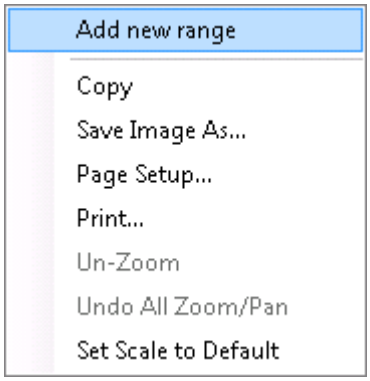


Figure 6-22. Survey Scan Settings context menu

   The context menu offers several items to copy, save, print, zoom and scale the graphic, and to add a new range.

6. Click **Add new range**.
   A new scan region is added to the graphic.
7. Drag the scan region borders in the graphic above the table to define the **Start mass** and **End mass** of the scan region.
   A new row is added to the table below and the values are displayed immediately.
8. Click  to save the changes to your Template.

❖ **To define the number of sweeps**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click  in the list of Method Parameters to open the **Survey scan settings** view in the Template.
5. In the **Advanced Parameters** section at the bottom, enter the **Number of sweeps** to be performed during one survey scan.
6. Click  to save the changes to your Template.

Interference Correction

For all Template types, the **Interference Correction** view in Experiment Editor allows you to enable mathematical interference correction for the analytes in the Template.

NOTICE Interference Correction must be enabled prior to running the measurement to be used to correct data. ▲

Elements selected for analysis in the **Analytes** view are listed in the Interference Correction view, see Figure 6-23.

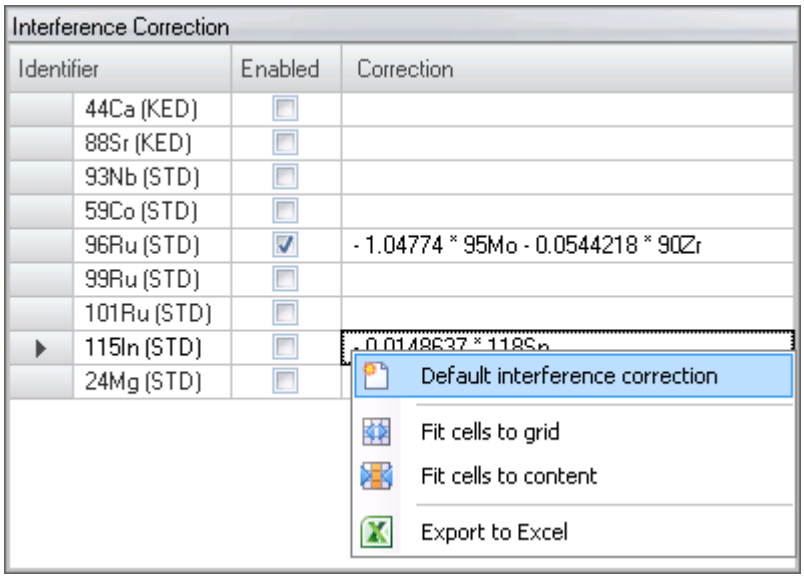


Figure 6-23. Interference Correction view

By default, isobaric interference corrections are displayed but not **Enabled**. Interference Correction can be activated individually for each analyte. The column **Corrections** allows you to enter equations for interference correction. The **Default interference correction** value for the analyte can be selected from the context-menu.

NOTICE Interference correction can always be edited or disabled during and after running a measurement. ▲

If the isotopes used in the interference correction equation are not part of the selected analytes, Qtegra uses the settings for the Identifier belonging to this equation in Interference Correction also for the isotope not listed.

❖ **To open the Interference correction view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Interference correction** view.

❖ **To select analytes for interference correction in Experiment Editor**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  in the list of Method Parameters to open the **Interference correction** view in the Template.
5. Select the **Enabled** check box next to the analyte to activate interference correction.
   By default, all analytes are disabled.
6. Right-click in the **Correction** cell to open the context menu and select **Default interference correction** from the context menu.
   The default formula defined for this isotope is added.
   You can also click in the cell **Correction** to enter the formula via the keyboard.
7. Define the interference correction for all analytes.
8. Click  to save the changes to your Template.

Standards

For all Template types, the **Standards** view in Experiment Editor allows you to define standards. 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 6-24.

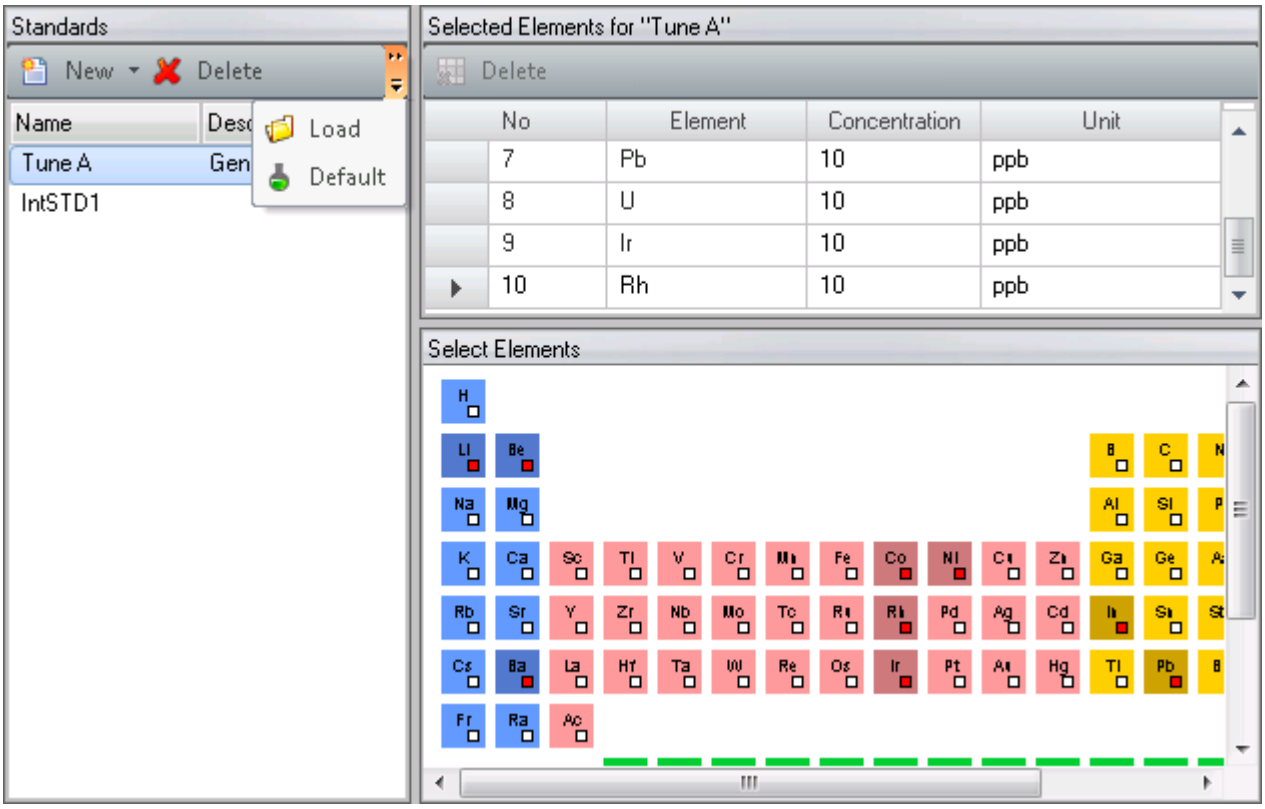


Figure 6-24. Standards view of a Template

For a tQuant Template, compound standards are defined that will subsequently be used to create compound-specific calibrations and compound-specific quantifications. You can create a compound standard from the compound list if you define the compounds first, see "Compounds (tQuant only)" on page 6-41.

The columns of the table above the periodic table define the properties of the elements, see Table 6-6.

Table 6-6. Specification of standard elements

Column	Description
No	Automatically assigned number in ascending order.
Element/Isotope/Compound	Displays the symbol for the chemical element contained in this standard file.

Table 6-6. Specification of standard elements

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 "Setting the Default Concentration" on page 6-38. 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, which has a similar mass and ionization potential to the analyte to be corrected and is at a concentration similar to the expected concentrations of analytes in the sample.
Unit	Displays the concentration unit for the element in the standard file. By default, the unit is set to *ppb*. This default can be changed and stored. See "Setting the Default Concentration" on page 6-38.

The commands of the **Standards** view of a Template are summarized in Table 6-7.

Table 6-7. Commands of the Standards view of a Template

Commands	Description
	To create a new standard (for eQuant and trQuant also Internal Standard).
	To delete the selected standard(s).
	To load all standards from the standard database.
	To edit the default concentration. The **Default Concentration** of the isotopes in the solutions is set to *10 ppb*.

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 (or less commonly enriched isotopes of an analyte). Internal standards are used to correct for instrumental drifts in sensitivity and sample specific signal suppression or enhancement.

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 6-117. When defining the calibration standards in that section, dilution factors can be applied to the standard.

Internal standards which are used for quantification are also created here. Their definition as internal standards is done in the **Quantification** view, see "Quantification" on page 6-62.

❖ **To open the Standards view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Standards** view.

Creating a New Standard

Standards created in the **Standards** view of a Template (or LabBook) in Experiment Editor are created for the current Template (or LabBook) but can be saved to the global database.

For eQuant and trQuant Templates, it is possible to create internal standards.

For rQuant Templates, isotope dilution standards can be created.

NOTICE Global database standards are created in the Configurator applet "Standard Editor" on page 3-35. ▲

❖ **To create a new standard**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Standards** view.

5. Click  to open the **Add New Standard** dialog.

6. For eQuant or trQuant Templates, click  to open the drop-down menu, see Figure 6-25.

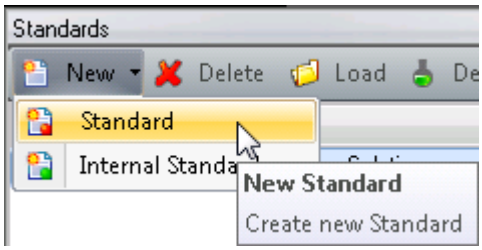


Figure 6-25. Creating a new standard

7. Click  **Standard** to open the **Add New Standard** dialog, see Figure 6-26.

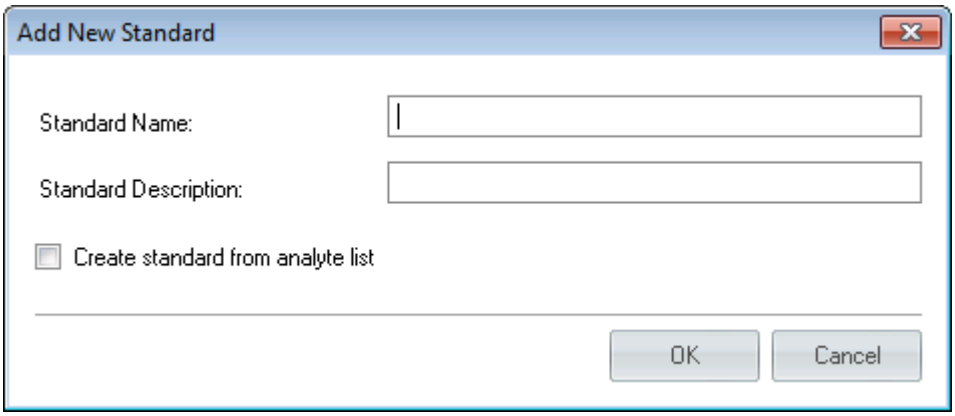


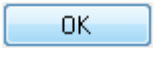
Figure 6-26. Add New Standard dialog

8. Enter the **Standard Name**.

9. Enter a **Standard Description**.

10. Select the check box **Create standard from analyte list** to create the standard from the list of analytes.

NOTICE For tQuant Templates, it is possible to create a new standard from the compound list as soon as the compounds have been defined. ▲

11. Click  .

12. Click elements in the periodic table to add or remove analytes.

13. Define the properties of the analytes as required.

14. Click to save the standard to your Template.

❖ **To create a new internal standard**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click to select the **Standards** view.
5. For eQuant or trQuant Templates, click New to open the drop-down menu, see Figure 6-25.

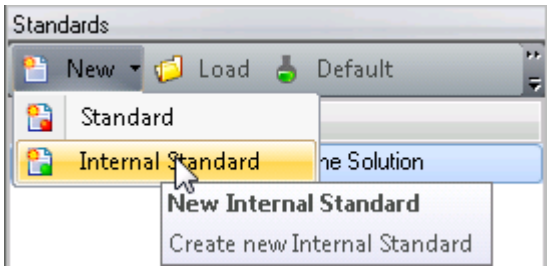


Figure 6-27. Creating a new internal standard

6. Click **Internal Standard** to open the **Add New Standard** dialog, see Figure 6-26.

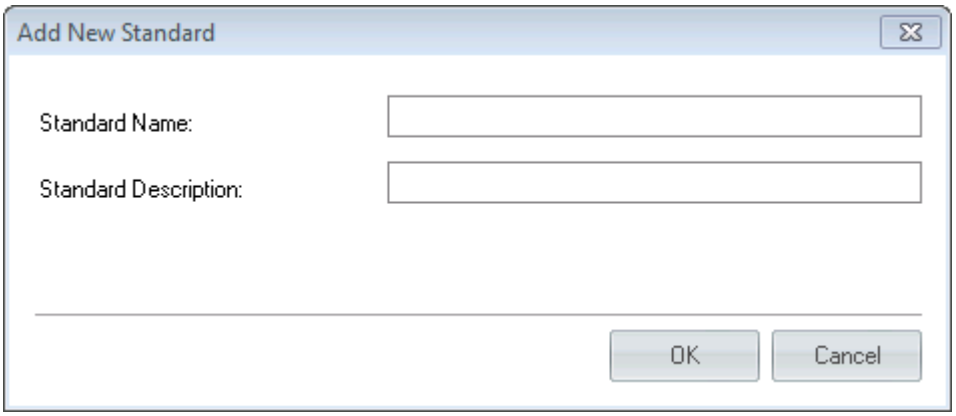


Figure 6-28. Add New Standard dialog for internal standards

7. Enter the **Standard Name**.
8. Enter a **Standard Description** for the new internal standard.

9. Click OK.
10. Click elements in the periodic table to add or remove analytes.
11. Define the properties of the analytes as required.
12. Click to save the internal standard to your Template.

❖ **To create a new isotope dilution standard**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation rQuant.
4. Click to select the **Standards** view.
5. Click New to open the **Add New Standard** dialog, see Figure 6-26.

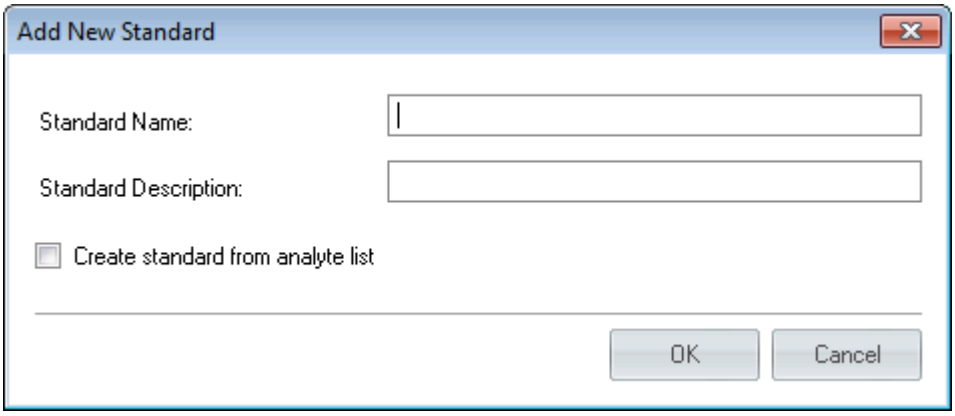


Figure 6-29. Add New Standard dialog

6. Enter the **Standard Name**.
7. Enter a **Standard Description**.
8. Select the check box **Create standard from analyte list** to create the standard from the list of analytes.
9. Click OK to add the file.
   The new isotope dilution standard is added to the list on the left. An

empty page opens containing the table columns **No**, **Element**, **Concentration**, **Unit**, **Isotope 1**, **Isotope 2**, **Abundance 1**, **Abundance 2** and **Atomic Weight**, and the periodic table of elements with all available isotope information.

10. Click elements in the periodic table to add or remove analytes.
11. Select the isotope of interest from the drop-down list of column **Isotope 1**.
12. Select the isotope of interest from the drop-down list of column **Isotope 2**.
13. Define the properties of the analytes as required.
14. Click  to save the isotope dilution standard to your Template.

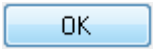
Loading a Standard from the Global Database

It is possible to load global standards created in the Configurator tool to your Template in Experiment Editor.

❖ **To load a standard from the global database**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Standards** view.
5. In the **Standards** view, click 

to open the **Load Standard** dialog.
6. Select a file from the list and click 

or double-click to load the file.
The selected file is loaded to the **Standards** view.

Setting the Default Concentration

For each Template in Experiment Editor, a default concentration for the standards can be defined.

❖ **To set the default concentration**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Standards** view.
5. In the **Standards** view, click 

to open the **Set Default Concentration** dialog, see Figure 6-30.

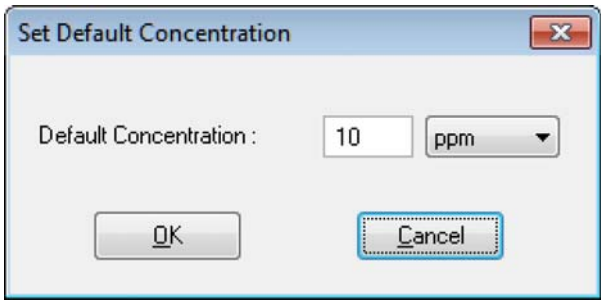


Figure 6-30. Set Default Concentration dialog

6. Enter the new **Default Concentration**.
7. Click  to display the list of unit.
8. Select a unit from the list and click 

.
This default concentration is used for each new analyte added to the table.
9. Click  to save this default concentration to your Template.

Editing an Existing Standard File

Existing standards can be edited and saved to your Template in Experiment Editor.

❖ **To edit an existing standard file**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Standards** view.
5. In the **Standards** view, click the standard to be edited.
6. If required, change the default concentration 

.
7. Click the elements in the periodic table to add or remove analytes.
8. Click  to save your Template.

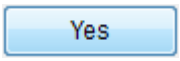
Deleting a Standard

Standards can be deleted from a Template in Experiment Editor.

❖ **To delete a standard**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Standards** view.
5. In the **Standards** view, click the standard to be deleted.
6. Click 

to delete the standard.
7. Click 

to confirm the message dialog.
8. Click  to save your Template.
The standard is deleted from the Template.

Saving a Standard to the Global Database

Standards that have been created in your Template in Experiment Editor can be transferred to the global database.

❖ **To save a standard to the global database**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Standards** view.
5. In the **Standards** view, right-click the standard to be saved to the global database to open the context menu, see Figure 6-31.

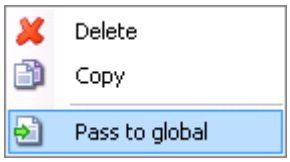


Figure 6-31. Standard context menu

6. Select **Pass to global**.
   The standard is saved to the global database.

Compounds (tQuant only)

The **Compounds** view of a tQuant Template in Experiment Editor allows you to define compounds for the measurement.

Once **Internal Standardization** is activated in the **Compounds** view, you can define compounds as Internal Standard, see Figure 6-32.

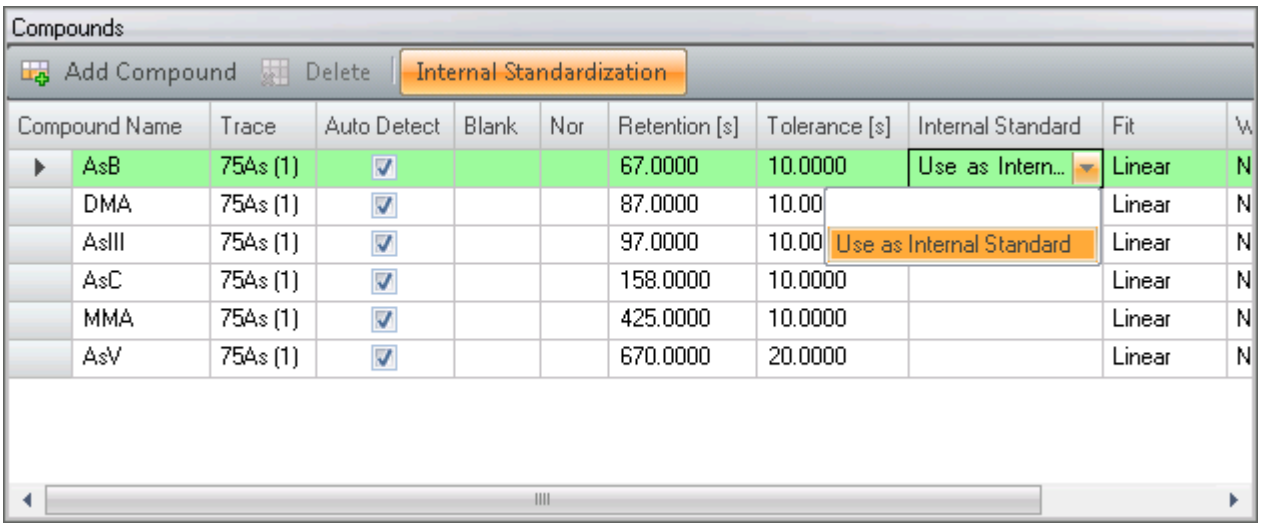


Figure 6-32. Compounds view for tQuant

The columns that define the properties of the Compounds are listed in Table 6-8.

Table 6-8. Columns to define Compounds in tQuant Templates

Column	Description
Internal Standardization	Activates the column **Internal Standard**.
Compound Name	Identifier automatically assigned with continuous number. Identifier can be changed.
Trace	Analyte (isotope) trace used for the compound defined in the row. The drop-down list includes all isotopes selected in the Analytes view.
Auto Detect	Automatically searches for peaks and applies properties as defined in "Peak Detection (tQuant only)" on page 6-44.
Blank	Compound area in the chromatogram to be subtracted from all other compounds.
Normalize Trace	Normalization of the compound trace with another analyte (continuous internal standard correction). The trace used for Normalization can only be selected here if defined in the Analytes list.
Retention [s]	Expected retention time of the compound.
Tolerance [s]	Search window for the compound; compound retention time +/- Tolerance/2.
Internal Standard	Defined compounds can be selected as Internal Standards for correction purposes. If **Use as Internal Standard** is selected from the drop-down list, the background color of this row changes to green when you click in another cell. In the rows of the other compounds, the defined Internal Standard can then be selected from the drop-down list in all cells of this column.

Table 6-8. Columns to define Compounds in tQuant Templates

Column	Description
Fit	By default the calibration fit is set to **Linear**. All concentration calibrations should be linear with the signal response in the iCAP Q instrument.
	In the rare case that a non-linear calibration is acquired, you can define a **2nd Order** calibration fit.
Weighting	By default set to **None**.
	If **Absolute SD** is selected, absolute standard deviation is used to weight the signals.
	If **Relative SD** is selected, relative standard derivation is used to weight the signals.
Forcing	By default set to **No**. If set, defines whether the calibration curve should be forced through the blank value (**Blank**) or through the origin of the coordinate system (**Zero**).

❖ **To open the Compounds view of a Template**

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation tQuant.
4. Click  to select the **Compounds** view.

❖ **To define compounds**

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Compounds** view in the Template.
5. Click 

to add a line to the table.

6. Enter a name for the compound in the column **Compound Name**.
7. Select a **Trace** for the compound from the drop-down list.
   The check box for **Auto Detect** is selected by default.
8. Enter an expected **Retention Time** if it is known.
   This can also be performed once the chromatogram has been acquired or when the LabBook is still running.
9. Modify the default settings of the other columns if desired.
10. Click  to save your Template.

❖ **To activate Internal Standardization**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to select the **Compounds** view in the Template.
5. Click 

.
   Internal Standardization is activated.
6. In the row of a compound, select **Use as Internal Standard** from the drop-down menu for the column **Internal Standard**.
7. In the rows of the other compounds, select the defined Internal Standard from the drop-down list in all cells of this column **Internal Standard**.
8. Click  to save your Template.

Peak Detection (tQuant only)

For tQuant Templates only, the **Peak Detection** view in Experiment Editor allows you to define Peak Detection and Integration Algorithms for compounds to specify the content of an analyte. Furthermore, you have the option to smooth the obtained chromatograms.

Peak detection is applied to compounds if the check box **Auto Detect** is selected for the compound in "Compounds (tQuant only)" on page 6-41. The same peak detection properties are applied to all compounds.

Smoothing, Peak Detection and Peak Filter parameters (see Figure 6-33) can be defined.

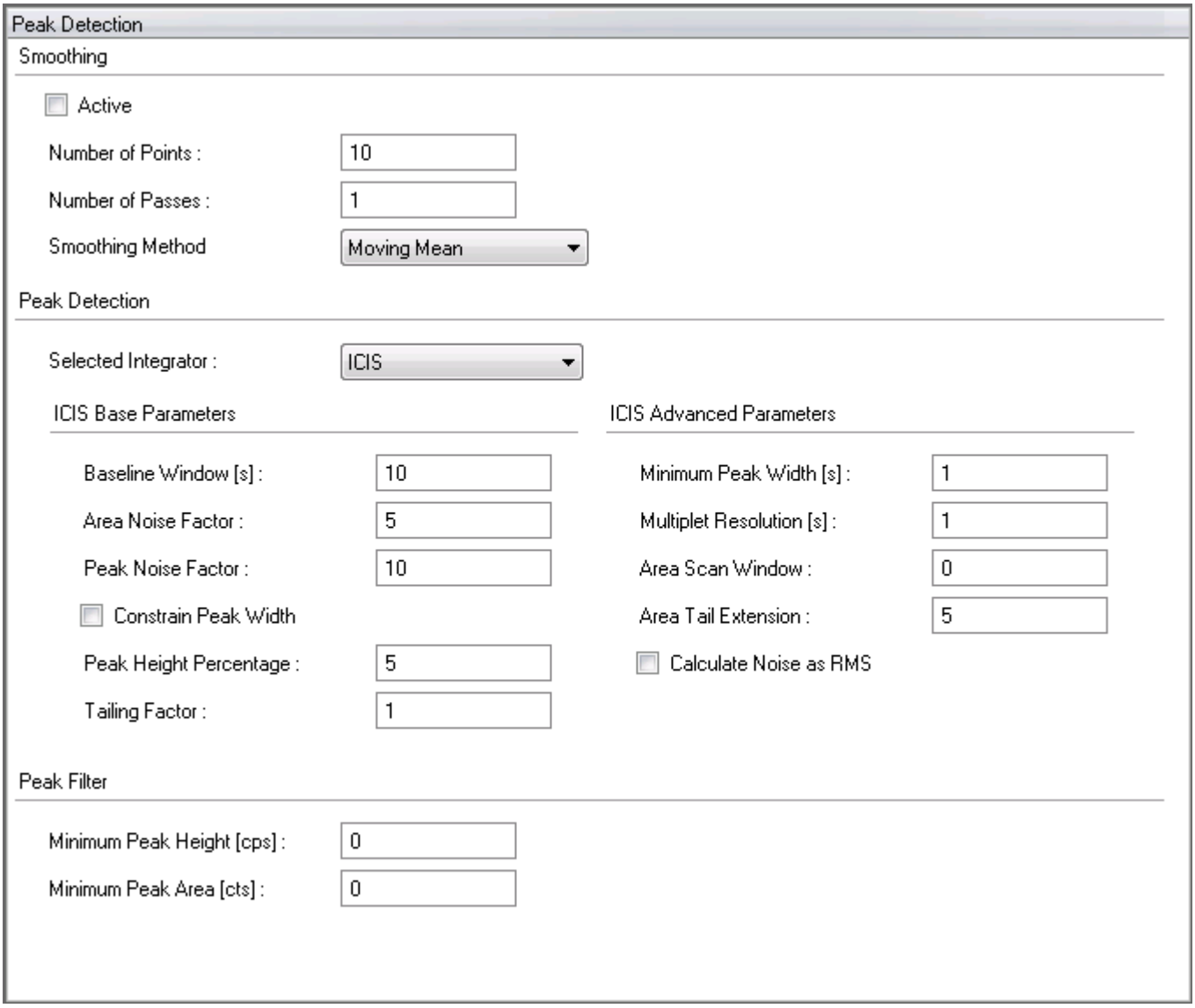


Figure 6-33. Peak Detection for tQuant

NOTICE If you do not wish to define Peak Detection, select **None** from the drop-down list **Selected Integrator**. ▲

NOTICE All settings except instrument scan dependent parameters can still be changed after measurement. ▲

❖ **To open the Peak Detection view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation tQuant.
4. Click  to select the **Peak Detection** view.

❖ **To define Smoothing in Peak Detection**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation tQuant.
4. Click  to select the **Peak Detection** view in the Template.
5. For **Smoothing**, select the check box **Active** to activate **Smoothing**.
The smoothing settings are applied to the traces.
6. Enter the **Number of Points**.
Determines the number of points to be used to calculate the average value.
7. Enter the **Number of Passes**.
Number of times the smoothing algorithm is run.
8. Select the **Smoothing Method** from the drop-down menu.
Mainly used is the smoothing method **Moving Mean** which uses the rolling average of the given number of points.
9. Click  to save your Template.

❖ **To define peak filter parameters**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation tQuant.
4. Click  to select the **Peak Detection** view in the Template.
5. For **Peak Filter**, enter the **Minimum Peak Height [cps]**.
   Only peaks that meet this condition are automatically integrated.
6. For **Peak Filter**, enter the **Minimum Peak Area [cts]**.
   Only peaks that meet this condition are automatically integrated.
7. Click  to save your Template.

Defining ICIS Peak Detection Parameters

Peak integration and detection criteria for the ICIS (Interactive Chemical Information System) peak detection algorithm are defined in the **Peak Detection** view of a Template in Experiment Editor.

❖ **To define ICIS Peak Detection parameters**

1. Click 

   to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation tQuant.
4. Click  to select the **Peak Detection** view in the Template.
5. For **Peak Detection**, select **ICIS** from the drop-down list **Selected Integrator**.

The parameters for the ICIS integrator are displayed, see Figure 6-34.

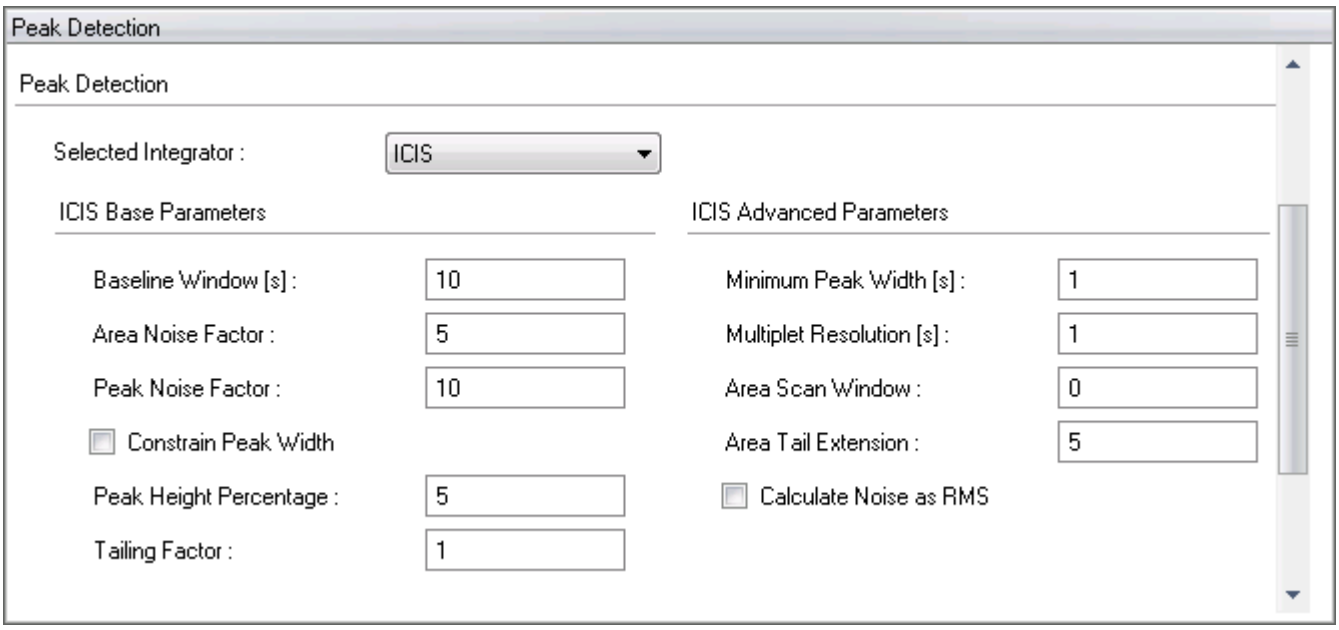


Figure 6-34. Peak Detection Integrator ICIS

6. For **ICIS Base Parameters**, enter the value for **Baseline Window [s]** to review for a local minima.

7. Enter the value for **Area Noise Factor** to determine the peak edge after the location of the possible peak.
   Valid range is *1* to *500*.

8. Enter the **Peak Noise Factor** to determine the potential peak signal threshold.
   Valid range is *1* to *1000*.

9. Select the check box **Constrain Peak Width** to limit the peak width of a component during peak integration of a chromatogram according to the values set for Peak Height Percentage and Tailing Factor.

10. Enter the **Peak Height Percentage**.
    The signal value must reach the given percentage above the baseline before integration is turned on.

11. Enter the **Tailing Factor** to control how the tail of the peak is integrated.
    This factor is the maximum ratio of the tailing edge to the leading side of a constrained peak.

12. For **ICIS Advanced Parameters**, enter the **Minimum Peak Width [s]**.

13. Enter the **Multiplet Resolution [s]**.
    This is the minimum separation between the apexes of two potential peaks and is used as a criterion for the separation.

14. Enter the value for **Area Scan Window**.
    Enter the time on each side of the peak apex to be included in the area integration. The valid range is *0* to *100* s. A value of *0* s specifies that all scans from peak start to peak end are to be included in the area integration.

15. Enter the value for **Area Tail Extension**.
    Type the time past the peak endpoint to use in averaging the intensity. The valid range is *0* to *100* s.

16. Select the check box **Calculate Noise as RMS** if you wish to calculate the noise according to the root mean square method.

17. Click  to save your Template.

Defining PPD Peak Detection Parameters

Peak integration and detection criteria for the PPD (parameter-less peak detection) peak detection algorithm are defined in the **Peak Detection** view of a Template in Experiment Editor without the need of entering additional parameters.

❖ **To define PPD Peak Detection parameters**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation tQuant.

4. Click  to select the **Peak Detection** view in the Template.

5. For **Peak Detection**, select **PPD** from the drop-down list **Selected Integrator**, see Figure 6-35.

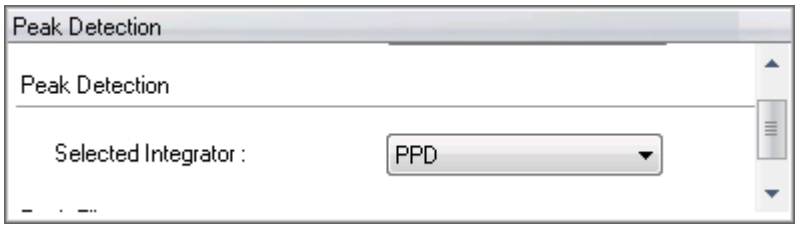


Figure 6-35. Peak Detection Integrator PPD

6. Click to save your Template.

Defining Avalon Peak Detection Parameters

Peak integration and detection criteria for the Avalon peak detection algorithm are defined in the **Peak Detection** view of a Template in Experiment Editor. This peak detection algorithm that has been designed for chromatographic data and is also used for detectors other than MS.

❖ **To define Avalon Peak Detection parameters**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation tQuant.
4. Click to select the **Peak Detection** view in the Template.
5. For **Peak Detection**, select **Avalon** from the drop-down list **Selected Integrator**.
   The parameters for the Avalon integrator are displayed, see

Figure 6-36.

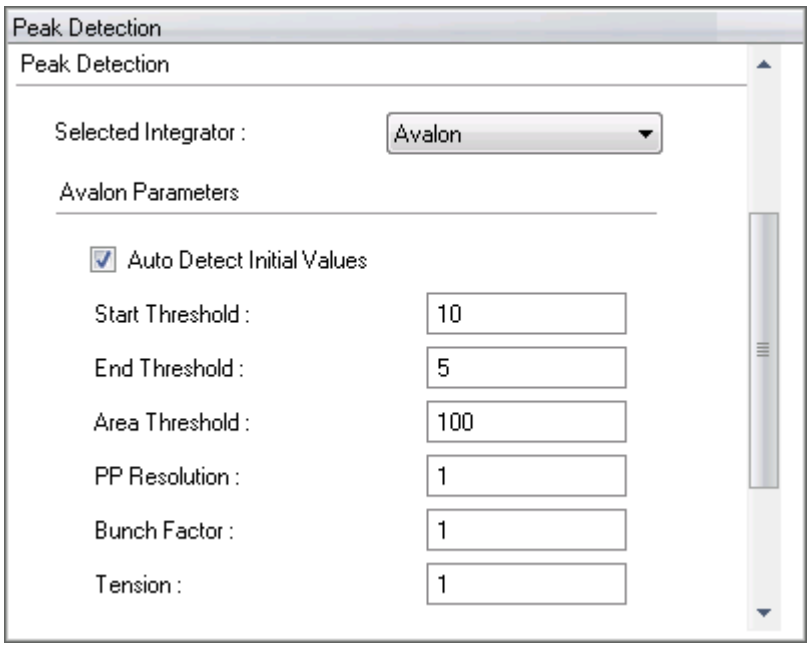


Figure 6-36. Peak Detection Integrator Avalon

6. Select the check box **Auto Detect Initial Values**.
   Searches for the best values of initial events that detect peaks in the data. When you select this check box, Avalon automatically estimates the initial values for the detection of peaks based on the data.

7. Enter the value for **Start Threshold** and **End Threshold**.
   Directly related to the RMS noise in the chromatogram, these values control the fundamental peak detection.

8. Enter the value for **Area Threshold**.
   Controls the area cutoff. Avalon does not detect any peaks with a final area less than the area threshold.

9. Enter the value for **PP Resolution**.
   The peak to peak resolution threshold controls how much peak overlap must be present before two or more adjacent peaks create a peak cluster. Peak clusters have a baseline drop instead of valley to valley baselines. This option is specified as a percent of peak height overlap.

10. Enter the value for **Bunch Factor**.
    The Bunch Factor is the number of points grouped together during peak detection. It controls the bunching of chromatographic points during integration and does not affect the final area calculation of the peak. The Bunch Factor must be an integer between *1* and *6*. A high bunch factor groups peaks into clusters.

11. Enter the value for **Tension**.
    Controls how closely the baseline should follow the overall shape of the chromatogram. A lower tension traces the baseline to follow changes in the chromatogram more closely. A high baseline tension follows the baseline less closely over longer time intervals.

12. Click  to save your Template.

Defining Genesis Peak Detection Parameters

Peak integration and detection criteria for the Genesis peak detection algorithm are defined in the **Peak Detection** view of a Template in Experiment Editor.

❖ **To define Genesis Peak Detection parameters**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation tQuant.

4. Click  to select the **Peak Detection** view in the Template.

5. For **Peak Detection**, select **Genesis** from the drop-down list **Selected Integrator**.

The parameters for the Genesis integrator are displayed, see Figure 6-37.

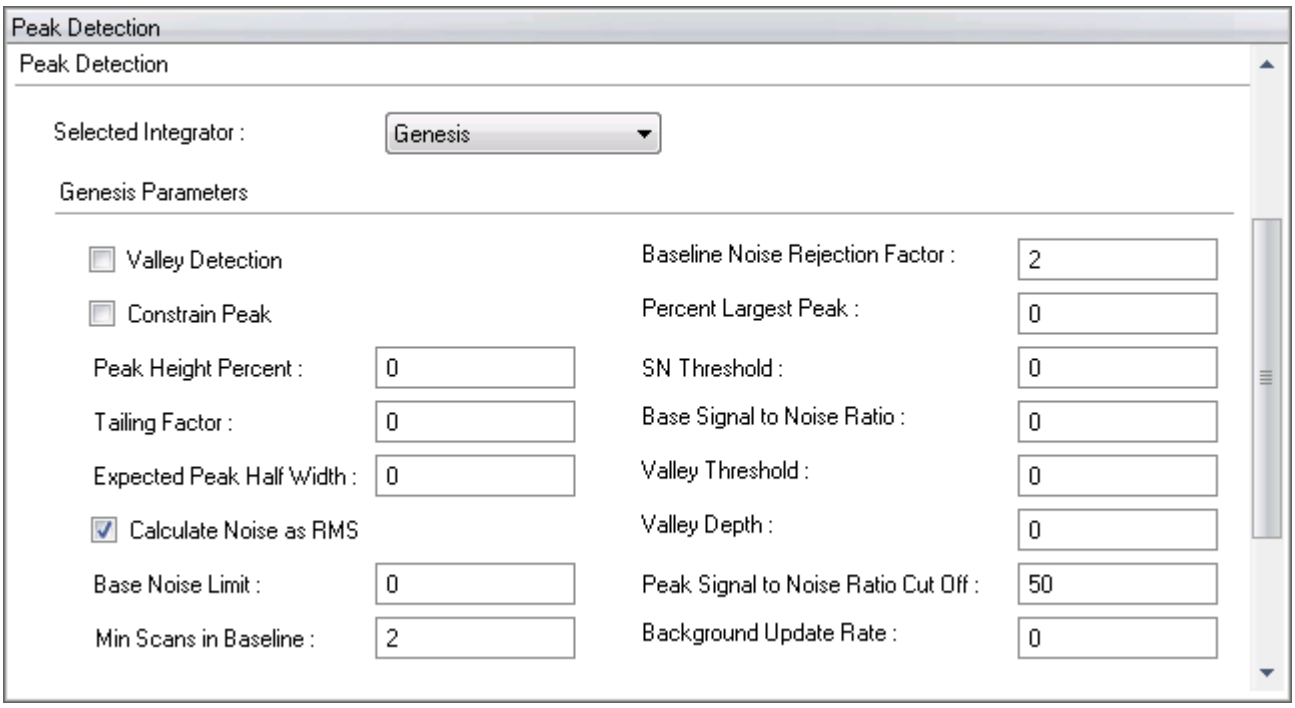


Figure 6-37. Peak Detection Integrator Genesis

6. Select the check box **Valley Detection**.
   Choose the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.

7. Select the check box **Constrain Peak** to limit the peak width of a component during peak integration of a chromatogram according to the values set for Peak Height Percentage and Tailing Factor.

8. Enter the **Peak Height Percent**.
   The signal value must reach the given percentage above the baseline before integration is turned on.

9. Enter the **Tailing Factor** to control how the tail of the peak is integrated.
   This factor is the maximum ratio of the tailing edge to the leading side of a constrained peak.

10. Enter the value for **Expected Peak Half Width**.
    This controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the [expected width]/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the peak is automatically terminated at that point.

11. Select the check box **Calculate Noise as RMS** if you wish to calculate the noise according to the root mean square method.

12. Enter the value for **Base Noise Limit**.
    This is the parameter that controls how the baseline is drawn in the noise data. The higher the baseline noise limit value, the higher the baseline is drawn through the noise data. The valid range is *0.0* to *100.0*.

13. Enter the value for **Min Scans in Baseline**.
    This parameter is used to calculate a baseline. A larger number includes more data in determining an averaged baseline. The valid range is *2* to *100.0*.

14. Enter the value for **Baseline Noise Rejection Factor**.
    This factor controls the width of the RMS noise band above and below the peak detection baseline. This factor is applied to the raw RMS noise values to raise the effective RMS noise used by the software during peak detection. Qtegra responds by assigning the left and right peak boundaries above the noise and therefore closer to the peak apex value in seconds. This action effectively raises the peak integration baseline above the RMS noise level. The valid range of this factor is *0.1* to *10.0*.

15. Enter the value for **Percent Largest Peak**.
    This limits the number of peaks submitted for further processing. Qtegra discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.

16. Enter the value for **SN Threshold**.
    The default value is *0.5* and the valid range is *0.0* to *999.0*. Qtegra calculates the signal-to-noise ratio using only the baseline signal. Any extraneous, minor, detected peaks are excluded from the calculation.

17. Enter the value for **Base Signal to Noise Ratio**.

18. Enter the value for **Valley Threshold**.

19. Enter the value for **Valley Depth**.

20. Enter the value for **Peak Signal to Noise Ratio Cut Off**.
    Qtegra defines this signal-to-noise level as the top of the peak edge. For example, if the signal-to-noise at the apex is *500* and the Peak S/N Cutoff value is *200*, Qtegra will define the right and left edges of the peak when the S/N reaches a value less than *200*. The valid range is *50.0* to *10000.0*.

21. Enter the value for **Background Update Rate**.
    Qtegra periodically recalculates the representative background signal it uses for background subtraction. This is to compensate for the possibility that the height of the background might change over the

course of a run. The Background Update Rate is the time interval in minutes between these recalculations. The valid range is *0.5* to *10.0* min.

22. Click  to save your Template.

Parameters

For rQuant and trQuant Templates, the **Parameters** view in Experiment Editor is provided to specify further settings.

For trQuant Templates, the Parameters view (see Figure 6-38) shows a table with the analytes defined for this Template.

Parameters

Internal Standardization active

Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing	Use for SemiQuant
137Ba	STD	Yes		Linear	None	Blank	Yes
223Ra	STD	Yes		Linear	None	Blank	Yes
223Fr	STD	Yes		Linear	None	Blank	Yes

Figure 6-38. Parameters for trQuant

For rQuant Templates, the Parameters view lists the selected isotopes and their natural abundances, see Figure 6-39.

Parameters

No	Element	Isotope 1	Isotope 2	Abundance 1	Abundance 2	Atomic Weight
1	Cu	63Cu	65Cu	69.17	30.83	63.5456
2	Hf	174Hf	178Hf	0.162	27.297	178.4864
3	Sn	114Sn	118Sn	0.65	24.22	118.7102
4	Ni	58Ni	61Ni	68.27	1.13	58.6878
5	Fe	54Fe	56Fe	5.8	91.72	55.8468

Figure 6-39. Parameters for rQuant Template with isotopes and their abundance

The values included in this table contain the natural isotopic abundances of the measured elements.

❖ **To open the Parameters view**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation rQuant or trQuant.
4. Click  to select the **Parameters** view of the Template.

❖ **To activate and define Internal Standardization for trQuant Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation trQuant.
4. Click  to select the **Parameters** view in the Template.
5. Select the check box **Internal Standardization active**.
6. In the column **Internal Standard**, select **Use as Internal Standard** from the drop-down list, see Figure 6-40.

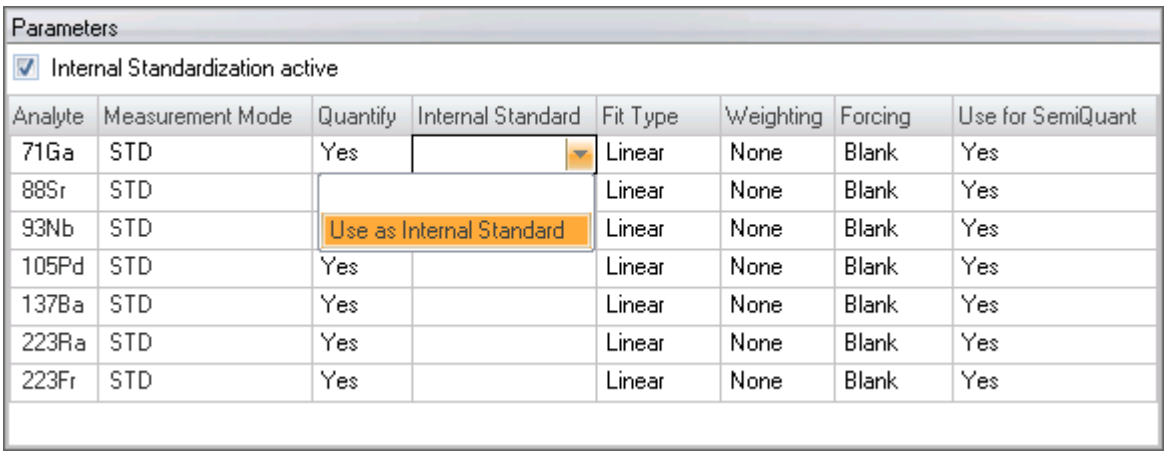


Figure 6-40. Parameters for trQuant Template with drop-down Internal Standard

The value for **Quantify** is set to **No** and the color of the entire row changes to green, see Figure 6-41.

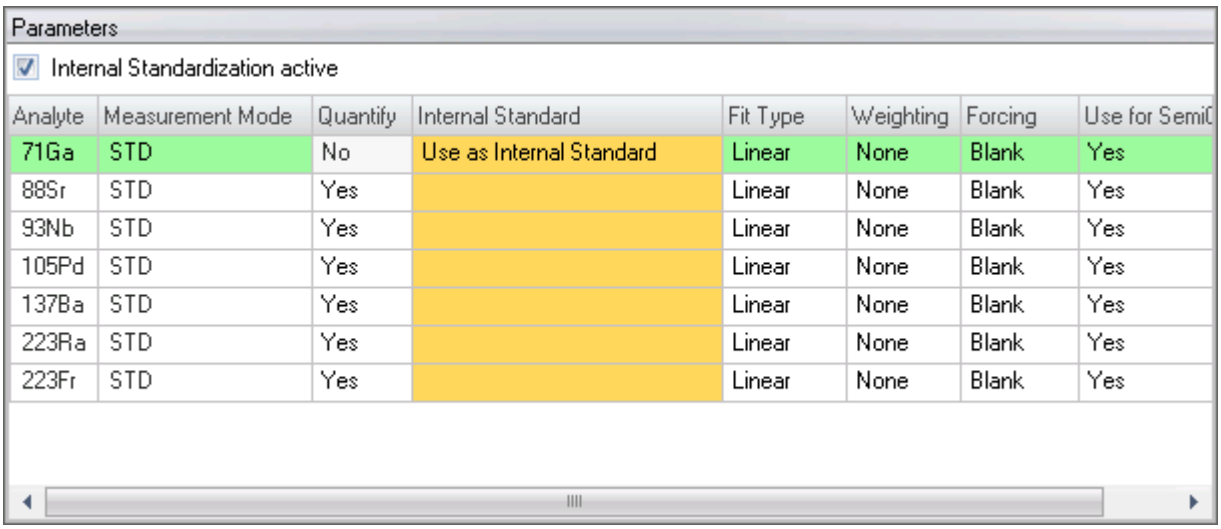


Figure 6-41. Parameters for trQuant Template with defined Internal Standard

7. Select a value for **Fit Type** from the drop-down list, see Figure 6-42.

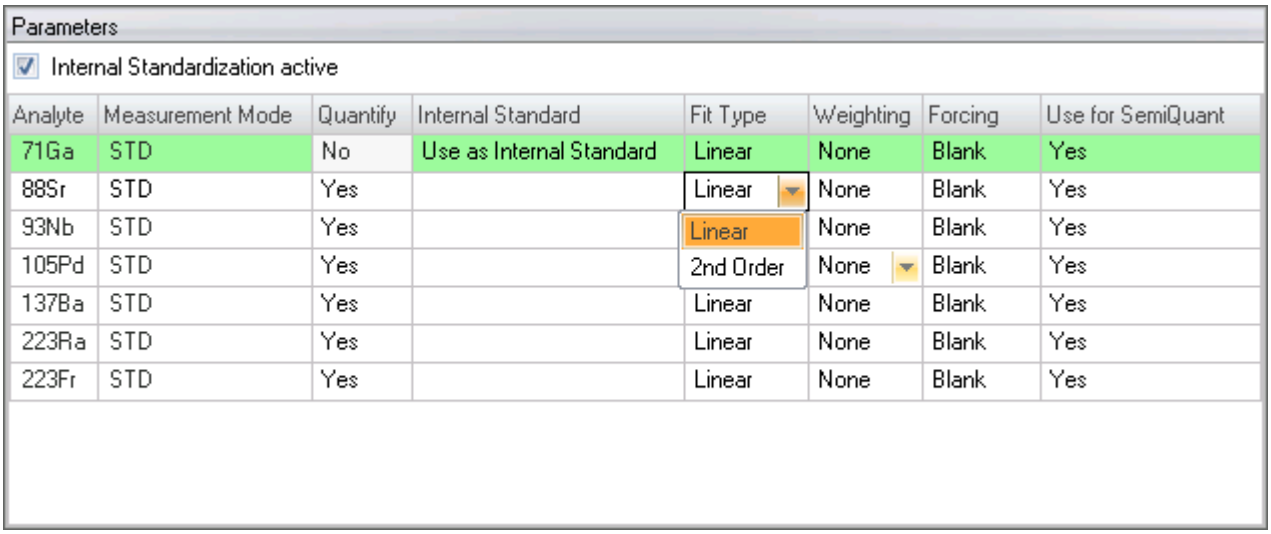


Figure 6-42. Parameters for trQuant Template drop-down Fit Type

8. Select a value for **Weighting** from the drop-down list, Figure 6-43 Figure 6-37.

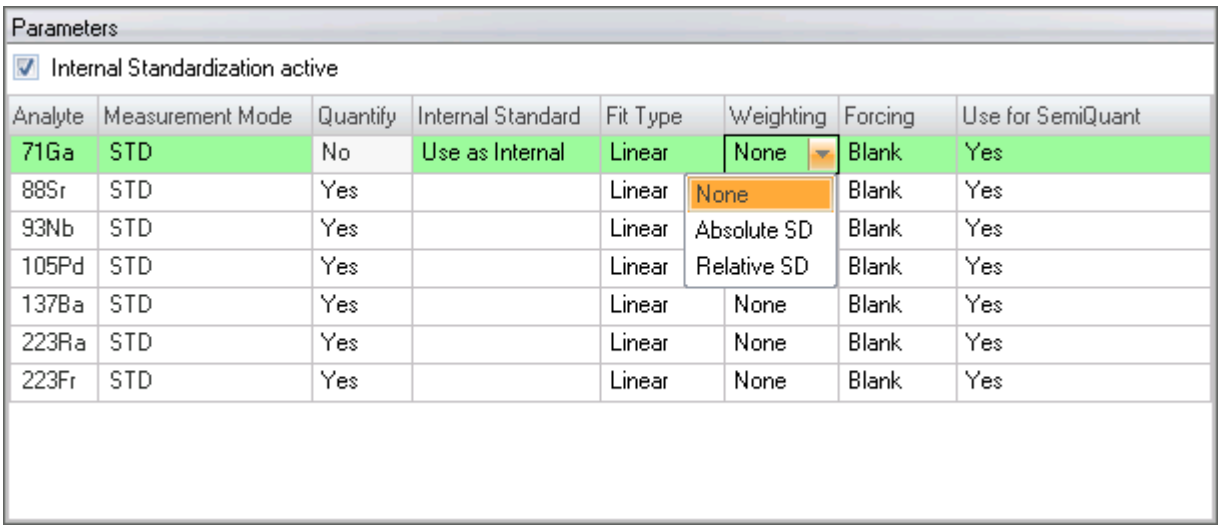


Figure 6-43. Parameters for trQuant Template drop-down Weighting

9. Select a value for **Forcing** from the drop-down list, see Figure 6-44.

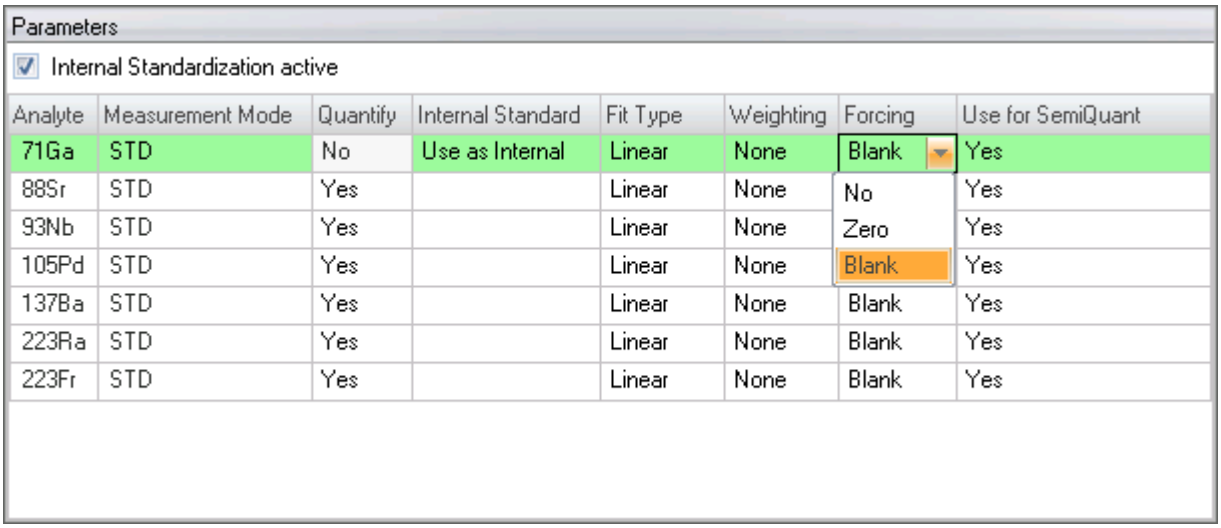


Figure 6-44. Parameters for trQuant Template drop-down Forcing

10. Select a value for **Use for SemiQuant** from the drop-down list, see Figure 6-45.

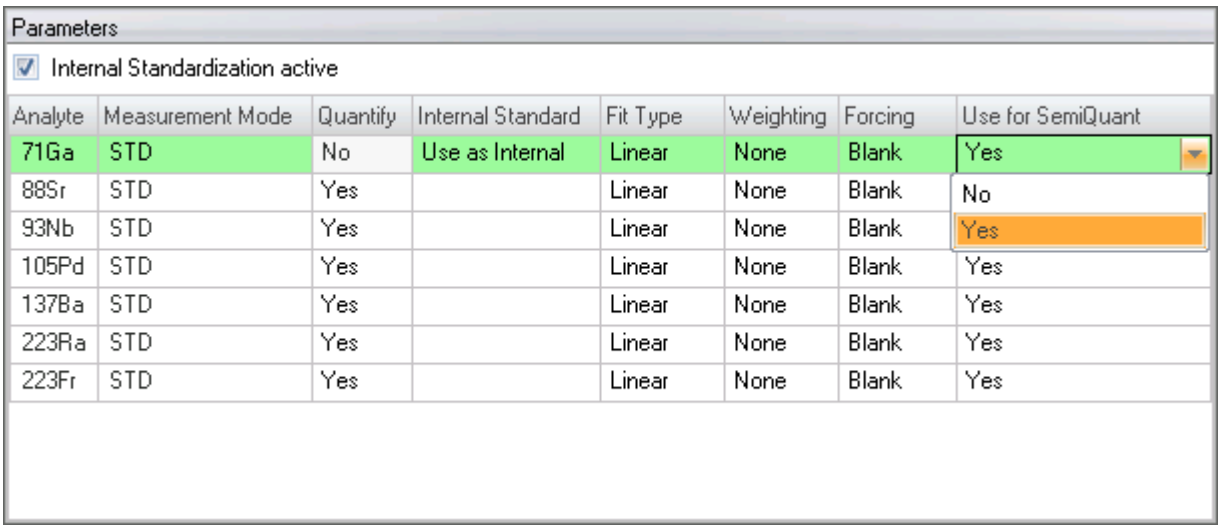


Figure 6-45. Parameters for trQuant Template drop-down Use for SemiQuant

11. Click to save your Template.

❖ **To define isotopes in rQuant Template**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation rQuant.
4. Click to select the **Parameters** view in the Template.

5. For each element row, select a value for **Isotope 1** from the drop-down list, see Figure 6-46.

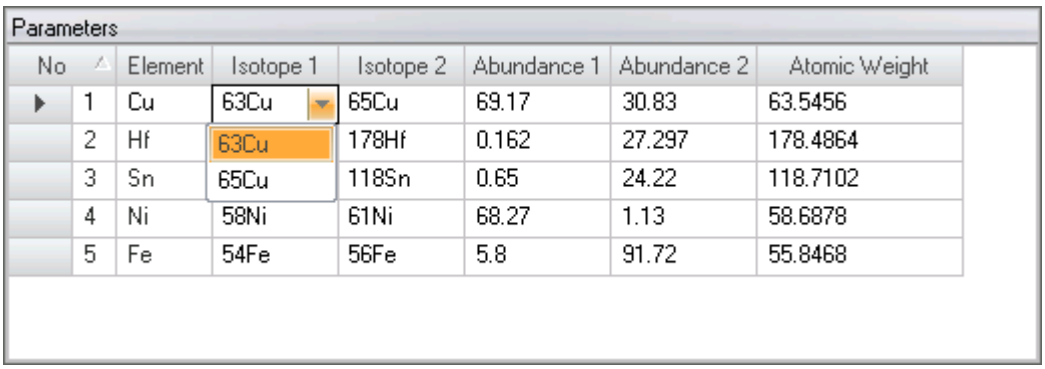


Figure 6-46. Parameters for rQuant Template drop-down Isotope 1

6. For each element row, select a value for **Isotope 2** from the drop-down list, see Figure 6-47.

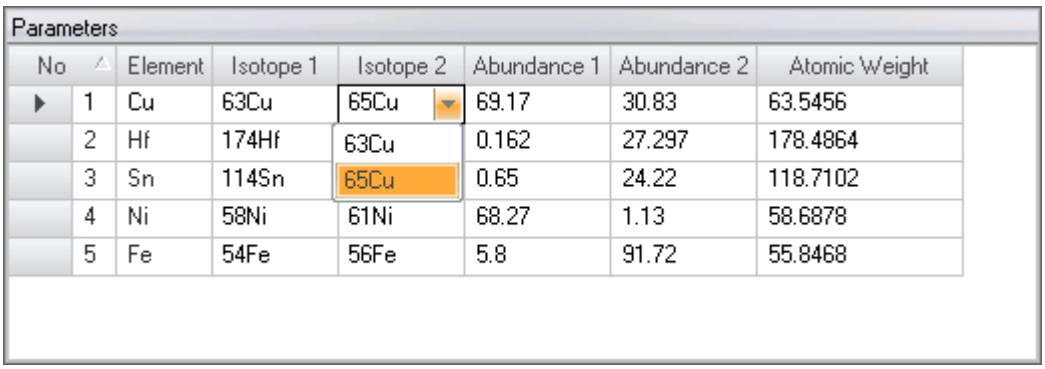


Figure 6-47. Parameters for rQuant Template drop-down Isotope 2

7. Click to save your Template.

Regions (trQuant only)

For trQuant Templates only, with the **Regions** view in the Experiment Editor tool you can define different time windows for certain regions of interest whose averaged signal is used for the subsequent data evaluation. Different time windows can be defined for regions like *gas blank* or *ablation* in experiments dealing with, for example, a coupling to a laser ablation system.

The Regions view (see Figure 6-48) allows you to define regions.

Regions

Region name	Blank name	Start (s)	End (s)	Quantify
region1		10.0000	30.0000	☐
region2		40.0000	80.0000	☑

Figure 6-48. Regions for trQuant

❖ **To open the Regions view**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation trQuant.
4. Click  to select the **Regions** view in the Template.

❖ **To add a row to the Regions table**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation trQuant.
4. Click  to select the **Regions** view in the Template.
5. Click 

in the Toolbar of the Template to add a row to the table.
6. Click in the cell **Region name** and enter a name.
7. Select a region for **Blank name** if appropriate.
The averaged signal of the selected region will be subtracted from the corresponding region in Region name.

8. Select the check box **Quantify** if appropriate.
9. Adjust the settings in each row as appropriate.
10. Click  to save your Template.

Quantification

The **Quantification** view of a eQuant or aQuant Template in the Experiment Editor tool 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 6-49.

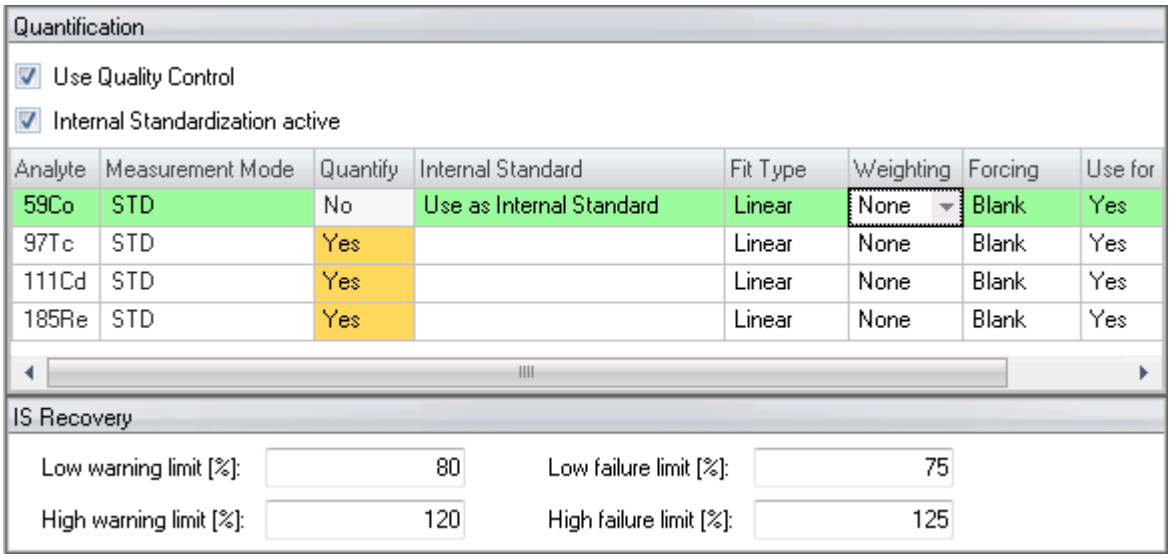


Figure 6-49. Quantification for eQuant and aQuant

The check box **Use Quality Control** is only available for eQuant Templates and enables the Quality Control Method Parameter of Qtegra, see "Quality Control (eQuant only)" on page 6-69.

The check box **Internal Standardization active** in the Quantification view must be selected if you wish to set internal standards for the measurement.

If an internal standard is used, warning limits and failure limits of its recovery in percent can be entered into the fields of the **IS Recovery** pane at the bottom of the page. This Internal Standard Test can also be found on the Quality Control page, see "Internal Standard Test" on page 6-77.

The parameters that can be defined for the Quantification table are summarized in Table 6-9.

Table 6-9. Parameters of Quantification table

Column	Description
Analyte	Displays analytes selected in the analytes view (see "Analytes" on page 6-15). 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 isotopes. **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 6-15.
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 isotope desired. If **Use as Internal standard** is selected, this row is shown with a green background.
	Use Interpolation enables a linear regression between two enshrouding internal standards that corrects the observed intensity of the analyte. If only one internal standard was chosen, Qtegra automatically selects the internal standard with the mass closest to the analyte.
Fit Type	By default the calibration fit is set to **Linear**. All concentration calibrations should be linear with the signal response in the iCAP Q instrument.
	In the rare case that a non-linear calibration is acquired, you can define a **2nd Order** calibration fit.
Weighting	By default set to **None**.
	If **Absolute SD** is selected, absolute standard deviation is used.
	If **Relative SD** is selected, relative standard derivation is used.

Table 6-9. Parameters of Quantification table

Column	Description
Forcing	**No** forcing for the calibration.
	If **Zero** is selected, the calibration is forced through zero.
	If **Blank** is selected, the forcing of the calibration is set to run through the blank. Default setting is Blank.
Use for SemiQuant	Allows rough estimation of the content in the sample. Default setting is **Yes** for analytes that are quantified with a concentration quantification standard. All signal responses from the analytes selected are plotted on a semi-quant calibration graph as a function of mass. This way a rough concentration of analytes not present in the standards used for external calibration can be obtained (if at least three semiquant providers have been defined and the mass of the unknown analyte lies between the defined analytes). If **No** is selected, this analyte is not used as semi-quant provider.

❖ **To open the Quantification view**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation eQuant or aQuant.
4. Click  to select the **Quantification** view in the Template.

❖ **To set the quantification parameters**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to open the **Quantification** view in the Template.

5. Select the check box **Internal Standardization active** to activate internal standards for the measurement.

6. Click  in the cell of the column **Internal Standard** to open the drop-down list.

7. Select **Use as Internal Standard** to define this analyte to be used as internal standard.
   In the column **Quantify** the value is automatically set to **No**. This isotope will not be quantified.

8. In the rows of the other isotopes, select the defined Internal Standard from the drop-down list in all cells of this column **Internal Standard**.

9. Select **Use Interpolation** to enable a linear regression between two enshrouding internal standards that corrects the observed intensity of the analyte.

10. Click  in the cell of the column **Fit Type** to open the drop-down list and select a value.

11. Click  in the cell of the column **Weighting** to open the drop-down list and select a value.

12. Select **Absolute SD** to weigh each point by the standard deviation of the analyte.

13. Select **Relative SD** to weigh each point by its standard deviation relative to the mean value.

14. Click  in the cell of the column **Forcing** to open the drop-down list.

15. Select **Zero** to define that calibration is forced through zero for this analyte.
    If you select **Blank**, the calibration is set to run through the blank for this analyte.

16. Click  in the cell of the column **Use for SemiQuant** to open the drop-down list.

17. Select **Yes** to select the analyte as semi-quant provider.

18. Repeat for all analytes or use the fill-down option to apply a setting to more than one analyte.

19. Click  to save your Template.
    The new parameters are saved to the Template.

Ratios

The **Ratios** view of a eQuant, aQuant and tQuant Template in the Experiment Editor tool allows you to define isotopic, elemental or compound ratios for the measurement.

For aQuant and eQuant Templates, the Ratios view shows a table with the isotopes selected for this Template, see Figure 6-50.

Ratios

No	Ratio	Isotope 1	Isotope 2
1	92Mo / 94Mo	92Mo	94Mo
2	92Mo / 96Mo	92Mo	96Mo
3			

Figure 6-50. Ratios for aQuant Template

For tQuant Templates, the Ratios view shows a table with the compounds selected for this Template, see Figure 6-51.

Ratios

No	Ratio	Compound 1	Compound 2
1	C1 / C2	C1	C2
2	C3 / C1	C3	C1
3	C2 / C4	C2	C4
4			

Figure 6-51. Ratios for tQuant Template

The parameters that can be defined for the Ratios table are summarized in Table 6-10.

Table 6-10. Columns of Ratios table

Column	Description
No	Automatically assigned number in ascending order.
Ratio	Displays the ratio of columns **Isotope 1** and **Isotope 2** (eQuant and aQuant Templates) or **Compound 1** and **Compound 2** (tQuant Template).

Table 6-10. Columns of Ratios table

Column	Description
Isotope 1 or Compound 1	First isotope or compound to be selected for Ratio (numerator). All isotopes/compounds selected for this Template in the Analytes view are displayed in the drop-down list.
Isotope 2 or Compound 2	Second isotope or compound to be selected for Ratio (denominator). All isotopes/compounds selected for this Template in the Analytes view are displayed in the drop-down list.

❖ **To open the Ratios view**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template with the Evaluation eQuant, aQuant or tQuant.
4. Click  to select the **Ratios** view in the Template.

❖ **To define isotope ratios (aQuant and eQuant)**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to open the **Ratios** view in the Template.
5. Click  in a cell of the column **Isotope 1** to display the list of available isotopes.
6. Select an isotope or compound for column **Isotope 1**.
The isotope selected in column **Isotope 1** is the numerator in column **Ratio**.

7. Click in a cell of the column **Isotope 2** to display the list of available isotopes.
8. Select an isotope for column **Isotope 2**.
   The isotope selected in column **Isotope 2** is the denominator in column **Ratio**.

   The ratio of both isotopes is displayed in the column **Ratio**.
9. Click to save your Template.

❖ **To define compound ratios (tQuant only)**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click to open the **Ratios** view in the Template.
5. Click in a cell in the column **Compound 1** to display the list of available compounds.
6. Select a compound for column **Compound 1**.
   The compound selected in column **Compound 1** is the numerator in column **Ratio**.
7. Click in a cell in the column **Compound 2** to display the list of available compounds.
8. Select a compound for column **Compound 2**.
   The compound selected in column **Compound 2** is the denominator in column **Ratio**.

   The ratio of both compounds is displayed in the column **Ratio**.
9. Click to save your Template.

❖ **To delete rows**

1. Click Experiment Editor to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  to open the **Ratios** view in the Template.
5. Right-click the cell at the beginning of a row.
   A context menu opens, see Figure 6-52.

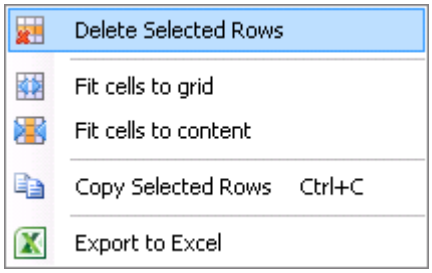


Figure 6-52. Ratio table context menu

6. Select **Delete Selected Rows**.
7. Click **Yes** to delete the selected row.
8. Click  to save your Template.

Quality Control (eQuant only)

For eQuant Templates only, the **Quality Control** view in the Experiment Editor 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.

The Quality Control view of the eQuant Template in Experiment Editor, see Figure 6-53, allows you to set quality control tests for the measurement.

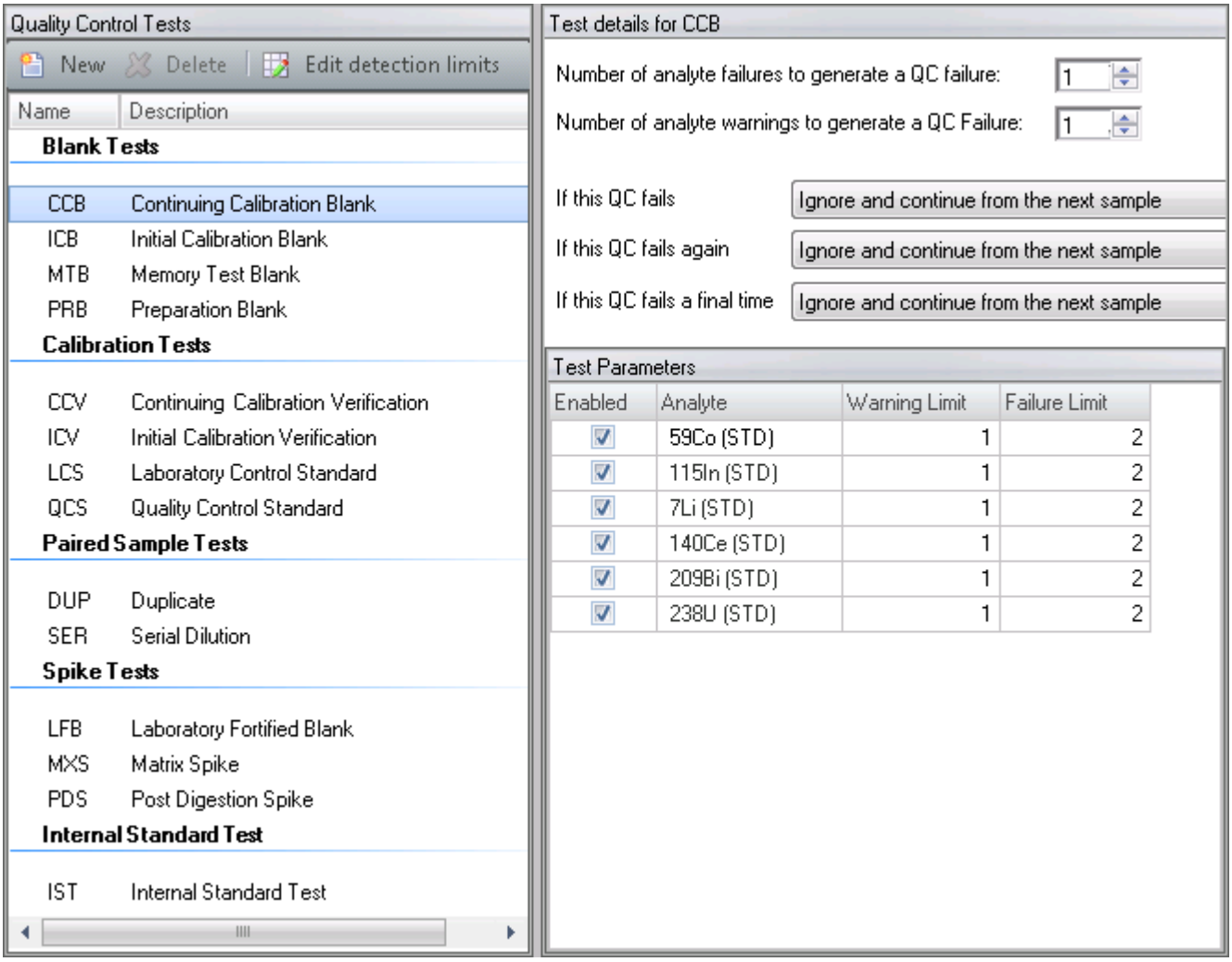


Figure 6-53. Quality Control page of eQuant Template in Experiment Editor

NOTICE This method parameter only becomes available after the check box **Use Quality Control** has been selected in the parameter "Quantification" on page 6-62. ▲

❖ **To open the Quality Control view**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template with the Evaluation eQuant.
4. Select the check box **Use Quality Control** in **Quantification**.
5. Click  to select the **Quality Control** view in the Template.

Blank Verification

In Experiment Editor, the Quality Control method parameter of the eQuant Template offers several types of blank verification, see Figure 6-54.

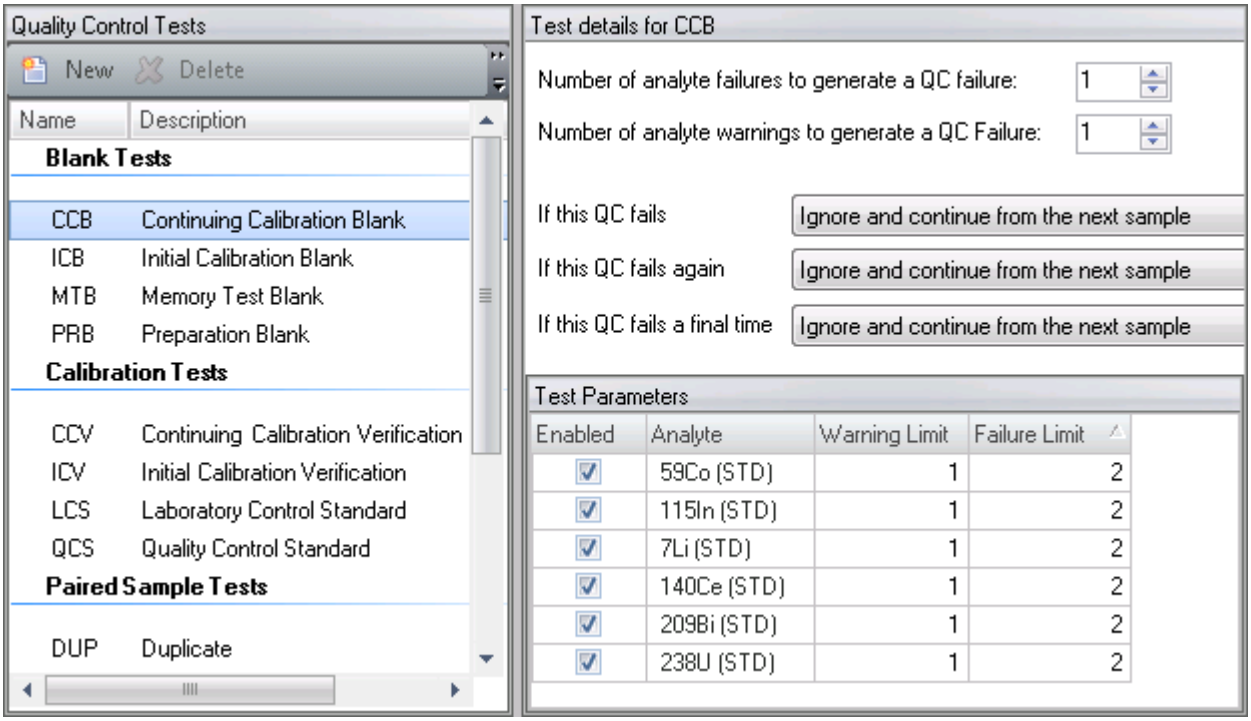


Figure 6-54. QC settings for blank verification

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 6-11. The last two columns show typical QC requirements of the US EPA.

Table 6-11. Quality control blank tests

Test type	Description	Purpose	Frequency	Limits
CCB	Continuing Calibration Blank	a continuing periodic check on the signal at blank levels	after each calibration and every 10 samples	< 3 x IDL
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 (LRB in Method 200.8)	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* ppt, 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 *0* ppt respectively.

Calibration Verification

In Experiment Editor, the Quality Control method parameter of the eQuant Template offers several types of calibration verification, see Figure 6-55.

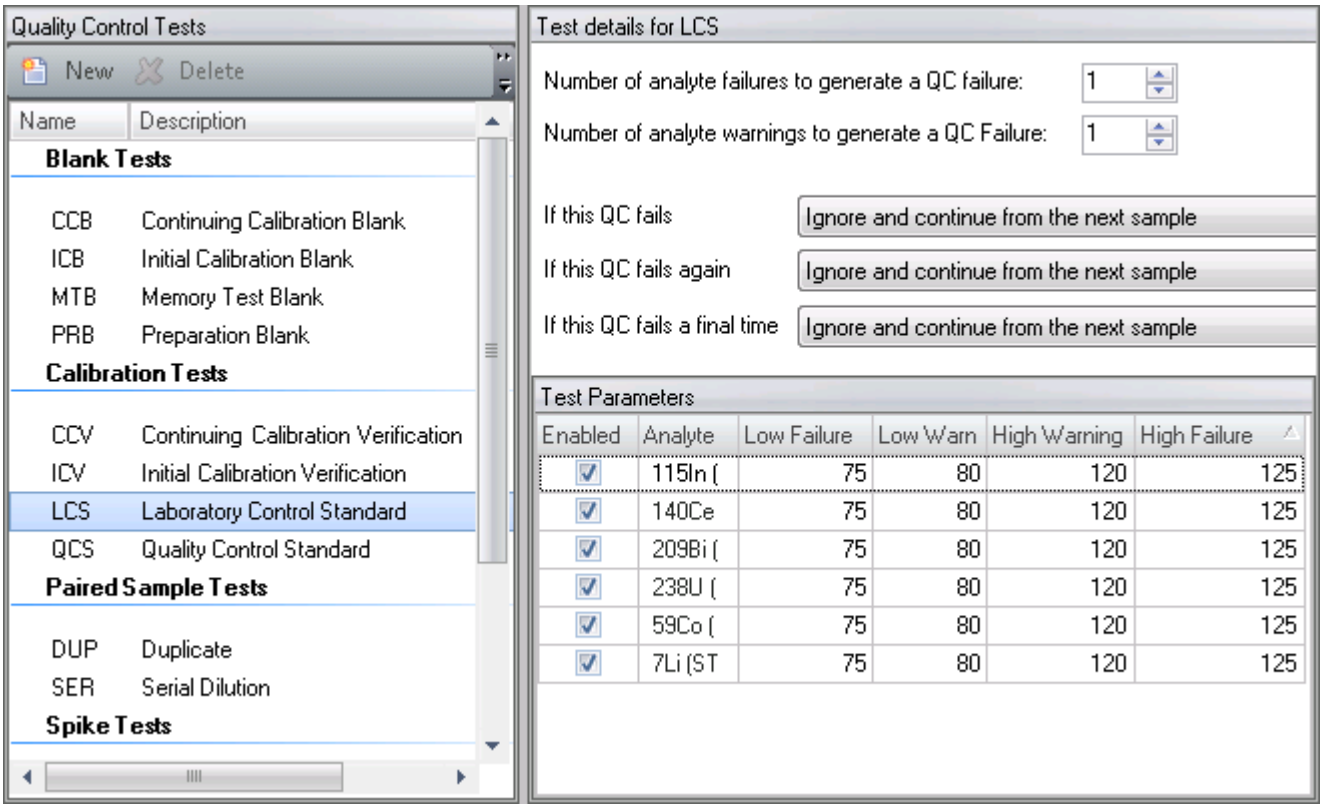


Figure 6-55. Table of QC settings for external calibration verification

Standards of known concentration, usually in the mid dynamic range of the calibration, 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 or warnings to generate a QC failure.

The **Calibration Tests** available for the external calibration verification are summarized in Table 6-12. The last two columns show typical QC requirements of the US EPA.

Table 6-12. Quality control calibration tests

Test type	Description	Purpose	Frequency	Limits
CCV	Continuing Calibration Verification	a continuing periodic check on accuracy and drift	after each calibration and 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 % (6020A 2007) 30-70 % (ism 12d 2010)
QCS	Quality Control Standard	checks the accuracy of the entire analytical process	once per batch	±10% (Method 200.8)

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.

Paired Sample

In Experiment Editor, the Quality Control method parameter of the eQuant Template offers several types of **Paired Sample Tests**, see Figure 6-56.

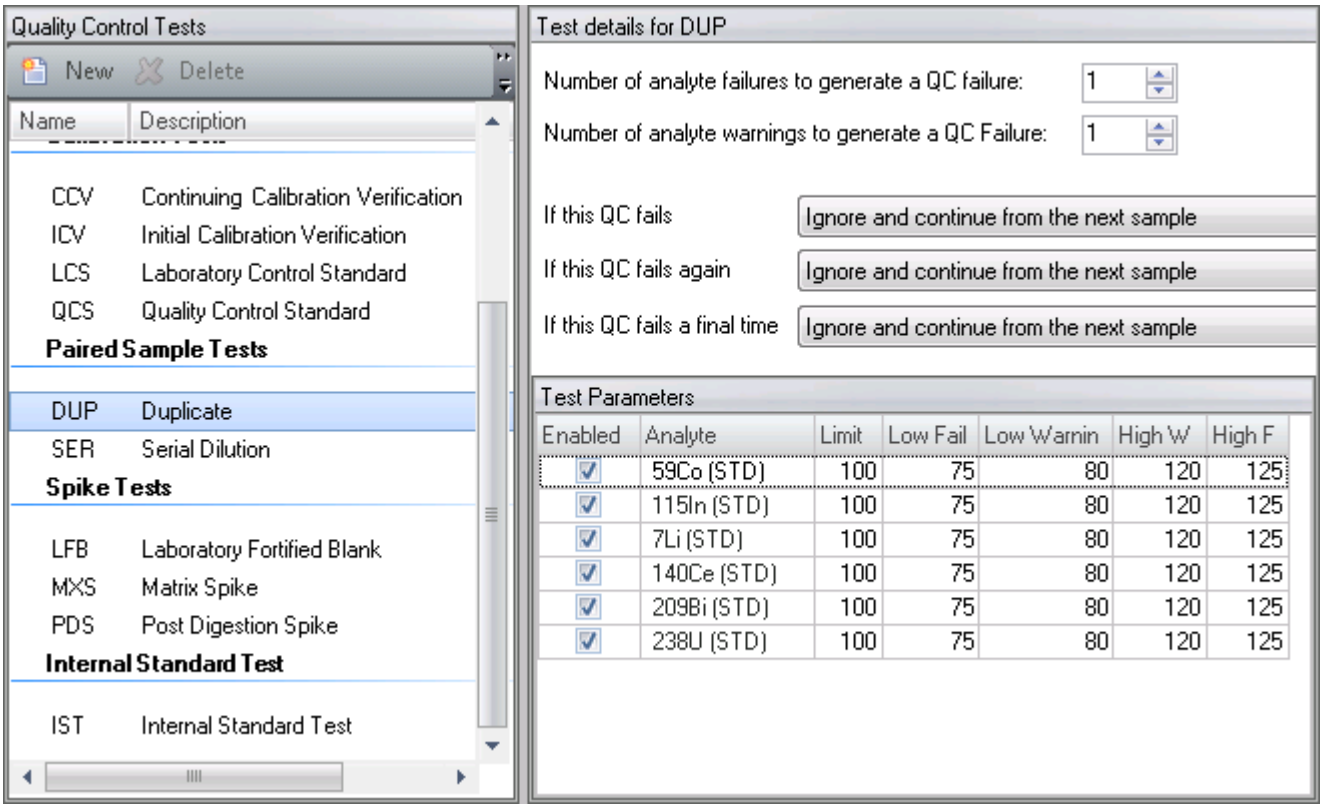


Figure 6-56. Table of QC settings for paired sample

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.

In order to do an analytically meaningful comparison between the two samples, the concentration in the original sample must be at least a certain multiple of the detection limit, for example, 200 times higher. 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.

The **Paired Sample Tests** available are summarized in Table 6-13. The last two columns show typical QC requirements of the US EPA.

Table 6-13. 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	±10 % of the original undiluted result after dilution correction

Warning and Failure Limits

The same rules as for other QC tests apply for setting the lower and higher warning and failure limits.

Spike Recovery

In Experiment Editor, the Quality Control method parameter of the eQuant Template offers several types of **Spike Tests**, see Figure 6-57.

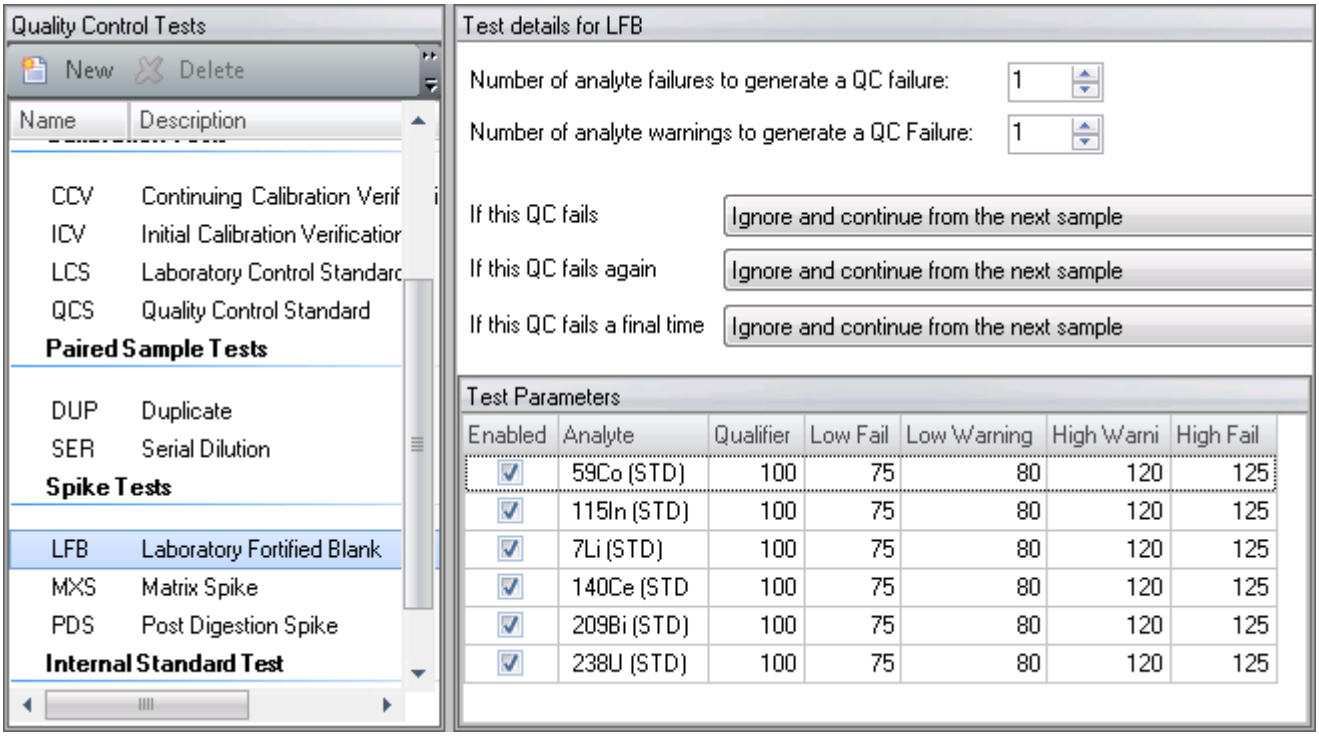


Figure 6-57. Table of QC settings for spike recovery

Spike recovery samples are used to determine the recovery of a known addition of analyte to a particular sample.

Three different **Spike Tests** are available. The last two columns in Table 6-14 show typical QC requirements of the US EPA.

Table 6-14. Quality control spike recovery

Test type	Description	Purpose	Frequency	Limits
LFB	Laboratory Fortified Blank	checks the recovery of analytes at a level close to the detection limit	every 20 to 30 samples	85-115% (Method 200.8)
MXS	Matrix Spike	checks the recovery of a spike in the sample matrix	every 20 samples	80-120 % (6020A 2007) 30-70 % (ism 12d 2010)
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 %

Warning and Failure Limits

The same rules as for other QC tests apply for setting the lower and higher warning and failure limits.

Internal Standard Test

In Experiment Editor, the Quality Control method parameter of the eQuant Template offers an **Internal Standard Test**, see Figure 6-58.

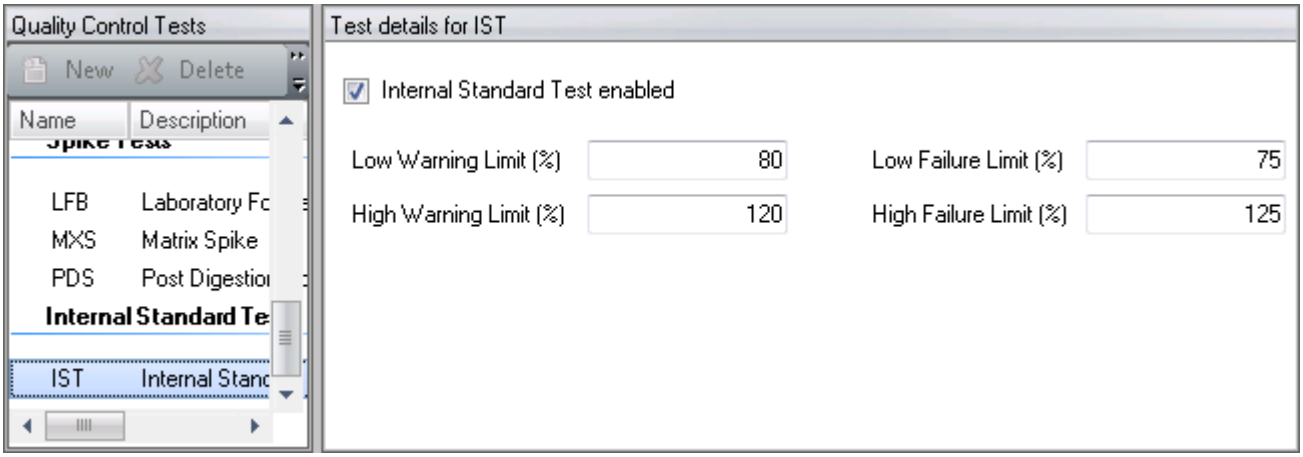


Figure 6-58. Quality control test details for IST

If an internal standard is used, warning limits and failure limits of its recovery in percent can be entered.

NOTICE 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 6-62. ▲

Quality Control Failure Rules

Failure rules for QC tests are defined in the method parameter Quality Control of the eQuant Template in Experiment Editor, see Figure 6-59.

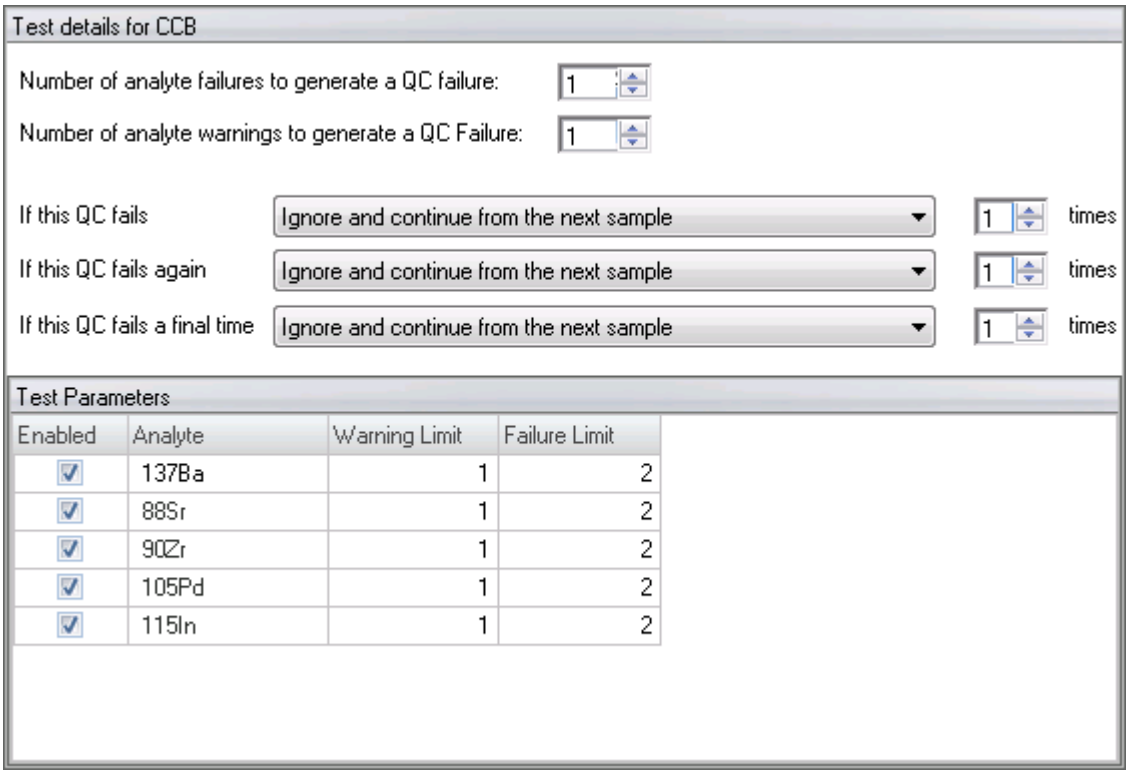


Figure 6-59. Quality control details and parameters for CCB

In the first part of **Test details**, the number of failures can be defined, see Table 6-15.

Table 6-15. 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. **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. **Recommended setting:** 3

When the QC test fails, there are a number of options that 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 6-15.

Table 6-16. 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 named 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 Sample Definition section.
Autotune, recalibrate, recalculate and reacquire from a previous sample	Upon QC failure this action will automatically run the autotune program followed by a copy of the calibration block and the 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 Sample Definition section.
Abort the Experiment and continue with the queue	Upon QC failure, the LabBook will be aborted and the Scheduler will continue with other scheduled LabBooks.
Dilute and repeat line	If an autodilution system is available, a copy the QC sample will be inserted immediately following the QC failure and autodiluted or diluted by a pre-defined factor.

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.

Defining or Changing Quality Control Test Settings (eQuant only)

Qtegra is supplied with predefined settings for QC test types. If not changed and saved separately, these default settings will be applied when adding a QC test to the eQuant Template or LabBook in Experiment Editor.

❖ **To activate quality control (QC) test settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template for eQuant Evaluation.
4. Select the check box **Use Quality Control** in the **Quantification** view to activate the method parameter **Quality Control**.

❖ **To define QC settings for blank tests**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.
4. Click  to select the **Quality Control** view.
On the left, the available **Quality Control Tests** are listed, see

Figure 6-60.

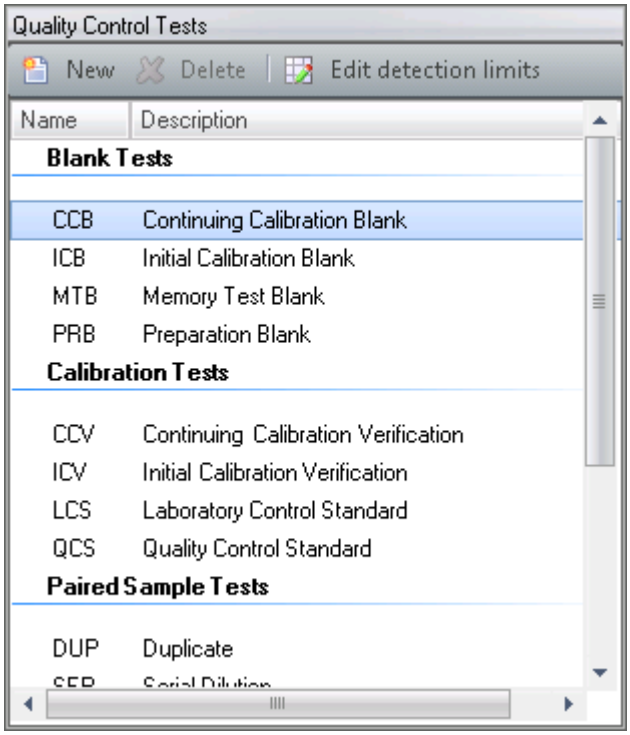


Figure 6-60. Quality Control Blank Test types

5. Click the **Quality Control Test** you wish to define.
   On the right, the corresponding **Test details** and **Test Parameters** are shown.

6. Click  to change the **Number of analyte failures to generate a QC failure** or enter the new value directly.

7. Click  to change the **Number of analyte warnings to generate a QC failure** or enter the new value directly. For details, see "Quality Control Failure Rules" on page 6-78.

8. Select the action to take place **If this QC fails**.

9. Select the action to place **If this QC fails again**.

10. Select the action to take place **If this QC fails a final time**.

11. Deselect the check box next to the analyte in the **Enabled** column to skip this analyte, see Figure 6-61.

Test Parameters

Enabled	Analyte	Warning Limit	Failure Limit
☑	59Co (STD)	1	2
☑	115In (STD)	1	2
☑	7Li (STD)	1	2
☑	140Ce (STD)	1	2
☑	209Bi (STD)	1	2
☑	238U (STD)	1	2

Figure 6-61. Quality Control Blank Test Parameters

By default, all analytes defined in the Template are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.

12. Define the **Warning Limit** and **Failure Limit** for the analytes. Set the limits for each analyte individually or set the limits for the first analyte in the grid and fill down the values to the grid.

13. In the tab for your **Template**, click  to save your Template.

❖ **To define QC settings for calibration tests**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.

4. Click  to select the **Quality Control** view.
On the left, the available **Quality Control Tests** are listed, see

Figure 6-62.

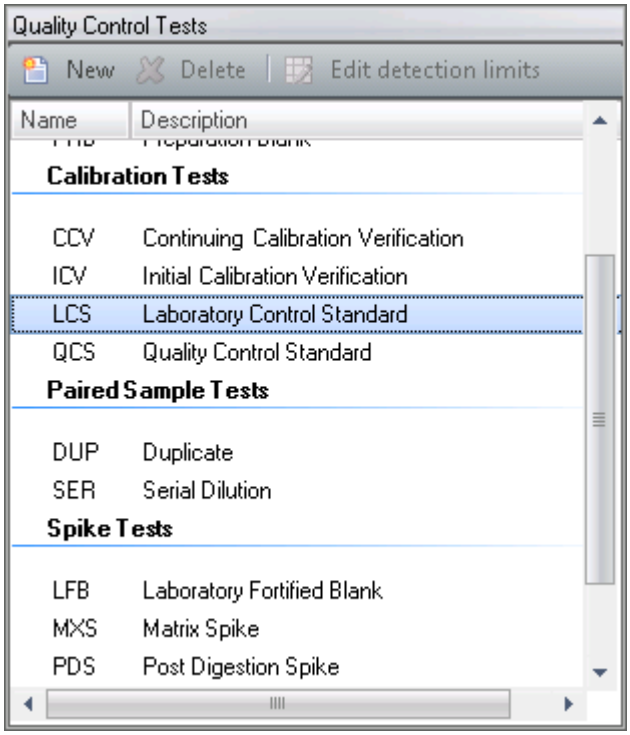


Figure 6-62. Quality Control Calibration Test types

5. Click the **Quality Control Test** you wish to define.
   On the right, the corresponding **Test details** and **Test Parameters** are shown.

6. Click  to change the **Number of analyte failures to generate a QC failure** or enter the new value directly. For details, see "Quality Control Failure Rules" on page 6-78.

7. Click  to change the **Number of analyte warnings to generate a QC failure** or enter the new value directly.

8. Select the action to take place **If this QC fails**.

9. Select the action to place **If this QC fails again**.

10. Select the action to take place **If this QC fails a final time**.

11. Deselect the check box next to the analyte in the **Enabled** column to skip this analyte, see Figure 6-63.

Test Parameters

Enabled	Analyte	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)
☑	115In (STD)	75	80	120	125
☑	140Ce (STD)	75	80	120	125
☑	209Bi (STD)	75	80	120	125
☑	238U (STD)	75	80	120	125
☑	59Co (STD)	75	80	120	125
☑	7Li (STD)	75	80	120	125

Figure 6-63. Quality Control Calibration Test Parameters

By default, all analytes defined in the Template are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.

12. Define the **Low Failure Limit** and **Low Warning Limit** for the analytes.
    Set the limits for each analyte individually or set the limits for the first analyte in the grid and fill down the values to the grid.

13. Define the **High Warning Limit** and **High Failure Limit** for the analytes.
    Set the limits for each analyte individually or set the limits for the first analyte in the grid and fill down the values to the grid.

14. In the tab for your **Template**, click  to save your Template.

❖ **To define QC settings for paired sample tests**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.

4. Click  to select the **Quality Control** view.
   On the left, the available **Quality Control Tests** are listed, see

Figure 6-64.

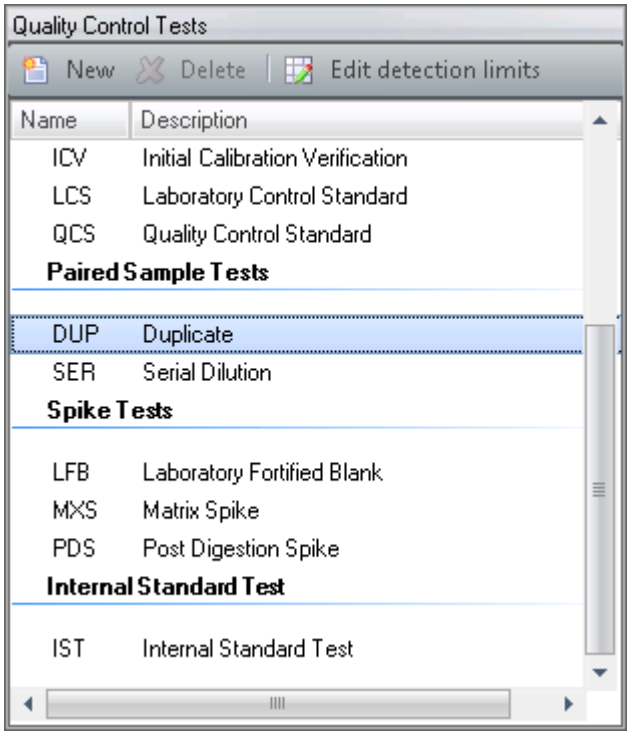


Figure 6-64. Quality Control Paired Sample Test types

5. Click the **Quality Control Test** you wish to define.
   On the right, the corresponding **Test details** and **Test Parameters** are shown.

6. Click  to change the **Number of analyte failures to generate a QC failure** or enter the new value directly. For details, see "Quality Control Failure Rules" on page 6-78.

7. Click  to change the **Number of analyte warnings to generate a QC failure** or enter the new value directly.

8. Select the action to take place **If this QC fails**.

9. Select the action to place **If this QC fails again**.

10. Select the action to take place **If this QC fails a final time**.

11. Deselect the check box next to the analyte in the **Enabled** column to skip this analyte, see Figure 6-65.

Test Parameters

Enabled	Analyte	Limit	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)
☑	59Co (STD)	100	75	80	120	125
☑	115In (STD)	100	75	80	120	125
☑	7Li (STD)	100	75	80	120	125
☑	140Ce (STD)	100	75	80	120	125
☑	209Bi (STD)	100	75	80	120	125
☑	238U (STD)	100	75	80	120	125

Figure 6-65. Quality Control Paired Sample Test Parameters

By default, all analytes defined in the Template are included for the QC test. If not set, by default the software only looks for those analytes that are included in the standard solution.

12. Define the **Limit** for each analyte.
Default value is *100*.

13. Define the **Low Failure Limit** and **Low Warning Limit** for the analytes.
Set the limits for each analyte individually or set the limits for the first analyte in the grid and fill down the values to the grid.

14. Define the **High Warning Limit** and **High Failure Limit** for the analytes.
Set the limits for each analyte individually or set the limits for the first analyte in the grid and fill down the values to the grid.

15. In the tab for your **Template**, click  to save your Template.

❖ **To define QC settings for spike tests**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.

4. Click  to select the **Quality Control** view.
   On the left, the available **Quality Control Tests** are listed, see Figure 6-66.

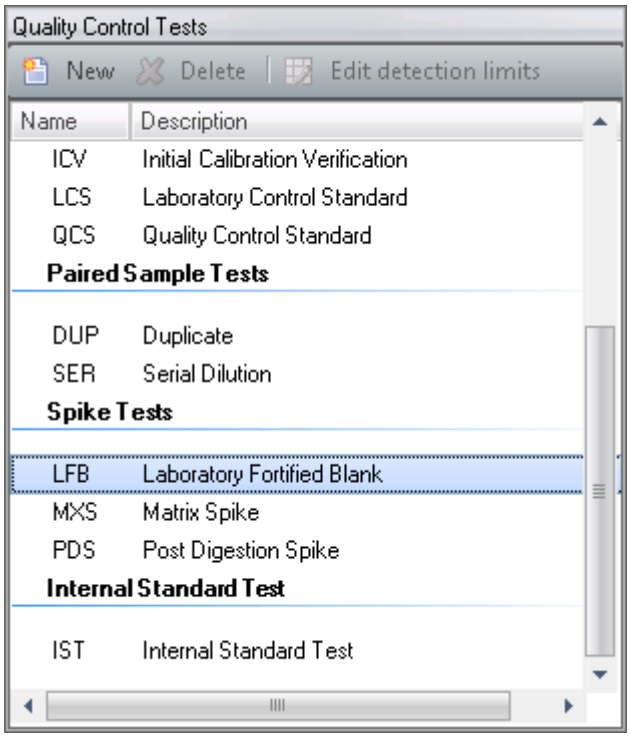


Figure 6-66. Quality Control Spike Test types

5. Click the **Quality Control Test** you wish to define.
   On the right, the corresponding **Test details** and **Test Parameters** are shown.

6. Click  to change the **Number of analyte failures to generate a QC failure** or enter the new value directly. For details, see "Quality Control Failure Rules" on page 6-78.

7. Click  to change the **Number of analyte warnings to generate a QC failure** or enter the new value directly.

8. Select the action to take place **If this QC fails**.

9. Select the action to place **If this QC fails again**.

10. Select the action to take place **If this QC fails a final time**.

11. Deselect the check box next to the analyte in the **Enabled** column to skip this analyte, see Figure 6-67.

Test Parameters

Enabled	Analyte	Qualifier	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)
☑	59Co (STD)	100	75	80	120	125
☑	115In (STD)	100	75	80	120	125
☑	7Li (STD)	100	75	80	120	125
☑	140Ce (STD)	100	75	80	120	125
☑	209Bi (STD)	100	75	80	120	125
☑	238U (STD)	100	75	80	120	125

Figure 6-67. Quality Control Spike Test Parameters

By default, all analytes defined in the Template are included for the QC test. Although, by default the software only looks for those analytes that are included in the standard solution.

12. Define the **Qualifier** for each analyte.
Default value is *100*.

13. Define the **Low Failure Limit** and **Low Warning Limit** for the analytes.
Set the limits for each analyte individually or set the limits for the first analyte in the grid and fill down the values to the grid.

14. Define the **High Warning Limit** and **High Failure Limit** for the analytes.
Set the limits for each analyte individually or set the limits for the first analyte in the grid and fill down the values to the grid.

15. In the tab for your **Template**, click  to save your Template.

❖ **To define QC settings for internal standard tests**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.

4. Click  to select the **Quality Control** view.
   On the left, the available **Quality Control Tests** are listed, see Figure 6-68.

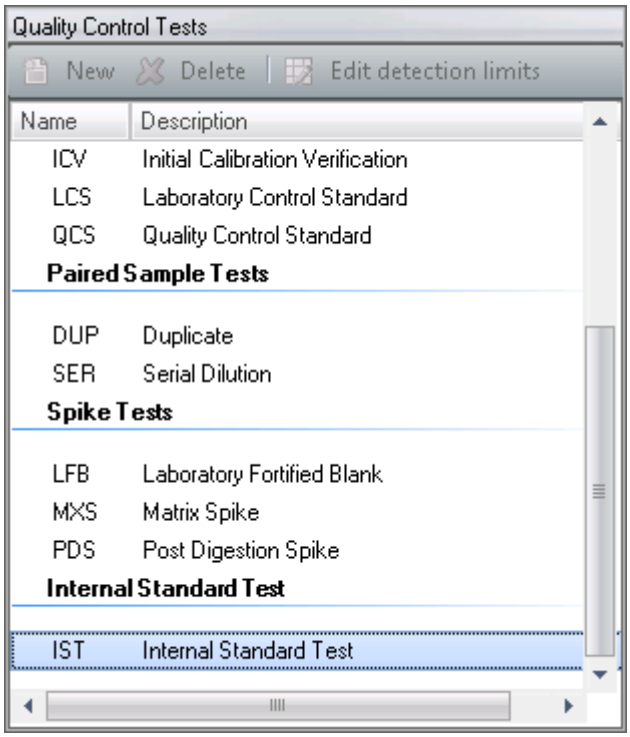


Figure 6-68. Quality Control Internal Standard Test types

5. Click the **Quality Control Test** you wish to define.
   On the right, the corresponding **Test details** are shown, see Figure 6-69.

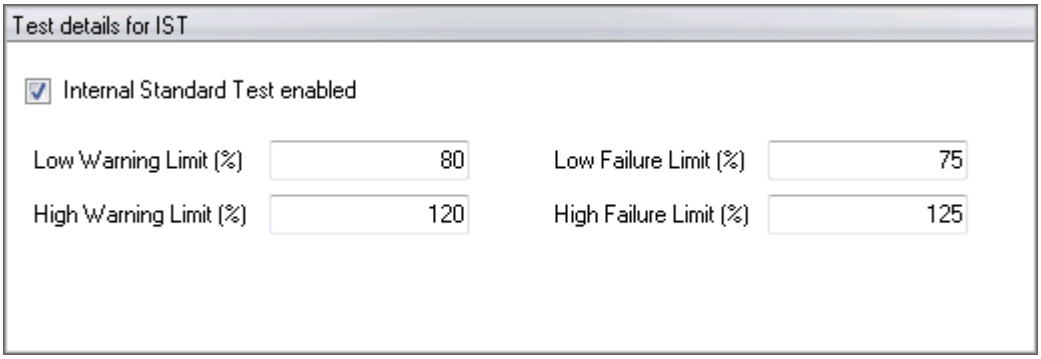


Figure 6-69. Quality Control Internal Standard Test details

6. Select the check box **Internal Standard Test enabled** to activate this feature.

7. Define the **Low Warning Limit** and **High Warning Limit** for the analytes.

8. Define the **Low Failure Limit** and **High Failure Limit** for the analytes.

9. In the tab for your **Template**, click  to save your Template.

❖ **To copy a set of values to the grid**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.

4. Click  to select the **Quality Control** view.
On the left, the available Quality Control Tests are listed.

5. Click the **Quality Control Test** you wish to define.
On the right, the corresponding **Test details** and **Test Parameters** are shown.

6. In the **Test Parameters** table, complete the entries you wish to fill down/up.

7. Click anywhere next in the table.

8. Click and drag the mouse from this first entry you wish to copy over all cells of the column to be changed with this value.

9. Right-click in the cell of the table to where you wish to copy the value.
A context menu opens, see Figure 6-70.

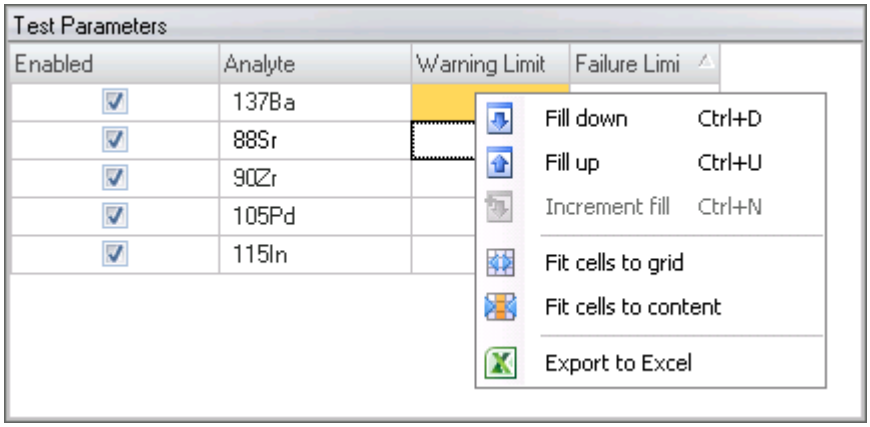


Figure 6-70. Quality Control Test Parameter context menu

10. Select **Fill down** or **Fill up**, as appropriate.
    The entries from the first selected cell are copied down or up to all cells selected.

11. Click  to save your Template.

❖ **To create a new quality control test**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.

4. Click  to select the **Quality Control** view.
   On the left, the available Quality Control Tests are listed.

5. Click the **Quality Control Test** you wish to duplicate and define.

6. Click 

.
   A dialog box opens, see Figure 6-71.

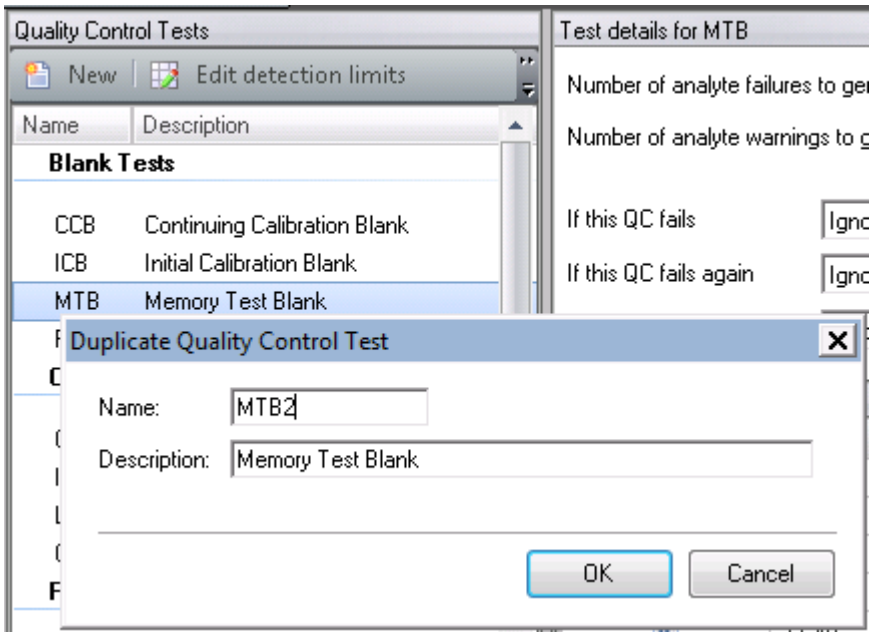


Figure 6-71. Duplicate Quality Control Test window

7. Enter a **Name** and **Description** for the new quality control test.

8. Click **OK**.
   The new test is added to the list.

9. Click  to save your Template.

❖ **To delete a new quality control test**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.

4. Click  to select the **Quality Control** view.
   On the left, the available Quality Control Tests are listed.

5. Click the **Quality Control Test** you wish to delete.
   Predefined quality control tests cannot be deleted.

6. Click 

.
   The selected quality control test is deleted from the list.

7. Click  to save your Template.

Defining Detection Limits (eQuant only)

The Quality Control view of the eQuant Template in Experiment Editor allows the definition of contract-required detection limits for the measurement.

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 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 6-17.

Table 6-17. Detection limits

Column	Description
Symbol	Displays the Analytes selected for the Template.
Concentration	Defines the detection limit for this analyte/isotope.
Unit	This column defines the units 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.
Export	Export Contract Required Detection Limits.

NOTICE Any analytes (cells) that are not required for the LOD checks can be left blank. ▲

❖ **To enter detection limits for the defined analytes**

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template for eQuant Evaluation with activated **Quality Control**.
4. Click  to select the **Quality Control** view.

5. Click 

.
A dialog opens, see Figure 6-72.

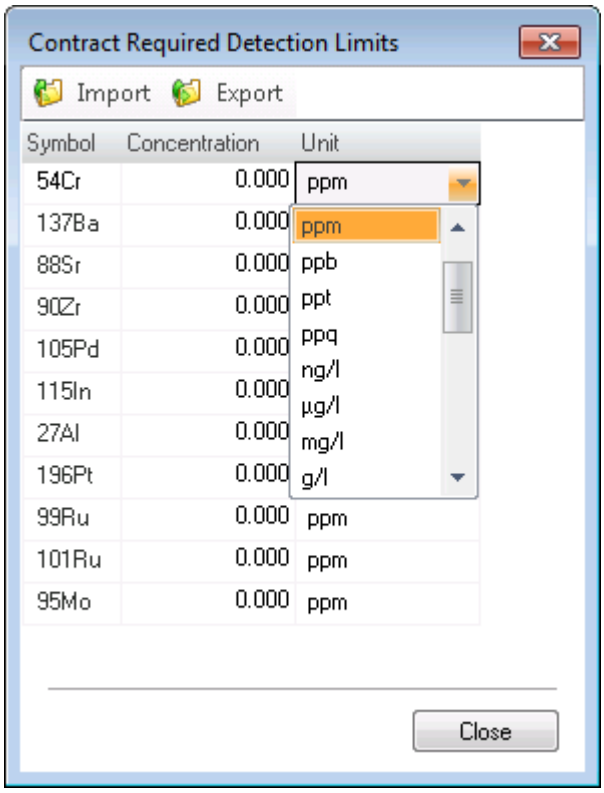
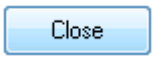


Figure 6-72. Contract Required Detection Limits window

6. Click the cell **Concentration** next to an analyte and type in a value for the detection limit.

7. Click  in the cell of column **Unit** to open the drop-down list and select a unit.
The default unit is *ppm*.

8. Repeat until all detection limits are set.

9. Click 

.

10. Click  to save your Template.
The detection limits are saved to the Template.

❖ **To import an existing analyte list**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click  to select the **Quality Control** view.

5. Click 

.
A dialog opens, see Figure 6-72.

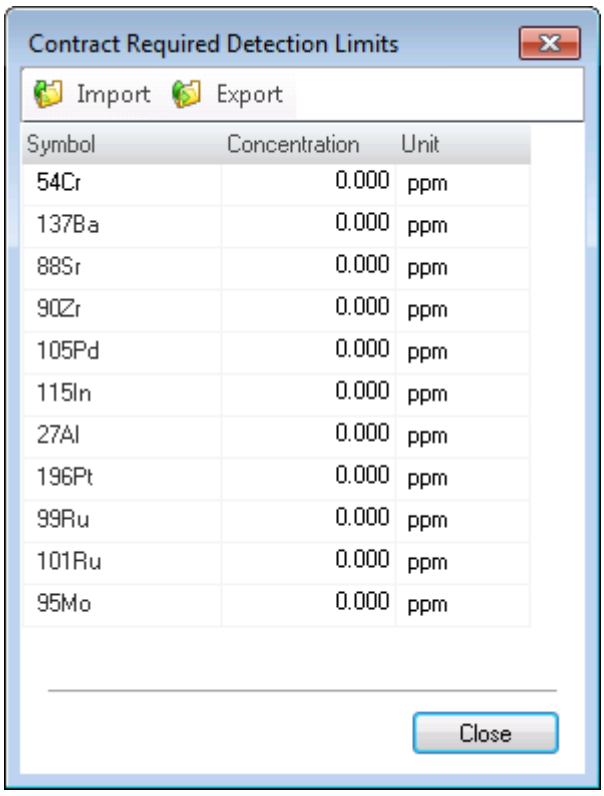


Figure 6-73. Contract Required Detection Limits window

6. Click Import to open the **Import detection limits** dialog, see Figure 6-74.

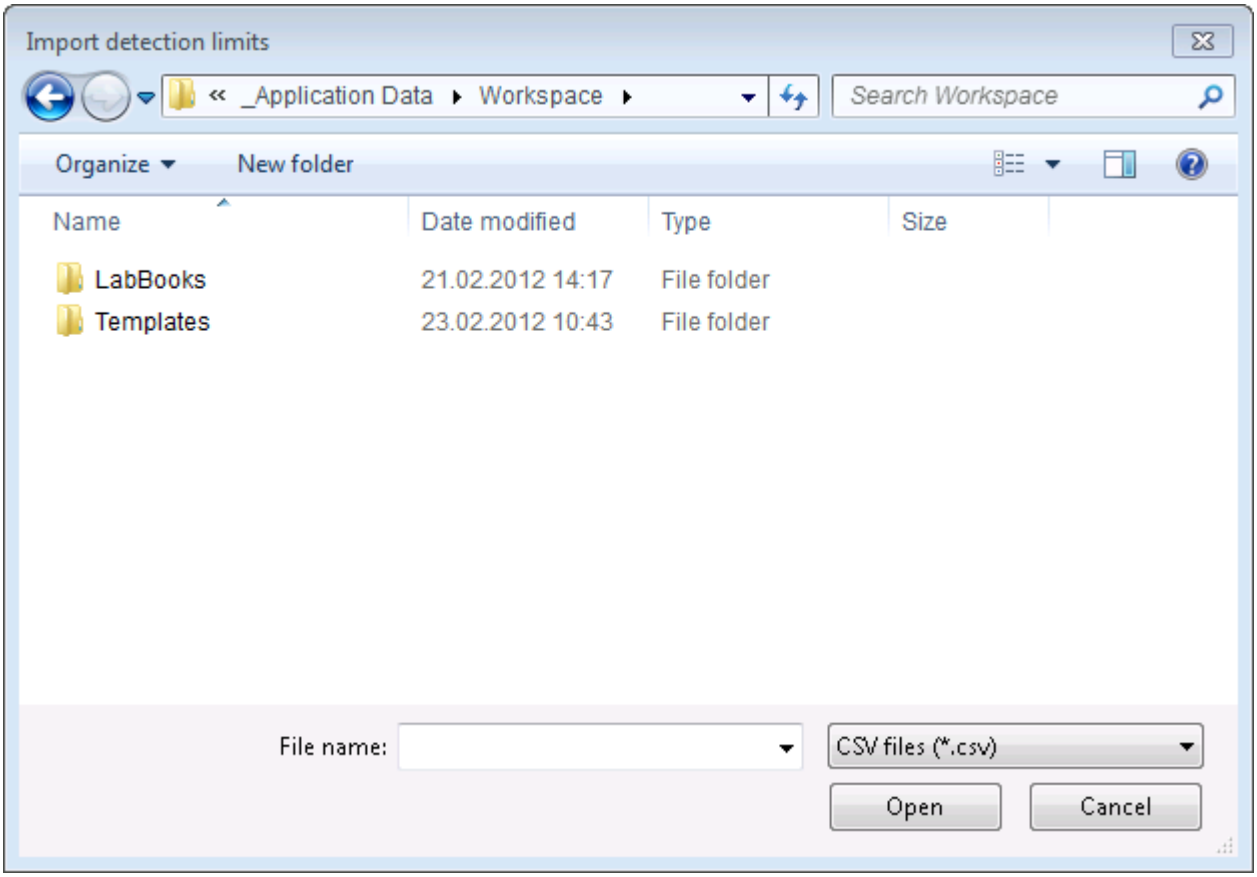


Figure 6-74. Import detection limits window

7. Select the directory of your *.csv file.
8. Select the *.csv file you wish to import.
9. Click Open to load the file.
   The *.csv file is imported into the table to be edited as required.

❖ **To export the currently loaded analyte list**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click to select the **Quality Control** view.

5. Click Edit detection limits.
   A dialog opens, see Figure 6-75.

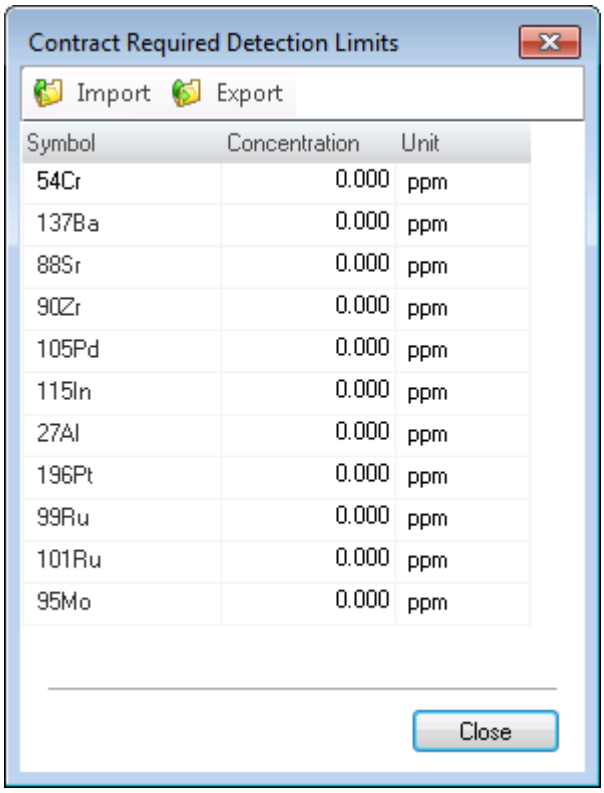


Figure 6-75. Contract Required Detection Limits window

6. Click Export to open the **Export detection limits** dialog, see Figure 6-76.

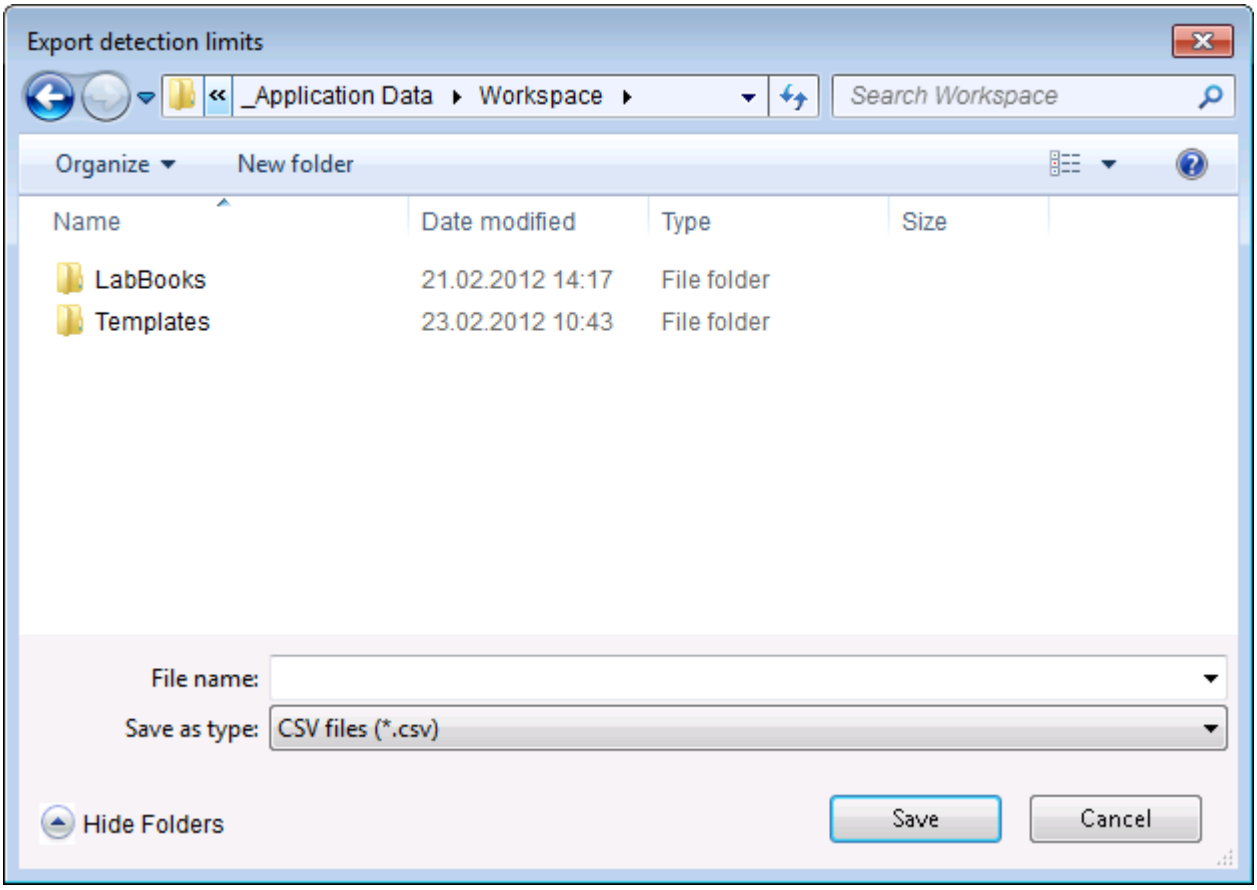


Figure 6-76. Export detection limits window

7. Select the directory of your *.csv file.
8. Enter a name for the *.csv file you wish to export.
9. Click Save to save the file.

Defining QC Settings in Sample Definition (eQuant only)

The QC settings are specified for each sample in the Sample Definition section of the eQuant Template in Experiment Editor. The Sample List of the LabBook is generated from the definition given in this section.

❖ **To define QC settings in Sample Definition**

1. Click Experiment Editor to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select a Template for eQuant Evaluation with activated **Quality Control**, see "Defining or Changing Quality Control Test Settings (eQuant only)" on page 6-80.
4. Click  **Sample Definition** to open the Sample Definition view of the Template.
5. Define **Header**, **Body** and **Footer** as appropriate.
6. Add as many rows as you need for your experiment.
7. Enter a **Label** for each row.
8. For QC, typically in the Footer select **QC** for **Sample Type** for a sample.
9. For the column **QC Action**, select a QC test type from the drop-down list, see Figure 6-77.

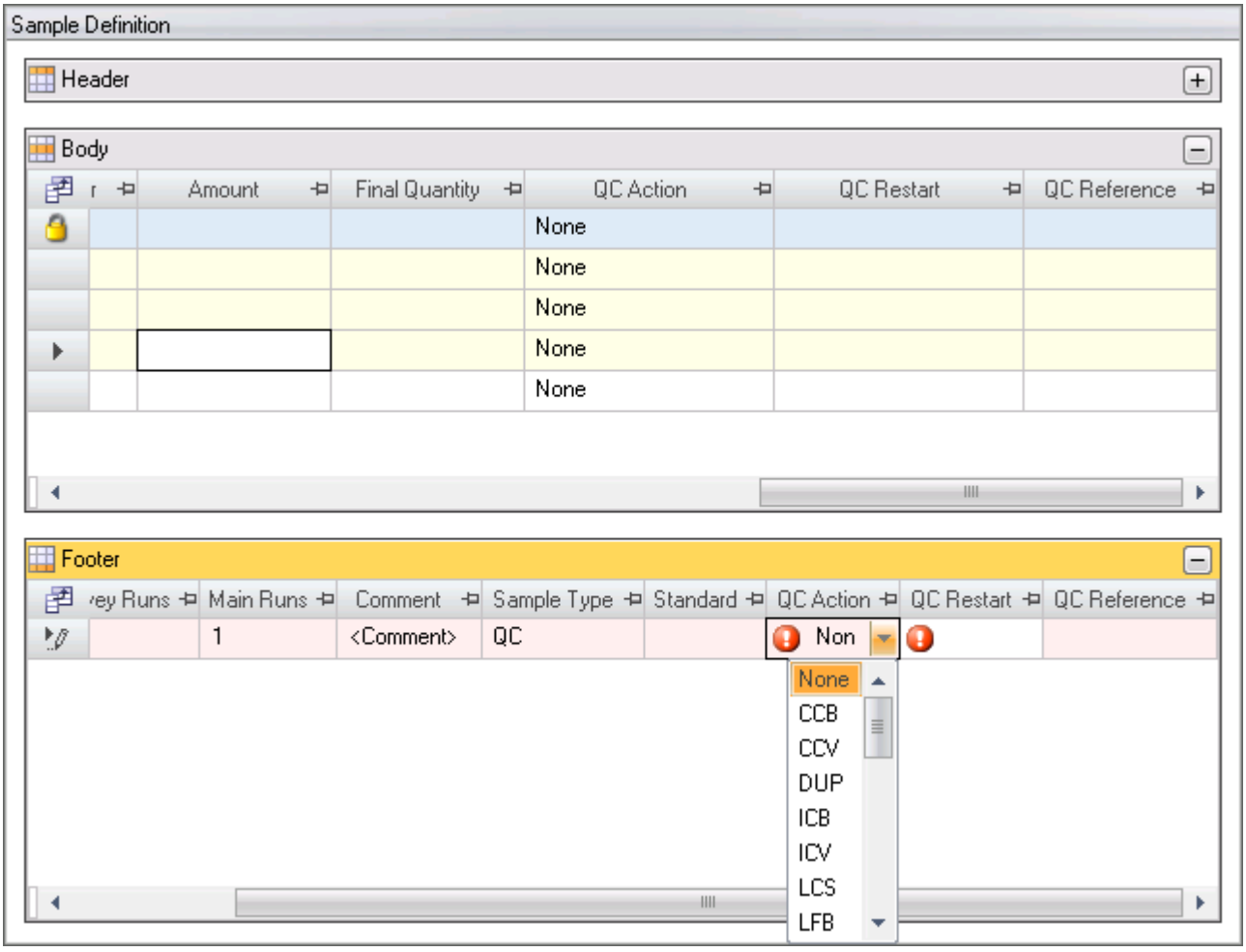


Figure 6-77. QC Action drop-down in eQuant Template Sample Definition Footer

NOTICE For details on Quality Control, see "Quality Control (eQuant only)" on page 6-69. ▲

10. Select a **Standard** for the sample row, if appropriate.

11. For the column **QC Restart**, select an option from the drop-down list, see Figure 6-78.

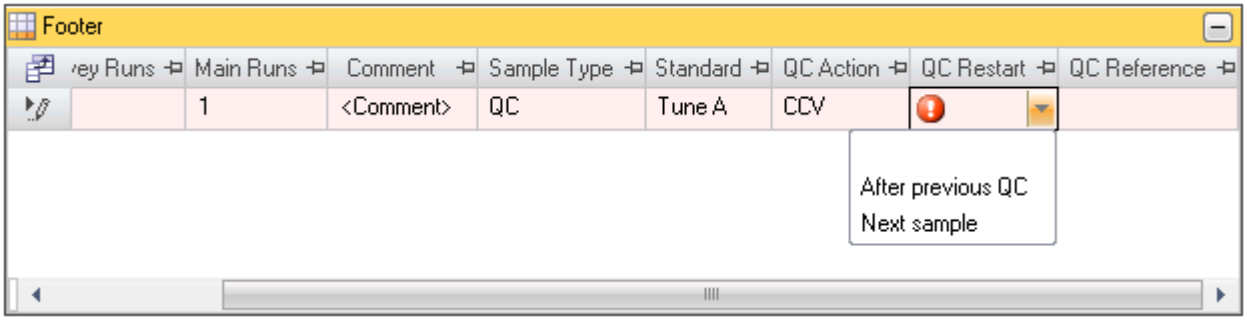


Figure 6-78. QC Restart drop-down in eQuant Template Sample Definition Footer

12. Continue to enter a value for each column or select an item from the drop-down list, as appropriate.

13. If you worked with paired measurements, enter the same indicators in **QC Reference** for both sample lines.

NOTICE For details on the columns, see "Sample Definition for a Template" on page 6-117. ▲

14. Click  to save the changes to your Template.

Peripherals

The settings for peripherals such as LC pumps or LC autosamplers can be adjusted in the corresponding view of the Template in Experiment Editor.

NOTICE Peripherals are added to the Configuration in the Configurator tool of Qtegra (see "Experiment Configurator" on page 3-13). ▲

Cetac ASX-520 Autosampler

The Cetac™ ASX-520 autosampler offers four racks.

❖ **To adjust the Cetac ASX-520 autosampler settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to open a Template with a Configuration including the Cetac ASX-520 autosampler.

4. Click Cetac ASX-520 to open the autosampler view, see Figure 6-79.

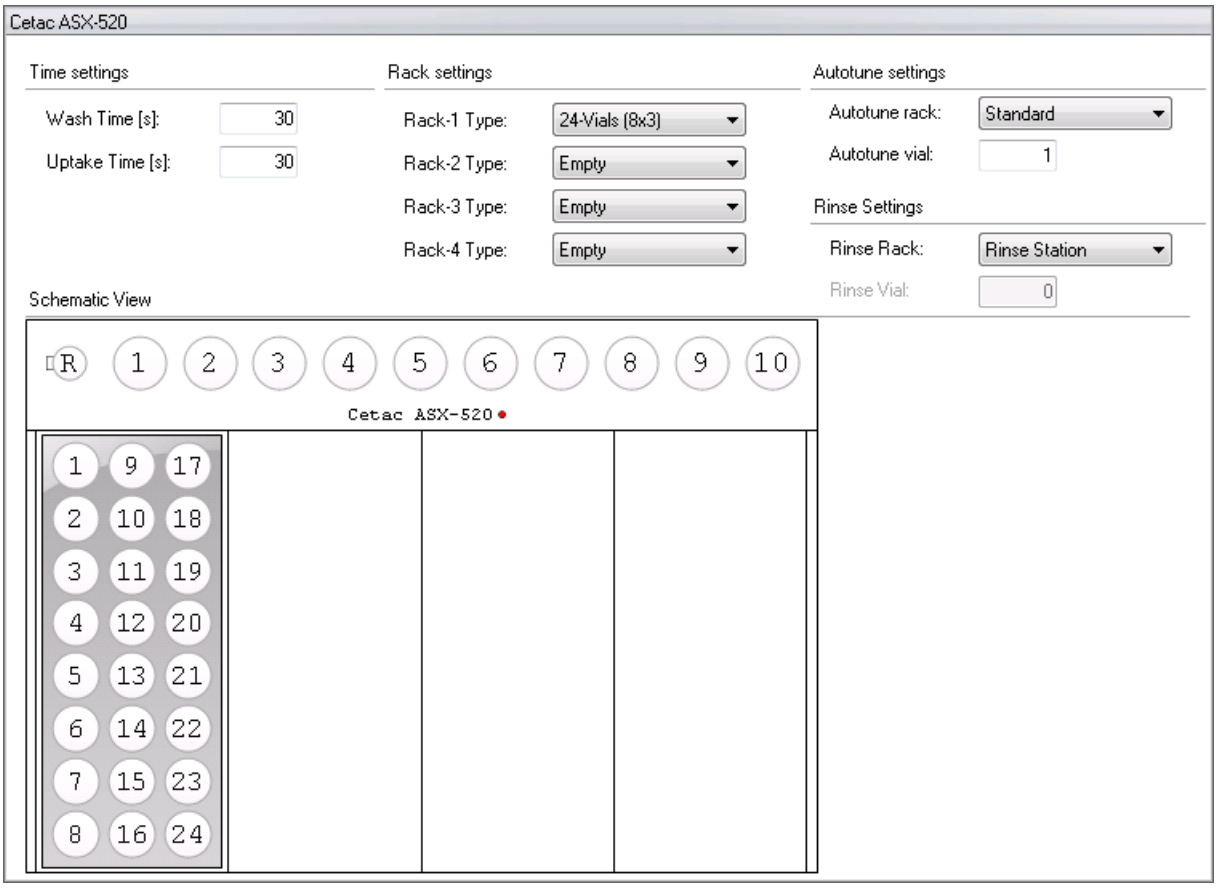


Figure 6-79. Cetac ASX-520 settings

5. Enter the **Wash Time [s]**.
6. Enter the **Uptake Time [s]**.
7. Select the **Rack settings** from the drop-down menus.
   The **Schematic View** shows the selected rack configuration.
8. Select the **Autotune settings** from the drop-down menu **Autotune rack**.
9. Enter the **Autotune vial** number.
10. Select the **Rinse Settings** from the **Rinse Rack** drop-down menu.
    Enter the Rinse Vial only if the setting is not Rinse Station.
11. Click to save your Template.

Cetac ASX-260 Autosampler

The Cetac™ ASX-260 autosampler offers two racks.

❖ **To adjust the Cetac ASX-260 autosampler settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to open a Template with a Configuration including the Cetac ASX-260 autosampler.
4. Click 

to open the autosampler view, see Figure 6-79.

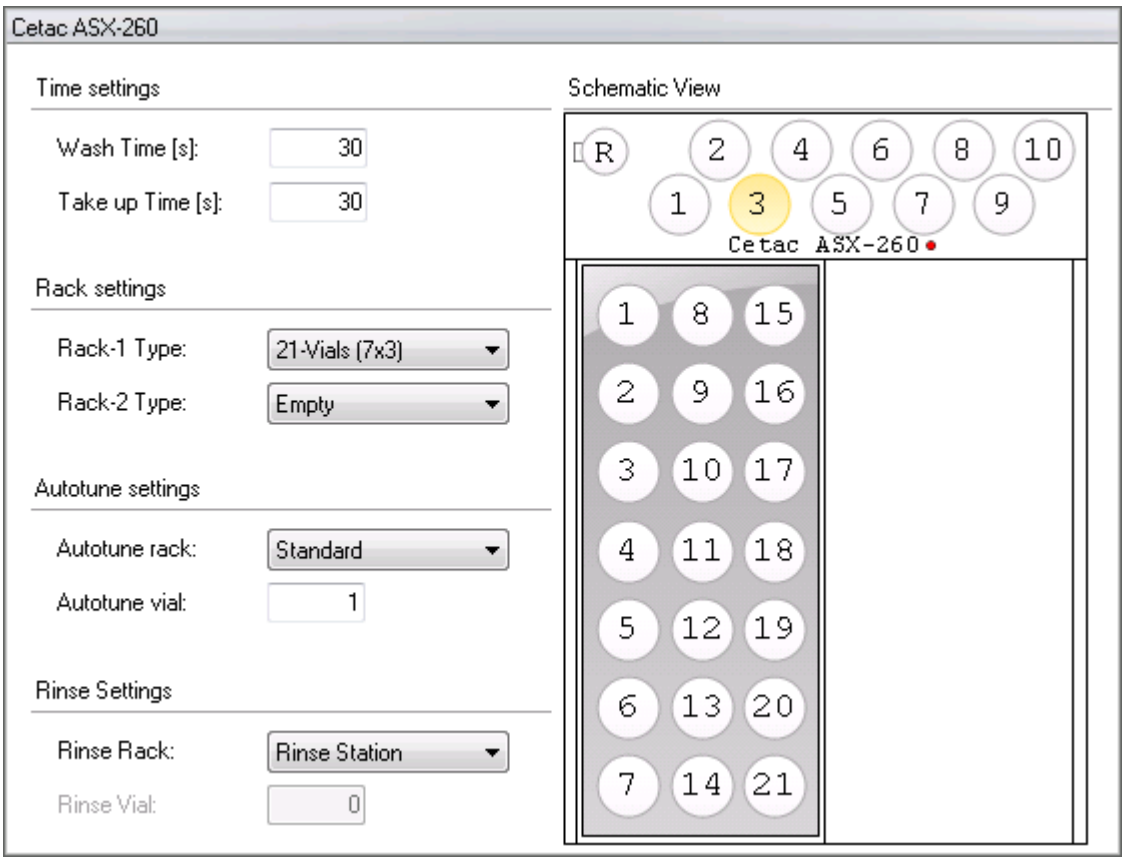


Figure 6-80. Cetac ASX-260 settings

5. Enter the **Wash Time [s]**.
6. Enter the **Take Up Time [s]**.
7. Select the **Rack settings** from the drop-down menus.
The **Schematic View** shows the selected rack configuration.
8. Select the **Autotune settings** from the drop-down menu **Autotune rack**.

9. Enter the **Autotune vial** number.
10. Select the **Rinse Settings** from the **Rinse Rack** drop-down menu. Enter the Rinse Vial only if the setting is not Rinse Station.
11. Click  to save your Template.

ESI SC-4S Autosampler

The ESI SC-4S autosampler offers four racks.

NOTICE The settings for Uptake and Wash in the Monitor Analytes view of Experiment Editor will overwrite these settings for the autosampler. ▲

❖ **To adjust the ESI SC-4S autosampler settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to open a Template with a Configuration including the ESI SC-4S autosampler.

4. Click ESI SC-4S to open the autosampler view, see Figure 6-81.

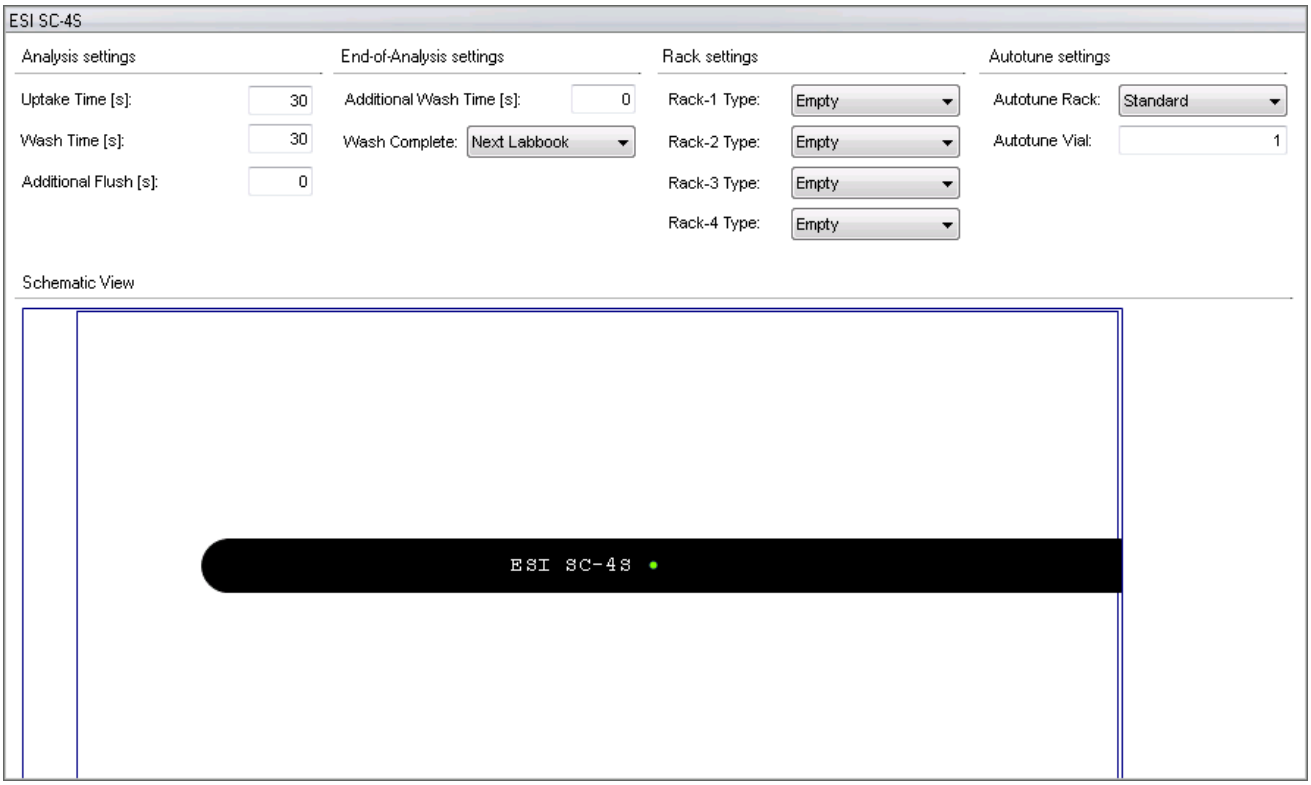


Figure 6-81. ESI SC-4S settings

5. Enter the **Uptake Time [s]**.
6. Enter the **Wash Time [s]**.
7. Enter **Additional Flush [s]**.
8. Enter **Additional Wash Time [s]**.
9. Select the action after **Wash Complete** from the drop-down menu, see Figure 6-82.

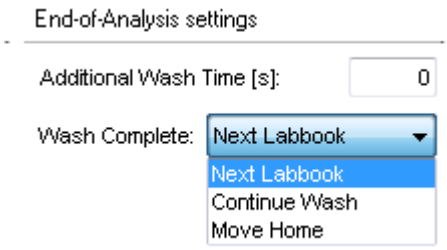


Figure 6-82. Wash Complete drop-down menu

10. Select the **Rack settings** from the drop-down menus.
    The **Schematic View** shows the selected rack configuration.

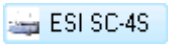
11. Select the **Autotune settings** from the drop-down menu **Autotune Rack**.
12. Enter the **Autotune Vial** number.
13. Click  to save your Template.

ESI FAST Option

The ESI FAST option is available as part of the ESI SC-4S. Several models are offered with different valves and vacuum pumps.

❖ **To adjust the ESI FAST settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to open a Template with a Configuration including the ESI autosampler.
4. Click 

.

5. Click ESI FAST to open the ESI FAST view, see Figure 6-83.

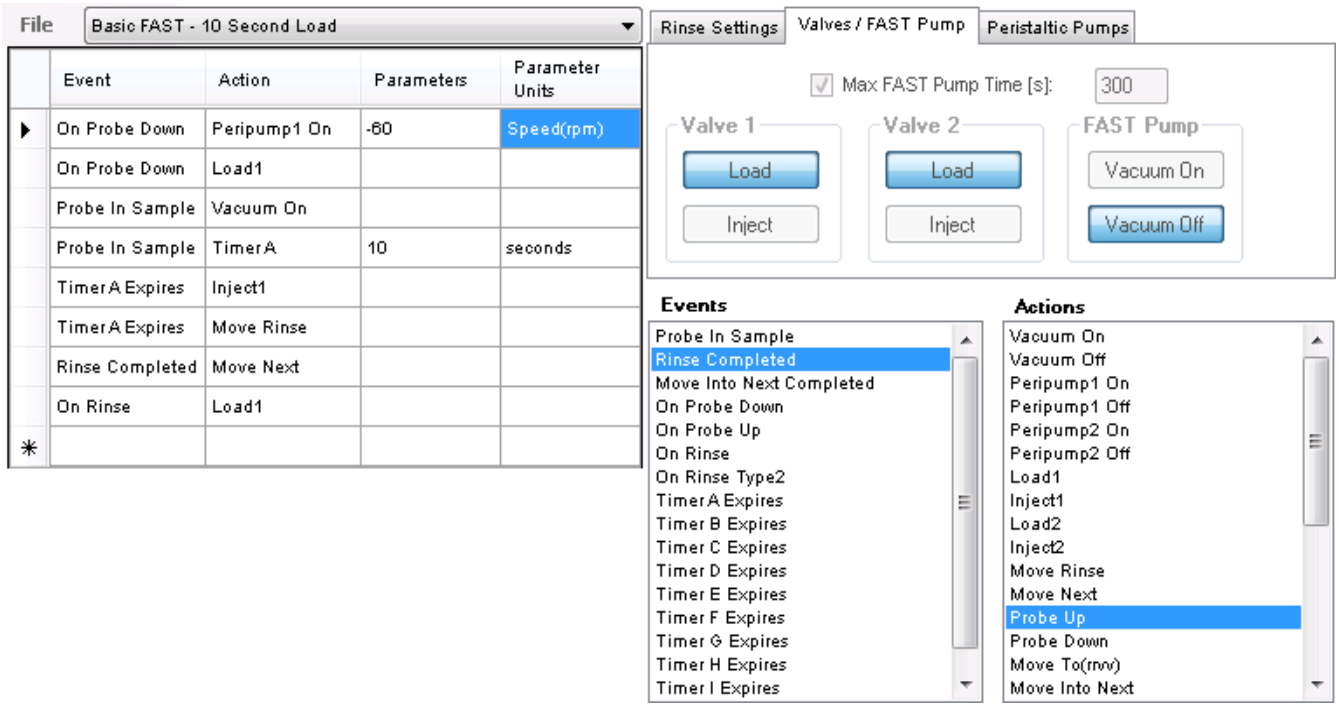


Figure 6-83. ESI FAST settings

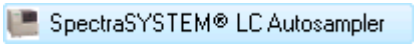
6. Select a **File** from the drop-down menu.
7. Add **Events** and **Actions** to your need.
   Changing these settings might only be possible in Instrument Control, ask your Administrator.
8. Click the tab **Rinse Settings** and adjust the settings to your needs.
9. Click the tab **Valves / FAST Pump** and adjust the settings to your needs.
10. Click the tab **Peristaltic Pumps** and adjust the settings to your needs.
11. Click  to save your Template.

SpectraSystem LC Autosampler

The SpectraSystem™ LC autosampler can be operated in combination with the SpectraSystem LC pump.

❖ **To adjust the SpectraSystem LC autosampler settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to open a Template with a Configuration including the SpectraSystem LC autosampler.
4. Click 

, see Figure 6-84.

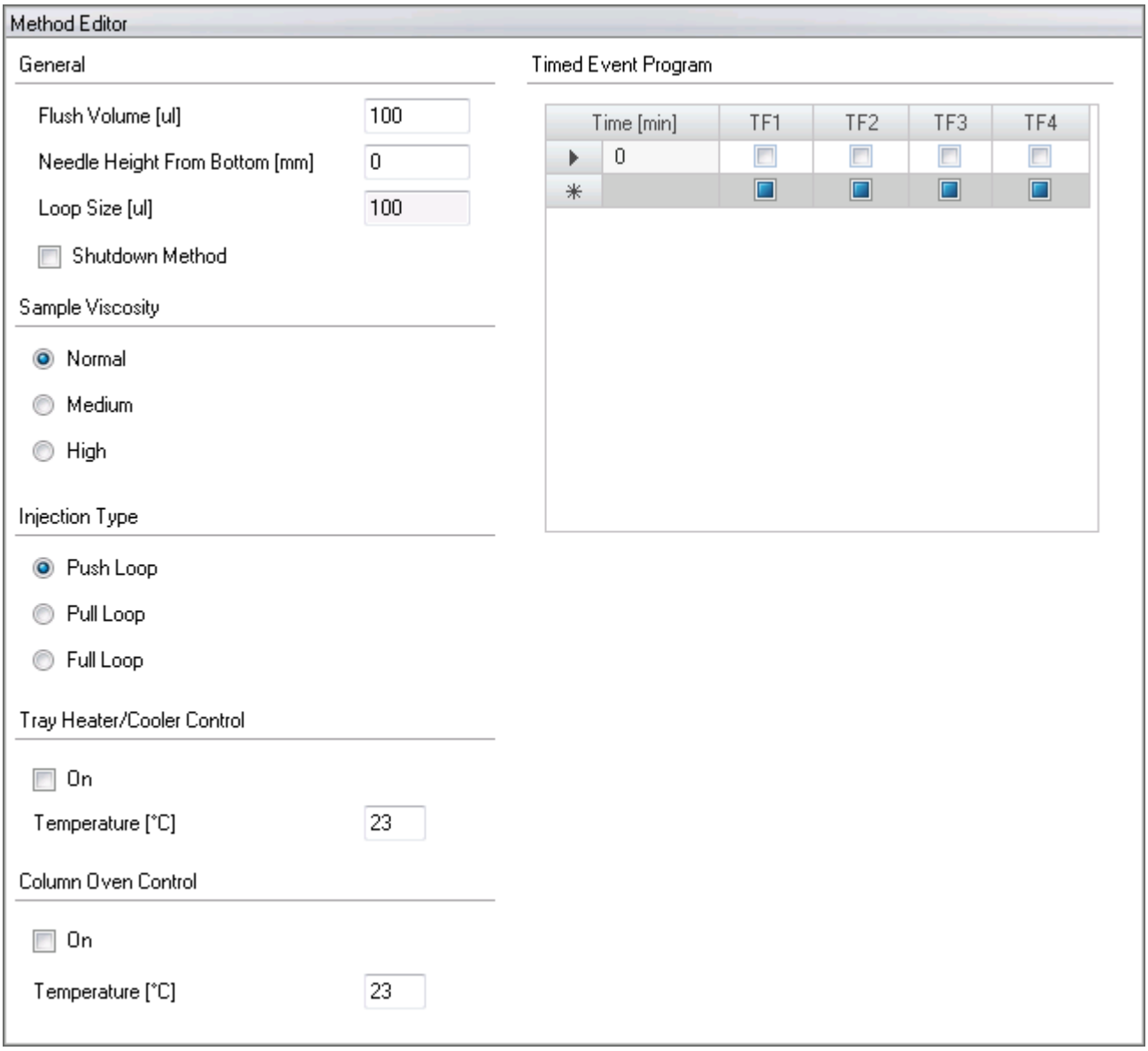


Figure 6-84. SpectraSystem LC autosampler settings

5. Enter the **Flush Volume [ul]** (µL).
6. Enter **Needle Height From Bottom [mm]**.
7. Enter **Loop Size [ul]** (µL).
8. In the table **Time Events Program**, add **Events** and **Actions** to your need.
9. Select the check box **Shutdown Method** if desired.
10. Select **Sample Viscosity** (**Normal**, **Medium** or **High**).
11. Select the **Injection Type** (**Push Loop**, **Pull Loop** or **Full Loop**).
12. Select the check box **On** for **Tray Heater/Cooler Control** and enter the **Temperature [°C]**, if desired.
13. Select the check box **On** for **Column Oven Control** and enter the **Temperature [°C]**, if desired.
14. In the **Time Event Program** table, select the check box in the desired column (TF1 to TF4) and enter the desired value in the column **Time [min]**.
15. Click  to add a row to the **Time Event Program** table.
16. Click  to save your Template.

SpectraSystem LC Pump

The SpectraSystem™ LC pump can be operated in combination with the SpectraSystem LC autosampler.

❖ **To adjust the SpectraSystem LC pump settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to open a Template with a Configuration including the SpectraSystem LC pump.

4. Click SpectraSYSTEM® LC Pump, see Figure 6-85.

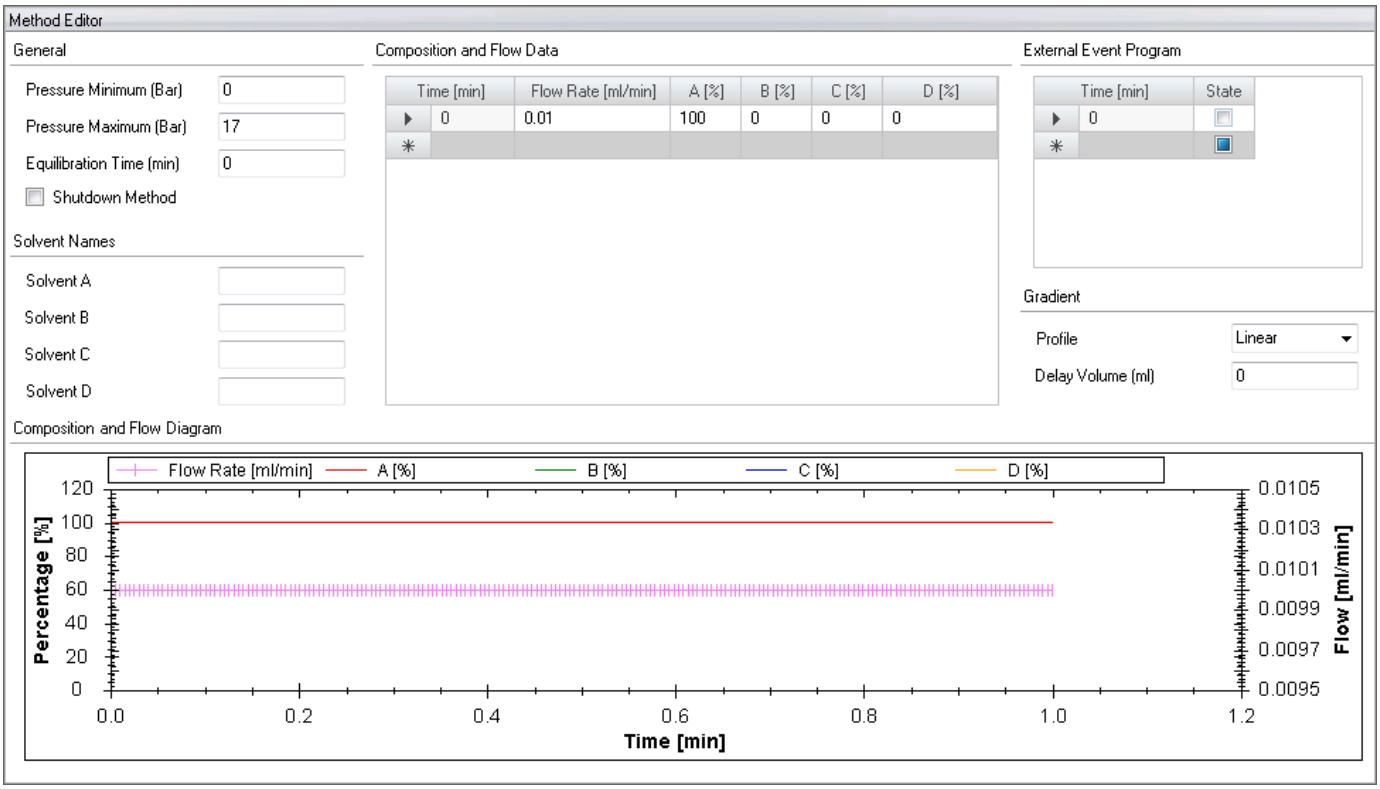


Figure 6-85. SpectraSystem LC pump settings

5. Enter **Pressure Minimum (Bar)**.
6. Enter **Pressure Maximum (Bar)**.
7. Enter the **Equilibration Time (min)**.
8. Select the check box **Shutdown Method** if desired.
9. Enter **Solvent Names**.
   The descriptions entered here immediately show in the table **Composition and Flow Data** and the legend of the diagram **Composition and Flow Diagram**.
10. In the table **Composition and Flow Data** click a cell in the column **Time [min]** and enter a value.
    The effect is immediately shown in the diagram below.
11. Click in the cell below and enter a value to add a row to the table.
12. Enter or changes values as appropriate.
13. In the table **External Event Program** click a cell in the column **Time [min]** and enter a value.
14. Select the check box **State** if appropriate.

15. Click  to add a row to the **External Event Program** table.
16. Select a **Profile** from the drop-down menu.
17. Enter a value for **Delay Volume (ml)** (mL).
18. Click  to save your Template.

Accela LC Autosampler

The Accela™ LC autosampler (600, 1000, 1250) can be operated in combination with the Accela LC pump.

NOTICE Settings for Syringe size and Tray Type must be selected in the Configurator tool by your Administrator (see "How to Edit the Settings of Instruments" on page 3-17). ▲

❖ To adjust the Accela LC autosampler settings

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to open a Template with a Configuration including the Accela LC autosampler.

4. Click Accela LC Autosampler, see Figure 6-86.

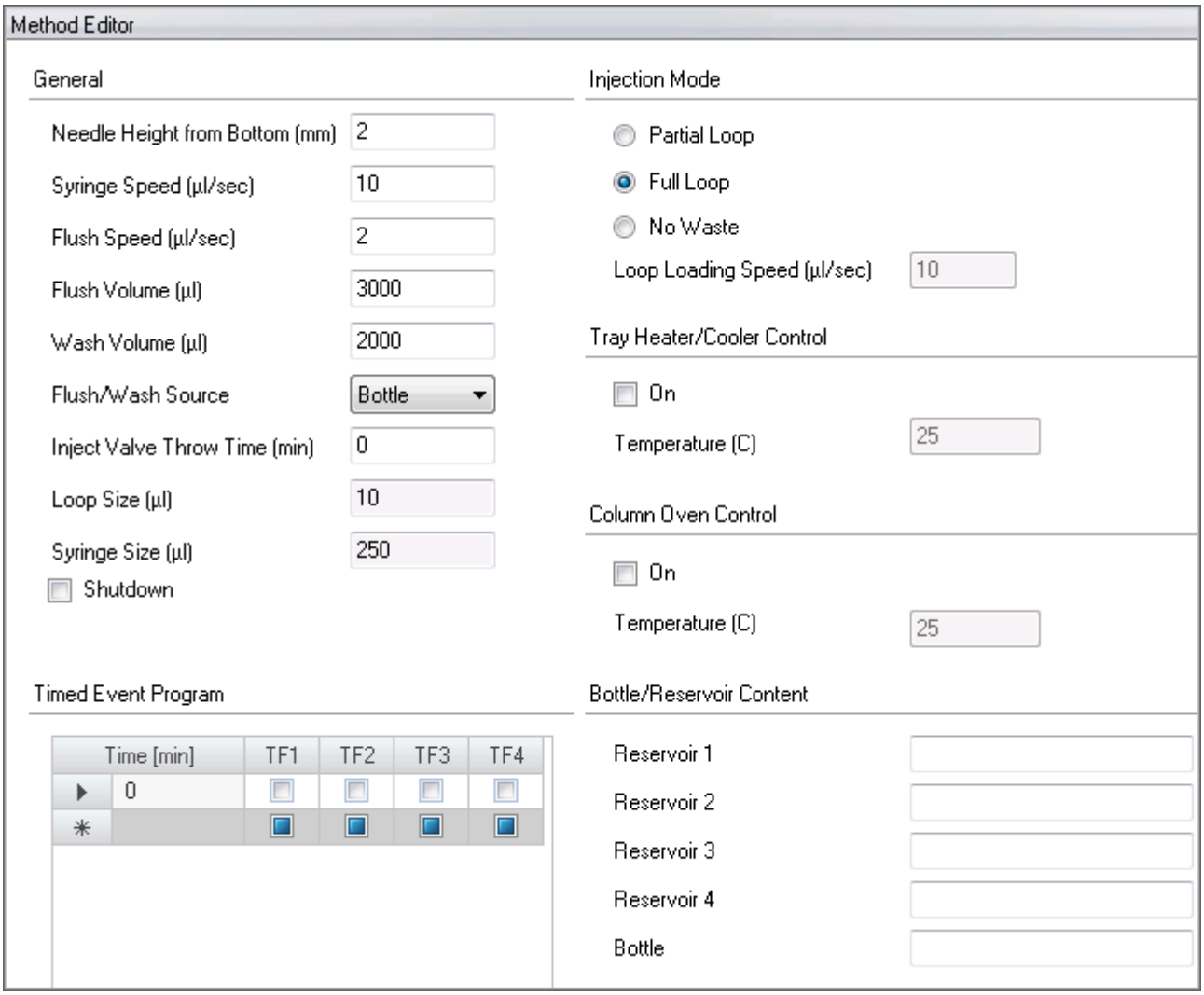


Figure 6-86. Accela LC autosampler settings

5. Enter the **Needle Height from Bottom [mm]**.
6. Enter the **Syringe Speed [µl/sec]** (µL/s).
7. Enter the **Flush Speed [µl/sec]** (µL/s).
8. Enter the **Flush Volume [µl]** (µL).
9. Enter the **Wash Volume [µl]** (µL).
10. Select the **Flush/Wash Source** from the drop-down menu.
11. Enter the **Inject Valve Throw Time (min)**.
12. Enter the **Loop Size [µl]** (µL).
13. Enter the **Syringe Size [µl]** (µL).
14. Select the check box **Shutdown Method** if desired.

15. In the **Time Event Program** table, select the check box in the desired column (TF1 to TF4) and enter the desired value in the column **Time [min]**.

16. Click  to add a row to the **Time Event Program** table.

17. Select the **Injection Mode** and enter the **Loop Loading Speed [µl/sec]** (µL/s).

18. Select the check box **On** for **Tray Heater/Cooler Control** and enter the **Temperature** (°C), if desired.

19. Select the check box **On** for **Column Oven Control** and enter the **Temperature** (°C), if desired.

20. Enter **Bottle/Reservoir Content**.

21. Click  to save your Template.

Accela LC Pump

The Accela™ LC pump can be operated in combination with the Accela LC autosampler.

NOTICE Pump model must be selected and Serial number must be entered in the Configurator tool by your Administrator (see "How to Edit the Settings of Instruments" on page 3-17). ▲

❖ To adjust the Accela LC pump settings

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
Be sure to open a Template with a Configuration including the Accela LC pump.

4. Click Accela LC Pump, see Figure 6-87.

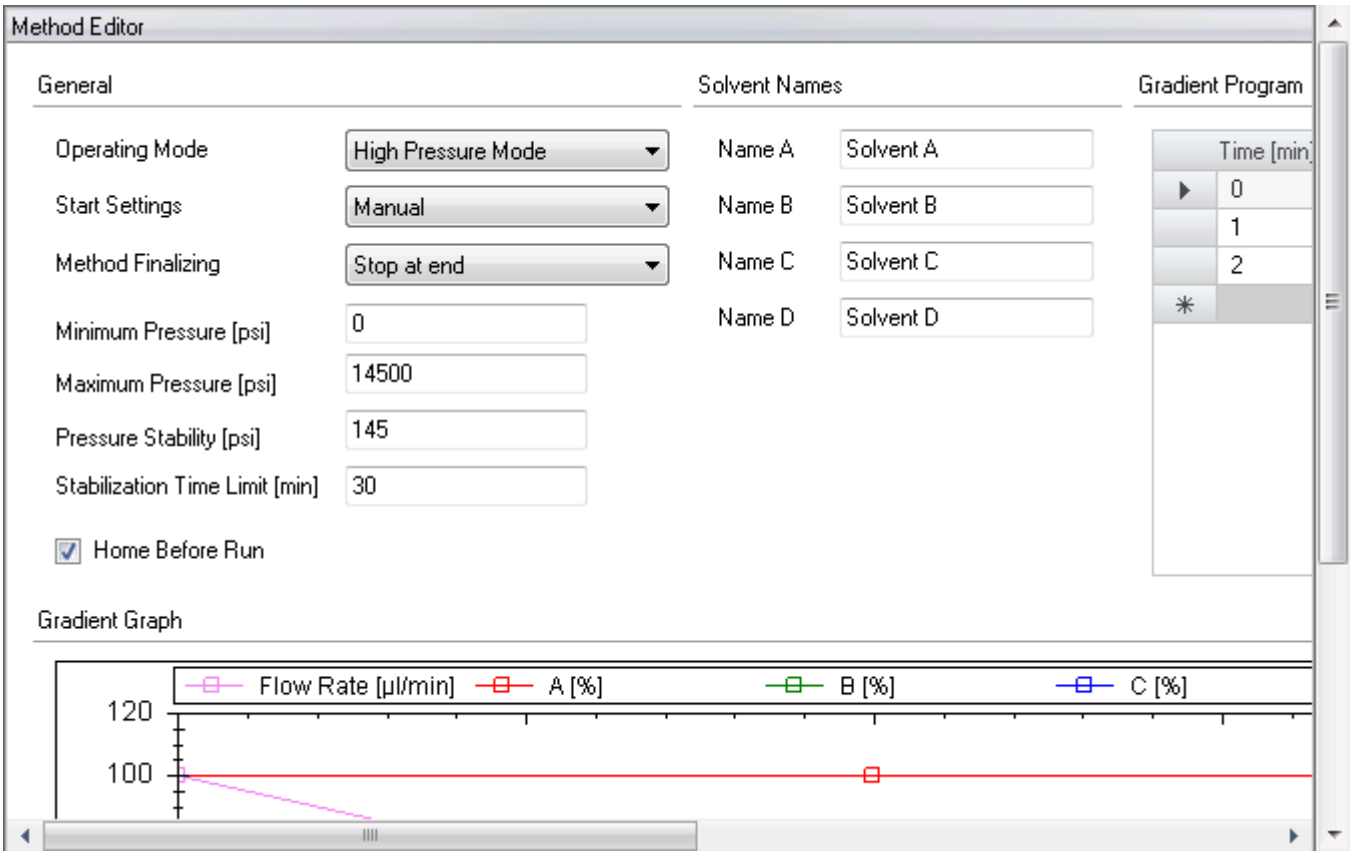


Figure 6-87. Accela LC pump settings

5. Select the **Operating Mode**, the **Start Settings**, and **Method Finalizing** each from the drop-down menus.
6. Enter **Minimum Pressure (psi)**.
7. Enter **Maximum Pressure (psi)**.
8. Enter **Pressure Stability (psi)**.
9. Enter the **Stabilization Time Limit [min]**.
10. Select the check box **Home Before Run** if desired.
11. Enter **Solvent Names**.
12. In the table **Gradient Program** click a cell and enter a value.
13. Click in the cell below and enter a value to add a row to the table.
14. Enter or changes values as appropriate.
    The effect is immediately shown in the diagram **Gradient Graph** below.
15. Click to save your Template.

Manual Sample Control

Manual Sample Control can be added to your Configuration in the Configurator to enter samples without autosampler.

NOTICE Configurations are created by your Administrator or Manager, see "Experiment Configurator" on page 3-13. ▲

In the Manual Sample Control view of a Template in Experiment Editor, Uptake and Wash Time can be defined, see Figure 6-88.

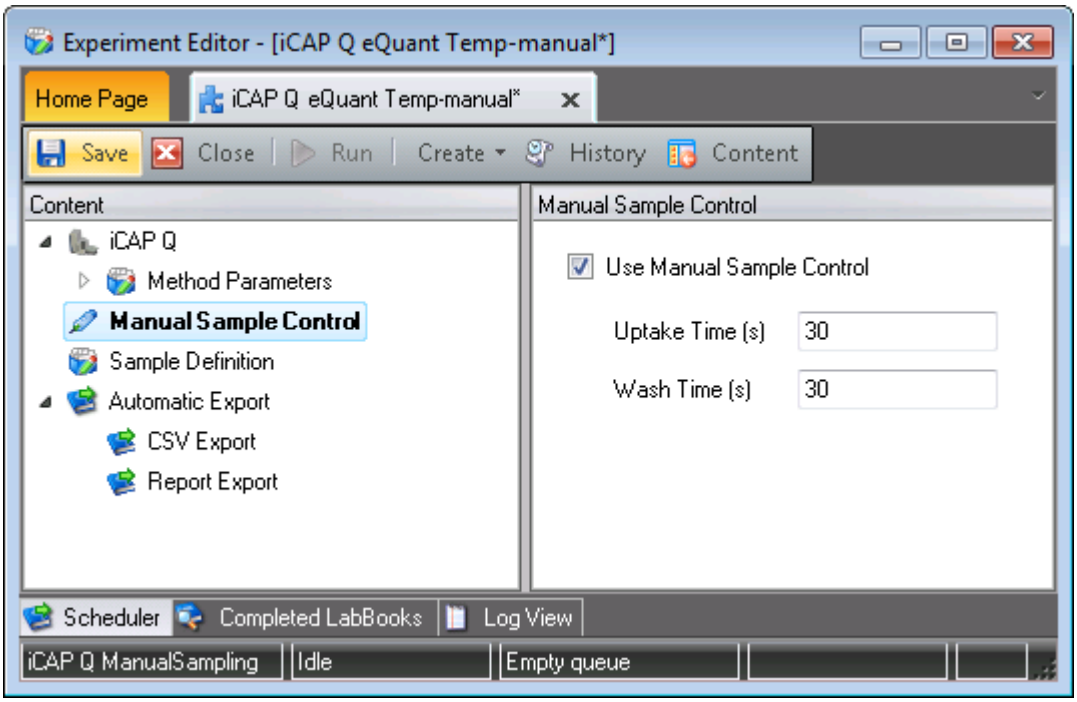


Figure 6-88. Manual Sample Control view in Template

❖ **To define Uptake and Wash Time for manual sampling**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to open a Template with a Configuration including Manual Sample Control and no other peripheral.
4. Click **Manual Sample Control** to open the Sample Definition view of the Template.
5. Select the check box **Use Manual Sample Control**.

6. Enter 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.

7. Click  to save your Template.

Sample Definition for a Template

Sample Definition is a sub-section in the Template view in Experiment Editor. In this section the parameters of the measurements are defined, see Figure 6-89.

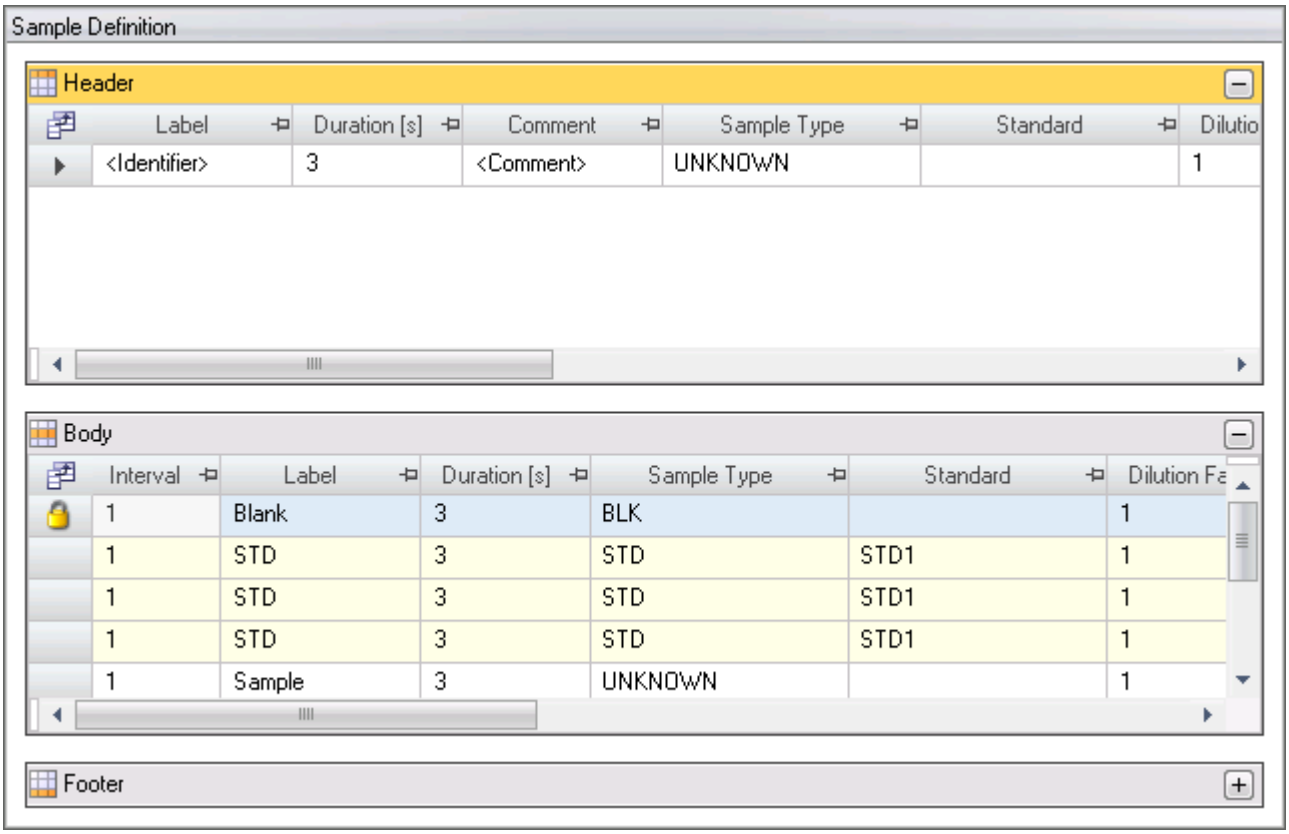


Figure 6-89. Sample Definition view

The Sample List of the LabBook is generated from the definition given in this section. For example, when eight Body items are defined in the Sample Definition section of the Template and 100 samples are defined when creating a New LabBook (see "LabBooks" on page 7-1), the Body section of the Template will be repeated 100 times if **Interval** has been set to 1.

In the **Header** you enter samples to be inserted once at the start of the sample list.

The **Body** rows make up a repeating unit of the Sample List when creating a LabBook. Typically standard and unknown sample types are defined here. The **Body** rows unit is repeated with the number of samples desired for the LabBook.

The **Footer** rows are for samples (such as QC samples) to be inserted at the end of the sample list.

Depending on the evaluation method selected for the Template, the columns of the components may differ. All columns that may be shown in Sample Definition are explained in Table 6-18.

Table 6-18. Columns of Sample Definition

Column	Description
Interval	Number of times this sample line is repeated for each sequence. For an **Interval** 3 and 3 samples, this line is inserted once. For an **Interval** 3 and 6 samples, this line is inserted twice.
Label	User-defined identification (name) for the sample line.
Duration	For tQuant and trQuant Templates. To set the time for acquiring the data.
Injection Volume	For tQuant Templates. Volume of the sample which is withdrawn from the vial and injected into the sample loop according to chosen mode of injection.
Survey Runs	For aQuant, eQuant, and rQuant Templates. Number of survey runs (mass spectrum scans) 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 the survey run are defined in the method parameters view "Survey Scan Settings" on page 6-26. **Recommended Settings:** It is recommended to run at least one survey run per sample when eQuant was selected as evaluation method. **NOTICE** Be aware of high concentration matrix components that are present in the mass spectral region of the survey run and that can saturate the detector. ▲
Main Runs	For aQuant, eQuant, and rQuant Templates. Number of main runs (peak jumping acquisition) performed. The number of runs can be set from *1* to *1,000,000*. By default, the number is set to *1*. **Recommended Settings:** It is recommended to run at least three main runs per sample.
Comment	Additional pertinent information about sample can be entered here.
Sample Type	For all except rQuant Templates. Definition of the sample type. See also "Data Evaluation" on page 10-1.
Internal Standard	For eQuant and trQuant Templates. 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 6-32.
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 6-32.

Table 6-18. Columns of Sample Definition

Column	Description
Dilution Factor	Dilution of sample. Can be used to define different calibration concentrations. Factors can be integers (dilution) or fractions (concentration).
Sample Amount	For rQuant Template to calculate concentrations.
Spike Amount	For rQuant Template to calculate concentrations.
Amount	Volume or mass of initial sample (enter unit, for example, <ml>).
Final Quantity	Volume (if volume is entered for Amount) or mass of final volume.
QC Action	For eQuant Templates. 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 (eQuant only)" on page 6-69.
QC Restart	For eQuant Templates. Defines restart of QC. Value is selected from drop-down list.
QC Reference	For eQuant Templates. If QC test type DUP or SER is selected for Template.
Special Blank	Added column in Sample List. To be selected from a drop-down list.
Rack Number/Tray/Block	Rack/Tray/Block number of peripheral.
Vial Number/Vial	Vial number of peripheral.

After creation of a LabBook from the Template (see "Template Toolbar" on page 6-2 and "Creating a LabBook" on page 5-16), the column **Special Blank** is added to the Sample List.

With **Special Blank**, see sample list example in Figure 6-90, it is possible to subtract the calculated concentrations of a sample from those of one or more others.

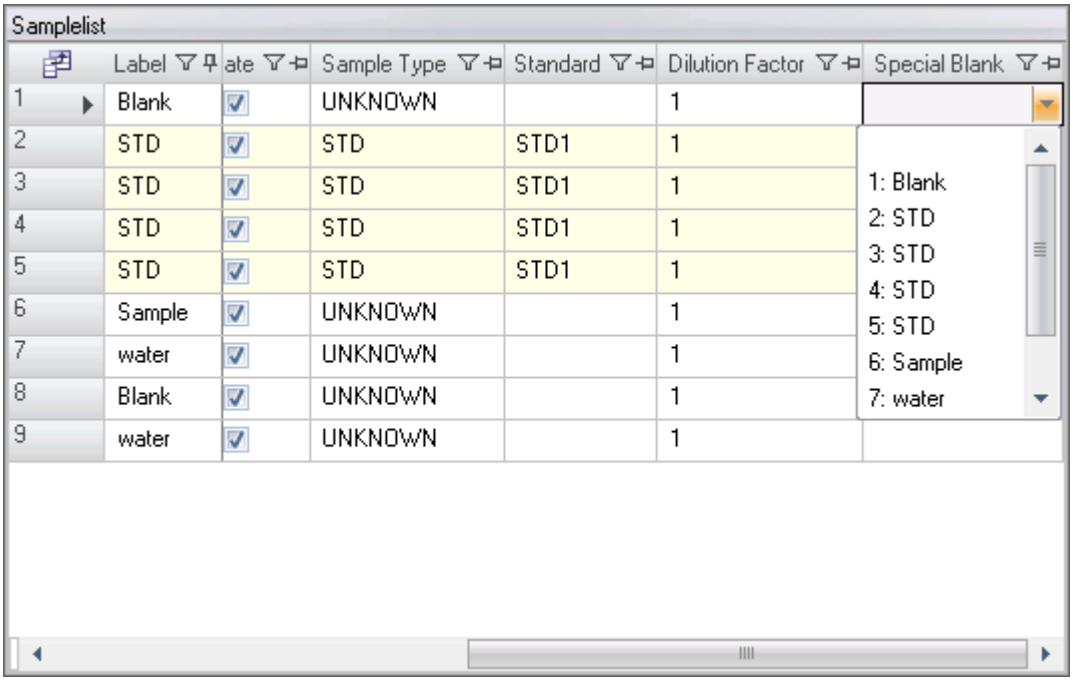


Figure 6-90. Sample List view with Special Blank

❖ **To open the Sample Definition view of a Template**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  **Sample Definition** to open the Sample Definition view of the Template.

Customizing the Columns for Sample Definition

In Experiment Editor, the columns for Header, Body and Footer of the Sample Definition view differ according to the evaluation method selected for the Template. You can show or hide columns and change the order in the table.

❖ **To customize the appearance of columns**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  **Sample Definition** to open the Sample Definition view of the Template.
5. In the Header, Body or Footer section you wish to change, click  to open the **Choose Columns** window, see Figure 6-91.

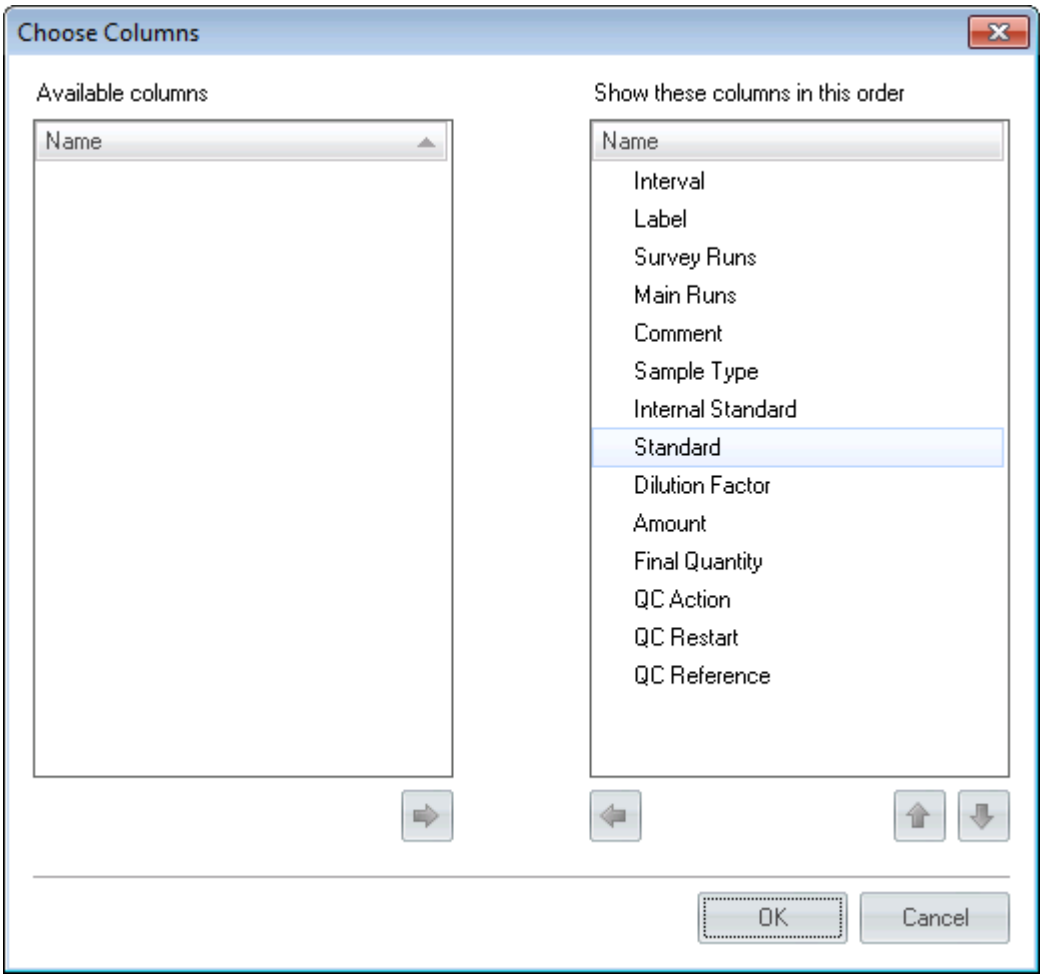


Figure 6-91. Choose Columns window of Sample Definition

6. Click  to move the column headings up or down.

7. Select a column in the right list and click  to move it to the left list.
   This column is hidden in the Sample Definition view.
   Double-clicking also moves the columns in the lists.

8. Click 

   .
   The columns are arranged accordingly.

Defining the Body, Footer and Header

In the Sample Definition view of Experiment Editor, Header, Body and Footer items are defined. Additional rows can be added and values can be defined.

❖ **To define Body, Footer and Header**

1. Click 

   to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click  **Sample Definition** to open the Sample Definition view of the Template.

5. In the Toolbar of the Template, click 

   to open the drop-down menu, see Figure 6-92.

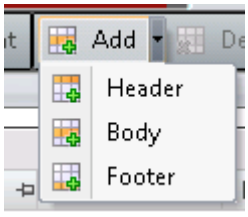


Figure 6-92. Add rows for Sample Definition

6. Select the item you wish to add a row for.
   A row is added to the selected item.

7. Adjust 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 6-117.

8. Click to save the Template.

Defining the Settings in Sample Definition

The settings for your experiment are defined in Experiment Editor in the Sample Definition section of your Template.

❖ **To define the settings of your experiment**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Define **Header**, **Body** and **Footer** as appropriate.
5. Add as many rows as you need for your experiment.
6. Enter a **Label** for each row.
7. Select a **Sample Type** from the drop-down list, see Figure 6-93.

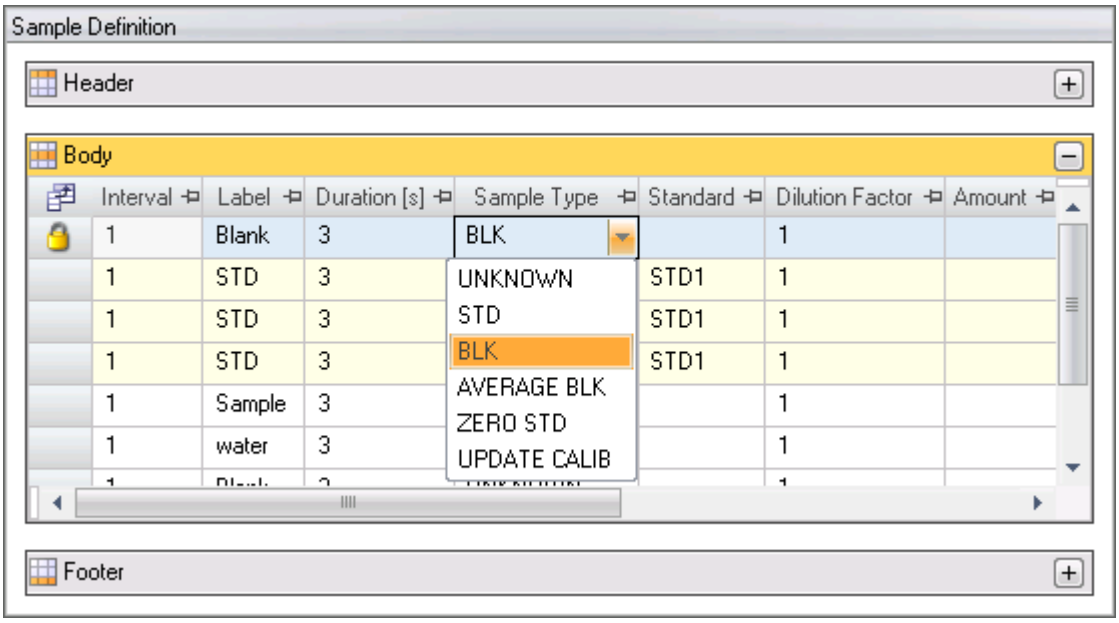


Figure 6-93. Sample Type drop-down in Template Sample Definition

For example, select **STD** for the calibration solution, **UNKNOWN** for the samples, and **BLK** or **AVERAGE BLK** for blanks. See also "Data Evaluation" on page 10-1.

8. Enter a value for each column or select an item from the drop-down list, as appropriate.

NOTICE For details on the columns, see "Sample Definition for a Template" on page 6-117. ▲

9. Click  to save the changes to your Template.

Automatic Export - Template

In the **Automatic Export** view of a Template in Experiment Editor, you define the export settings for your data as *.csv or *.xml file and for reports, see Figure 6-94.

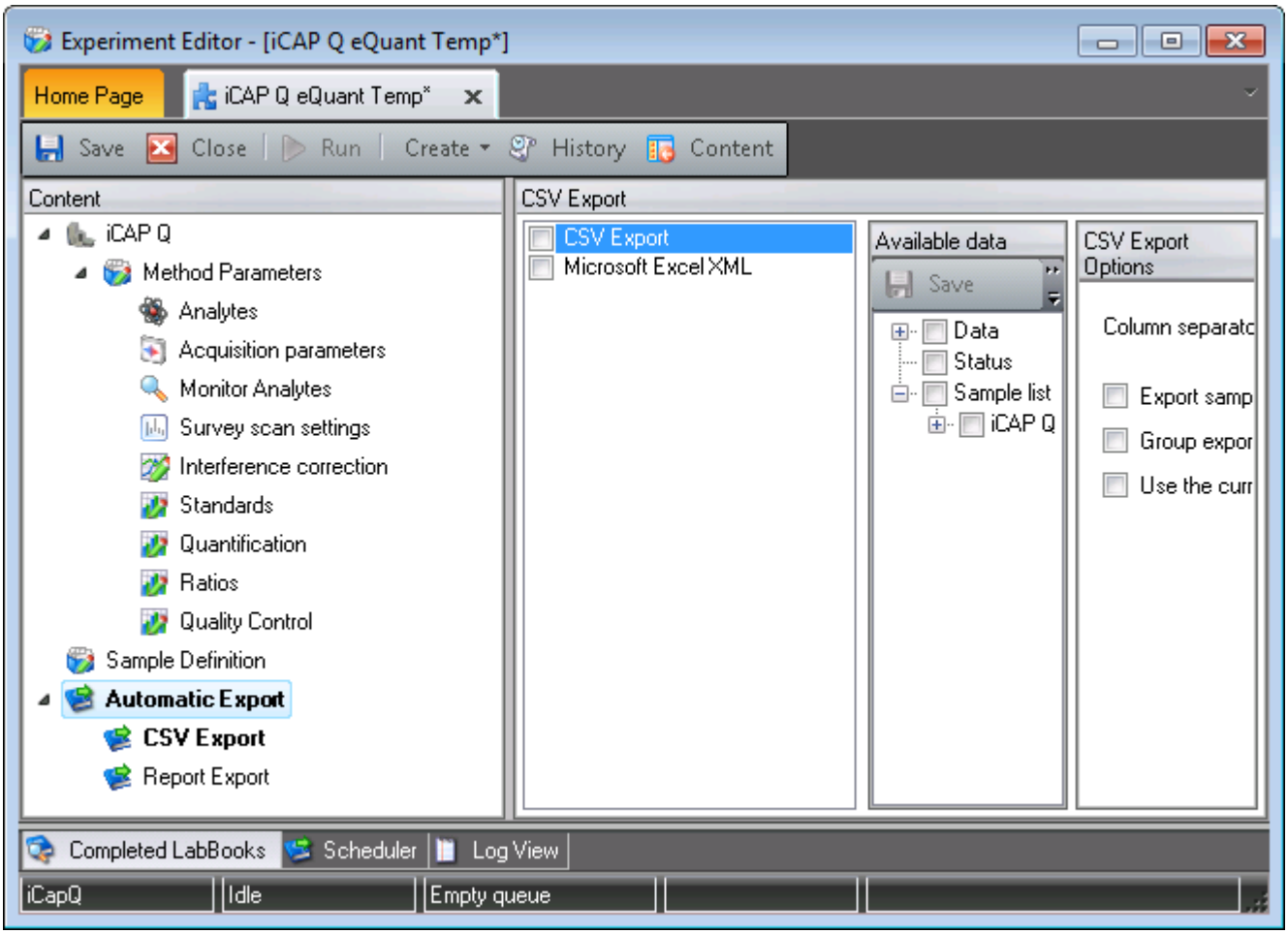


Figure 6-94. Template Automatic Export settings

Upon completion of the LabBook, the data are automatically exported as defined.

❖ **To define automatic export settings**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
4. Click  **CSV Export** to select this **Automatic Export** view.

5. Select the check box **CSV Export** to define these export settings, see Figure 6-95.

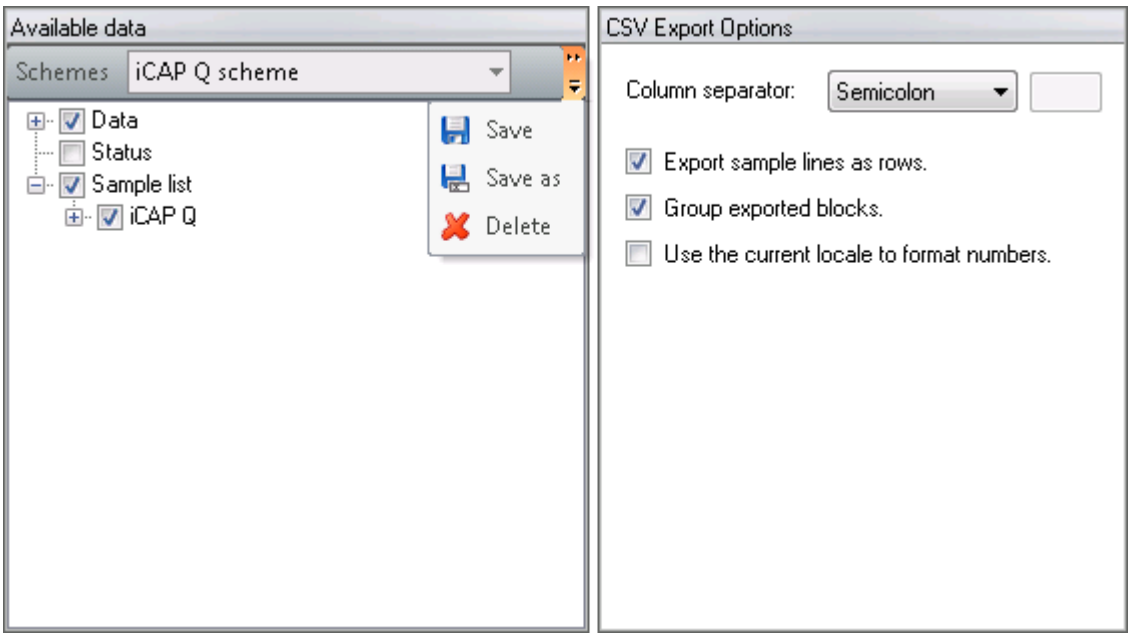


Figure 6-95. Automatic Export, CSV settings

6. For **Available data**, select the check boxes for the data you wish to export.
7. For **CSV Export Options**, select a **Column separator** from the drop-down list.
8. Select the check box **Export sample lines as rows** to show the sample lines as rows.
   If you do not select this check box, the sample lines are exported as columns.
9. Select the check box **Group exported blocks** to group the data output.
10. Select the check box **Use the current locale to format numbers** if you wish to format numbers as defined on your locale computer.

11. Click  to save the setting to a scheme.
    The **Save Export Scheme** dialog opens, see Figure 6-96.

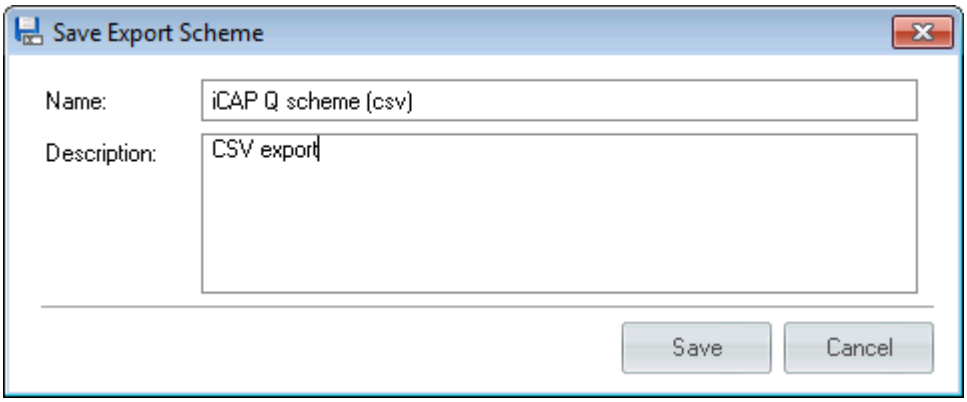


Figure 6-96. Save Export Scheme dialog (CSV)

12. Enter a **Name** and **Description**.

13. Click  .
    The settings for **CSV Export** are saved to this scheme.

14. Click **Microsoft Excel XML**.
    The corresponding CSV Export view opens, see Figure 6-97.

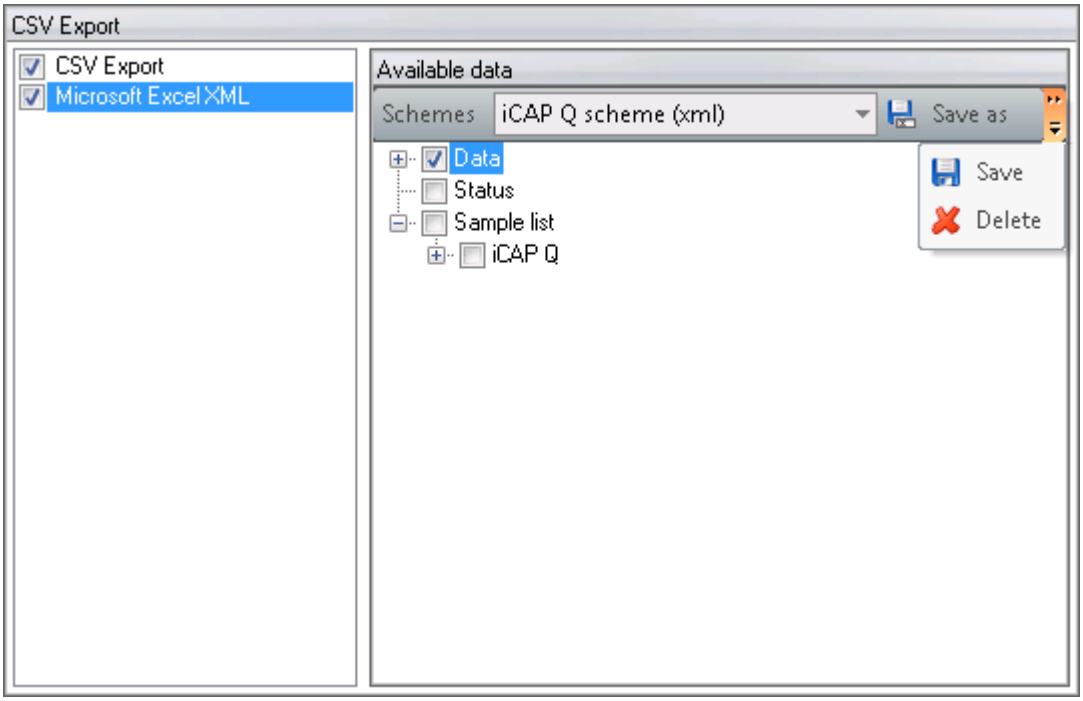


Figure 6-97. Automatic Export, XML settings

15. Select the check boxes for **Available data** to select the data you wish to export.

16. Click  to save the setting to a scheme.
    The **Save Export Scheme** dialog opens, see Figure 6-98.

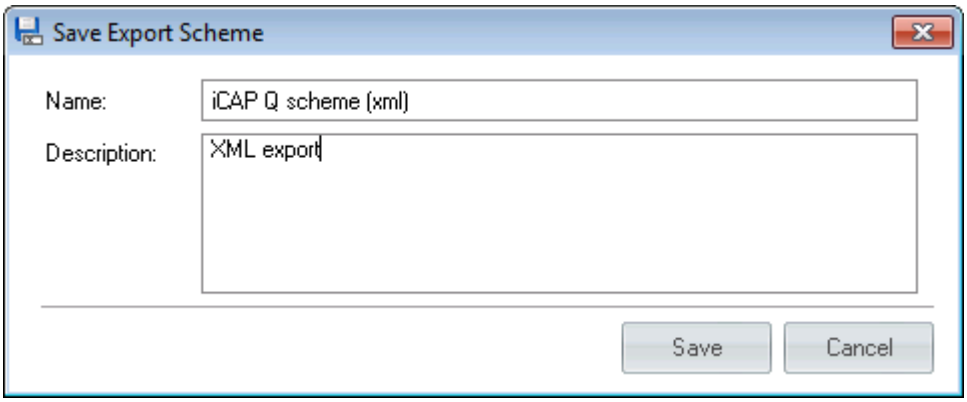


Figure 6-98. Save Export Scheme dialog (XML)

17. Enter a **Name** and **Description**.

18. Click  .
    The settings for **Microsoft Excel XML** are saved to this scheme.

19. Select the check boxes for the formats you wish to automatically export the data.

20. In the toolbar, click  to save the settings to the Template (or LabBook).

❖ **To define report export settings**

1. Click  to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.

4. Click  **Report Export** to select this **Automatic Export** view.

5. Click **Report Export** to define the settings.
   The Report Export view opens, see Figure 6-99.

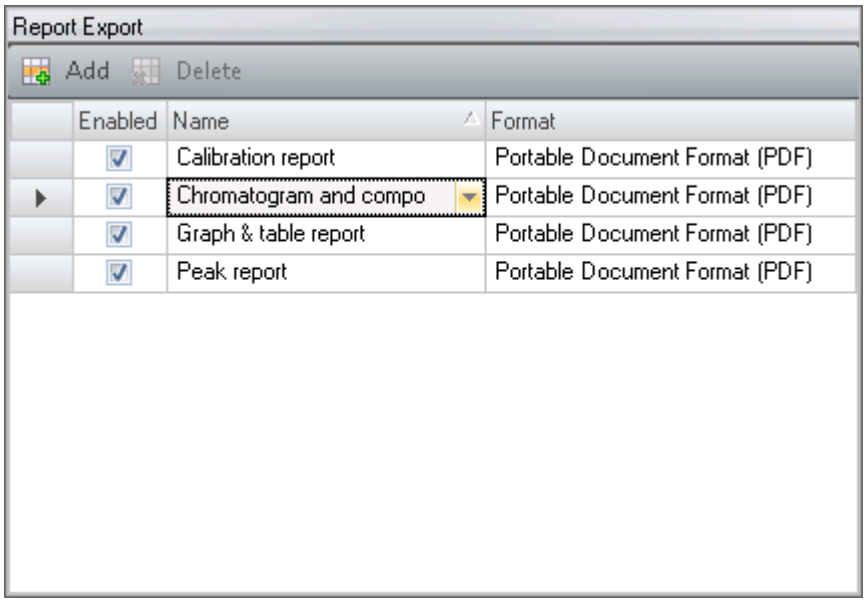


Figure 6-99. Automatic Export, Report Export active

6. Click  to add a row.

7. In the column **Name**, click  to open the drop-down menu, see Figure 6-100.

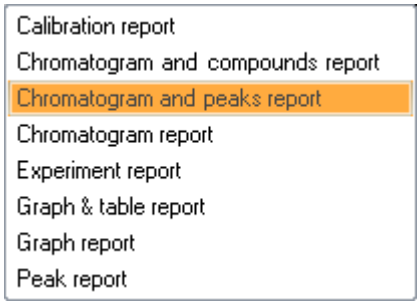


Figure 6-100. Report names

8. Select a **Name** for the report, for example, **Chromatogram and peaks report**.

9. In the column **Format**, click  to open the drop-down menu, see Figure 6-101.

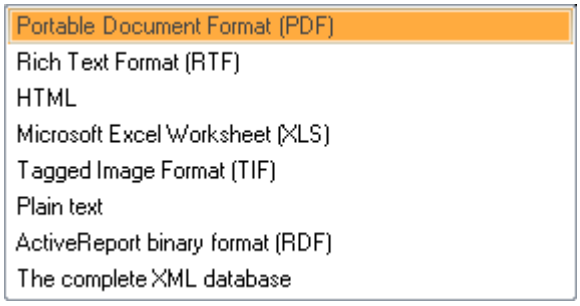


Figure 6-101. Report formats

10. Select a **Format** for the report, for example, **Portable Document Format (PDF)**.

11. Click the **Enabled** check boxes for the reports you wish to automatically export.

12. In the toolbar, click 

to save the settings to the Template (or LabBook).

Chapter 7 LabBooks

LabBooks are based on the settings specified in the "Templates" on page 6-1 in Experiment Editor. These setting can still be adjusted in the LabBook before the measurements is run.

Contents

- LabBook Toolbar
- Method Parameters LabBook
- Color Scheme of the Periodic Table
- Summary of LabBook
- Sample List - LabBook
- Automatic Export - LabBook
- Scheduling a LabBook
- Viewing the Result of a Measurement
- Log Messages
- Signing
- Query

❖ **To open a LabBook in the Experiment Editor tool**

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

LabBook Toolbar

In the LabBook tab of Experiment Editor, Qtegra offers buttons to save, close, run or export a LabBook, see Figure 7-1.

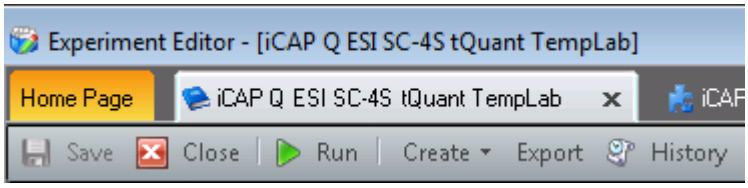


Figure 7-1. LabBook toolbar

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.

❖ **To save a LabBook**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Change the settings as appropriate.
5. Click  to save the LabBook.

❖ **To close a LabBook**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click  in the toolbar to close the LabBook.

   You can also click  in the tab of the LabBook.

❖ **To run a LabBook**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click  to run the LabBook.
The LabBook is added to the Scheduler and executed immediately.

❖ **To create a LabBook or Template from an existing LabBook**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click **Create**.
The **Create** drop-down menu opens, see Figure 7-2.

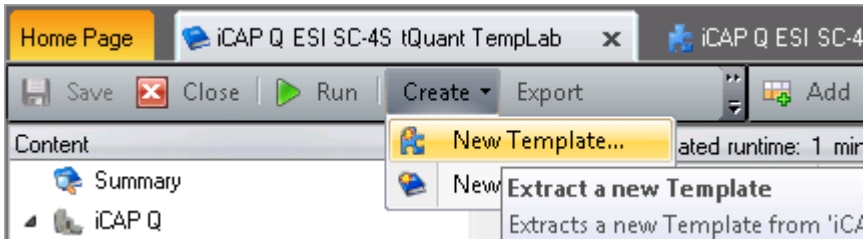


Figure 7-2. Create button in LabBook toolbar

5. 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 5-24 for further details.
6. 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 a LabBook" on page 5-16 for further details.

❖ **To export LabBook data**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. In the toolbar of the LabBook, click Export.
The **Export data** dialog opens, see Figure 7-3.

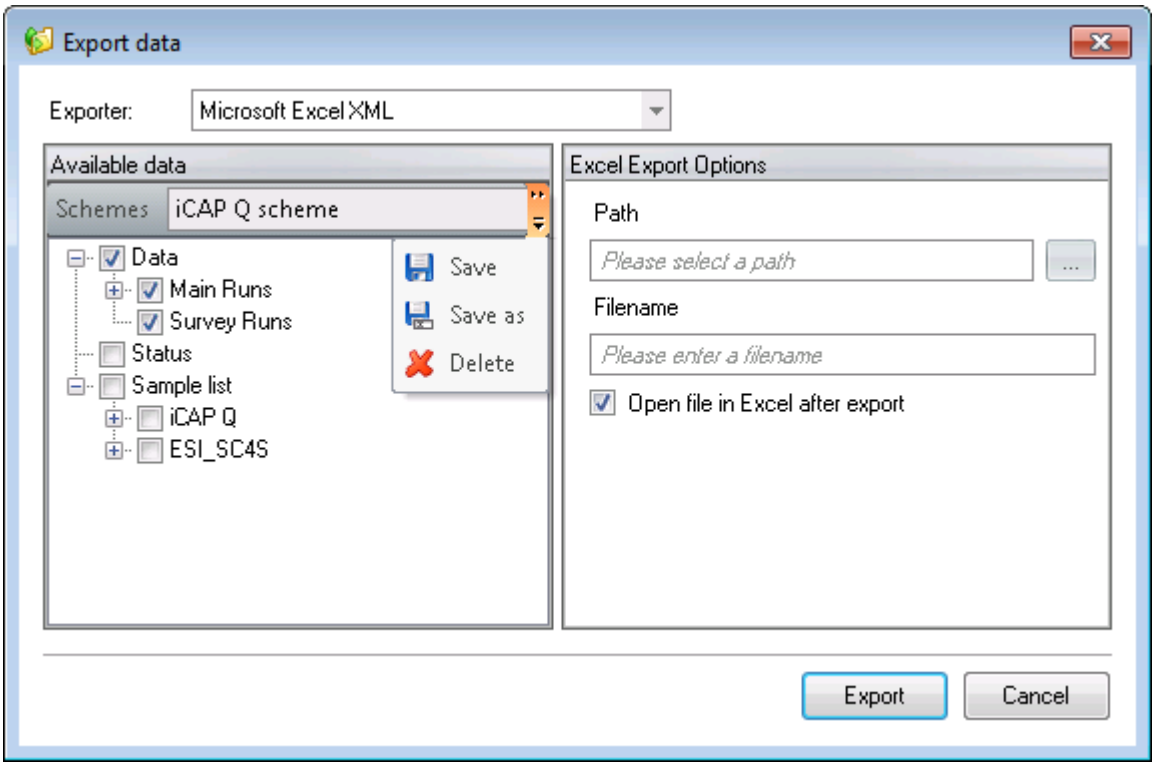


Figure 7-3. Export data dialog of LabBook

5. Select the check boxes for the data you wish to export.

6. Click Save as to save the settings as your scheme. The **Save Export Scheme** dialog opens, see Figure 7-4.

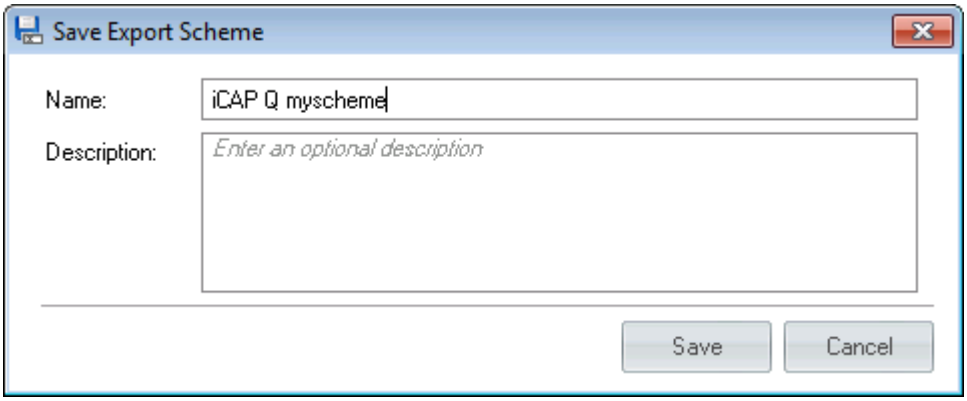


Figure 7-4. Export scheme of LabBook

7. Enter a **Name** and a **Description**.
8. Click Save.
9. In the **Excel Export Options** section on the right, select a **Path** and enter a **Filename**.
10. If you wish, select the check box **Open file in Excel after Export**.
11. Click Export.

❖ **To view the history of a LabBook**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

4. Click History.
   The **History** dialog for this LabBook opens, see Figure 7-5.

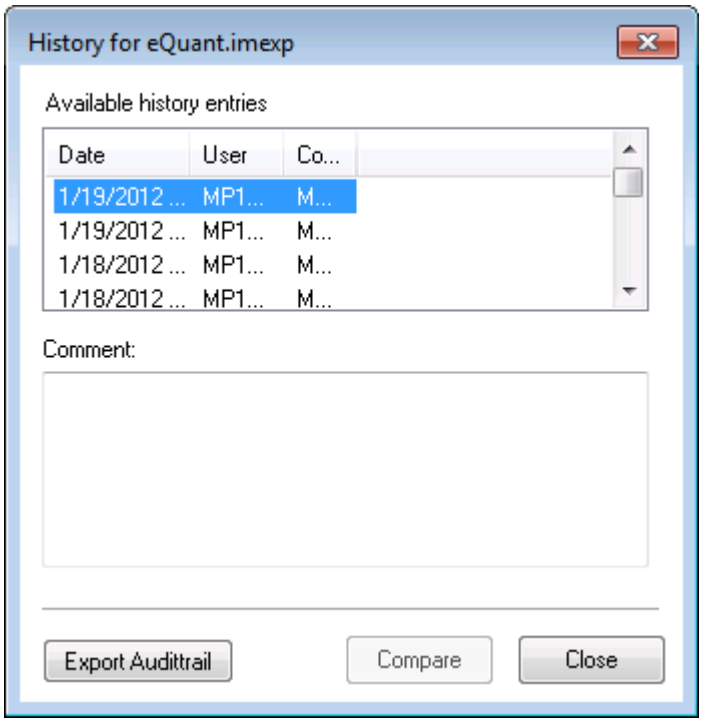


Figure 7-5. History dialog for LabBooks

5. Click Close to close the **History** dialog for this LabBook.

❖ **To compare the history entries of a LabBook**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

4. Click History.
   The **History** dialog for this LabBook opens, see Figure 7-6.

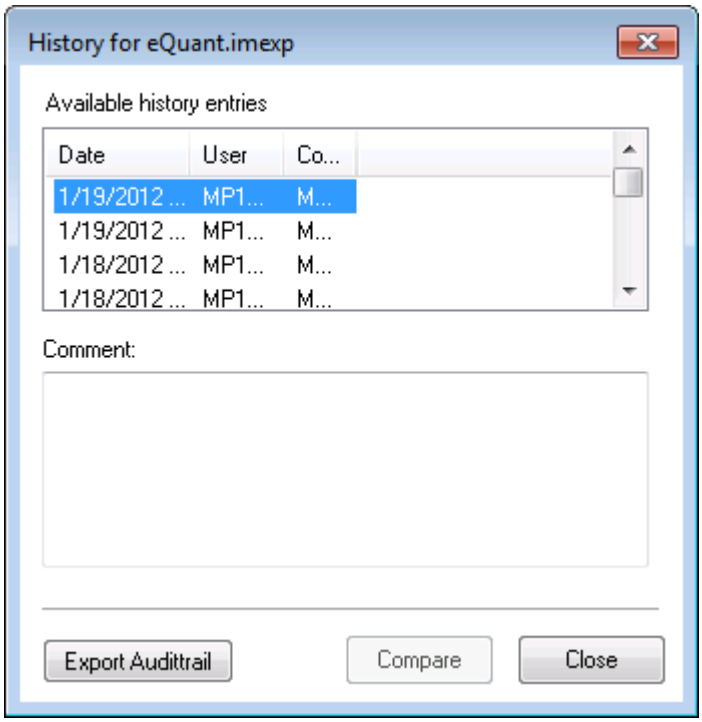


Figure 7-6. History dialog for LabBooks

5. Press <**Ctrl**> and select the entries you wish to compare.

6. Click Compare to compare the selected entries.
   The **Comparison** dialog opens, see Figure 7-7.

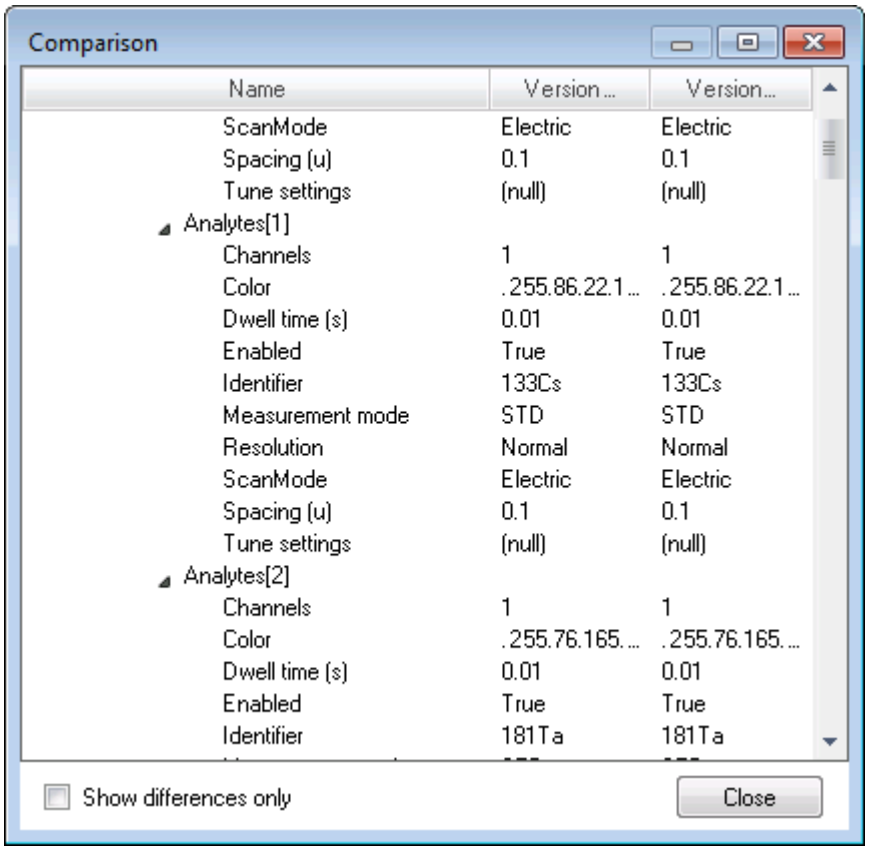


Figure 7-7. History Compare dialog for LabBook

7. Select the check box **Show differences only** if you wish to view only the differences.

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

9. Click Close to close the **History** dialog for this LabBook.

❖ **To export the audit trail of a LabBook**

1. Click Experiment Editor to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

4. Click History.
   The **History** dialog for this LabBook opens, see Figure 7-8.

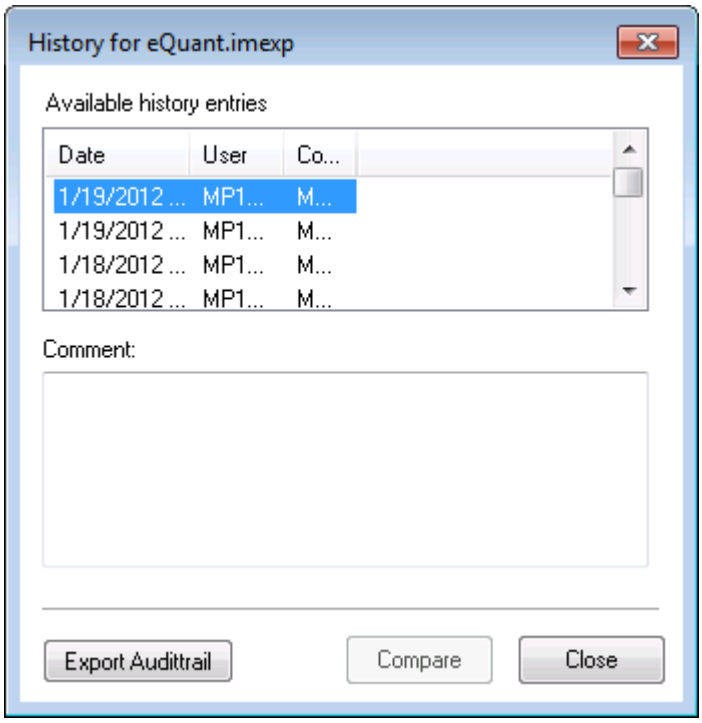


Figure 7-8. History LabBook dialog

5. To export the History audit trail, click Export Audittrail.
   The **Export Audittrail** dialog opens, see Figure 7-9.

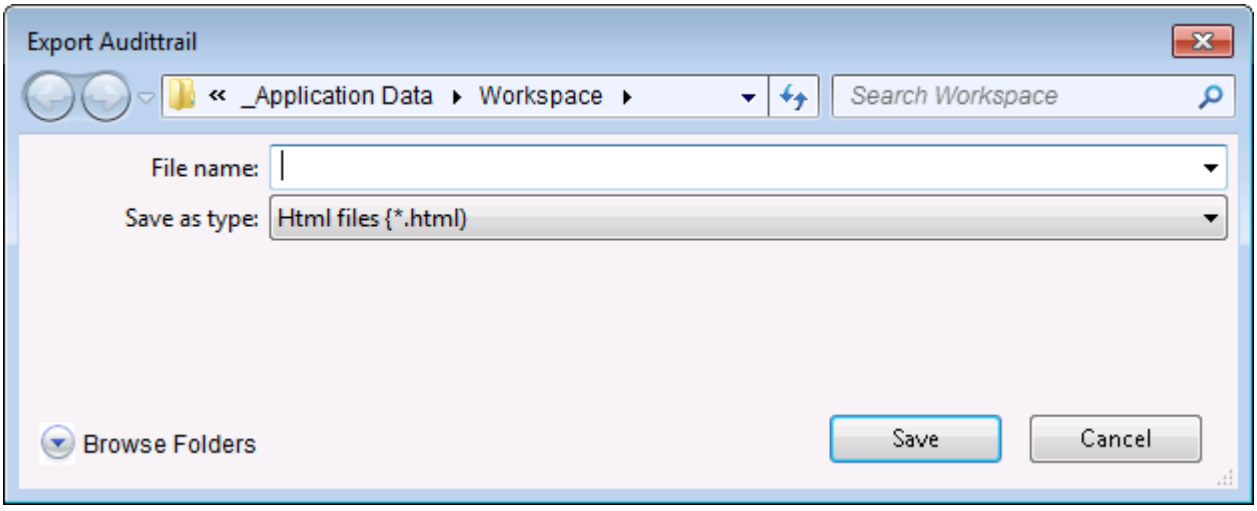


Figure 7-9. History Export Audittrail dialog

6. Click **Browse Folder** if you wish to change the pre-configured location of the file and select the directory.

7. Enter a **File name** for the HTML file, and click Save.
   Your standard web browser opens displaying the audit trail information.

8. Click Close to close the **History** dialog for this LabBook.

❖ **To hide Content pane**

1. Click Experiment Editor to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
   The **Content** pane of the LabBook is shown on the left, see Figure 7-10.

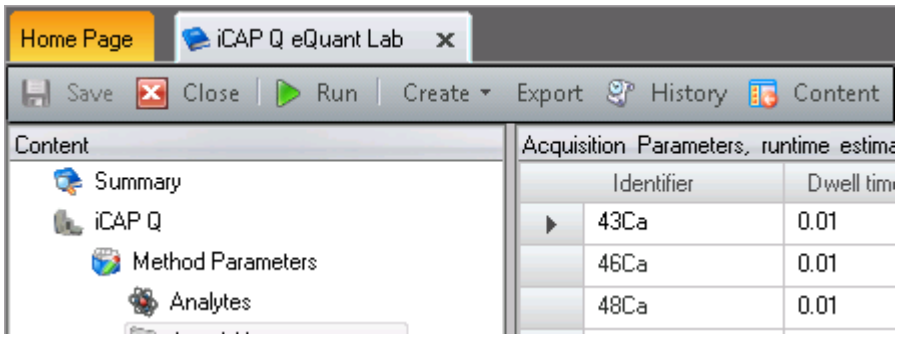


Figure 7-10. Content pane of LabBook visible

4. Click Content.
   The **Content** pane is hidden, see Figure 7-11.

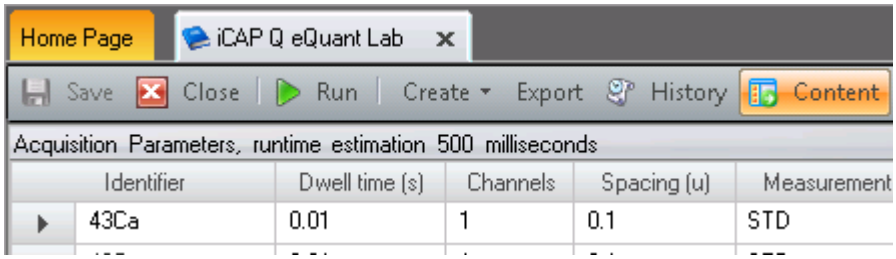


Figure 7-11. Content pane of LabBook hidden

5. Click Content to show the **Content** pane again.

Color Scheme of the Periodic Table

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 6-12. These settings can be changed in the LabBook.

Method Parameters LabBook

Method Parameters differ for each LabBook and are inherited from the Template from which the LabBook is created in Experiment Editor. 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 a tQuant Template is shown in Figure 7-12.

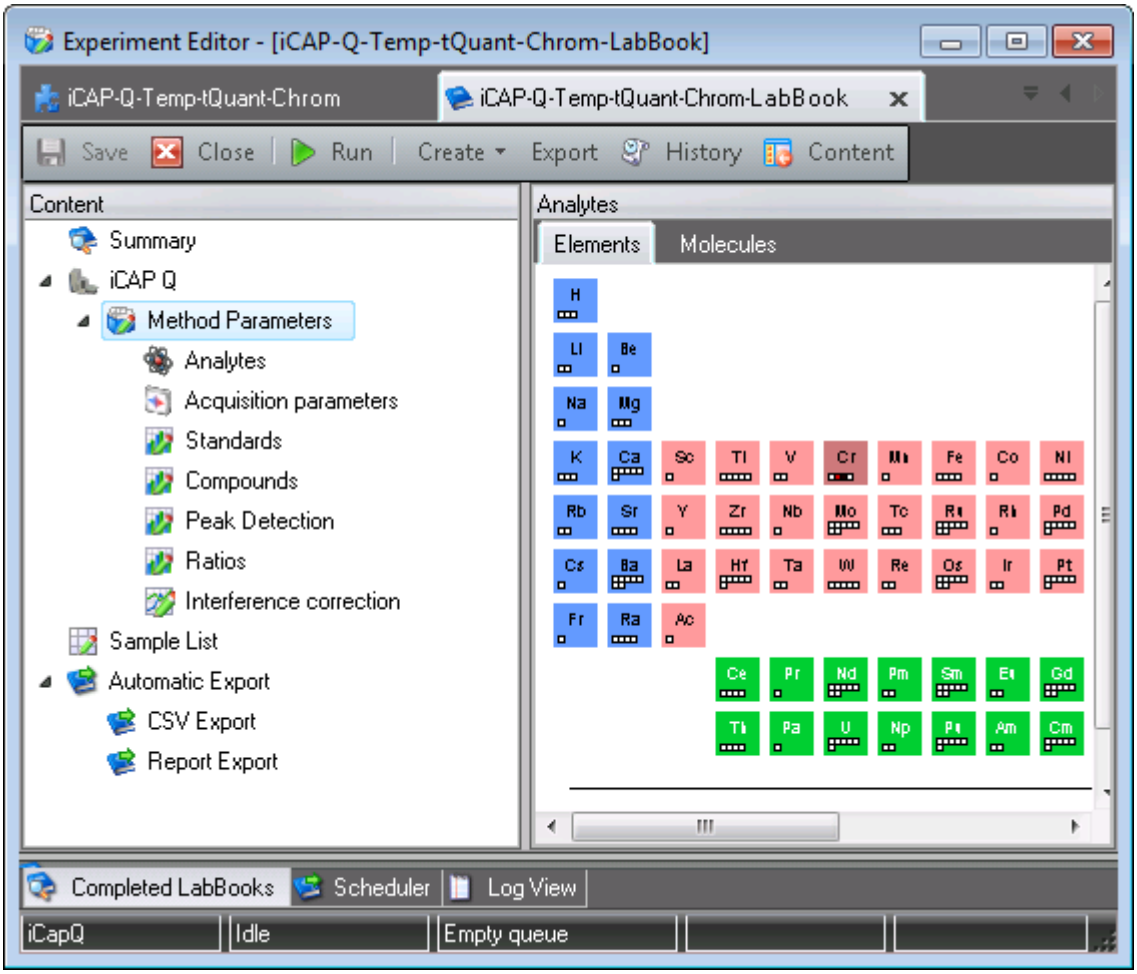


Figure 7-12. LabBook Method Parameters

All settings of the Method Parameters can be still be changed in the LabBook in Experiment Editor. For details, see "Method Parameters" on page 6-15.

NOTICE 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 6-117. ▲

Summary of LabBook

A summary page is added to each LabBook in Experiment Editor. This page shows the file name, and information about Properties, Date and People for the LabBook, see Figure 7-13.

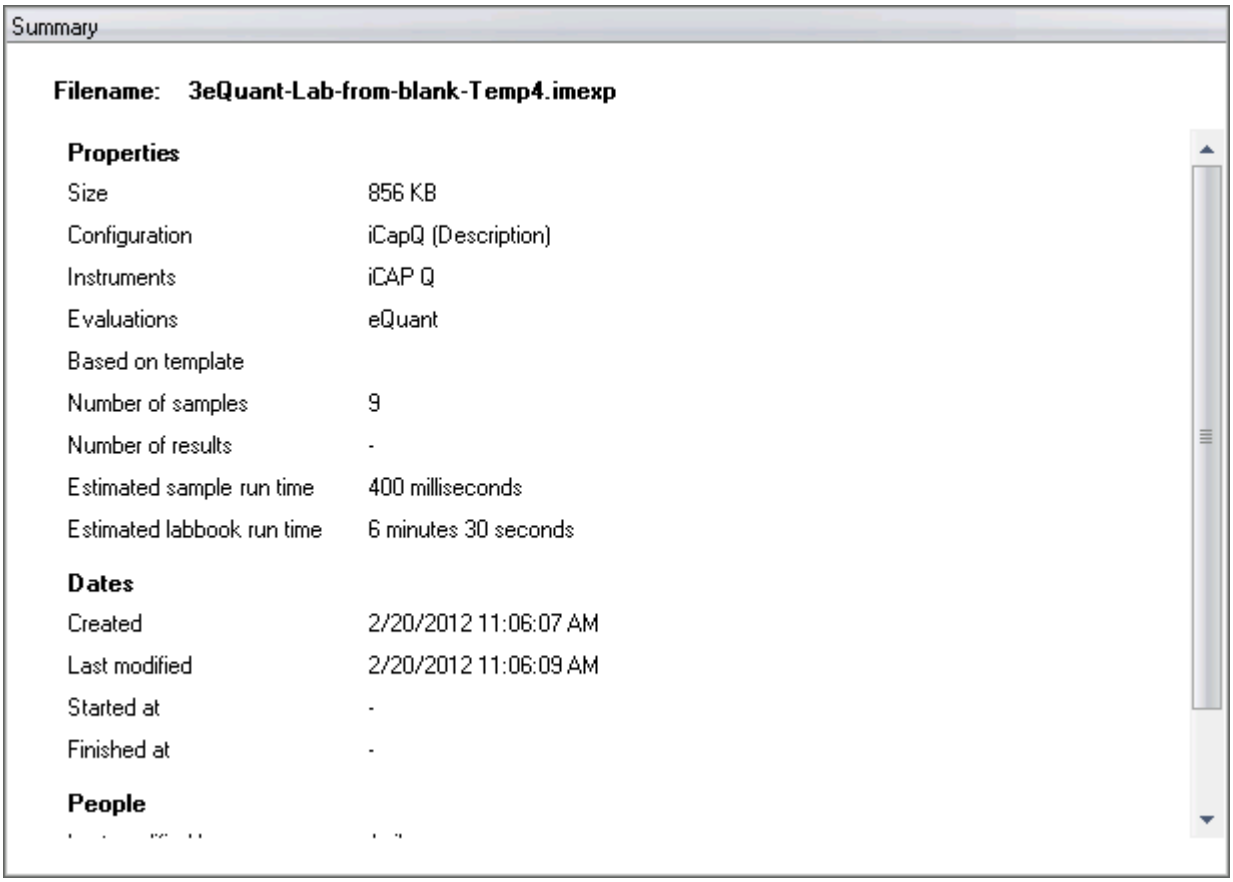
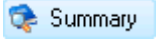


Figure 7-13. Summary of LabBook

❖ **To show the summary of a LabBook**

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click 

to view the summary of the LabBook.

Sample List - LabBook

The Sample List of a LabBook in Experiment Editor is based on the number of samples selected for analysis, and the structure of the Header, Body and Footer items defined in the section of the Templates (see "Sample Definition for a Template" on page 6-117).

An example of a sample list in a LabBook created from a tQuant Template is shown in Figure 7-14.

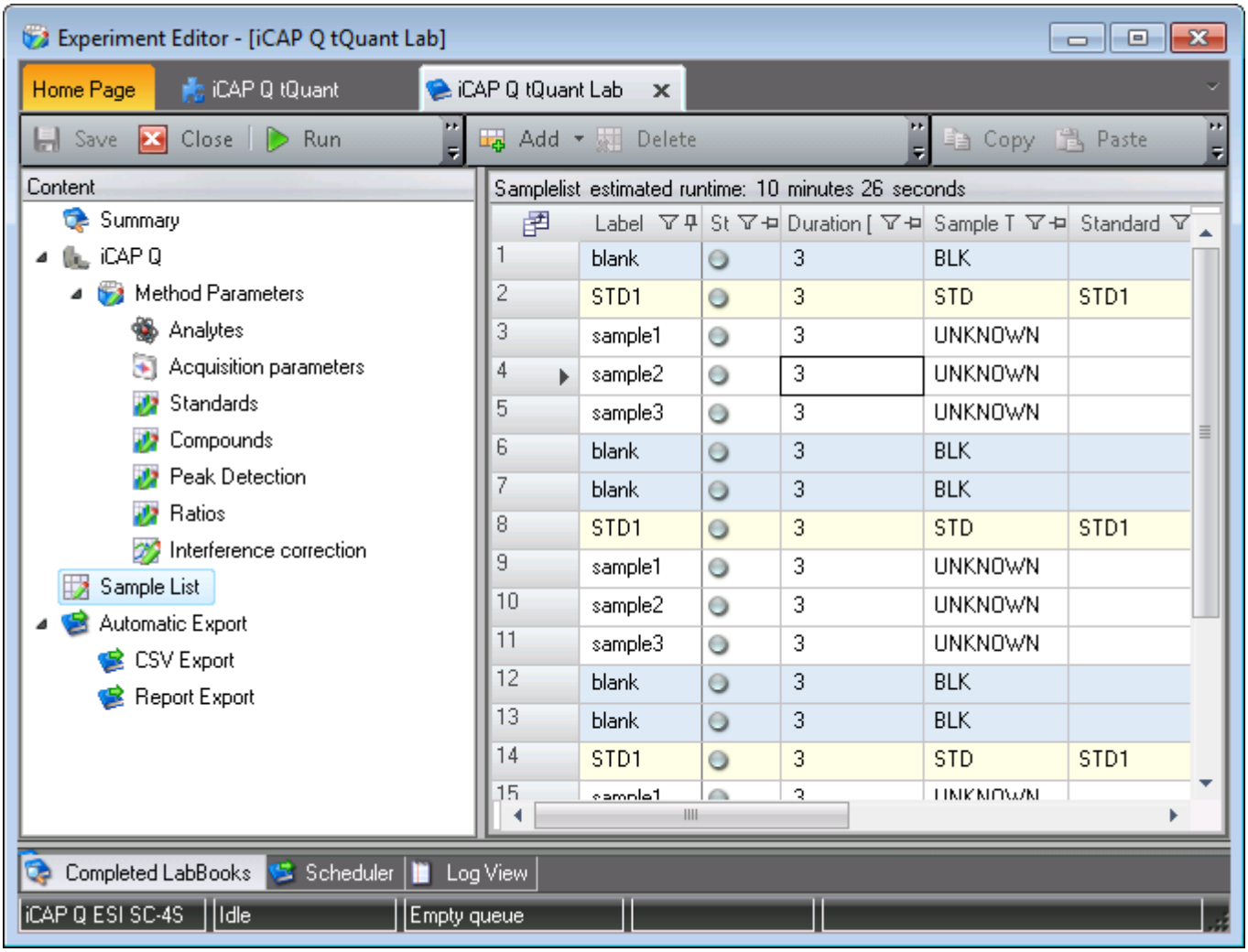


Figure 7-14. Sample list of LabBook

❖ **To view the Sample List**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

4. Click Sample List to view the **Sample List** of the LabBook.

❖ **To add a row to the Sample List**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click Sample List to view the **Sample List** of the LabBook.
5. Click Add to add a row below the Sample List.

❖ **To delete a row to the Sample List**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click Sample List to view the **Sample List** of the LabBook.
5. Click the gray field in front of the row you wish to delete.
6. Click Delete to delete the selected row.

❖ **To show comments of the Sample List**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click Sample List to view the **Sample List** of the LabBook.

5. 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. Click Experiment Editor to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click Sample List to view the **Sample List** of the LabBook.
5. Click Comments to show the comment for the selected row. The list of comments opens below the sample list.
6. Click Add Comment to add a comment for the selected row. The **User Comment** window opens, see Figure 7-15.

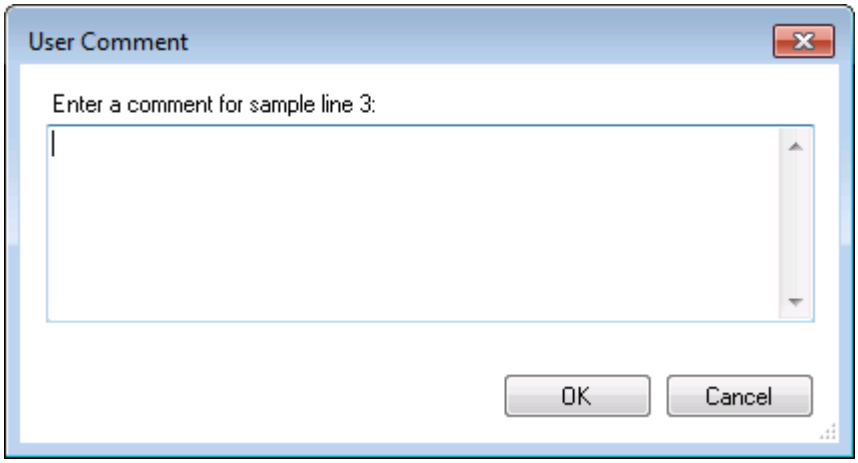


Figure 7-15. Add user comment to sample list row

7. Enter your comment.
8. Click OK.
   The comment is added and the User comment window closes.

❖ **To hide comments of the Sample List**

1. Click Experiment Editor to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.
4. Click 

to view the **Sample List** of the LabBook.
5. Click 

to hide the comment for the selected row. The list of comments is hidden.

Automatic Export - LabBook

Before measurement, you can define **Automatic Export** settings for a LabBook in Experiment Editor. Upon completion of the LabBook, the data are automatically exported.

You define the export settings for your data as *.csv or *.xml file and for reports, see Figure 7-16.

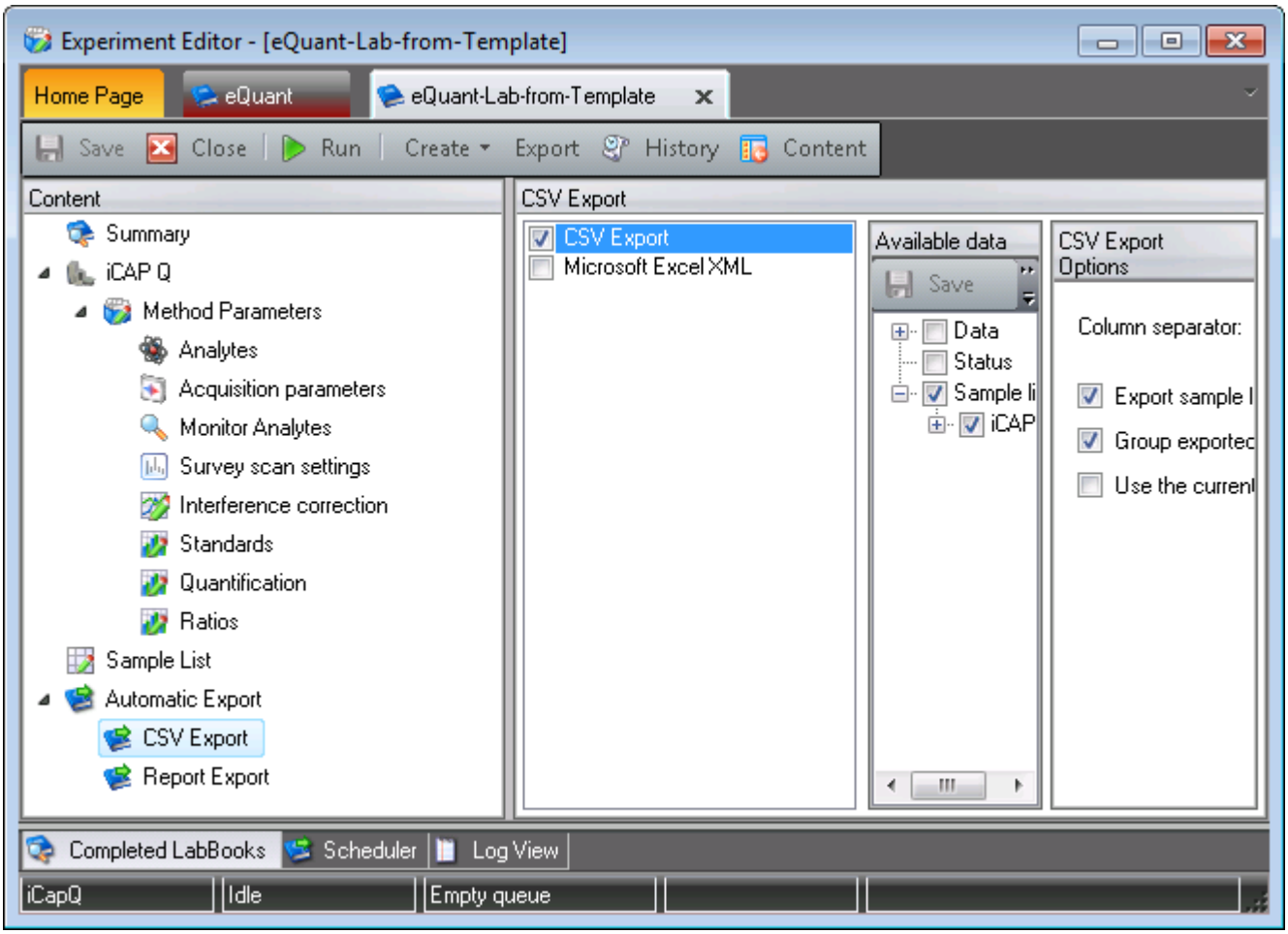


Figure 7-16. LabBook Automatic Export settings

LabBooks inherit the Automatic Export settings from the Template. See "Automatic Export - Template" on page 6-125 for details.

NOTICE 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 7-2. ▲

Scheduling a LabBook

To schedule a measurement, you open a LabBook in Experiment Editor and run it. Evaluation results can be accessed in a running LabBook so results can be viewed in real time, see "Evaluation Results" on page 7-22.

In the **Tools** section on the **Help** page of Experiment Editor, you define your **Scheduler** settings, see "Customizing Scheduler Settings" on page 5-49.

NOTICE To customize the Options of the Scheduler, you can also click the 

button. ▲

❖ To run a LabBook

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

4. Click  to schedule the LabBook for execution.
The LabBook is added to the Scheduler and the measurement is started, see Figure 7-17.

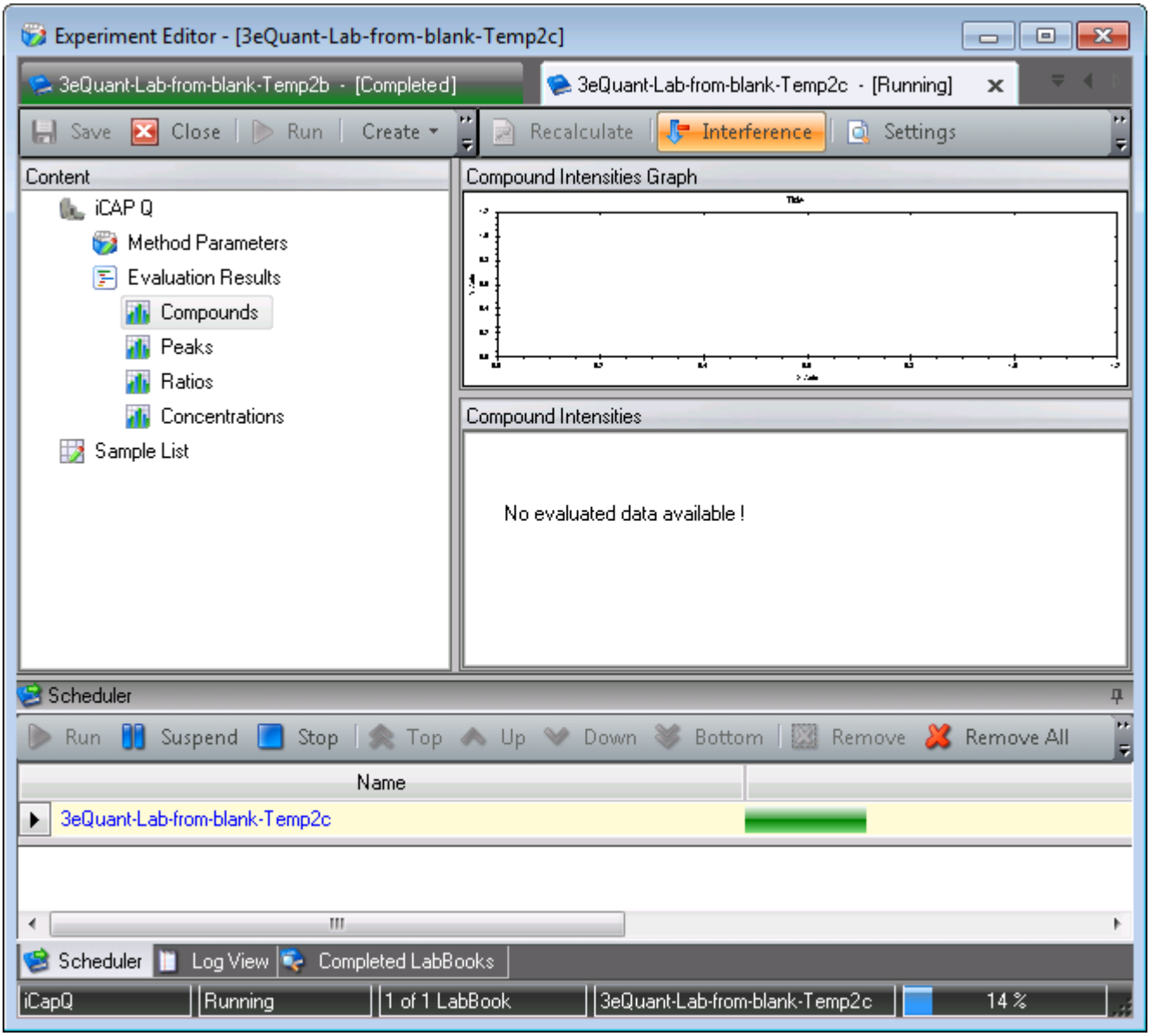


Figure 7-17. Measurement started for scheduled LabBook

The completed LabBook is automatically deleted from the Scheduler and added to **Completed LabBooks**.

5. Click  .
The list of completed LabBooks opens, see "Completed LabBooks" on page 5-54.

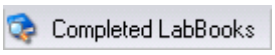
Viewing the Result of a Measurement

The results of the measurement are added to the completed LabBook and can be viewed in Experiment Editor.

❖ **To view the results of a measurement**

1. Click 

to open **Experiment Editor**.

2. Click 

.

3. In the **Completed LabBooks** tab, click the LabBook you wish to view.
In Experiment Editor, the completed LabBook opens in a separate tab, see Figure 7-18.

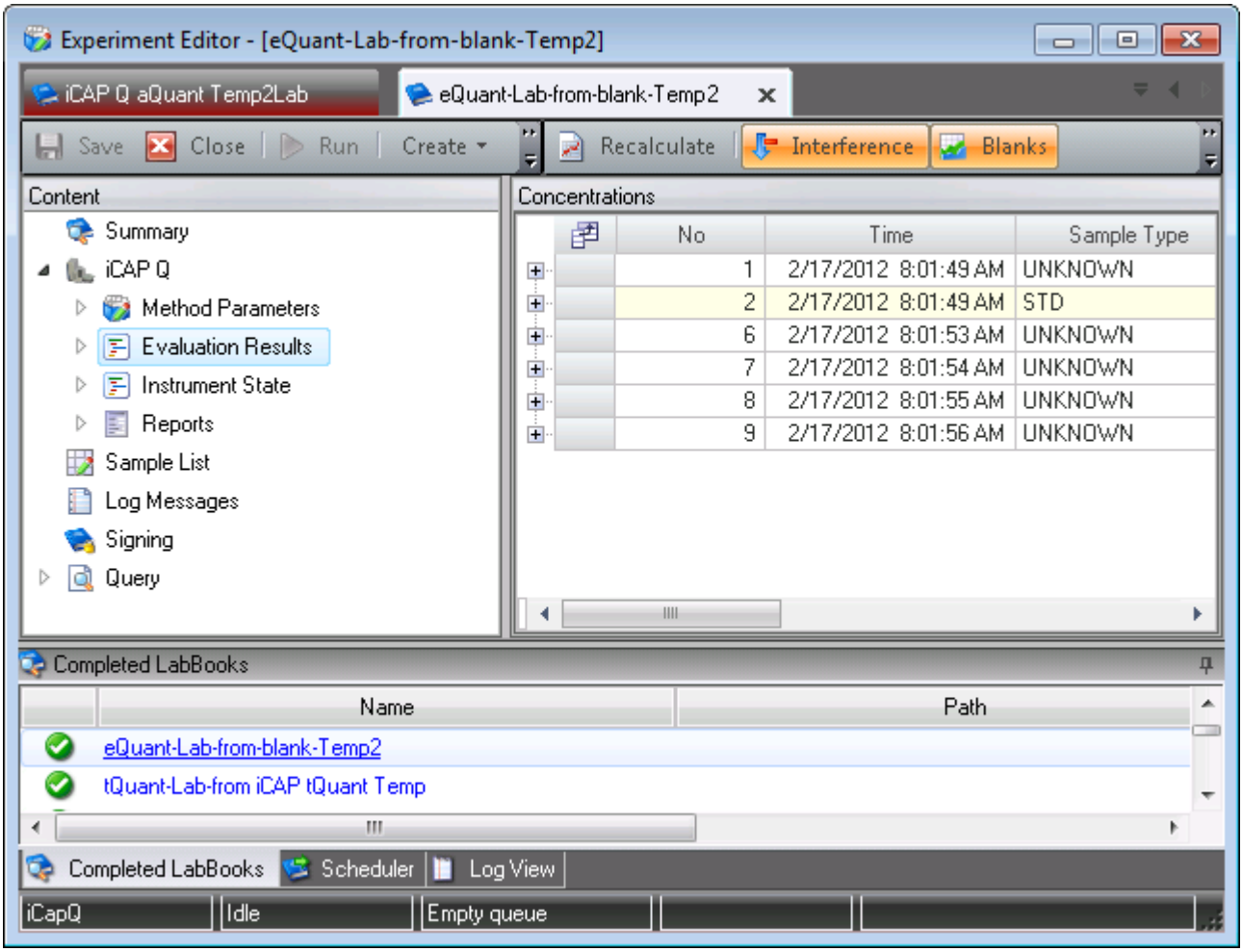


Figure 7-18. Completed LabBook

4. Click **iCAP Q** to show the items added to the LabBook after measurement, see Figure 7-19.

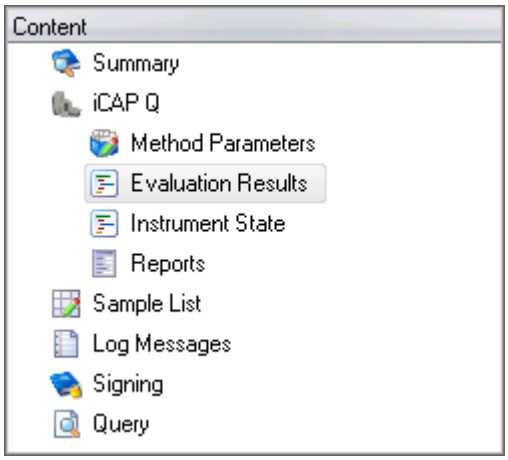


Figure 7-19. Added items of a completed LabBook

The menus **Evaluation Results**, **Instrument State** and **Reports**, and the items **Log Messages**, **Signing** and **Query** 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 Experiment Editor.

The presentation of the evaluation results differs, according to the "Method Parameters" on page 6-15 defined. In that way, Compounds will only be shown for tQuant LabBooks whereas Survey Intensities may be found in a variety of measurements.

❖ **To open the Evaluation Results view**

1. Click 

to open **Experiment Editor**.

2. Click 

.

3. In the Completed LabBooks list, click the LabBook you wish to view the result of.
The completed LabBook is opened in a new tab.

4. Click Evaluation Results to open the **Evaluation Results** view, for example, see Figure 7-20.

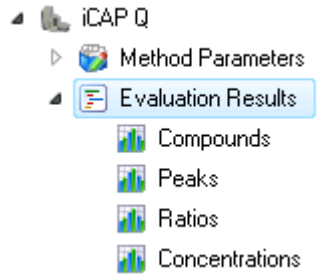


Figure 7-20. Evaluation Results submenus in completed tQuant LabBook

A number of functions that differ according to the evaluation method are available in the toolbar of this view, see Figure 7-21.

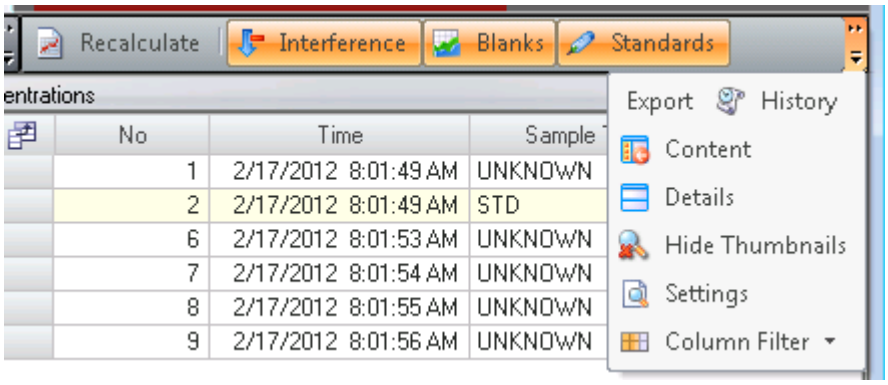


Figure 7-21. Added functions in toolbar of completed LabBook

Instrument State

The **Instrument State** view of a LabBook in Experiment Editor shows readback/status values for the instrument parameters of the iCAP Q system for each sample in the sample list.

❖ **To open the Instrument State view**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click Completed LabBooks.
3. In the Completed LabBooks list, click the LabBook you wish to view the result of.
   The completed LabBook is opened in a new tab.

4. Click Instrument State to open the **Instrument State** view, see Figure 7-22.

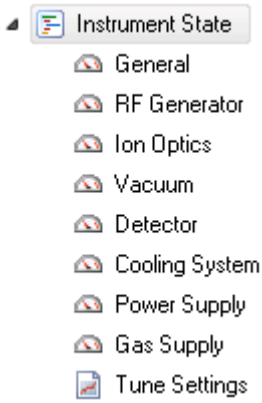


Figure 7-22. Instrument State submenus in completed LabBook

Reports

The **Reports** view of a LabBook in Experiment Editor displays the reports of the measurement. The availability of the reports differs, according to the "Evaluation Methods" on page 6-10. In that respect, a **Chromatogram report** will be available for a tQuant LabBook, whereas a **Quality Control** report shows for an eQuant LabBook.

The **Calibration report** (eQuant and tQuant LabBooks) displays in report format the quantitative calibration curves for each analyte defined as a standard and selected for quantification.

The **Experiment report** (also aQuant LabBooks) displays in report format the Acquisition Parameters for each analyte and the concentration data for each sample and for each analyte specified as a standard and selected for quantification.

❖ **To open the Reports view**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click Completed LabBooks.
3. In the Completed LabBooks list, click the LabBook you wish to view the result of.
   The completed LabBook is opened in a new tab.
4. Click Reports to open the **Reports** view.

Log Messages

The **Log Messages** view of a LabBook in Experiment Editor 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. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
4. In the **Completed LabBooks** tab, click the LabBook you wish to view.
5. Click 

to view the **Log Messages** of the completed LabBook, see Figure 7-23.

Log Messages

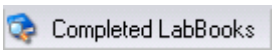
Logged at	Level	Message	Time	Category	Sub Category
Line no. 1: BLK	ⓘ	Total evaluation time [msec] : 16, Data loading time [msec] : 0, Peak detection time [msec] : 0	2/21/2012 13:46:5	ExperimentE	ChromBase.Ev
Line no. 2: sam	ⓘ	Total evaluation time [msec] : 47, Data loading time [msec] : 47, Peak detection time [msec] : 0	2/21/2012 13:47:1	ExperimentE	ChromBase.Ev
Line no. 3: sam	ⓘ	Total evaluation time [msec] : 16, Data loading time [msec] : 16, Peak detection time [msec] : 0	2/21/2012 13:47:2	ExperimentE	ChromBase.Ev

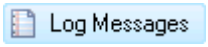
Figure 7-23. Log Messages in completed LabBook

❖ **To filter Log Messages**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Click 

.
4. In the **Completed LabBooks** tab, click the LabBook you wish to view.
5. Click 

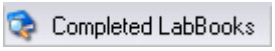
to view the **Log Messages**.
6. Click  in the header of the column you wish to filter the display of.
A drop-down menu opens, see, for example, Figure 7-24.

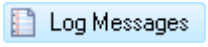
Figure 7-24. Log Messages filter drop-down menu in completed LabBook

7. Select an item from the drop-down menu.
The column only shows the selected values.

❖ **To customize filters in Log Messages**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Click 

.
4. In the **Completed LabBooks** tab, click the LabBook you wish to view.
5. Click 

to view the **Log Messages**.
6. Click  in the header of the column you wish to filter the display of.
A drop-down menu opens, see, for example, Figure 7-25.

Figure 7-25. Log Messages filter drop-down menu in completed LabBook

7. Select **(Custom)** from the drop-down menu.
   The **Custom Filter** dialog opens, see Figure 7-26.

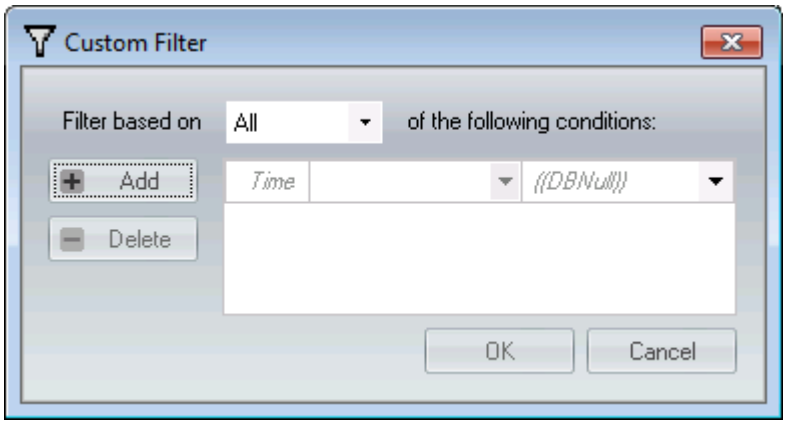


Figure 7-26. Custom Filter dialog of Log Messages in completed LabBook

8. Select **Any** or **All** from the drop-down menu **Filter based on**.

9. Click of the left column to open the drop-down menu for **Level**, see Figure 7-27.

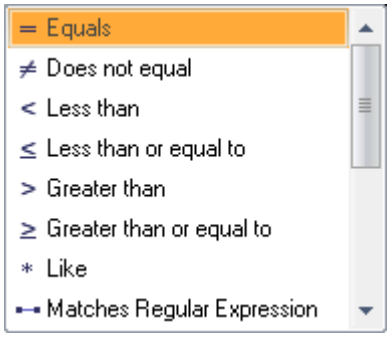


Figure 7-27. Level drop-down menu of Custom Filter dialog

10. Select a rule from the drop-down menu.

11. Click of the right column to open the drop-down menu, see Figure 7-28.

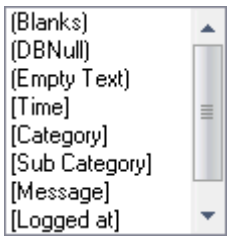


Figure 7-28. Drop-down menu of Custom Filter dialog with arguments

12. Select an argument from the drop-down menu.

13. Click 

.

    The specified rules are immediately applied to the table.

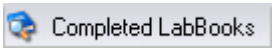
Signing

The **Signing** view of a LabBook in Experiment Editor is added to the LabBook after a measurement has been run for this LabBook.

Signing is used to protect the acquired data and verify the operator. Certificates are required to activate the Signing feature. These Digital SSL certificates are issued by Trusted CA Certificate Authorities and applied by your Administrator.

❖ **To open the Signing view**

1. Click 

to open **Experiment Editor**.
2. Click 

.
3. In the **Completed LabBooks** tab, click the LabBook you wish to view.
The completed LabBook is opened in a new tab.
4. Click 

to open the **Signing** view, see Figure 7-29.

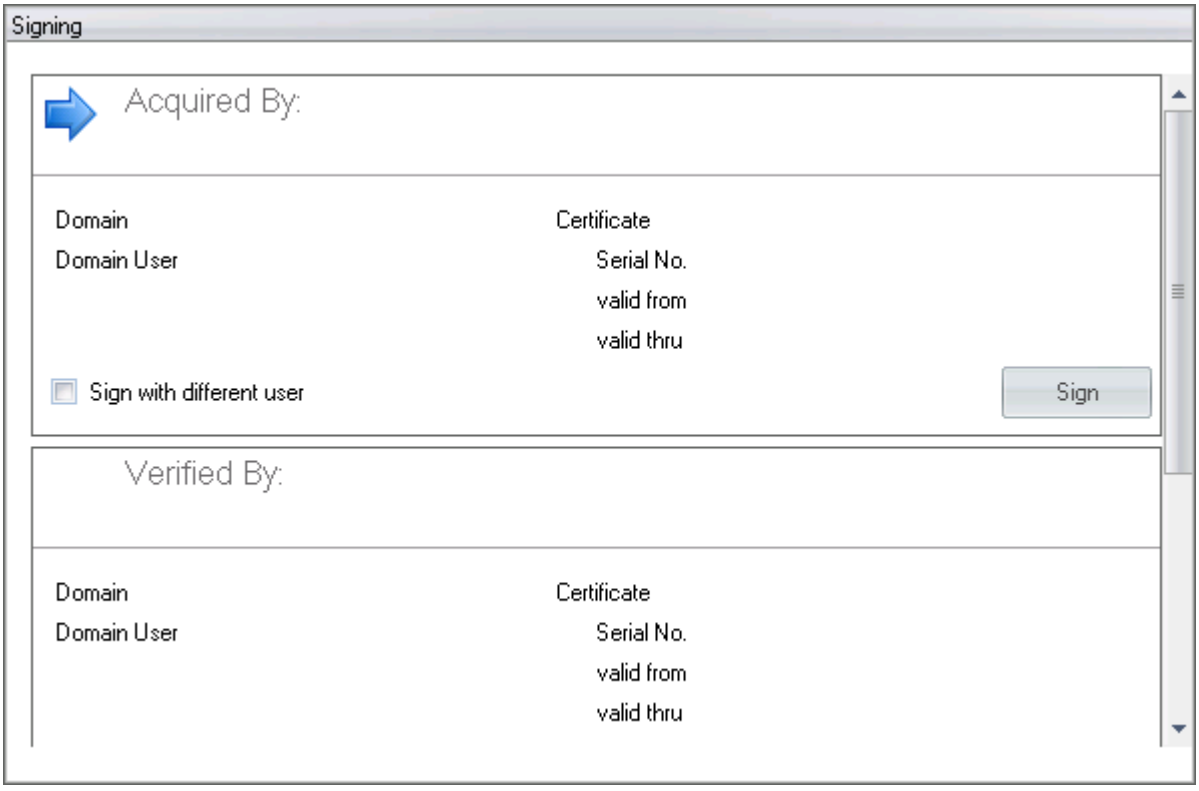


Figure 7-29. Signing in completed LabBook

❖ **To sign the LabBook**

1. Click 

to open **Experiment Editor**.

2. Click 

.

3. In the **Completed LabBooks** tab, click the LabBook you wish to sign.
The completed LabBook is opened in a new tab.

4. Click 

to open the **Signing** view.

5. In the **Acquired By** field, click 

.
The **Select certificate for signature** window opens, see Figure 7-30.

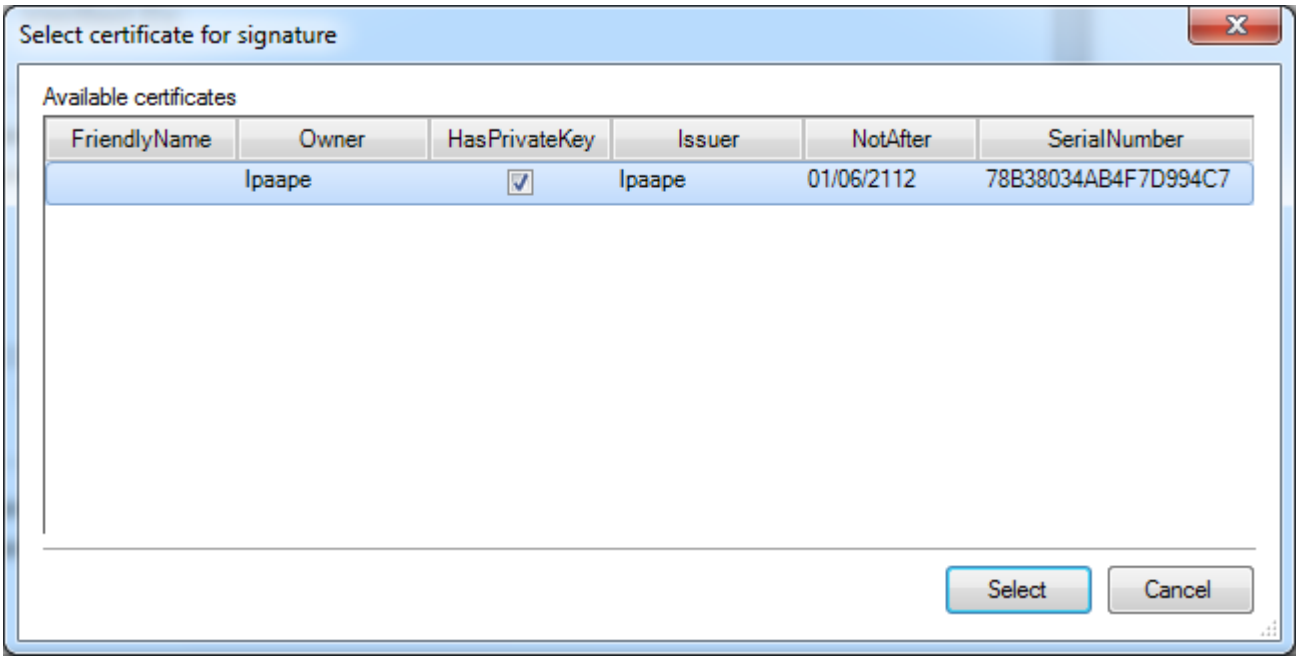


Figure 7-30. Select certificate for signature window

6. Select your certificate from the list and click **Select**.

7. Follow the instructions.
The fields **Verified By** and **Approved By** must now subsequently be signed by the Manager and the Administrator, or as defined in your company by the Administrator of Qtegra.

Query

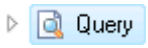
The **Query** view of a LabBook in Experiment Editor is added to the LabBook after a measurement has been run for this LabBook. A statistical breakdown of the intensity and concentration results can be displayed at a glance and can easily be exported to Microsoft™ Excel™.

NOTICE See also "Results Page" on page 5-30. ▲

❖ **To open the Query view**

1. Click 

to open **Experiment Editor**.
2. Click 

.
3. In the **Completed LabBooks** tab, click the LabBook you wish to view the result of.
The completed LabBook is opened in a new tab.
4. Click 

to open the **Query** view, see Figure 7-31.

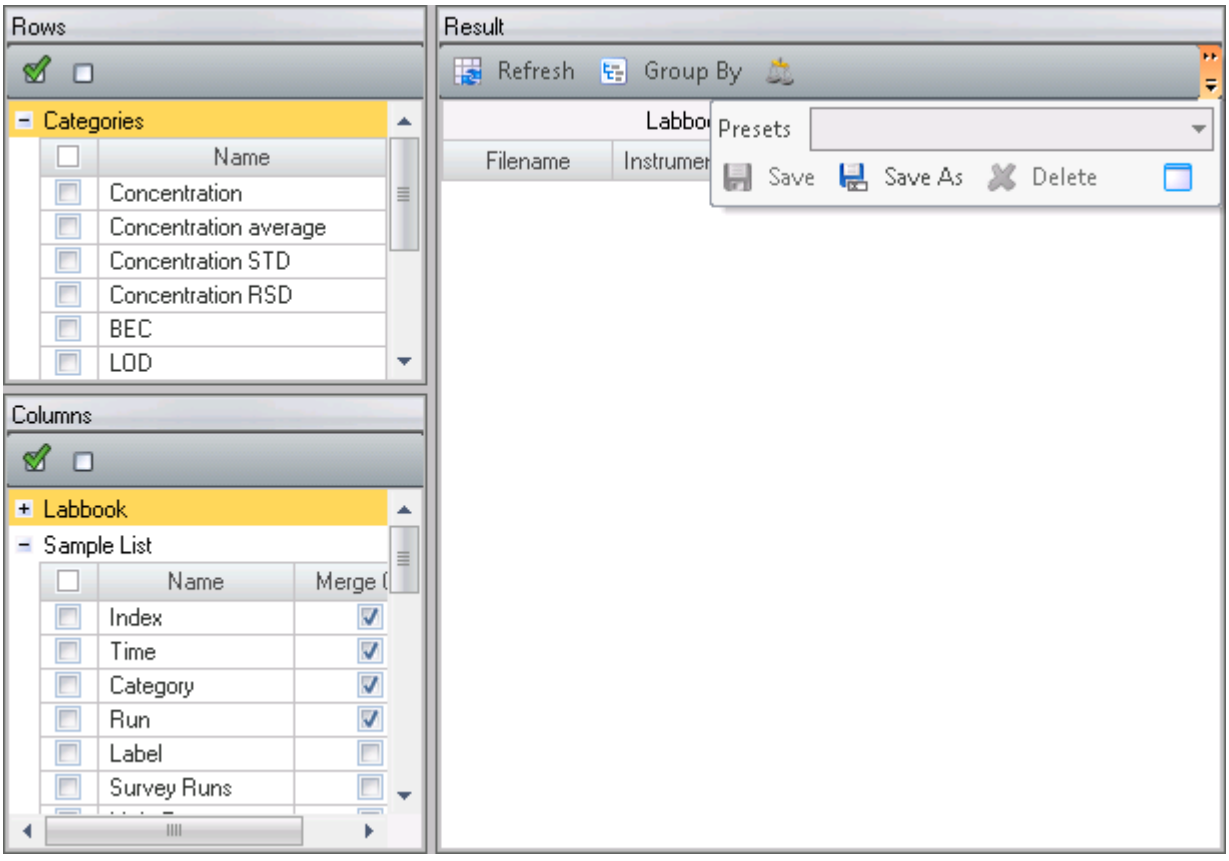


Figure 7-31. Query view in completed LabBook

❖ To place a Query

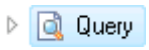
1. Click 

to open **Experiment Editor**.

2. Click 

.

3. In the **Completed LabBooks** tab, click the LabBook you wish to view the result of.
   The completed LabBook is opened in a new tab.

4. Click 

to open the **Query** view.

5. In the field **Rows**, select the check boxes for **Categories** you wish to display.
   Click  to select all check boxes.

6. In the field **Columns**, select the check boxes for **Labbook**, **Sample List**, and **Results** you wish to display.
   Click  to select all check boxes.

7. In the field **Result**, click Refresh to display the selected result values, see Figure 7-32.

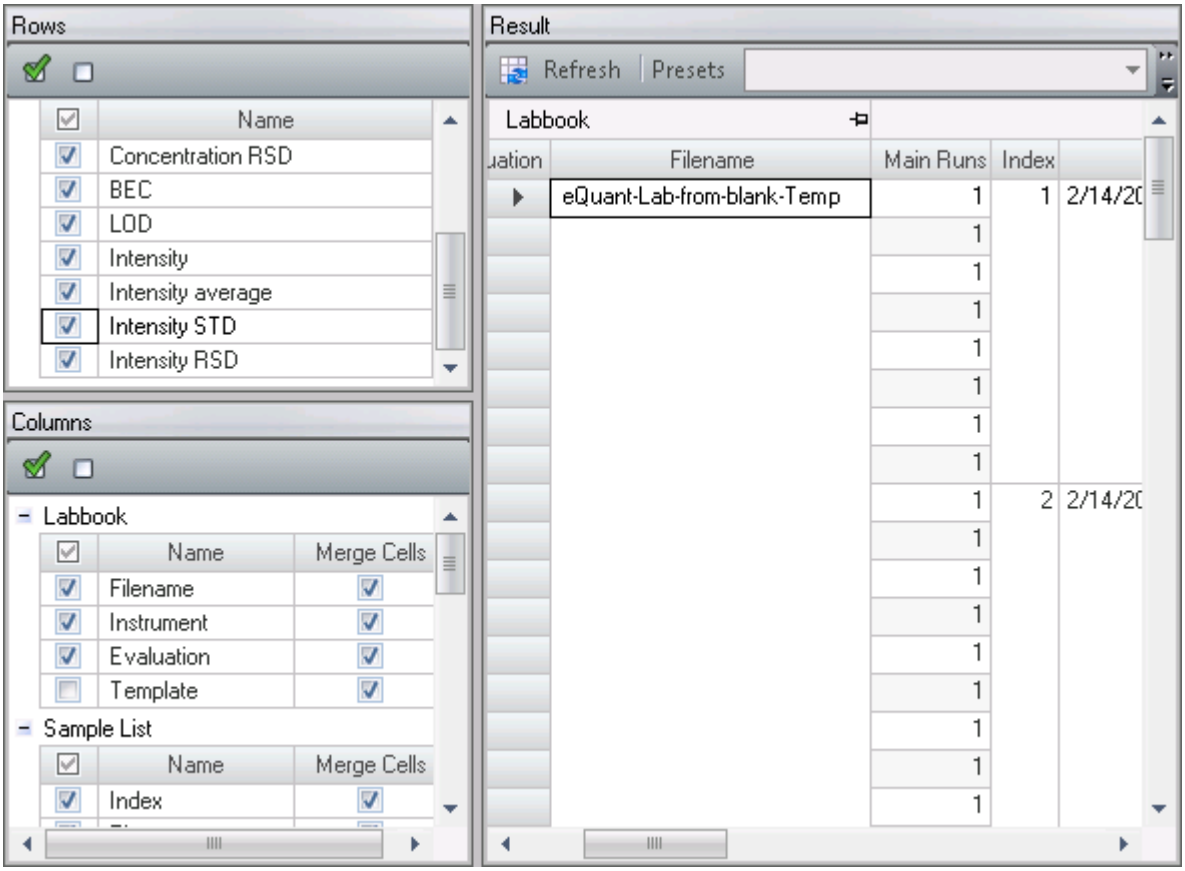


Figure 7-32. Query view with results in completed LabBook

❖ **To export Query result data**

1. Click Experiment Editor to open **Experiment Editor**.
2. Click Completed LabBooks.
3. In the **Completed LabBooks** tab, click the LabBook you wish to view the result of.
   The completed LabBook is opened in a new tab.
4. Click Query to open the **Query** view.
5. Select the check boxes for **Rows** and **Columns** you wish to display.
6. In the field **Result**, click Refresh to display the selected result values.

7. In the **Result** table, right-click to open the context menu, see Figure 7-33.

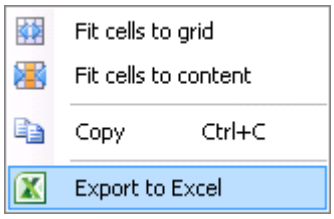


Figure 7-33. Query results context menu

8. Select **Export to Excel** from the context menu. The **Save As** window opens, see Figure 7-34.

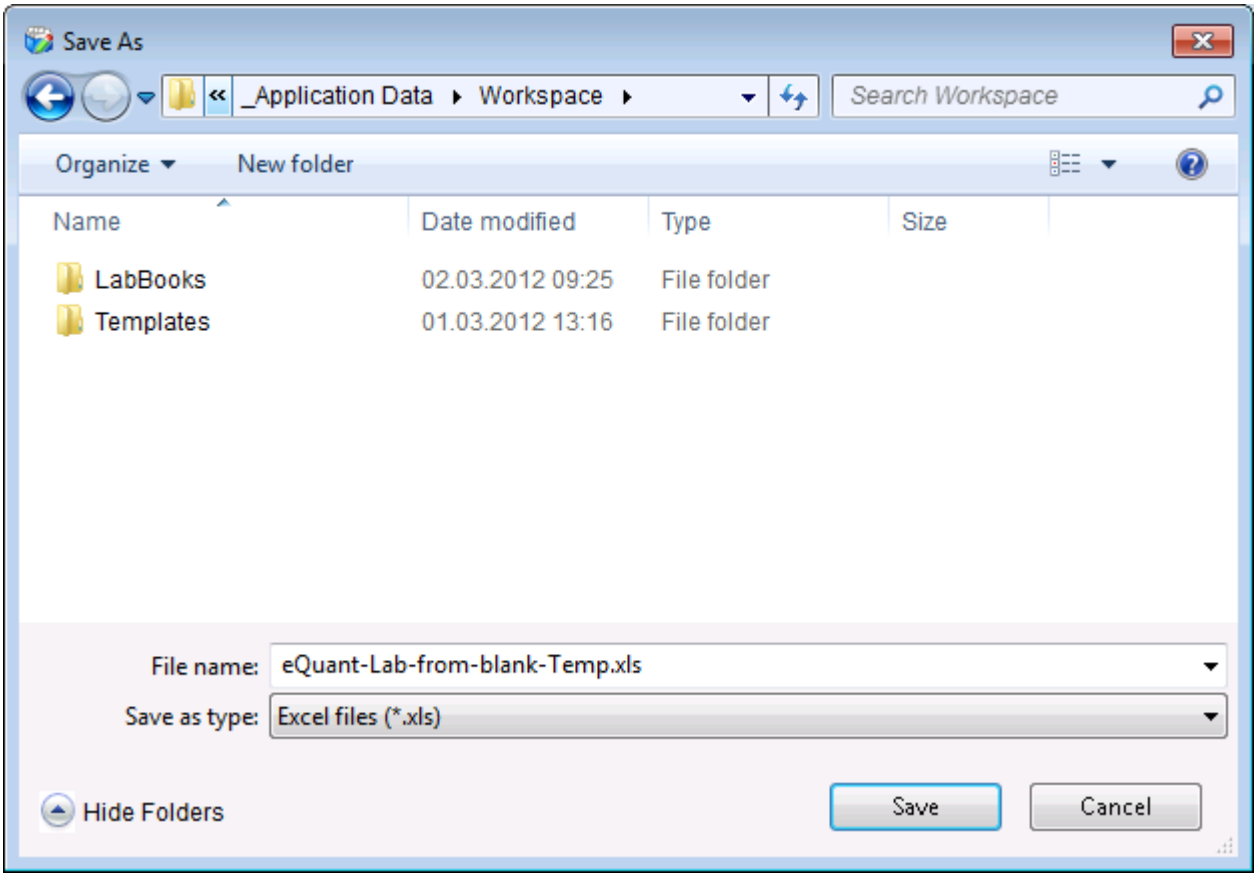


Figure 7-34. Export results window

9. Select a directory and enter a **File Name**.

10. Click 

.

Chapter 8 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 isotope of an analyte.

Employment of the iCAP Q instrument with an autosampler allows for high throughput of samples in the daily work of a laboratory.

Contents

- Setting Up the Template
- Creating LabBook for Analysis with eQuant Evaluation
- Run the Experiment of your Analysis with eQuant
- Results and Data Evaluation

NOTICE Be sure a Configuration has been created for your system setup, see "Experiment Configurator" on page 3-13. ▲

Setting Up the Template

In the Experiment Editor 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.

NOTICE For a detailed description of all parameters in a Template, see "Method Parameters" on page 6-15. ▲

❖ To define Template settings

1. Click to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Create a Template as described in "Creating a Template" on page 5-24.
   Be sure to select the Configuration for your system with iCAP Q, the Evaluation eQuant, and, for example, an autosampler.
4. Click  to select the **Analytes** view.
   See "Analytes" on page 6-15 for a general explanation.
5. 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.
6. Click  to select the **Acquisition Parameters** view.
   See "Acquisition Parameters" on page 6-19 for a general explanation.
7. Enter the **Dwell time (s)** for the elements of your calibration solution and your analytes.

   Typically, dwell times are related to the expected concentration of the analyte in the sample. Higher concentrations usually require shorter dwell times. Lower concentrations should be measured for a longer time to improve the signal-to-noise ratio. Short dwell times are often used for isotope dilution analysis.

NOTICE The more sweeps are averaged, the better the measured value should be. Drift effects might not be recognized with longer dwell times and a small number of sweeps. Very short dwell times might impair the duty cycle of the instrument. A good dwell time value to start from usually is 0.01 s. ▲

8. Enter the value for **Channels** and **Spacing (u)**.
   Usually with a good and stable mass calibration, the default values should be sufficient to measure on the apex of the mass peaks.

9. Select the **Measurement mode** for each analyte from the drop-down list, see Figure 8-1.

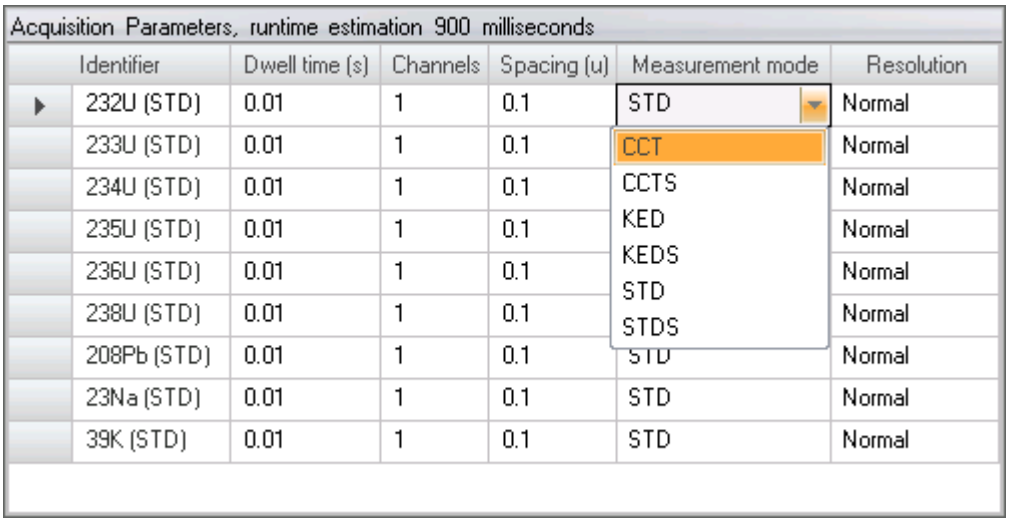


Figure 8-1. Acquisition Parameters view drop-down Measurement mode

For instrument models with a collision cell (QCell), CCT/CCTS or KED/KEDS mode can be used to suppress/eliminate polyatomic and isobaric interferences. If you suspect interferences from the analytes in the expected matrix, use KED, else STD.

NOTICE CCT mode and KED mode are only available with the instrument models iCAP Qc and iCAP Qs. ▲

10. Enter the **Resolution**.
    Default resolution is **Normal**. This setting can be used to reduce the count rate for analytes with high concentration (different linear scan slope of quadrupole) in order to increase the linear dynamic range for comparison of several analytes.

11. In **Advanced Parameters**, enter the **Number of sweeps** and arrange the **Measurement order** for your measurement modes, if appropriate.

12. Click  to select the **Monitor Analytes** view.

13. Add analytes to be monitored.
    One or more analytes can be entered which should be measured subsequently. The Qtegra software watches the intensities of the entered isotopes after the entered minimum uptake delay has elapsed. The software starts the measurement after all conditions are fulfilled, that is, the intensities are high and stable enough. If this condition is not passed within the entered maximum uptake time, the program performs the action defined for On Failure. The definition of conditions for wash are defined likewise.
    For details, see "Monitor Analytes" on page 6-24.

14. Click  to select the **Survey scan settings** view.

15. Define a complete or partial mass spectrum to get an overview of all elements and interferences potentially being present in a sample.
    For details, see "Survey Scan Settings" on page 6-26.

16. Enter dwell time and spacing for each survey scan region.

17. Select the number of sweeps the instrument should perform at the bottom of the page.

18. Click  to select the **Interference correction** view.
    Interference correction helps to minimize not-polyatomic isobaric interferences if no other interference-free isotope is available. This mathematical correction is suited for analytical measurements following EPA regulations.
    For details, see "Interference Correction" on page 6-30.

19. Click  to select the **Standards** view.

20. Click **New** to define a **Standard** as described in "Creating a New Standard" on page 6-34.
    See "Standards" on page 6-32 for details.

21. Click **New** to define an **Internal Standard** as described in "Creating a New Standard" on page 6-34.

    For definition of an internal standard, choose an element that is not 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. 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 mass of the elements in the Internal Standard (unless you can be sure to delete/eliminate these with KED/KEDS mode).

NOTICE For complex samples it is typically appropriate to select several elements to be used as internal standards. This way, Use Interpolation in Quantification can be applied. ▲

22. Click  to select the **Quantification** view in the Template.
23. Enter and select the values as described in "Quantification" on page 6-62.
    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**.
24. Select the check box **Use Quality Control** if you wish to use this feature.
    The additional Method Parameter **Quality Control** is shown immediately. For details on defining the test settings, see "Defining or Changing Quality Control Test Settings (eQuant only)" on page 6-80.

NOTICE For details on the Quality Control tests, see "Quality Control (eQuant only)" on page 6-69. ▲

25. Click  to open the **Ratios** view in the Template.
26. Select the **Isotope 1** and **Isotope 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 6-66.

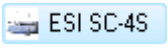
NOTICE For details on all parameters, see "Method Parameters" on page 6-15. ▲

27. Click  to save the changes to your Template.

❖ **To define settings of autosampler**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select the Configuration for your system with iCAP Q, the Evaluation eQuant, and, for example, the autosampler ESI SC-4S.
4. Click, for example, 

to open the autosampler view.
5. Define the settings of your autosampler as appropriate.
   See "Peripherals" on page 6-101 for details.
6. Click  to save the changes to your Template.

❖ **To define Sample Definition**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select the Configuration for your system with iCAP Q, the Evaluation eQuant, and, for example, an autosampler.
4. Define **Header**, **Body** and **Footer** as appropriate.
   To define Header and Footer rows is typically appropriate for a high amount of analyses with a routine method.
5. Enter a value for **Survey Runs**.
   The value **1** is typically appropriate.
6. Enter a value for **Main Runs**.
   The value **3** is typically appropriate.
7. For **Sample Type**, select **STD** for the calibration solution, **UNKNOWN** for the samples, and **BLK** or **AVERAGE BLK** for blanks.
8. 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.

NOTICE For details, see "Sample Definition for a Template" on page 6-117. ▲

9. Click  to save the changes to your Template.

Creating LabBook for Analysis with eQuant Evaluation

The LabBook should be based on the Template that you created for your eQuant analysis in Experiment Editor.

❖ **To create the LabBook for your eQuant analysis**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. On the **Home Page**, click **Analysis**.
   The **Analysis** view of Experiment Editor opens.
4. Enter a **Name** for the LabBook and select a **Location**, see Figure 8-2.

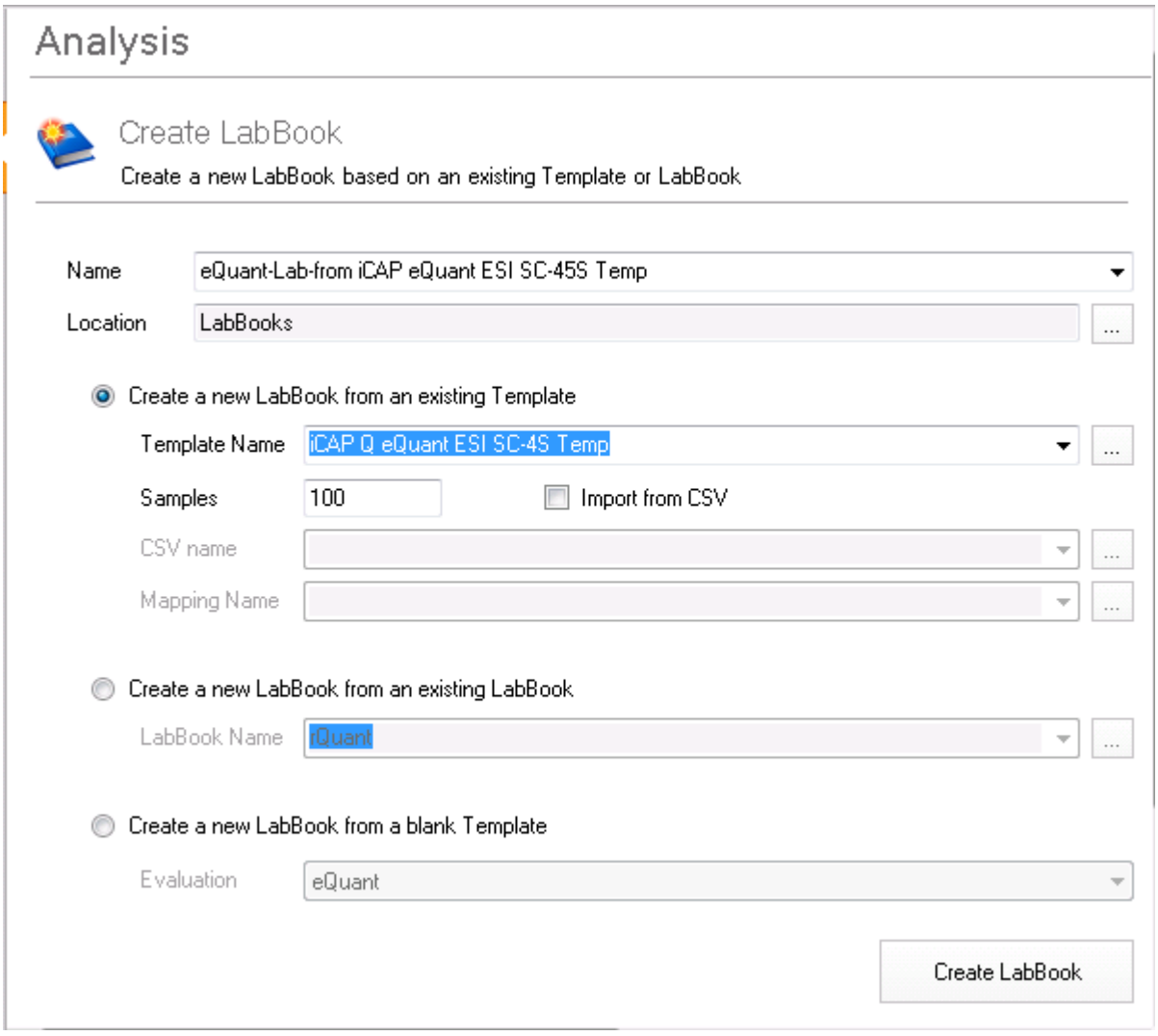
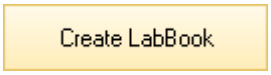


Figure 8-2. Enter Name for eQuant LabBook

5. Click the radio button **Create a new LabBook from an existing Template**.
6. Select the **Template Name** of your eQuant Template from the drop-down list.
7. Enter 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.
8. Click 

to create the new LabBook.
   A new tab opens for the new LabBook.
9. Check all settings.
10. Check the sample list.
11. Make sure that the settings for the autosampler are corresponding to the actual position of vials in the autosampler.
12. In the toolbar of your **LabBook** page, click 

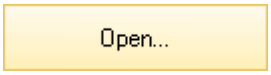
to save your LabBook.

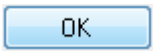
Run the Experiment of your Analysis with eQuant

After each measurement cycle, the signal intensities and measured concentrations can be observed in Experiment Editor. Spectra View furthermore offers the possibility to look at the mass spectra acquired during the Survey runs.

❖ **To run your eQuant LabBook**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. On the **Home Page**, click **Analysis**.
The **Analysis** view of Experiment Editor opens.
4. Below  , click 

.
The **Browse for LabBook** window opens.
5. Select your eQuant LabBook.
6. Click 

to open the LabBook.
The LabBook opens in a new tab of the Experiment Editor tool.
7. In the toolbar of your LabBook, click  to schedule the LabBook for execution.
The LabBook is added to the Scheduler. If the check box **Automatic** has been selected for **Start Queue** in the **Options** settings of the Scheduler (see "Customizing Scheduler Settings" on page 5-49), the measurement is started immediately.

Results and Data Evaluation

After measurement, the LabBook is added to the Completed LabBook tab in Experiment Editor. Intensities are shown of the measured values corrected by Interferences. The graphical display shows characteristics of the selected external calibration and corresponding concentrations. Results of QA/QC tests are shown. For details on viewing results, see "Viewing the Result of a Measurement" on page 7-21.

Depending on the need of your laboratory, data evaluation of results may be desired.

Inspecting the result data you can look for potential interferences, recognize drifts of the signals, look at the calculation of detection and determination limits, and estimate the calibration quality. The observation for carryovers and the rise of blank values might be desired.

Any changes in the LabBook are recorded and can be saved with comments. For a complete description of the toolbar functions of a LabBook, see "LabBook Toolbar" on page 7-2.

Concentrations

In the Evaluation Results **Concentrations** view of the LabBook in Experiment Editor, the results of the quantitative analysis are summarized. As with the sample list, blanks are displayed in blue, standards in yellow, QCs in red and unknowns in white. The mean values, standard deviations (SD) and relative standard deviations (RSD) as well as the results of each main run are shown when the line is

expanded by clicking . An entry can be added or removed from the calculation by right-clicking and selecting **Include entry** or **Exclude entry** from the context menu, see Figure 8-3.

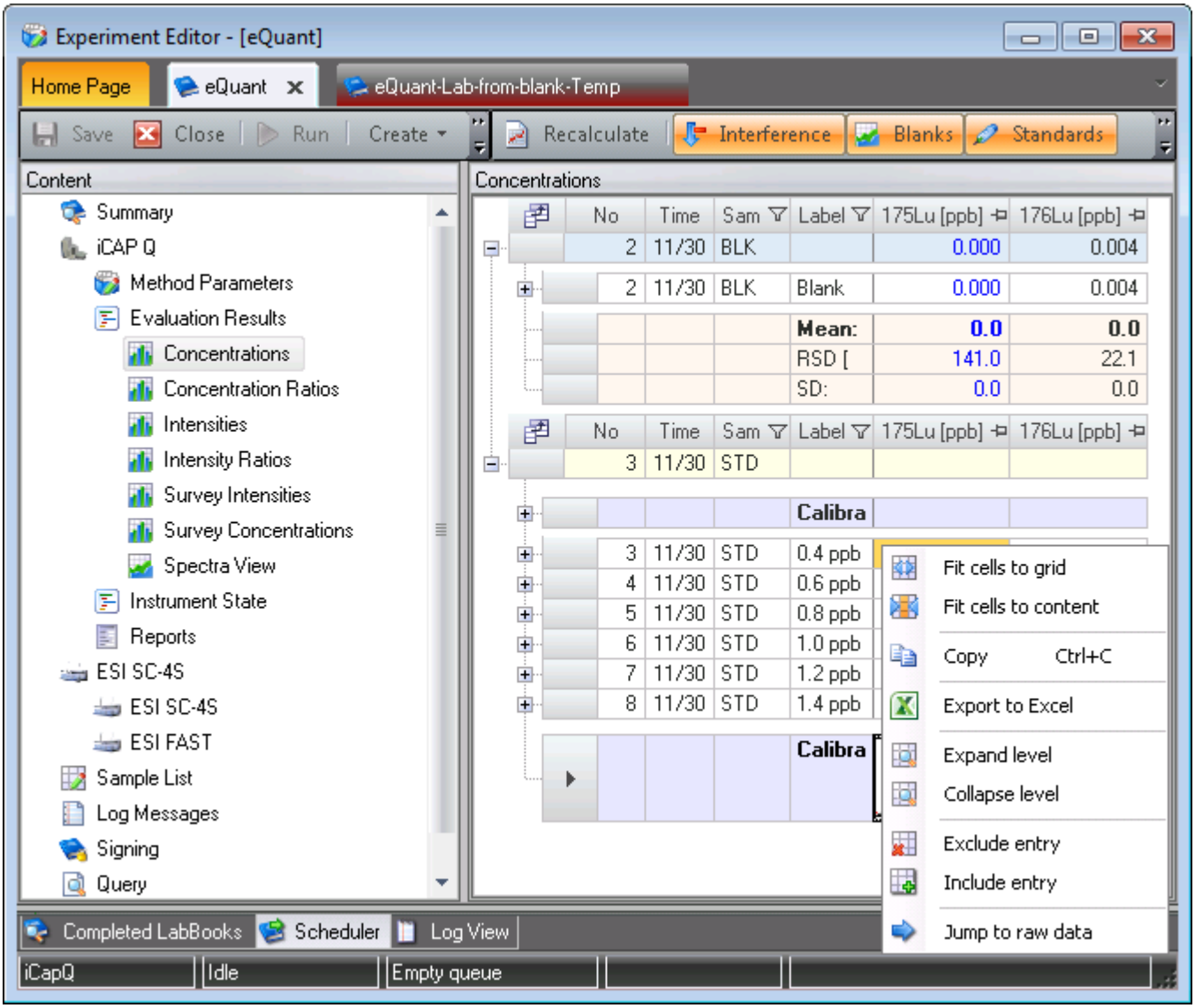


Figure 8-3. Evaluation results Concentrations with context menu

Values in brackets represent the expected concentration of the standard. The recovery of the internal standard is displayed in percent of the first sample line. Double-clicking one of these values displays a plot of the recovery against the sample number.

Double-clicking the thumbnails or selecting **Details** in the toolbar displays an enlarged graph of the calibration curve on the lower left side, 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 8-4.

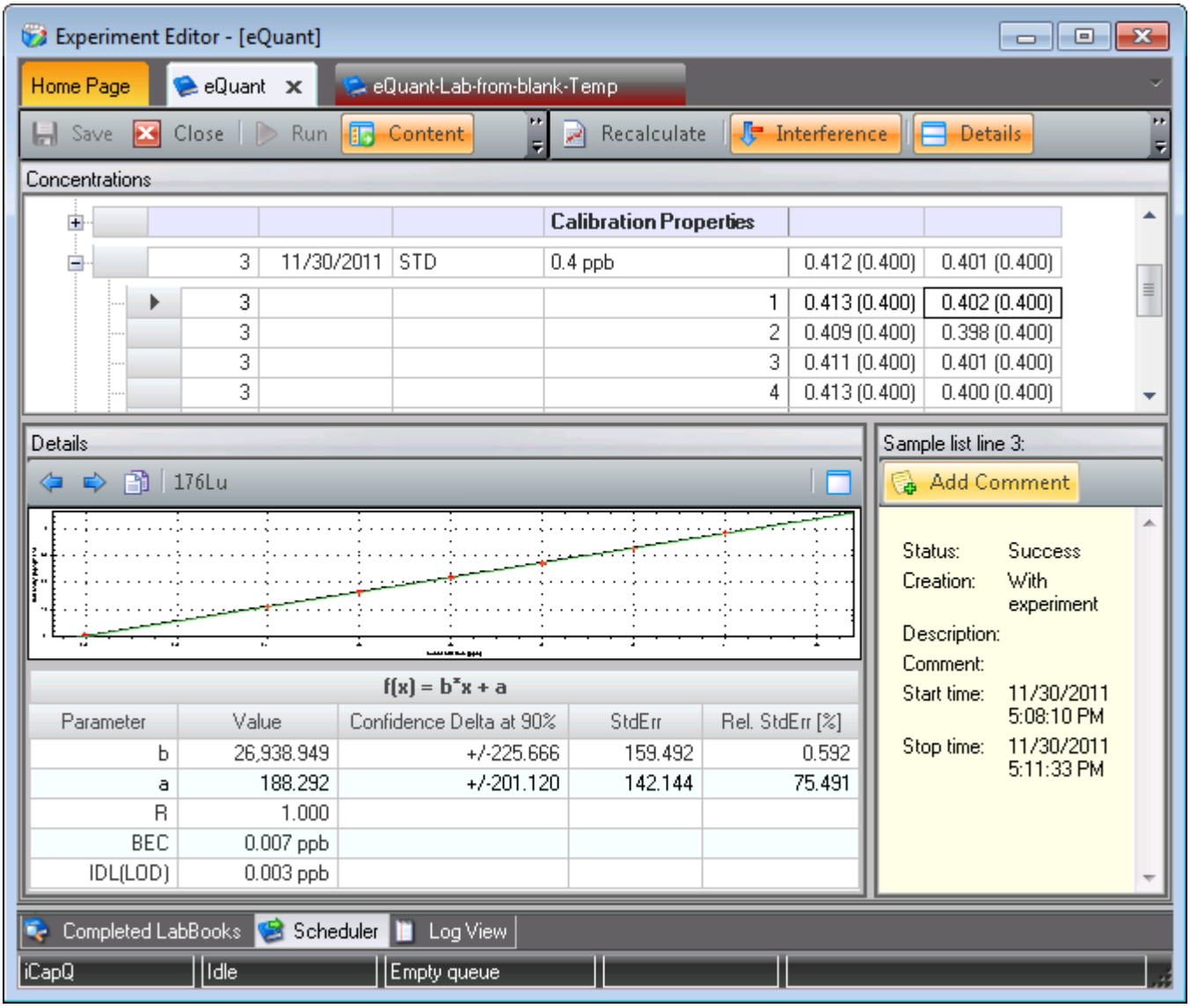
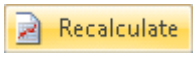


Figure 8-4. Evaluation results Concentrations details

The values are automatically updated when values are added or removed or the settings in the "Quantification" on page 6-62 view of the Method Parameters are changed. There is also the possibility to further enlarge the graph by clicking  **Maximize** in the upper right corner of the **Details** view. A right click on the graph opens a context menu with options to copy or save the graph or to display the data logarithmically. Comments for each sample line can be added by clicking the 

button in the lower right corner of the **Concentrations** view.

The toolbar of the **Concentrations** view includes options to perform a recalculation with 

, to switch on/off the mathematical interference correction 

and to switch on/off the use of internal standards 

. By clicking 

the blank correction is switched on/off. If no ZERO STD was selected, the blank correction is done by including the measured intensity of the different isotopes into the calibration plot with a concentration of *0*. 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.

Concentration Ratios

The Evaluation Results **Concentration Ratios** view of the LabBook in Experiment Editor shows the ratios for each pair of isotopes entered in the Method Parameters section related to the estimated concentrations, see Figure 8-5.

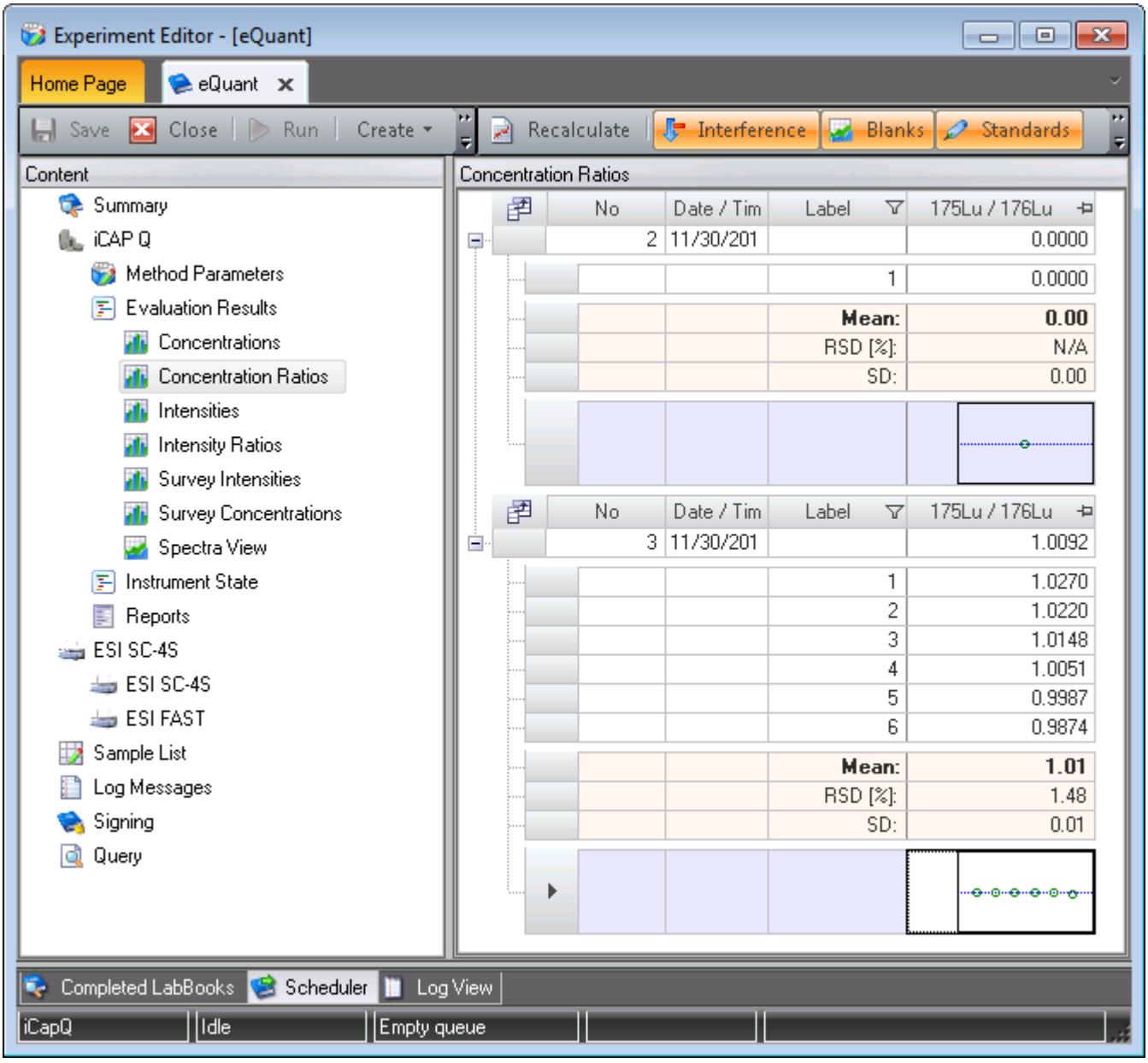


Figure 8-5. Evaluation results Concentration Ratios

Intensities

The Evaluation Results **Intensities** view of the LabBook in Experiment Editor displays the raw intensities. If the entries are shown in bold type, at least 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. Clicking displays the mean values as well as the SD and 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 enlarged graph represents the estimated mean value of the different main runs, see Figure 8-6.

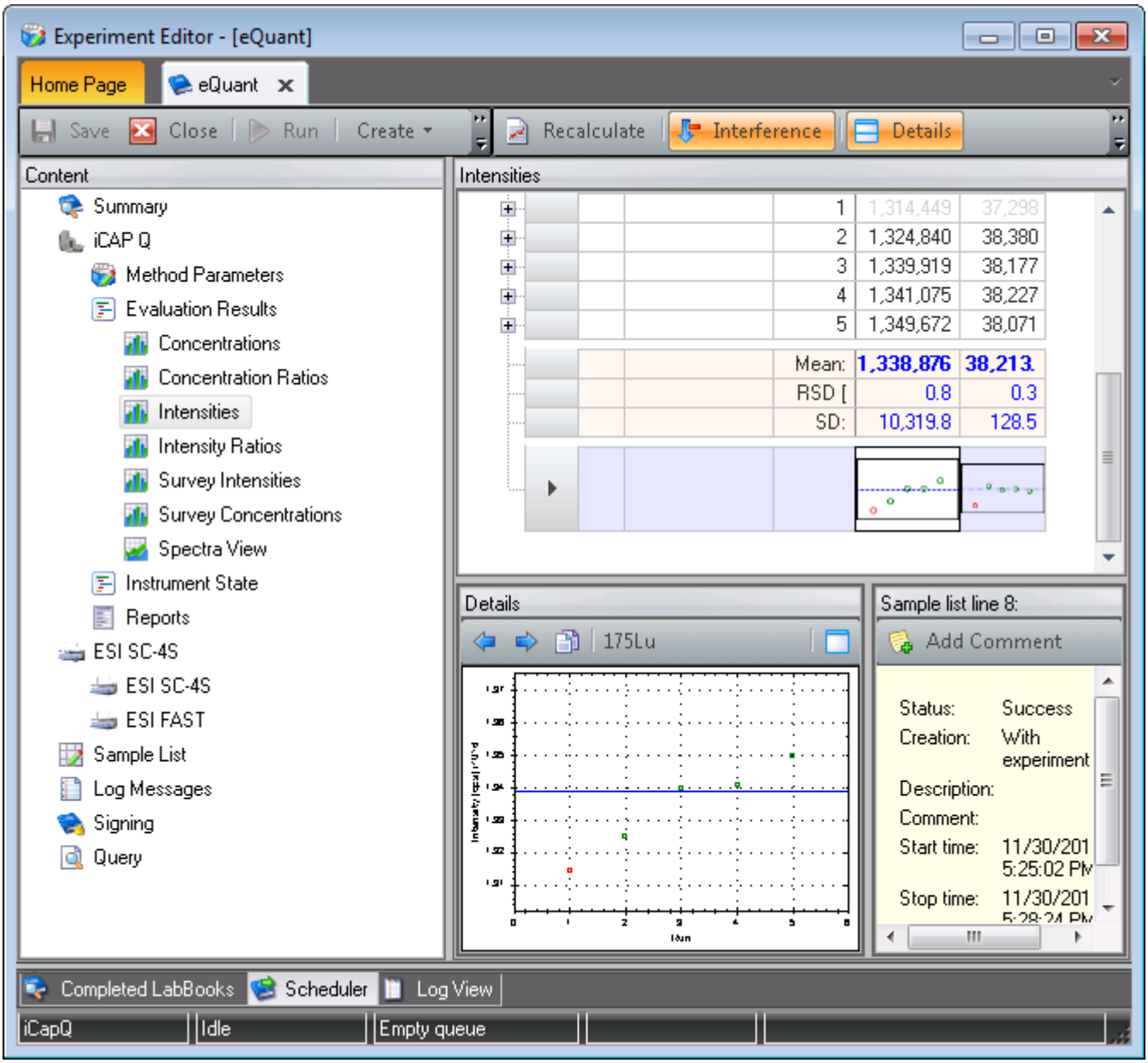


Figure 8-6. Evaluation results Intensities

If more than one channel was measured for any isotope, there is also the possibility to set the strategy how to handle the raw intensities, see Figure 8-7.

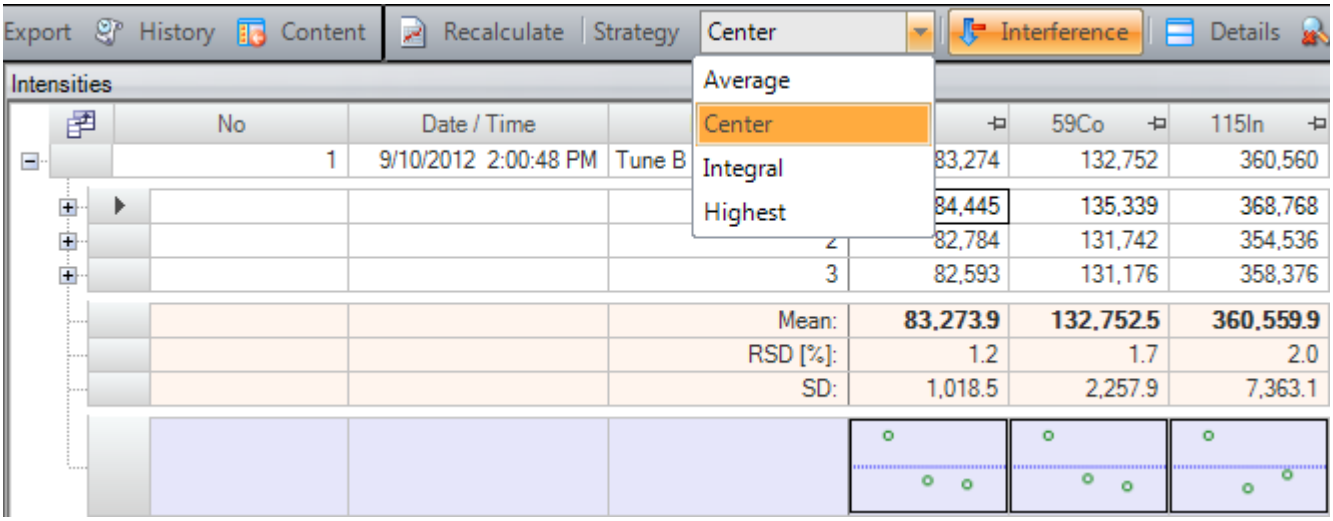


Figure 8-7. Evaluation results Intensities calculation strategies

The calculation strategies for **Strategy** are described in Table 8-1.

Table 8-1. Intensities calculation strategies

Strategy	Description
Average	Uses the average intensity value for each isotopes of the measured channels.
Center	Only uses the intensity of the middle channel.
Integral	Uses the sum of all channels measured for one isotope.
Highest	Selects the channel with the highest intensity for each main run.

Intensity Ratios

The Evaluation Results **Intensity Ratios** view of the LabBook in Experiment Editor shows the data with reference to the raw intensities. Again, the context menu offers functions to include or exclude single entries, see Figure 8-8.

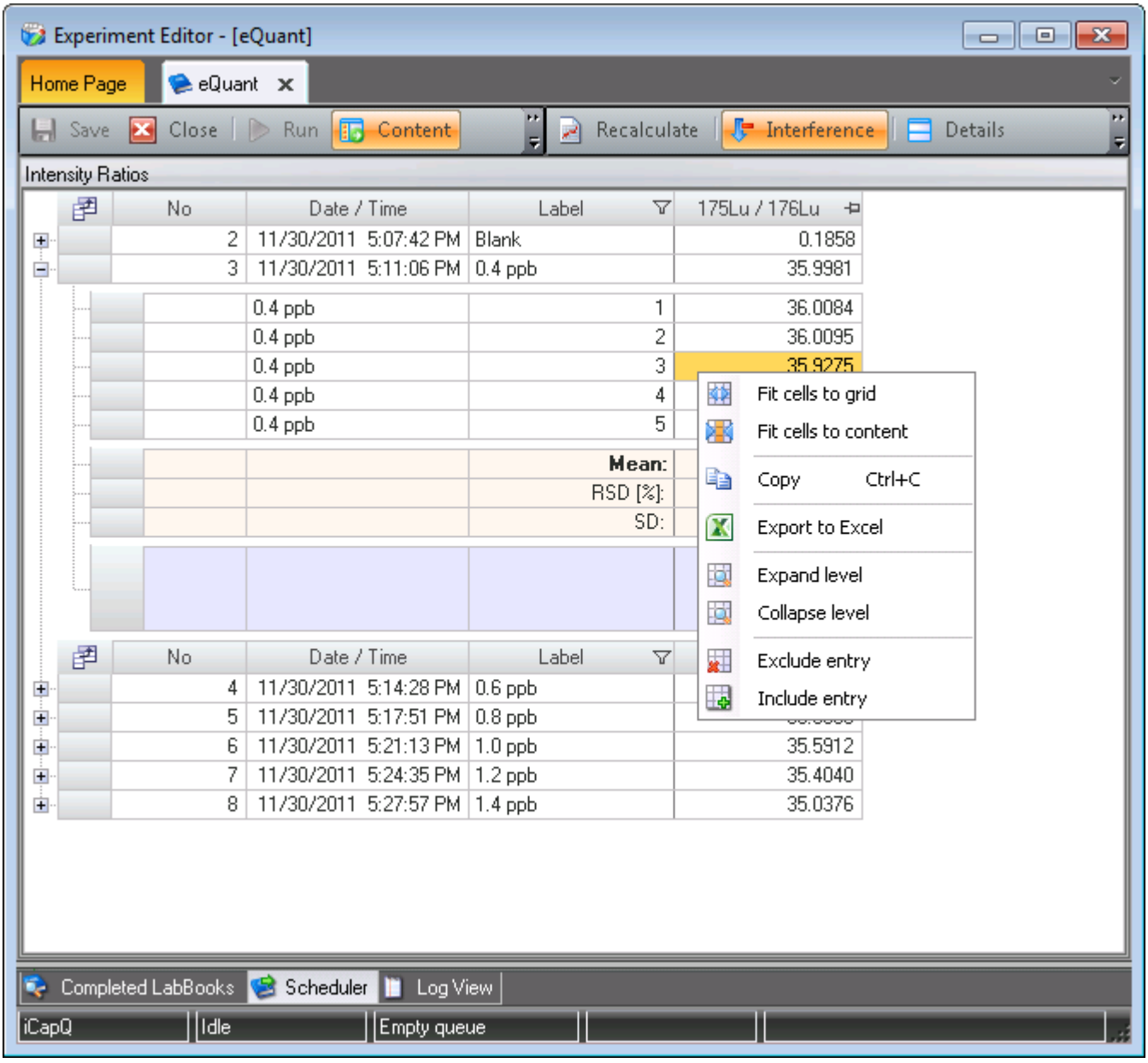


Figure 8-8. Evaluation results Intensity Ratios with context menu

Survey Intensities

When a survey scan was acquired, the Evaluation Results **Survey Intensities** view of the LabBook in Experiment Editor shows the measured intensities of all isotopes within the defined survey scan regions, see Figure 8-9.

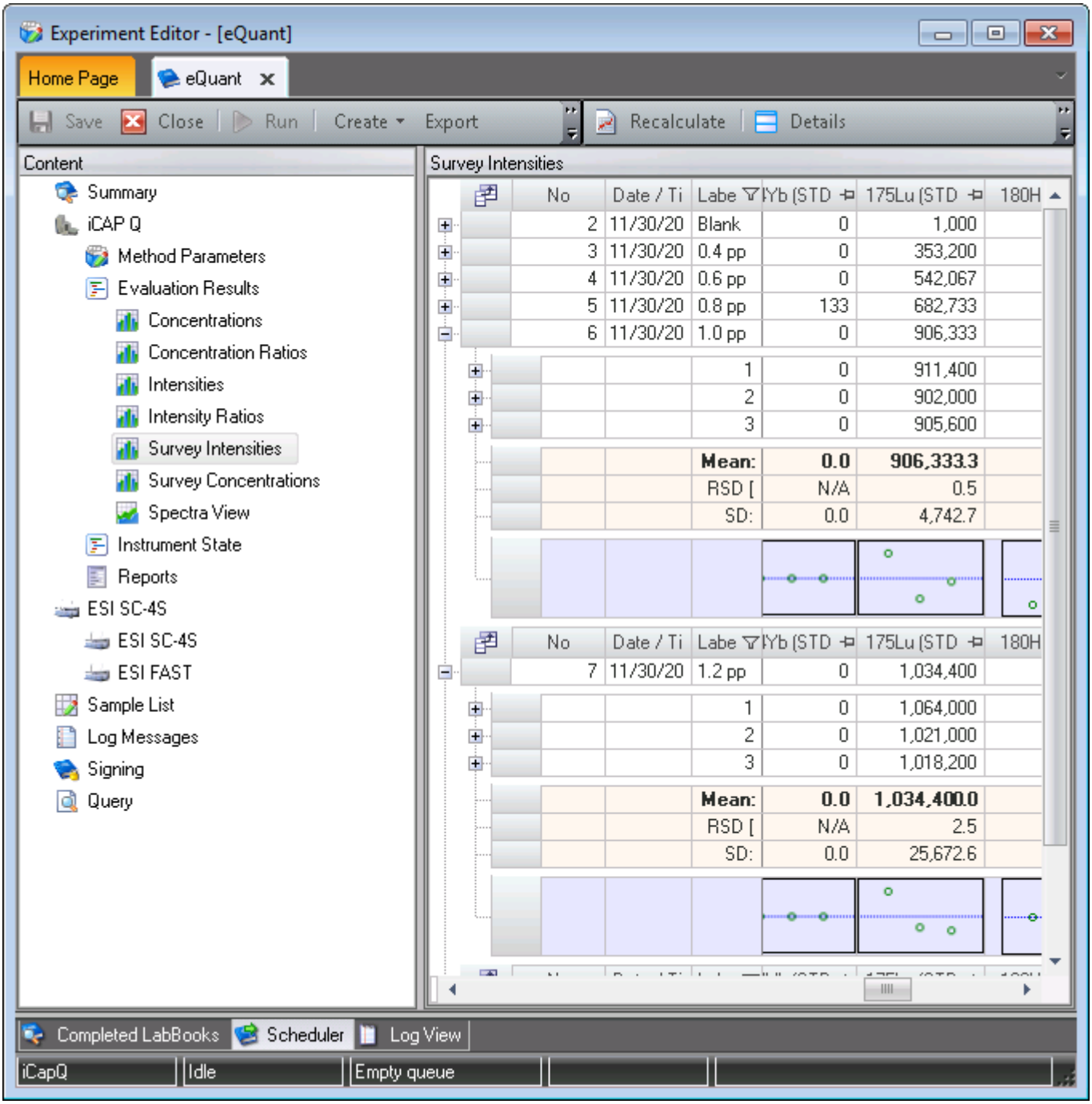


Figure 8-9. Evaluation results Survey Intensities

The display is comparable to that of the **Intensities** view.

Survey Concentrations

The Evaluation Results **Survey Concentrations** view of the LabBook in Experiment Editor is shown in Figure 8-10.

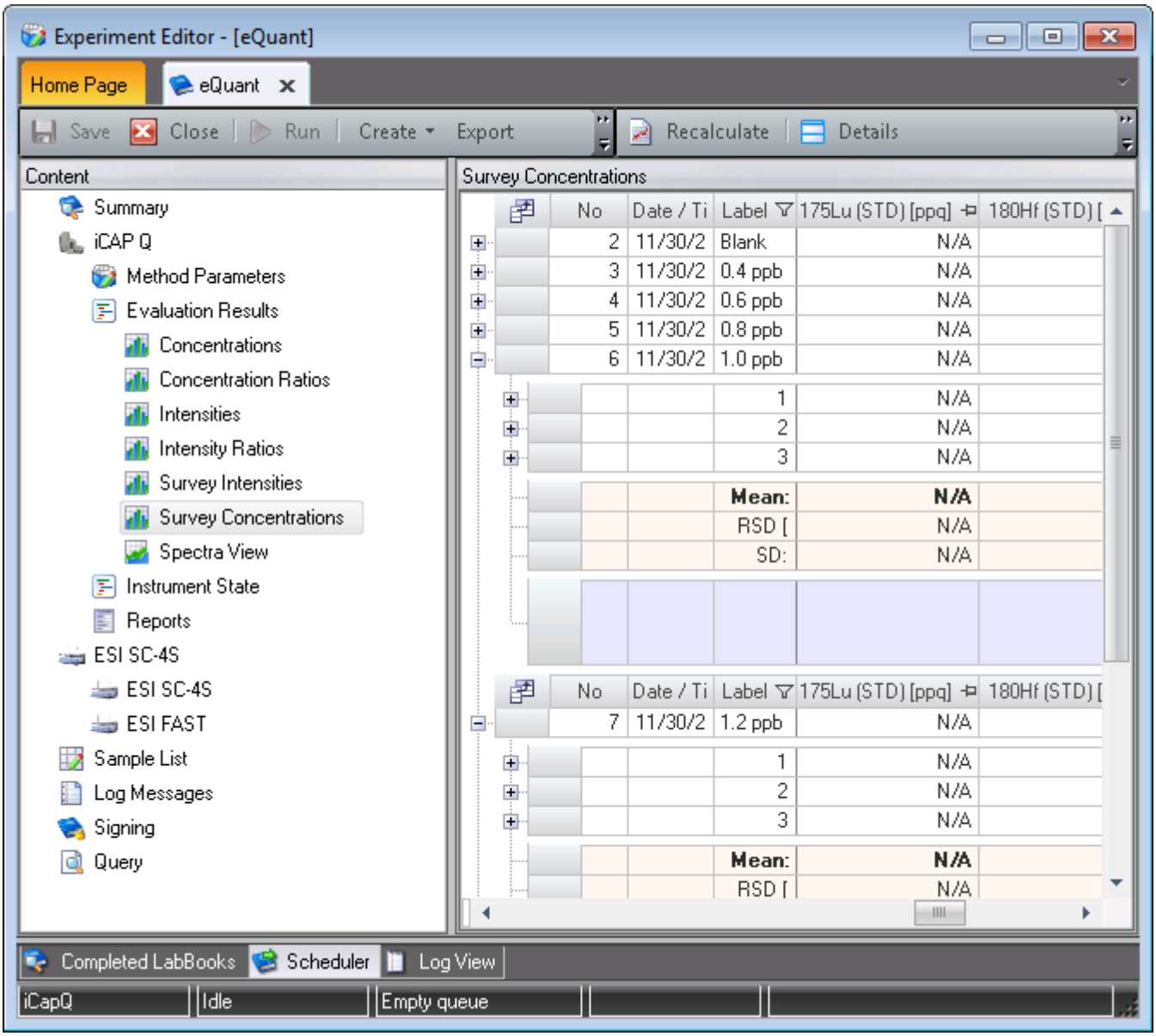


Figure 8-10. Evaluation results Survey Concentrations

This view only contains entries if a valid semi-quantitative evaluation was done.

Spectra View

The Evaluation Results **Spectra View** view of the LabBook in Experiment Editor displays the acquired mass spectra (plots of the measured intensities against the mass-to-charge ratio). Options to save, copy or print the graph are offered in the context menu, see Figure 8-11.

Figure 8-11. Evaluation results Spectra View with context menu

Already averaged intensities or the intensities of each single main or survey run can be displayed by expanding the sample line ⊞ and by selecting the check box for the spectrum of interest. The display options can be changed by clicking the buttons in the toolbar. There is, for example, the possibility to display the intensities not only as points but

also as sticks or profile or any combination of it. With the check boxes in the **Details** section it is possible to simulate the natural isotopic abundances of the elements as well as of common interferences.

Chapter 9 Analysis with tQuant Evaluation

Analysis with tQuant evaluation is used for chromatographic evaluations or for applications which require the recording and subsequent integration of transient signals.

This evaluation method should be used, for example, if all components in a sample have been previously separated to be detected and quantified individually using an appropriate separation technique.

Contents

- Setting Up the Template
- Creating LabBook for Analysis with tQuant Evaluation
- Run the Experiment of your Analysis with tQuant
- Results and Data Evaluation

NOTICE Be sure a Configuration has been created for your system setup, see "Experiment Configurator" on page 3-13. ▲

Setting Up the Template

In the Experiment Editor tool, all settings for your measurement are entered in the Template. For analysis with tQuant, you define elements that the species or compounds of interest contain, the retention time of every species/compound and the amounts of each of the compounds that are used in the calibration solutions.

NOTICE For a detailed description of all parameters in a Template, see "Method Parameters" on page 6-15. ▲

❖ To define Template settings

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Create a Template as described in "Creating a Template" on page 5-24.
   Be sure to select the Configuration for your system with iCAP Q, the Evaluation tQuant, and, for example, an LC autosampler and a LC pump.

4. Click  to select the **Analytes** view.
   See "Analytes" on page 6-15 for a general explanation.

5. In the periodic table, select the elements of interest for the species present in your calibration and sample solutions.
   First, the calibration curve of species with known concentrations must be acquired for later comparison of the peak areas of analytes with this calibration curve.

6. Click  to select the **Acquisition Parameters** view.
   See "Acquisition Parameters" on page 6-19 for a general explanation.

7. Enter the **Dwell time (s)** for the elements present in your calibration and sample solutions.

   The dwell time should be selected to be long enough to sufficiently improve the signal-to-noise ratio. Dwell times that are too long reduce the possibility to acquire enough points/values for the correct calculation and interpolation of the peak. Seven to nine points/values usually suffice to describe the peak shape correctly. A

good dwell time value to start from usually is 0.1 or 0.2 s. If you wish to analyze species containing many different elements in one measurement, the dwell times must be adjusted accordingly.

NOTICE Dwell times for very short peaks as, for example, with Ultra high pressure LC systems, are shorter than with customary LC systems but equal or slightly longer as with GC or CE systems. ▲

8. Enter the value for **Channels** and **Spacing (u)**.
   Default values are usually acceptable.

9. Select the **Measurement mode** the drop-down list, see Figure 9-1.

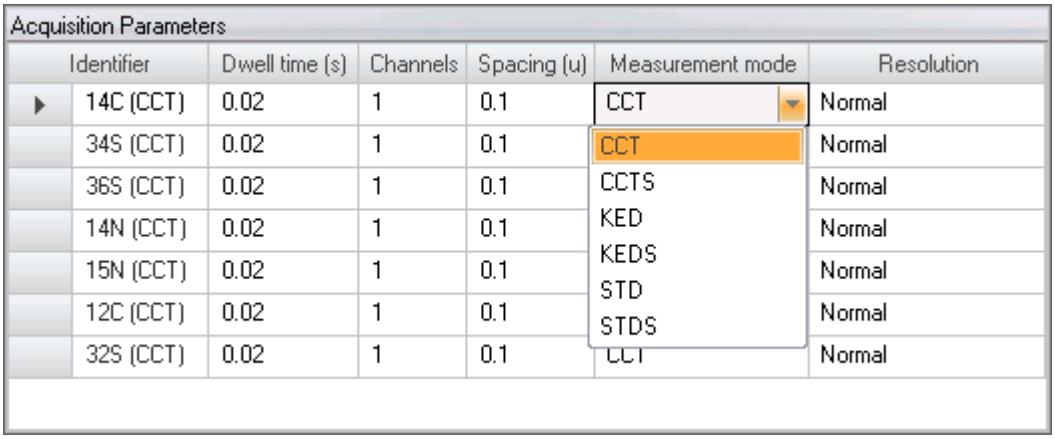


Figure 9-1. Acquisition Parameters view drop-down Measurement mode

The same Measurement mode must be selected for all analytes.

For model iCAP Qa (without QCell), only STD/STDS is possible. An example for a speciation analysis with this model would be the separation and subsequent detection and quantification of Hg and MeHg.
If you expect interferences, for models iCAP Qc and iCAP Qs, KED/KEDS is advisable or CCT/CCTS for dedicated applications. An example would be Cr speciation (Cr [III] and Cr [VI]).

NOTICE CCT/CCTS mode and KED/KEDS mode are only available with the instrument models iCAP Qc and iCAP Qs. ▲

10. Enter the **Resolution**.
    Default resolution is **Normal**.
    The setting **High** can be used to reduce the count rate for analytes with high concentration (different linear scan slope of quadrupole) in order to increase the linear dynamic range for comparison of several analytes.

11. In **Advanced Parameters**, configure the external trigger signals from, for example, the LC system, if appropriate, see Figure 9-2.

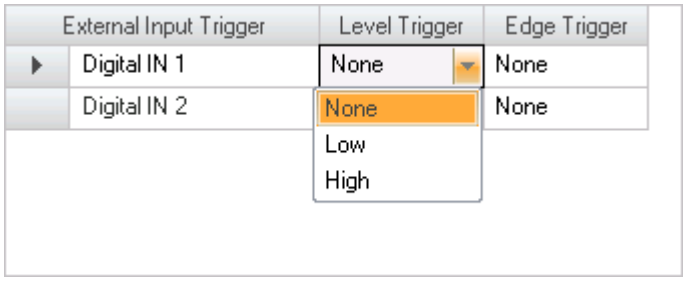


Figure 9-2. Advanced Parameters Trigger settings

12. Click  to select the **Standards** view.

13. Click **New** to define a **Standard** as described in "Creating a New Standard" on page 6-34.
See "Standards" on page 6-32 for details.

14. Define the Compounds you wish to use in your external calibration. You can create a compound standard from the compound list if you define the compounds first, see "Compounds (tQuant only)" on page 6-41.

15. Click  to select the **Compounds** view.

16. Click 

to add a line to the table and define your compound.
Your definitions for the column **Compound Name** will be used in the column **Compound** in **Standards** if you create a compound standard from the compound list. The names for **Compound Name** and **Compound** must be identical.
For details on defining compounds, see "Compounds (tQuant only)" on page 6-41.

NOTICE All settings except instrument scan dependent parameters can still be changed after measurement. ▲

17. Click  to select the **Peak Detection** view.

18. For **Smoothing**, select the check box **Active** and select **Moving Mean** from the drop-down list **Smoothing Method** to improve the signal-to-noise ratio.
For details, see "Peak Detection (tQuant only)" on page 6-44.

19. Click  to select the **Ratios** view.

20. Select the **Compound 1** and **Compound 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 6-66.

21. Click  to select the **Interference correction** view.
    This Method Parameter provides the option to minimize non-polyatomic isobaric interferences if no other interference-free isotope is available.
    For details, see "Interference Correction" on page 6-30.

NOTICE For details on all parameters, see "Method Parameters" on page 6-15. ▲

22. Click  to save the changes to your Template.

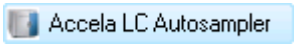
❖ **To define settings for hyphenated technique**

1. Click 

to open **Experiment Editor**.

2. Click the tab **Home Page**.

3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select the Configuration for your system with iCAP Q, the Evaluation tQuant, and, for example, the LC autosampler and LC pump.

4. Click, for example, 

to open the LC autosampler view.

5. Define the settings of, for example, your LC autosampler and LC pump(s), as appropriate.
   Depending on the autosampler or pump you use, these settings usually include flow rate, pump mode and gradient for LC pumps, needle height, speed of syringe pumps and injection mode for LC autosamplers.
   See "Peripherals" on page 6-101 for details.

6. Click  to save the changes to your Template.

❖ **To define Sample Definition**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. Open a Template as described in "Opening a Template" on page 5-22.
   Be sure to select the Configuration for your system with iCAP Q, the Evaluation tQuant, and, for example, an LC or IC system consisting of a pump system and an autosampler.
4. Define **Header**, **Body** and **Footer** as appropriate.
5. For **Sample Type**, select **STD** for the calibration solution, **UNKNOWN** for the samples, and **BLK** or **AVERAGE BLK** for blanks.
6. Enter the correct value for column **Duration**.
   The duration for the measurement should be as long as for the LC method.
7. In the columns for rack (block, tray) and vials, set the positions of the samples in the autosampler.
   The titles of these columns vary with the autosamplers.

NOTICE For details, see "Sample Definition for a Template" on page 6-117. ▲

8. Click  to save the changes to your Template.

Creating LabBook for Analysis with tQuant Evaluation

The LabBook should be based on the Template that you created for your tQuant analysis in Experiment Editor.

❖ **To create the LabBook**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. On the **Home Page**, click **Analysis**.
   The **Analysis** view of Experiment Editor opens.
4. Enter a **Name** for the LabBook and select a **Location**, see Figure 9-3.

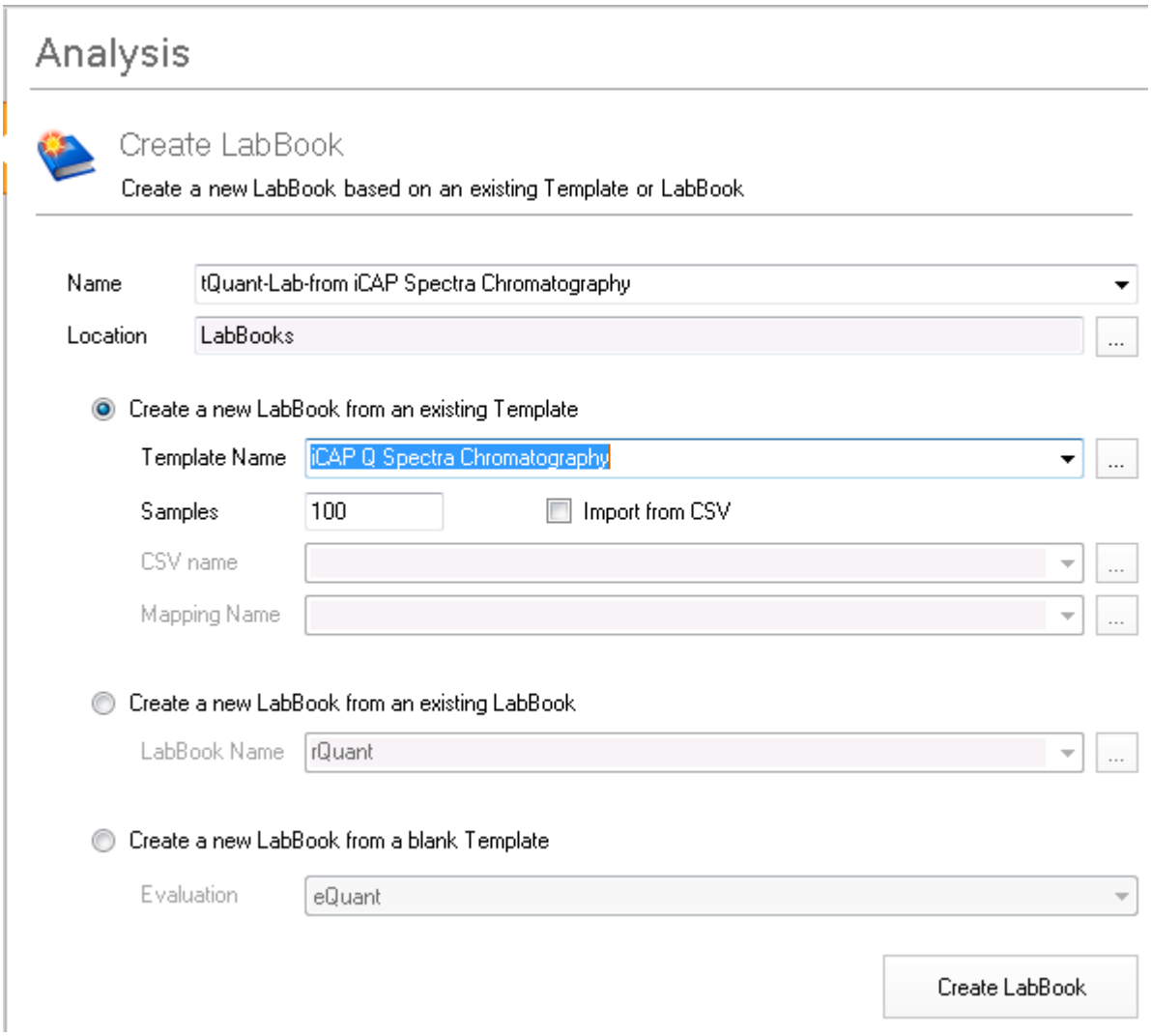
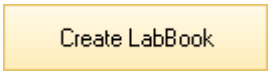


Figure 9-3. Enter Name for tQuant LabBook

5. Click the radio button **Create a new LabBook from an existing Template**.
6. Select the **Template Name** of your tQuant Template from the drop-down list.
7. Enter 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.
8. Click 

to create the new LabBook.
   A new tab opens for the new LabBook.
9. Check all settings.
   If external trigger signals are used make sure they are configured correctly. The settings are inherited from the Template.
10. Check the sample list.
    Pay special attention to Duration and Sample Type settings.
11. Make sure that the settings for the hyphenated technique are corresponding to the actual settings, for example, the position of vials in the LC autosampler.
12. In the toolbar of your **LabBook** page, click 

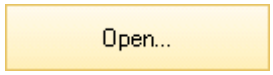
to save your LabBook.

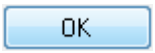
Run the Experiment of your Analysis with tQuant

During measurement, a range of settings can be observed in real time in Experiment Editor. A graphical representation shows the signal intensity of the traces over time. Peaks are shown with names, retention time integration limits as defined in the Method Parameters.

❖ **To run the tQuant LabBook**

1. Click 

to open **Experiment Editor**.
2. Click the tab **Home Page**.
3. On the **Home Page**, click **Analysis**.
The **Analysis** view of Experiment Editor opens.
4. Below  , click 

.
The **Browse for LabBook** window opens.
5. Select your tQuant LabBook.
6. Click 

to open the LabBook.
The LabBook opens in a new tab of the Experiment Editor tool.
7. In the toolbar of your LabBook, click  to schedule the LabBook for execution.
The LabBook is added to the Scheduler. If the check box **Automatic** has been selected for **Start Queue** in the **Options** settings of the Scheduler (see "Customizing Scheduler Settings" on page 5-49), the measurement is started immediately.

Results and Data Evaluation

After measurement, the LabBook is added to the Completed LabBook tab in Experiment Editor. The observed intensity is shown over time in the acquired graphical display. The graphical display shows characteristics of the selected external calibration and corresponding concentrations. For details on viewing results, see "Viewing the Result of a Measurement" on page 7-21.

NOTICE For the chromatogram, all peaks must have been aligned correctly and the areas must be correct. ▲

In the **Evaluation Results** section, the results can be monitored and quantitative data is calculated.

Any changes in the LabBook are recorded and can be saved with comments. For a complete description of the toolbar functions of a LabBook, see "LabBook Toolbar" on page 7-2.

Compounds

In the Evaluation Results **Compounds** view of the LabBook in Experiment Editor, the acquired time slices (chromatogram) are shown with the determined peak area for the defined compounds after automatic peak detection and integration, see Figure 9-4.

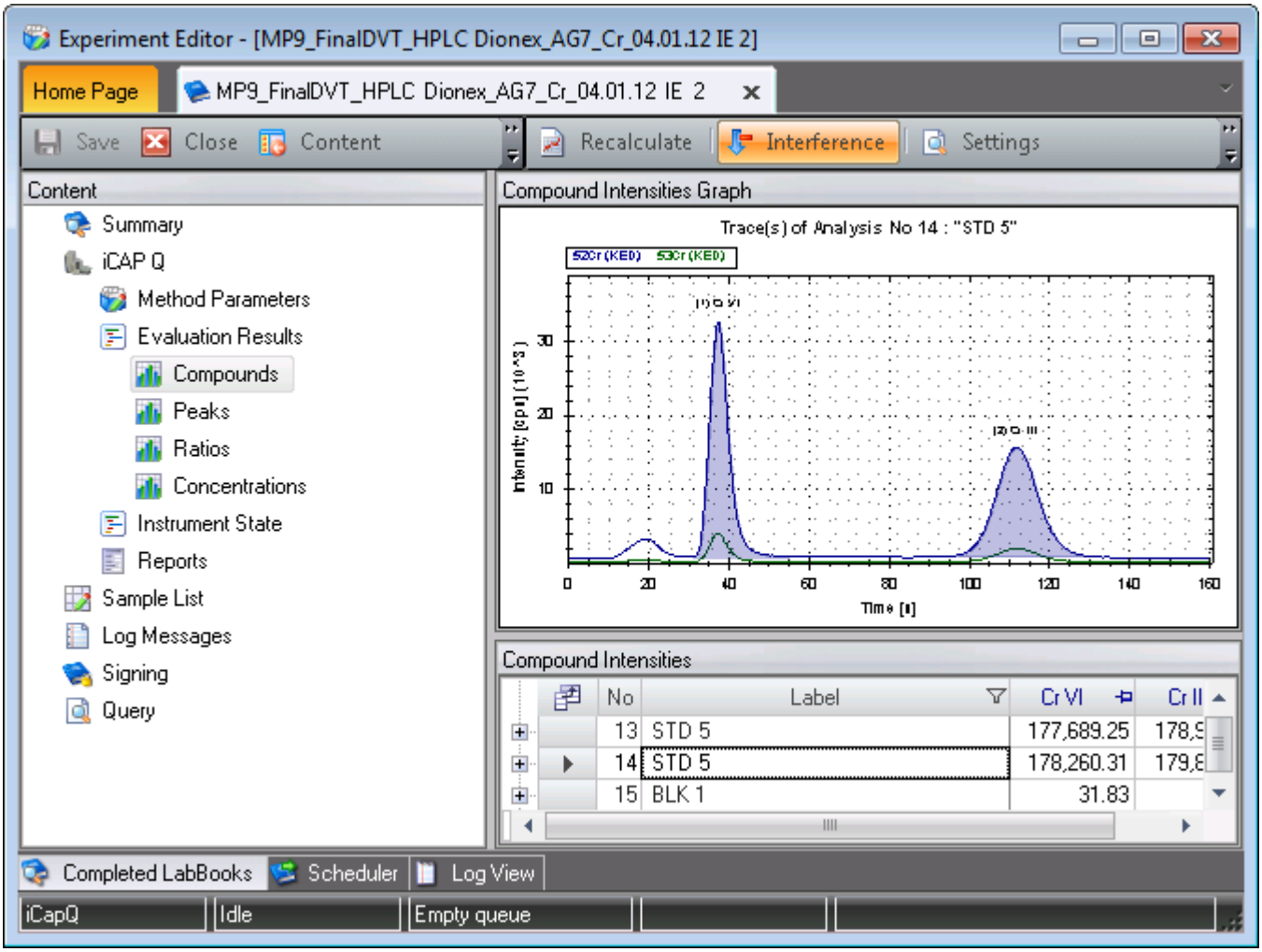


Figure 9-4. Result chromatogram

Values determined automatically by the software are displayed in black, values which have been changed or assigned manually are shown in blue.

Peaks can be selected by clicking into the table cell containing the respective peak area of a defined compound. The displayed time range in the chromatogram automatically refocuses to the time range of the selected peak, see Figure 9-5.

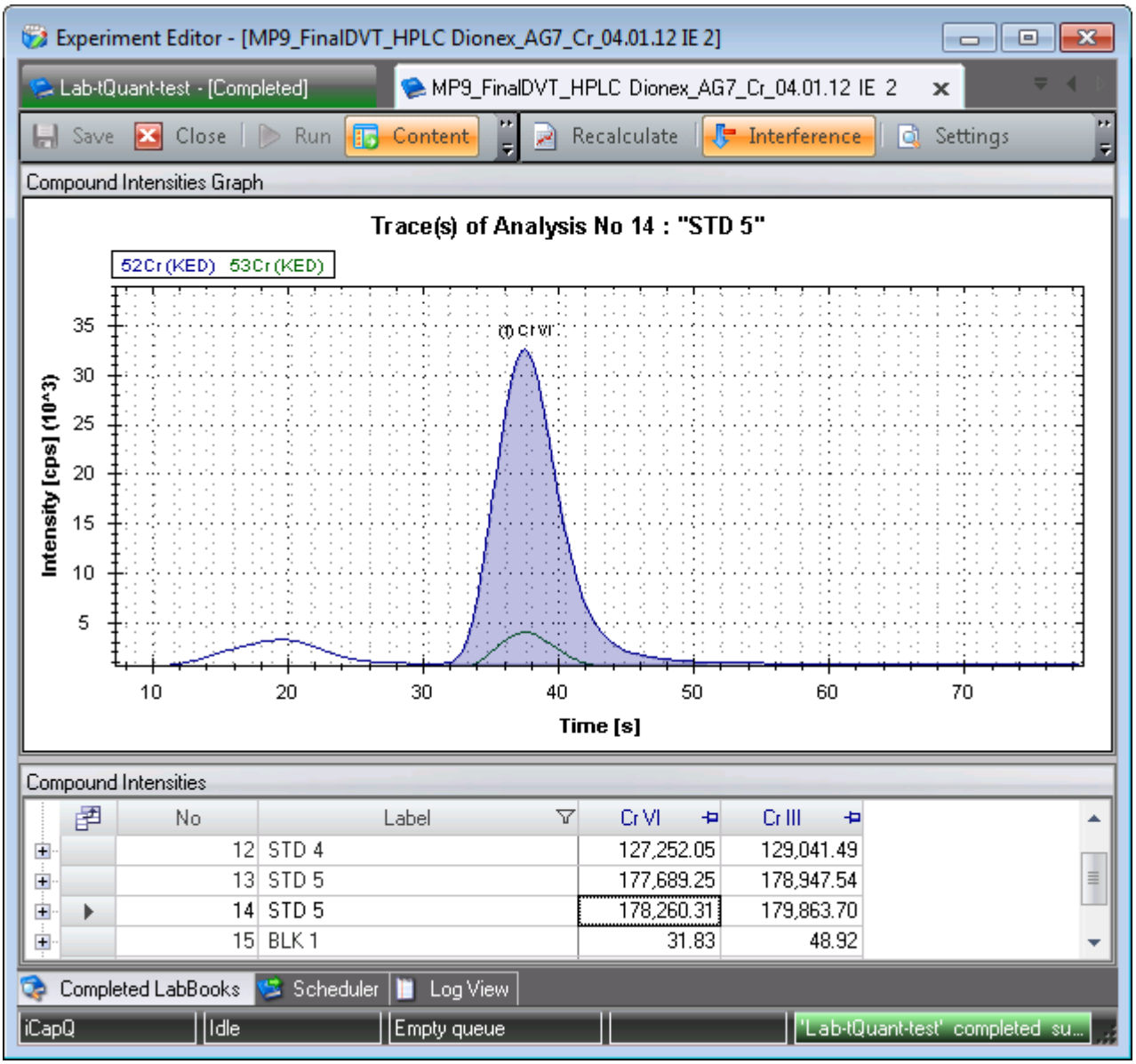


Figure 9-5. Result chromatogram of selected peak

Clicking the -sign at the front of a table row opens underlying information about the signal of interest, such as **Peak Start Time**, **Peak End Time**, **Apex Retention Time**, **Apex Baseline Height** and **Apex Height above Baseline**, see Figure 9-6.

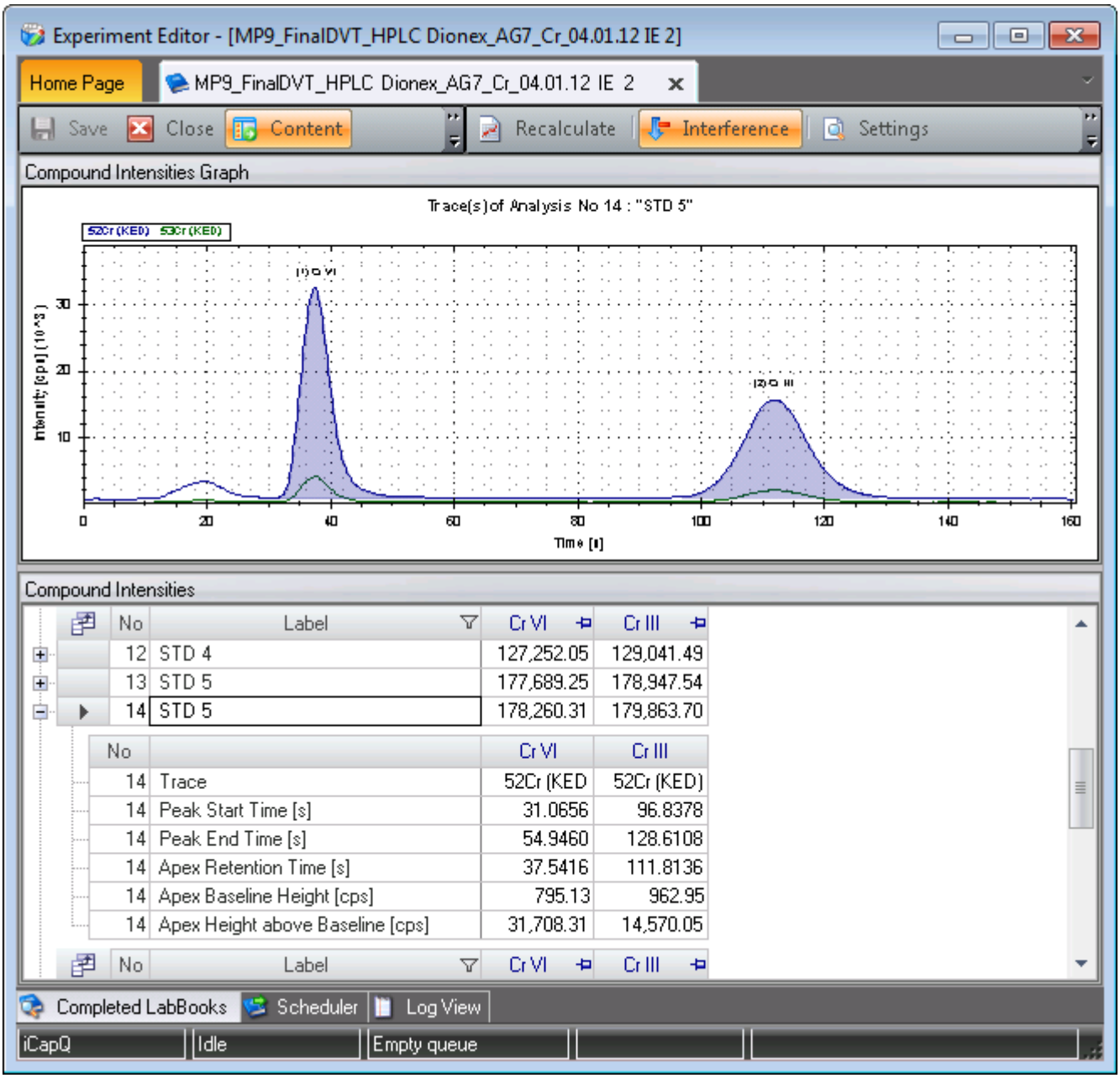


Figure 9-6. Result chromatogram and underlying information

Peak

In the Evaluation Results **Peaks** view of the LabBook in Experiment Editor, assignment of the peaks found in the chromatogram to the compounds to be quantified can be revised. Chromatographic peaks which were recognized but could not be associated to a compound are

also displayed here, see Figure 9-7.

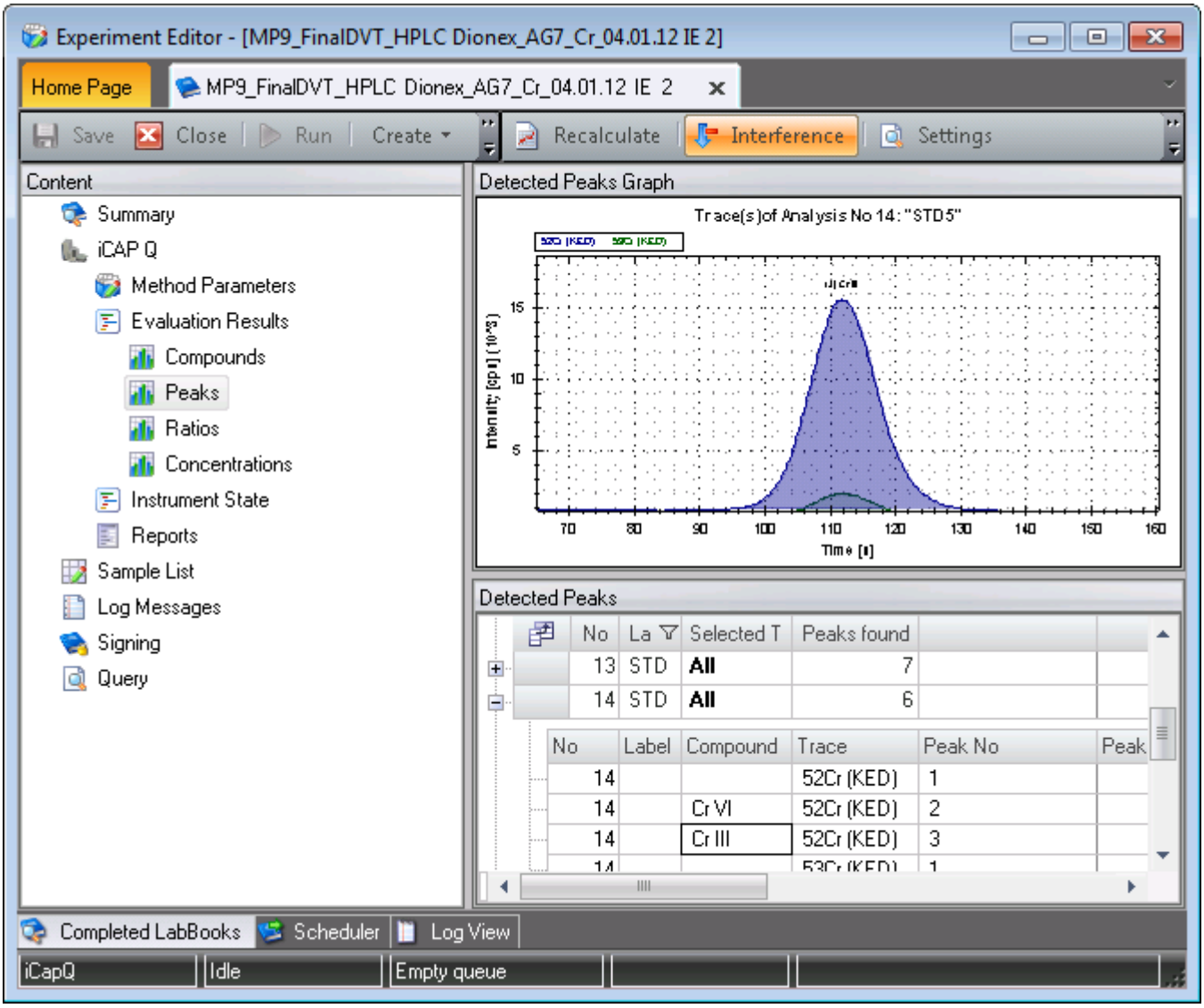


Figure 9-7. Result chromatogram Peaks view

In case that a peak for a defined compound has been detected, but was not assigned correctly, this can be done manually. By right-clicking a cell in the compound column a context menu opens, see Figure 9-8.

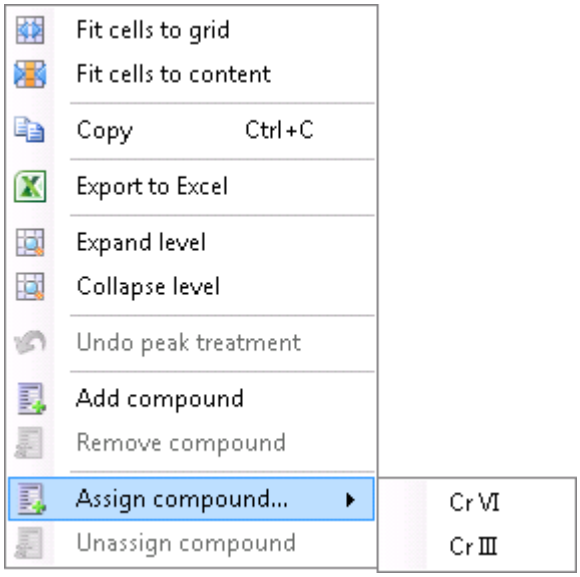


Figure 9-8. Peaks table context menu

With **Assign compound** the peak can be assigned to a compound selected from the list.

In addition, recognized peaks can be used for the creation of new compounds with **Add Compound**. The retention time and approximated tolerance of the compound are updated in the Method Parameters automatically.

If the peak identification and integration algorithm was not able to determine a peak correctly, the borders can be re-adjusted manually by clicking on  **Enable Modification** in the toolbar of the LabBook. The borders of the peak are shown and can be moved to the correct position.

Ratios

In the Evaluation Results **Ratios** view of the LabBook in Experiment Editor, ratios of the peak area between different compounds previously defined in the Method Parameters section are calculated and displayed, see Figure 9-9.

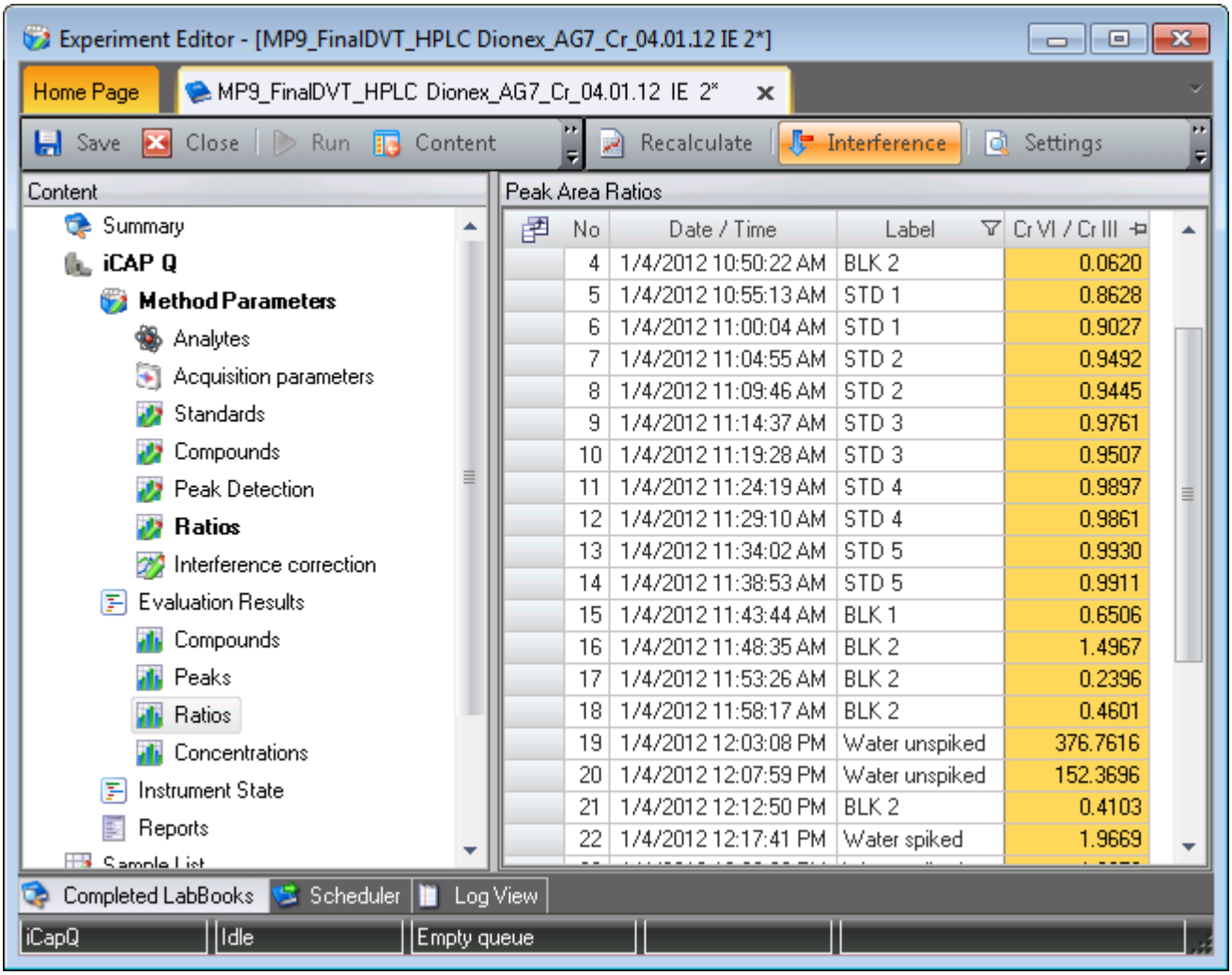


Figure 9-9. Result Ratios view

Concentration

In the Evaluation Results **Concentration** view of the LabBook in Experiment Editor, the acquired fully quantitative calibration can be revised, see Figure 9-10.

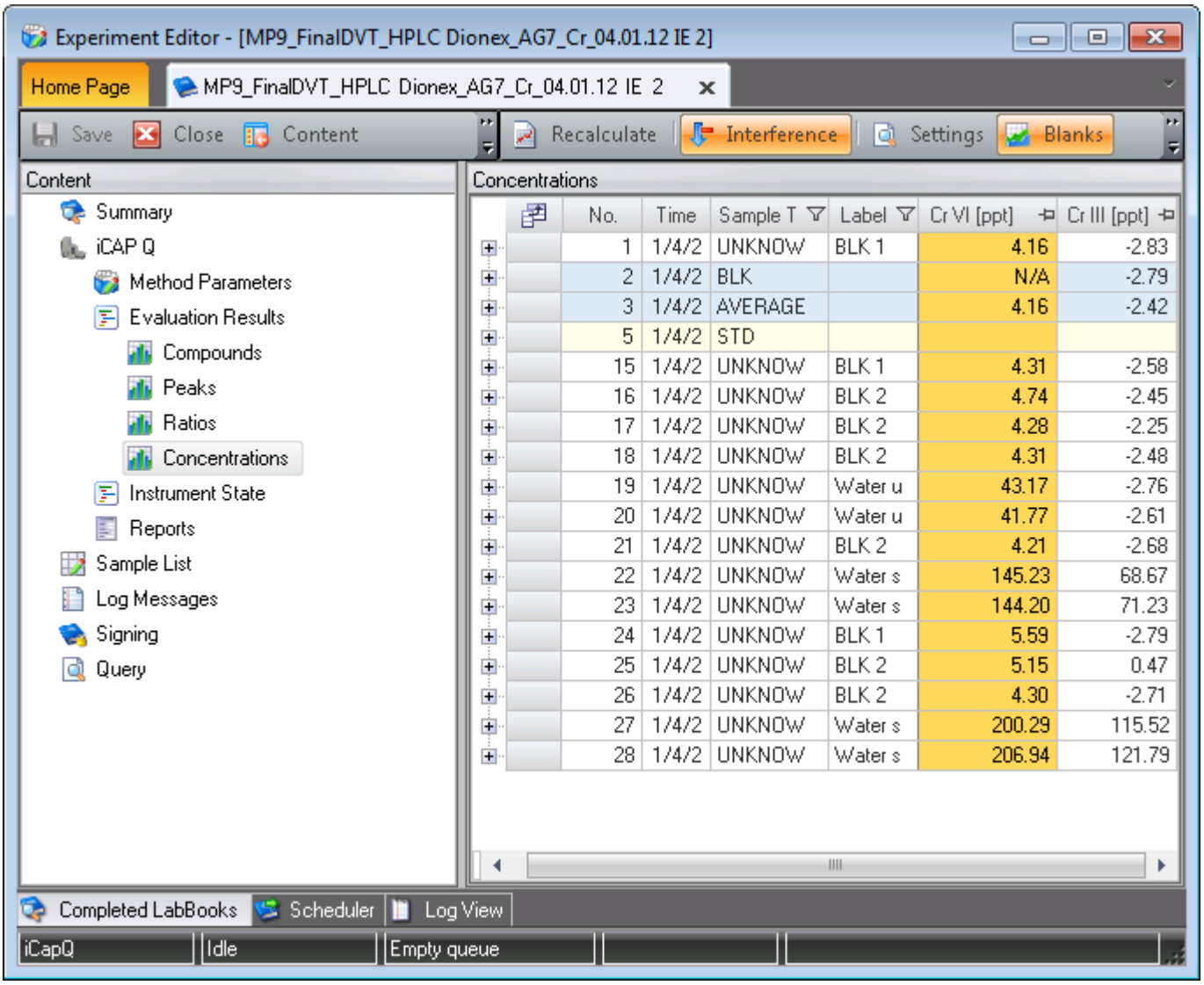


Figure 9-10. Result Concentration view

If any of the sample type UNKNOWN or fully quantitative standards should not be considered in the data evaluation process, the appropriate check box **Evaluate** has to be deselected in the Sample List. Another option is right-clicking onto the specific compound and choose **Exclude entry**, see Figure 9-11.

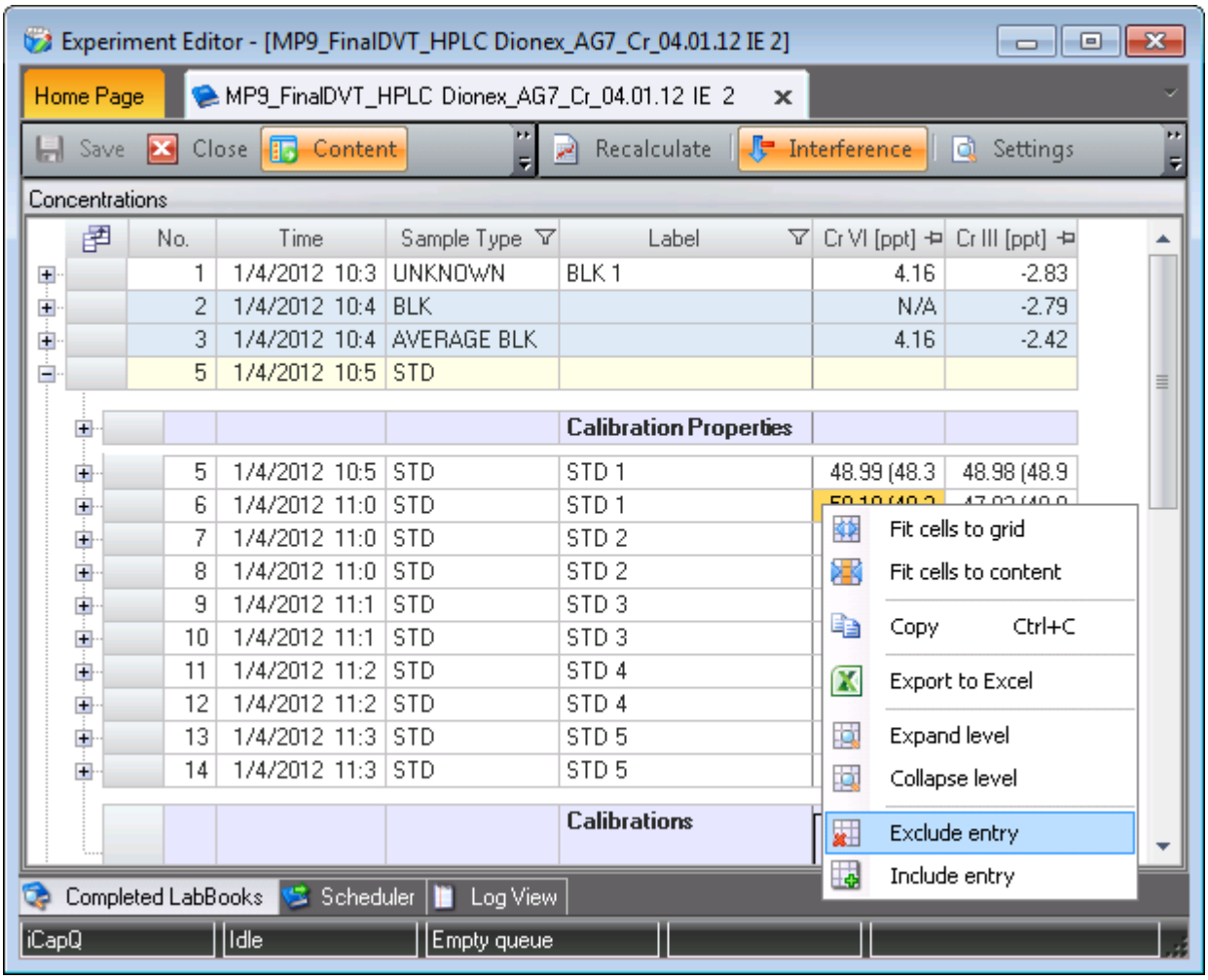


Figure 9-11. Result Concentration view with context menu to Exclude entry

The **Details** option is activated either by double-clicking the calibration graph or via the toolbar. The calibration graph for the selected compound is displayed in a larger size with related information such as

sensitivity or background equivalent concentration (BEC). The context menu of the **Details** window also offers **Display logarithmical**, see Figure 9-12.

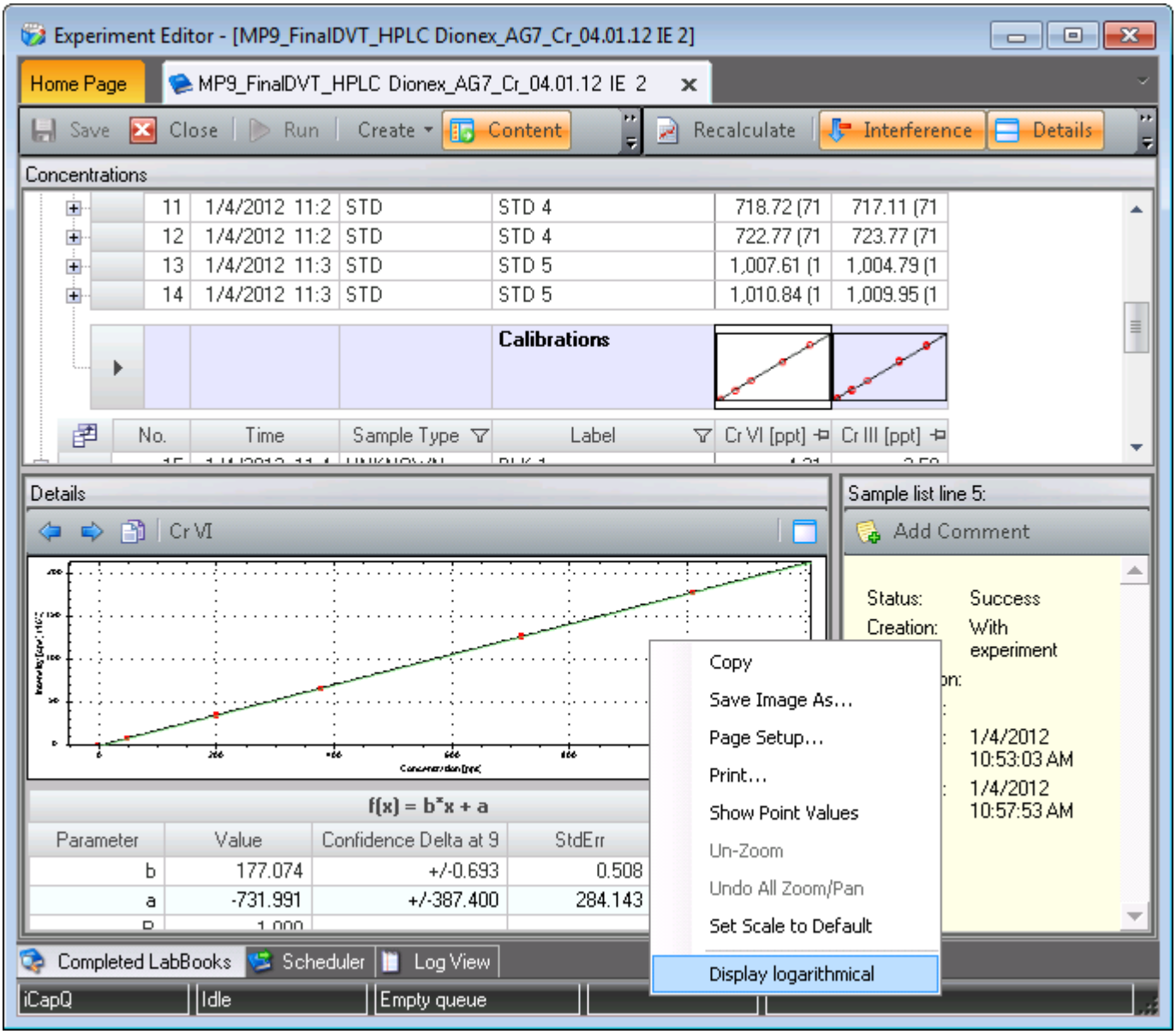


Figure 9-12. Result Concentration view Details

The determined fully quantitative results are shown in the same section. Interference correction or blank subtraction are not applied to the data if **Interference** or **Blanks**, respectively, is deactivated in the toolbar.

The history of the changes made to the Labbook are displayed by clicking **History** in the toolbar. Options to export the results are shown by clicking **Export**. 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 7-2.

NOTICE Print and exportable reports containing the previously selected information can be generated in the Query view, see "Query" on page 7-31. ▲

Chapter 10 Data Evaluation

Data Evaluations are calculation methods that are applied within the Qtegra software. These calculation or evaluation methods are selected when creating a Template in Experiment Editor (see "Evaluation Methods" on page 6-10).

The Qtegra data evaluation is handled by several evaluation modules (evaluation plug-ins) called virtual evaluation (VE). The system currently knows the following common evaluation modules for quantification:

Contents

- Integration - Raw Data Handling
- External Calibration
- Standard Addition
- Isotope Dilution

The raw data interface uses mathematical methods to manipulate the raw data acquired and serves as the basis for the data calculated by the modules.

Integration - Raw Data Handling

Raw data are based on the number of Main Runs shown in the corresponding line of the Samplelist in Figure 10-1 and are calculated for every amu (analyte) for which data has been collected. For semi-quant analyses, data of Survey Runs are also taken into account. For details on sample lists, see "Sample List - LabBook" on page 7-14.

Samplelist

	Label	Status	Survey Runs	Main Runs	Evaluate	Sample Type
1	Blank		0	1	☑	UNKNOWN
2	STD		0	1	☑	STD
3	STD		0	1	☑	STD
4	STD		0	1	☑	STD
5	STD		0	1	☑	STD
6	Sample		0	1	☑	UNKNOWN
7	water		0	1	☑	UNKNOWN
8	Blank		0	1	☑	UNKNOWN
9	water		0	1	☑	UNKNOWN

Figure 10-1. Sample list of LabBook

In the Acquisition Parameters table, see Figure 10-2, the operator defines the isotopes for the measurement, as well as measurement settings such as Dwell time. The number of channels corresponds directly to the number of measured intensities for a specified isotope in one run. For details, see "Acquisition Parameters" on page 6-19.

Acquisition Parameters, runtime estimation 40 milliseconds

Identifier	Dwell time (s)	Channels	Spacing (u)	Measurement mode	Resolution
44Ca	0.01	1	0.1	STD	Normal
24Mg	0.01	1	0.1	STD	Normal
23Na	0.01	1	0.1	STD	Normal
39K	0.01	1	0.1	STD	Normal

Figure 10-2. Acquisition parameters for analytes

In the background, the data adapter of the Qtegra software uses different mathematical strategies to calculate a raw data intensity value for a given isotope and a given run. For any strategy, the exact measured amu (analyte) is defined as the mean value of the amu for the measured channels:

- Average:

$$\text{Intensity } i = \left(\sum_{k=1}^{channel} i_k \right) / \text{channel}$$

- Centroid: Intensity $i = i_k$ with k = channel div 2
- Integral:

$$\text{Intensity } i = \left(\sum_{k=i}^{channel} i_k \right)$$

- Highest: Intensity $i = \max i_k$

  $\forall k \in \{1..channel\}$

External Calibration

The external calibration strategy is employed with the Evaluation methods eQuant (steady state signals), tQuant (transient signals), and trQuant (transient regions).

The External Calibration module is the most complex quantification module. It currently offers seven sample types to specify measurement blocks, see Table 10-1.

Table 10-1. Supported sample types

Name	Description
UNKNOWN	Defines a sample line where isotopes are quantified using the calibration curve from the preceding standard block or using the semi-quant methods.
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 values of all blanks in the current measurement block define the blank to be used for blank correction.
ZERO STD	Allows you to do work in standard addition mode inside the external calibration module.
UPDATE CALIB	Used to correct the current calibration curve.
QC	Defines a sample as quality control sample and applies the selected actions. A QC sample is handled the same way as an UNKNOWN.

Sample types can be defined for each sample line, see "Sample Definition for a Template" on page 6-117.

A minimal measurement block consists of at least one STD sample line and one UNKNOWN sample line. Only multiple measurement results assure statistically useful data. Typically, at least three main runs should be done. Valid measurement blocks are shown in Figure 10-3.

Samplelist estimated runtime: 9 minutes 50 seconds

	Label	Status	Surv	Main Runs	Evaluate	Sample Type
1	Blank		0	3	☑	BLK
2	STD		0	3	☑	STD
3	STD		0	3	☑	STD
4	STD		0	3	☑	STD
5	STD		0	3	☑	STD
6	Sample		0	3	☑	UNKNOWN
7	water		0	3	☑	UNKNOWN
8	Blank		0	3	☑	UNKNOWN
9	water		0	3	☑	UNKNOWN

Figure 10-3. Measurement blocks in a sample list

NOTICE Isotopes which cannot be quantified with a calculated calibration curve may be roughly quantified by using the semi-quant feature available in this module. ▲

Internal Standard Correction

The Method Parameter Standards (see "Standards" on page 6-32) is used for specifying standards as well as internal standards.

Global Internal Standards are created in the **Standard editor** of the Configurator tool. These can be loaded into the Method Parameter **Standards** of a Template or LabBook and are then used for internal standard correction if so defined.

Internal Standard Correction is available for methods based on eQuant, aQuant, tQuant or trQuant evaluation.

In a sample line, the internal standard to be used is specified in the column **Internal Standard**. All Internal Standards previously defined in the Method Parameter **Standards** of a Template or LabBook can be selected from a drop-down menu, see Figure 10-4.

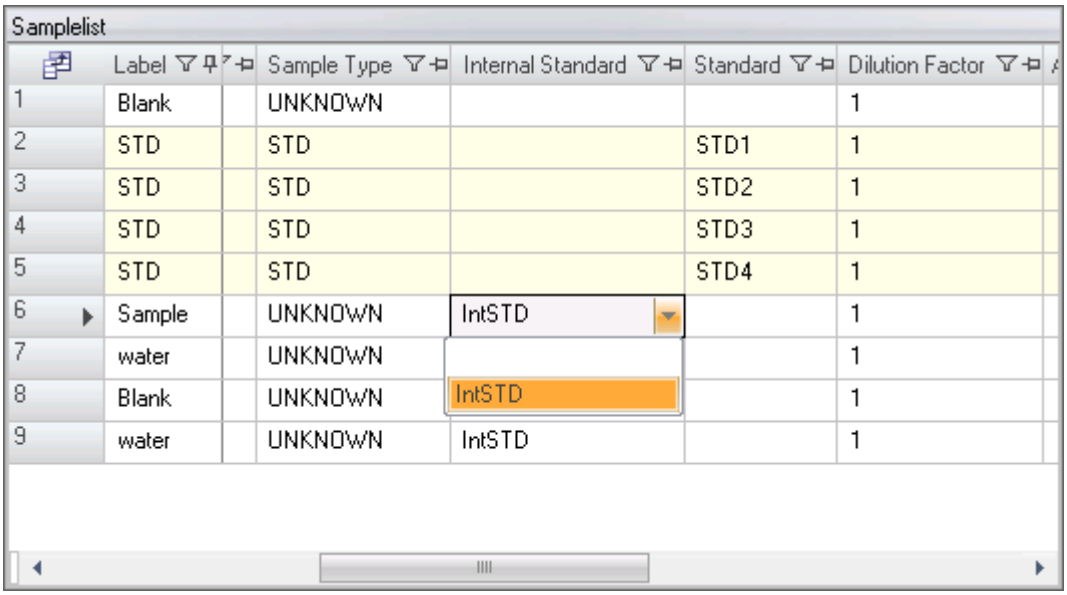


Figure 10-4. Selecting Internal Standard for sample line

For methods based on tQuant evaluation, **Internal Standardization** can be activated in the Compounds view, see "Compounds (tQuant only)" on page 6-41.

A specified mass is corrected with the isotope for that the **Use as Internal Standard** option is defined in the Method Parameter **Quantification** (eQuant or aQuant) or **Parameters** (trQuant). The check box **Internal Standardization active** must have been selected, see Figure 10-5.

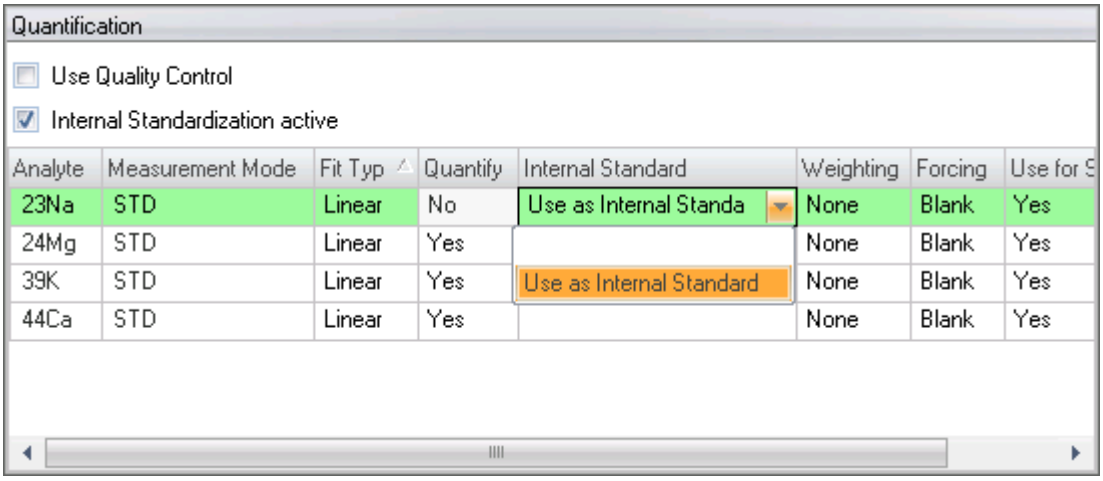


Figure 10-5. Internal standard correction activated

In case internal standard correction has been activated, all blank, standard, and unknown block sample lines are corrected. Every measured intensity i will be corrected with the appropriate internal standard correction factor:

$$g_{ISC} \text{ with } i_{corr} = i \cdot g_{ISC}$$

The other evaluation parameters (Forcing and Weighting) refer to the settings of the calibration properties used for the calibration curve of the isotope.

Using the first measurement line of the preceding standard block g_{ISC} is calculated as follows:

$$g_{ISC} = \frac{i_r^{ISC}}{i_t^{ISC}}$$

where i_t^{ISC} denotes the averaged intensity of the internal standard of all main runs in the first line of the preceding block corresponding to a certain chosen analyte, and i_r^{ISC} denotes the averaged intensity of the internal standard in each of the following sample lines.

NOTICE By definition, only one internal standard or internal standard mixture can be used for the whole experiment. Overlapping of internal standards and standards used for full-quantification is not allowed. ▲

Blanks

Consecutive blank sample lines are handled as so-called blank blocks. Each blank sample line generates one blank intensity value for each measured isotope. This intensity is defined as the mean value of all runs of the current sample. Depending on the sample type, each blank block is used in a different manner:

- AVERAGE BLK defines the blank value for the current measurement block as the average value of all blank intensities in the current blank block:

$$i_{Blank_{Isotope}} = \frac{\sum_{j=1}^{\#\text{ blank block lines}} i_{Blank_{jIsotope}}}{\#\text{ blank block lines}}.$$

- BLK uses the blank intensity last measured as the blank block intensity.

Blank correction is applied as a subtraction of intensity values or used as the zero intensity value for the calibration curve. The latter method is used as default.

Subtraction of intensity values is automatically chosen and only applied for a zero standard (ZERO STD) for quantification using the standard addition method.

NOTICE Blank correction is only done on non-internal standard isotopes. If a calibration curve is available, this curve will be used to quantify the measured intensities. Depending on the options used for calculating the calibration curve this will result in different values. For example, only forcing through Blank guarantees a zero concentration for the blank. ▲

Standards

Standards consisting of elements with known concentrations present the basis of any comparing quantification method. Consecutive standard sample lines are handled as a standard block. Each standard sample line generates one intensity value for each measured isotope. This value is combined with the known element concentration from the standard and forms a data point of the calibration curve.

Updating the Calibration Curve

With the sample type UPDATE CALIB, it is possible to recalculate your concentrations without running the standard measurement again if you realize, for example, drifts in the results. This sample type is used to calculate a correction value which will be applied to the preceding calibration block. Element concentration and dilution factor of the update calibration sample line must be identical to the one of the standard block.

The intensity of a measured isotope with the sample type UPDATE CALIB

$$i_{Isotope}^{UPDATECALIB}$$

for a certain concentration c_t is also measured inside one of the samples lines of the preceding standard block

$$i_{Isotope}^{STD}.$$

The factor obtained from the corresponding sensitivities

$$k_{UPDATECALIB} = \frac{s_r}{s_t}$$

is used for scaling any intensity value of the calibration curve applied to calculate the concentrations of the samples following the measurement of the UPDATE CALIB sample, where s_r and $\bar{s}_t$ are the reference and averaged target sensitivity in the preceding standard block of each standard isotope, respectively. The sensitivities are calculated using the equations:

$$s_r = \frac{i_{Isotope}^{UPDATECALIB}}{c_{Analyte}^{STD}}$$

$$\bar{s}_t = \frac{i_{Isotope}^{STD}}{c_{Analyte}^{STD}}$$

The sample type ZERO STD function can be combined with all other available sample types in the External Calibration module. For details, see "Standard Addition" on page 10-13.

NOTICE UPDATE CALIB samples can only compensate drifts affecting the sensitivity of the instrument. To compensate for increased or decreased blank values it is recommended to insert BLK or AVERAGE BLK sample types before the UPDATE CALIB sample and to use the QA/QC functionality of Qtegra. If a ZERO STD is used, all blank concentration is calculated by subtraction intensity values. ▲

Calculating the Calibration Curve

Based on the calibration curve, the original concentration c of the analyte in an UNKNOWN sample is calculated with

$c = f^{-1}(x)$ where x is the measured intensity.

NOTICE Depending on the evaluation method, different method parameters offer the options for calculating the calibration curve. See "Quantification" on page 6-62, "Compounds (tQuant only)" on page 6-41 and "Parameters" on page 6-55. ▲

The available options for calculating the calibration curve are listed in Table 10-2.

Table 10-2. Options for calibration curve calculation

Option	Description	
Fit Type	Linear	A linear regression curve with $f(x) = a_1 x + a_0$ is calculated given the data points.
	2nd order	A cubic regression curve with $f(x) = a_2 x^2 + a_1 x + a_0$ will be used.
Forcing	No	Value *y* for *x = 0 i*s 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 $f(0) = i_{Isotope}^{BLK}$ or $f(0) = i_{Isotope}^{AVERAGEBLK}$, depending on the current blank block mode.
Weighting	None	Value will not be weighted.
	Absolute SD	Weight $\omega_k = 1/\sigma_k^2$. Each point is weighted by the standard deviation σ_k of the analyte over the runs in the sample.
	Relative SD	Weight $\omega_k = 1/(\sigma_k/\bar{i}_k)$. Each point is weighted by the standard deviation σ_k of the analyte over the runs in the sample relative to the mean value $\bar{i}_k$.

If final quantity *q*, amount *a*, and dilution *d* are specified in the sample list, the concentration value is corrected by

$$c_{corr} = c \cdot d \cdot q / a .$$

Unspecified values are set to be 1. The dilution factor is in a comparable way also handled for standards.

NOTICE Unit selections are set for the complete experiment. ▲

Semi-Quant

The semi-quant feature is used for isotopes that cannot be quantified by using a calibration curve based on standards. For this type of analysis it is assumed that each isotope on a standard has a defined instrument-specific response. By default, any isotope calibration curve of the previous standard block will be used as input for the semi-quant methods.

A semi-quantitative response curve is produced for every standard block in the experiment. A semi-quantitative curve is a 2nd order line fit of sensitivity against mass. Each calibration curve in a standard block that has been selected for use in the response curve is included in the line fit. The sensitivity of each isotope is taken from the slope of its calibration curve and is corrected for relative sensitivity using the defined analyte RSF (relative sensitivity factor). Only linear curves may be used for semi-quantitative analysis and at least three calibration curves are needed to solve a 2nd order line fit problem. The semi-quant sensitivity s_{sq} is given by

$$s_{sq} = a_1^{isotope} / (RSF_{analyte} \cdot A_{isotope})$$

where $A_{isotope}$ defines the isotopic abundance (semi-quant curves are always defined in terms of isotopic sensitivity) and $a_1^{isotope}$ defines the slope given by the calibration curve.

The slope results lead directly to the quantification of a non-standard isotope with the measure intensity $i_{non\text{-}standard\ isotope}$

$$c_{sq} = i_{non\text{-}standard\ isotope} / a_i .$$

If final quantity q, amount a, and dilution d are specified in the sample list, the concentration value is corrected by $c_{corr} = c \cdot d \cdot q / a$. Unspecified values are set to be 1.

NOTICE In case of semi-quantitative analysis units are chosen automatically for best representation. ▲

Isotope Quantification

To fully quantify an isotope the preceding methods are applied. A full isotope quantification consists of the following steps:

- Calculation of internal standards, correction will only be applied if activated.
- Calculation of blanks.
- In case of the existence of zero standards, blank corrections directly corrects intensity values.
- Generation of calibration curves based on standards and zero standards.
- If necessary, semi-quant response curves for non-standard isotopes will be generated.
- Based on the pre-calculated information, the isotope quantification is executed.

Standard Addition

The Standard Addition module (aQuant) uses the sample type ZERO STD (defining the zero spike) and STD (for standards) to set up a measurement. For details on sample types see "Sample Definition for a Template" on page 6-117.

A valid sample list for standard addition consists of blocks of one ZERO STD measured at the beginning followed by a sequence of standards (STD). For each block, a first-order calibration curve is produced for every analyte. 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 square fit. The available options are listed in Table 10-3:

Table 10-3. 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.
Weighting	None	Value will not be weighted.
	Absolute SD	Weight $\omega_k = 1/\sigma_k^2$. Each point is weighted by the standard deviation σ_k of the analyte over the runs in the sample.
	Relative SD	Weight $\omega_k = 1/(\sigma_k/\bar{i}_k)$. Each point is weighted by the standard deviation σ_k of the analyte over the runs in the sample relative to the mean value $\bar{i}_k$.

Based on the calibration curve the original concentration c of the analyte in the standard (STD) samples is calculated with

$$c = f^{-1}(x)$$

where x is the measured intensity.

With

$$f(x) = a_1 x + a_0$$

the measured concentration of the zero standard is calculated as

$$i_{ZEROSTD} = a_0$$

$$c_{ZEROSTD} = i_{ZEROSTD} / a_1 .$$

If final quantity *q*, amount *a*, and Dilution *d* are specified in the sample list, the zero concentration value is corrected by

$$c_{ZEROSTDcorr} = c_{ZEROSTD} \cdot d \cdot q / a .$$

Unspecified values are set to be 1. The dilution factor is in a comparable way also handled for standards.

NOTICE 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. ▲

NOTICE Using 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 measuring the first zero standard will be ignored. ▲

Isotope Dilution

Due to the methodical structure of Isotope Dilution, this module has more complexity than the Standard Addition module. To quantify an element in a Isotope Dilution experiment, the standards for spiking must first be defined. The known concentration of an element as well as the known information about the specifying isotopes, their abundance values as well as atomic weight have to be entered.

A global Isotope Dilution Standard can be created in the applet **Standard editor** of the Configurator tool, see Figure 10-6.

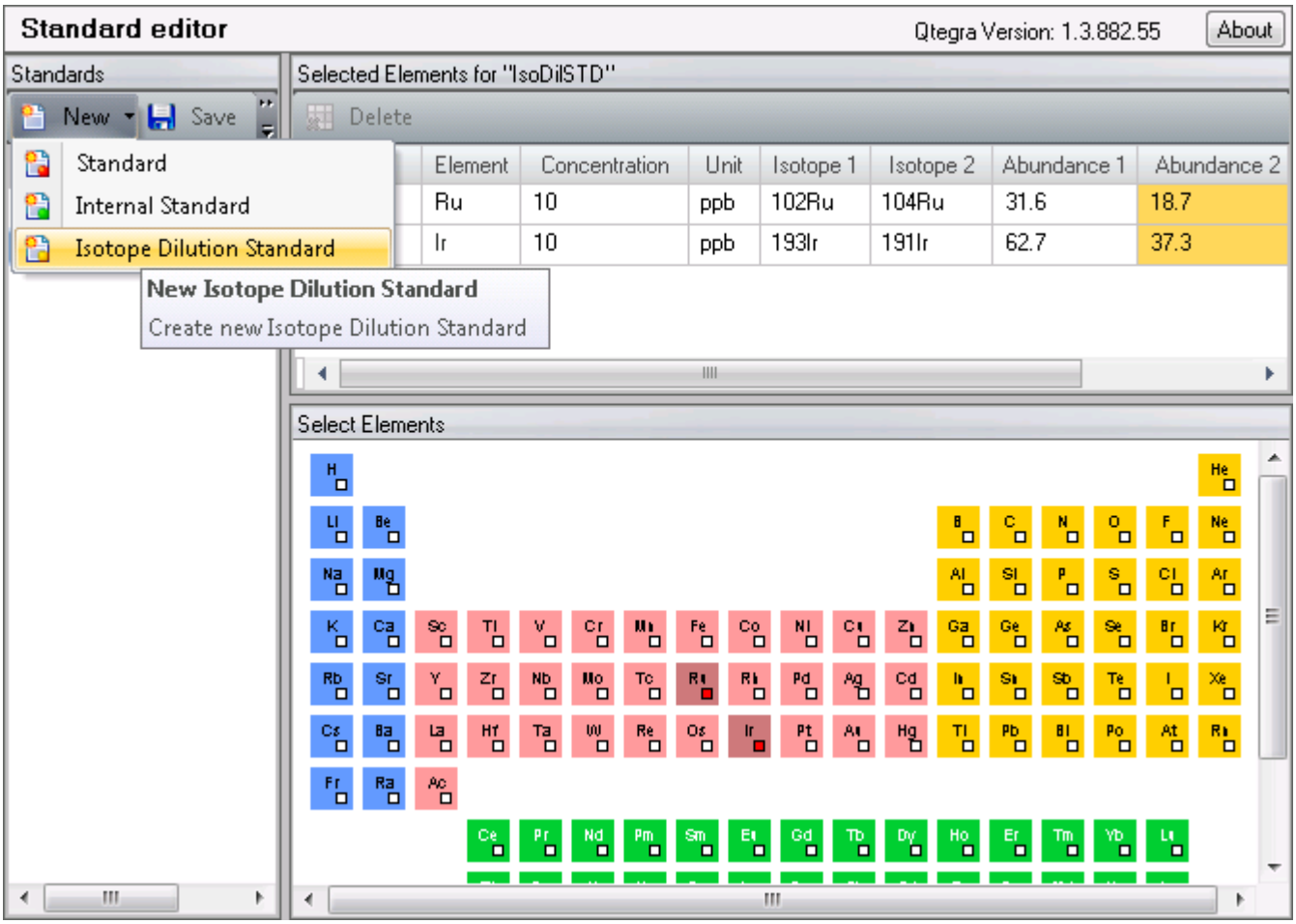


Figure 10-6. Isotope Dilution Standard in Configurator

NOTICE For details, see "Standard Editor" on page 3-35. ▲

Typically, isotope dilution standards are created in Templates or LabBooks with rQuant evaluation, see Figure 10-7.

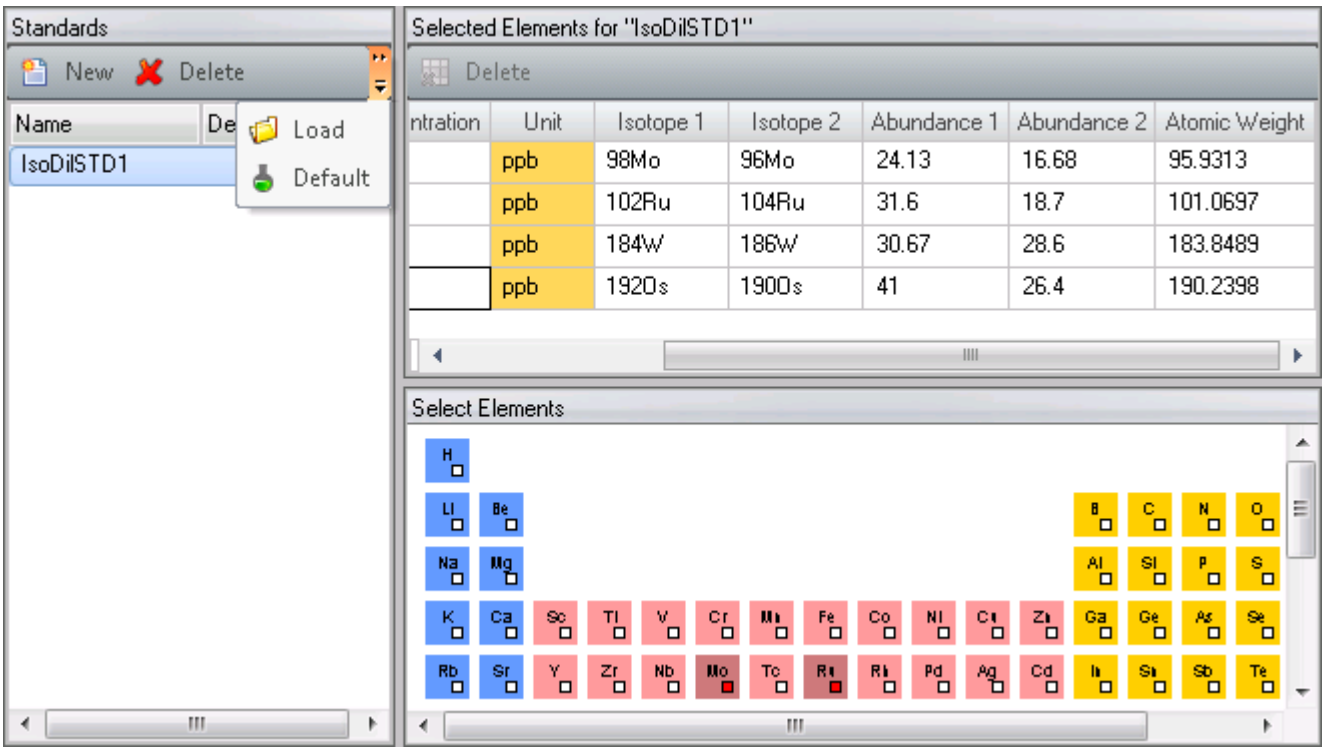


Figure 10-7. Isotope Dilution Standard in Template

NOTICE For details, see "Creating a New Standard" on page 6-34. ▲

The quantification of an element given by the concentration $c_{Element}$ is then based on the following equation:

$$c_{Element} = c_{Spike} \cdot \frac{M_{Spike}}{M_{Sample}} \cdot \left(\frac{a_{Spike}^{Isotope1} - (a_{Spike}^{Isotope2} \cdot R_{measured})}{(a_{Sample}^{Isotope2} \cdot R_{measured}) - a_{Sample}^{Isotope1}} \right) \cdot R_{ATW_{Element}}$$

where

c_{Spike} = element concentration in spike solution

M_{Spike} = amount of added spike

M_{Sample} = sample amount

$a_{Spike}^{Isotope\ k}$ with $k \in \{1, 2\}$ = abundance of isotope k in spike solution

$a_{Sample}^{Isotope\ k}$ with $k \in \{1, 2\}$ = abundance of isotope k in sample solution

$R_{measured} = \frac{i_{Isotope1}}{i_{Isotope2}}$ with the measured intensities $i_{Isotopes\ k}$ and

$k \in \{1, 2\}$

and

$$R_{ATW_{Element}} = \frac{ATW_{Element_{Sample}}}{ATW_{Element_{Spike}}}$$

with ATW as the atomic weight of the specified element.

If final quantity q, amount a, and dilution d are specified in the sample list, the element concentration value is corrected by

$$c_{\text{Element}corr} = c_{\text{Element}} \cdot d \cdot q / a .$$

Unspecified values are set to be 1.

NOTICE This measurement method quantifies the elements defined in the Evaluation Parameters tab control. Because of the structure of the Evaluation Parameters list, each element can be specified only once, even if there is theoretically the possibility to have different spiking standards including the same element. ▲

Glossary

This section lists and defines terms used in this manual. It also includes acronyms, metric prefixes, symbols, and abbreviations.

A

ac abbr. for alternating current, for example, an electric current that reverses its direction at regularly recurring intervals.

accurate mass The accurate mass is the theoretical ion mass of an isotope or molecule as given by IUPAC.

Acid Resistant Sample Inlet resistant inlet with a special nebulizer chamber and torch.

ADC abbr. for analog-to-digital converter; a device that converts data from analog to digital form.

AIM abbr. for Active Inverted Magnetron gauge used for vacuum (pressure) measurement; also referred to as Penning gauge.

AL/VI abbr. for Aluminum/Viton™; material used for gaskets.

amu see atomic mass unit.

analog mode the detection mode "Analog" can be used for high signals between 5×10^4 to 5×10^9 cps. The electrical current measured is converted into the intensity information, which is stored in the data file.

APG abbr. for Active Pirani Gauge used for vacuum (pressure) measurement.

atomic mass unit Atomic Mass Unit (u) defined by taking the mass of one atom of carbon12 as being 12 u; unit of mass for expressing masses of atoms or molecules.

aux gas auxiliary gas (argon), serves to generate the plasma.

B

BEC abbr. for Background Equivalent Concentration (normally in ppt); n=10, depends on the concentration in the blank.

$$\text{BEC} = \frac{(\text{blank intensities}) \times (\text{concentration of standard})}{(\text{intensity standard} - \text{average intensity blank})}$$

BLK abbr. for a blank (analyte).

C

°C degrees Celsius.

CE European conformity. Mandatory European marking for certain product groups to indicate conformity with essential health and safety requirements set out in European Directives.

cool gas serves to prevent the glass torch from melting.

counting mode the detection mode "Counting" is a digital measurement and counts electron pulses. It is very sensitive and can be used for the detection of low signals. During acquisition, the number of occurrences is used to generate the intensity information (in counts per seconds) that is stored in the data file. The operating range of the counting mode is between 0 and ~5×10^6 cps.

D

DAC abbr. for digital-to-analog converter; a device that converts data from digital to analog form.

dc abbr. for direct current, for example, an electric current flowing in one direction only.

DDS abbr. for direct digital synthesizer.

DSP abbr. for digital signal processor.

E

eV abbr. for electron volt; the energy gained by an electron which accelerates through a potential difference of one volt.

F

f femto (10^{-15}).

°F degrees Fahrenheit.

FTP file transfer protocol.

G

G Gauss; giga (10^{9})

GC gas chromatograph; gas chromatography.

GC/MS gas chromatograph / mass spectrometer.

GND electrical ground.

GUI graphical user interface.

H

h hour.

h height.

HPLC high-performance liquid chromatograph.

HR abbr. for High Resolution.

HV high voltage.

Hz hertz (cycles per second).

I

ICIS™ Interactive Chemical Information System.

ID inside diameter.

in. inch.

internal standards are used in ICP-MS analyses to compensate for drift effects in response or sensitivity caused by various processes in sample introduction or ion extraction.

I/O input/output.

ISO abbr. for International Organization for Standardization.

L

LAN local area network.

lb pound.

LC liquid chromatograph; liquid chromatography.

LC/MS liquid chromatograph / mass spectrometer.

LED light-emitting diode.

linear regression type: linear regression analyses.

LOD abbr. for Limit of Detection (normally in ppt); n = 10, depends on the stability of the blank measurement.

$$\mathrm{LOD} = \frac{(3 \times \text{stdev of BLK intensities}) \times (\text{concentration of STD})}{(\text{intensity STD} - \text{average intensity BLK})}$$

LR abbr. for Low Resolution.

M

M^+ molecular ion.

MH^+ protonated molecular ion.

MS mass spectrometer; mass spectrometry.

m/z mass-to-charge ratio.

O

OD outside diameter.

P

PCB printed circuit board.

PCL abbr. for Process Control Language.

P/N part number.

ppb abbr. for parts per billion. A unit of measure expressed as parts per billion. Equivalent to 1×10^{-9}. Similar to µg/L or micrograms per liter.

ppt abbr. for parts per trillion. A concentration unit of chemical constituents in solution, the weight of solute per unit volume of solvent.

psig pounds per square inch, gauge.

R

regression types are used in the creation of calibration curves during a sequence of analyses: the software offers four types: linear, thru zero, weighted, and square fit.

RF radio frequency.

S

s second.

square fit regression type: the fit is performed with a second order (quadratic) function.

STD abbr. for standard solution (analyte).

T

TCP/IP transmission control protocol / Internet protocol.

U

u symbol for atomic mass unit.

UPW abbr. for Ultra Pure Water.

V

V ac volts alternating current.

V dc volts direct current.

W

weighted regression type: linear regression weighted by the reciprocal of the standard deviation (1/standard deviation).

WEEE European Union Waste Electrical and Electronic Equipment Directive. Provides guidelines for disposal of electronic waste.

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