Thermo Fisher Scientific **iCAPTM Q Software Manual**

Revision B - 1288010





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Release History: Revision A released in April 2012 Revision B released in October 2012.

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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: Editors, Technical Documentation Thermo Fisher Scientific (Bremen) GmbH Hanna-Kunath-Str. 11

28199 Bremen

Germany

• 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 iCAPTM 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			
	<i>Left</i> and <i>right</i> 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 <i>F1</i>.</f1> 		
	• Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, "press <shift></shift> + <f1></f1> " means press and hold the <shift></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 Otegra

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:

- 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:

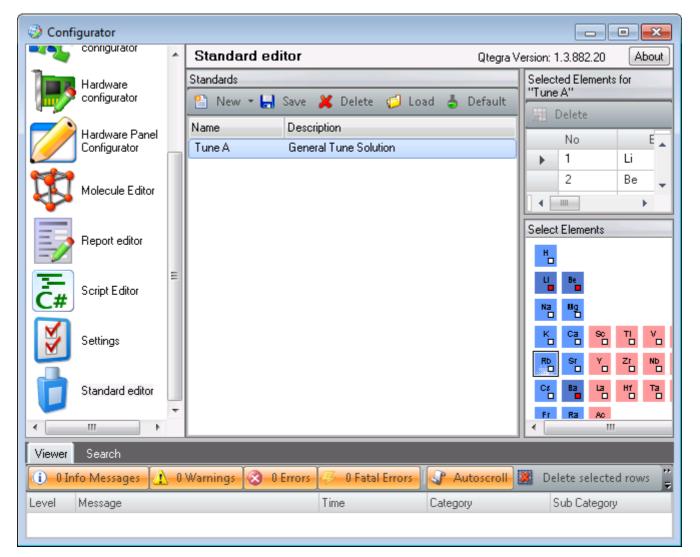


Figure 2-1. User interface of Configurator

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

Table 2-1.	Applets of the Configurator	
Applet		Description
2	Access Control Editor	Allows the Administrator/Manager to define the access permissions for the different programs and applications in the user interface.
2	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.
U	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.
C#	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.
b	Standard Editor	Central database editor for stock solutions and standards.

Table 2-1.Applets of the Configurator

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

* To open the Configurator tool



1. Click Configurator 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.

	Instrument Control	- = X		
Experiment Co	onfiguration ICAP Q Window			
🔽 👝 🕨 Run	Select STD 👻 🔯 Show Analog			
Stop	p 🧭 Edit 🎢 Spectrum Normal 👻			
On Off	tart 💋 Apply Tune Settings	Views		
Control	Measurement mode Display			
Control Panel 🛛 📮 📗	ICAP Q ESI_SC4S ESI FAST			
icap q	Analytes			
Major	Elements Molecules			
High Voltage	н	He		
Disable 🕨 Enable		œ Ne ⊟		
🔵 Hard 🎯 Soft		-		
Extraction	Na Mg Al Si P S Cl o co o co o	Ar		
-5.000	K Ca Sc TI V Cr Mi Fé Co NI Ci Zi Ga Ge As Se Br	Etter I		
CCT Focus	RD ST Y Zr ND NO TO RI RI PO Ag Cd II SI SD TE I	×.		
<u></u> 35.00				
Angular De	Enabled 🛆 Identifier 🛆 Dwell time (s) Channels Spacing (u) Resolu	tion 📘		
<u>1250.00</u> ■ 88Sr 0.01 1 0.1 Normal ■ ■				
CCT Bias [V]				
Major Add Analyte				
Minor	Analyte Table Formula Table			
Torch Position	Analytes Data Display			
Gas Flow	Average Intensities			
ССТ				
RF Generator	Value Identifier RSD [%] ▶ 0 95Mo 0	*		
Vacuum		_		
Valves	Properties	Ŧ		
Mass Calibration	alibration Average Intensities			
Mass Calibration D				
Inlet System	🕕 0 Info Messages 🛕 0 Warnings 🐼 0 Errors 🌾 0 Fatal Errors 🔐 Autosci	roll "		
*	Level Message Time Category Sub Cat			
Control Status P	Time Category Sub Cat			
		.:		

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



Instrument 1. Click Control 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:

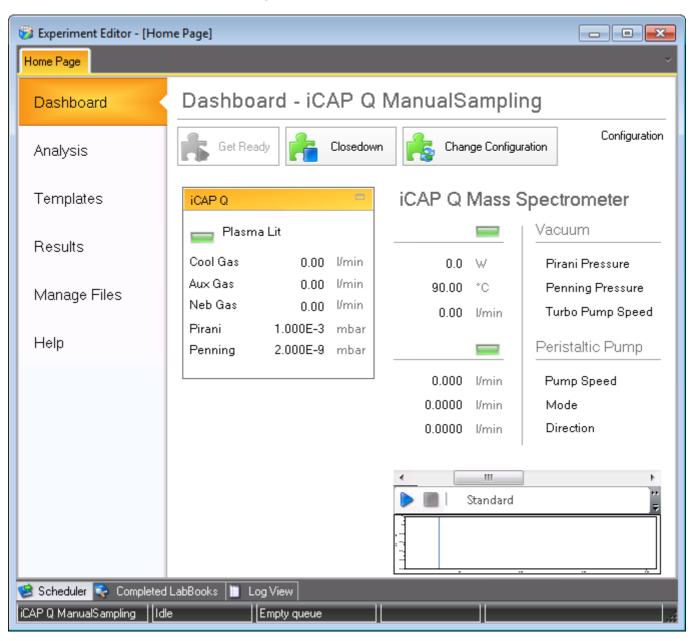


Figure 2-3. User interface of Experiment Editor

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

* To open the Experiment Editor tool

Experiment 1. Click Editor to open Experiment Editor. Introduction to Otegra Experiment Editor Overview

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:

3		1		
Configurator				
Access control	Element editor	Qtegra Version: 1.3	3.882.55 About	
editor				
Element editor	H He He Li ■			
Experiment configurator	. н. Ве 			
Hardware configurator	terner • • • • • • • • • • • • • • • • • • •			
Hardware Panel Configurator				
Molecule Editor	. Si 			
Viewer Search				
i) 0 Info Messages 🚺 0	Warnings 😣 0 Errors	🎸 0 Fatal Errors 🛛 🖓 Auto	scroll 🖁	
Level Message	Time	Category	Sub Category	
)		

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.

(i) 7	In	fo Messages 🚺 0 Warning	gs 🔕 O Err	ors 🔗 0 Fa	tal Errors
Level		Message	Time	Category	Autoscrol
	(j)	Communications with the iCAP Q instrument has been established!	4/13/2012 1	ControlMan	×

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.

Access control editor	Qtegra Version: 1.3.882.55	About		
Applications Configurators Virtual instruments ·· AccelaLCAutosampler ·· Control ·· Control ·· ProjectParameters ·· DefaultSettings	Access mode Administrator Full access Manager Full access Normal user Full access Unknown user Hidden			
 Settings Samplelist header definitions Samplelist body definitions Samplelist footer definitions Samplelist Samplelist CelaLCPump CAP Q CetacASX100 	Administrator Access mode for users with Administrator privileges. Thermo.Imhotep.AccelaLCAS.View.ControlView Image: Add to the second			
 CetacASX112FR CetacASX260 CetacASX520 ESI_SC4S GenericInstrument ID100Autodilutor ManualSampler MicroProbeIILaser SpectraSystemLCAS SpectraSystemLCPump TraceGC Virtual evaluations 	Accessibility AccessibleDescription AccessibleName AccessibleRole Default Appearance BackColor BackgroundImage Default Accessibility Accessibility	•		

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 Utegra
	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.

 Table 3-2.
 Access rights for Otegra

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





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 ^{Configurator} to open **Configurator**.



- 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.

Access control editor Qtegra Version: 1.3.882.43 About H ⊕ Applications ₿₽₽₽ 🚊 Configurators Access mode - Access control edit Administrator • Element editor None Experiment configu User Hardware configura Manager Hardware Panel Co Administrator Molecule Editor Report editor Minimum user level Script Editor The minimal user privilege level used to use the configurator. Settings - Standard editor Access control editor • Virtual instruments • Virtual evaluations ₿ 2↓ ш Þ

5. Click is 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 ^{Configurator} to open **Configurator**.



Access control editor.

- 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**.

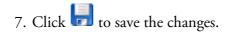
5. Click **I** to display the list of access rights, see Figure 3-5.

Access control e	ditor	Qtegra Version: 1.3.882.43	About
Applications Configurators Virtual instruments Virtual evaluations Ormatography Ormatography OrojectParar	 Access mode Administrator Manager Normal user Unknown user 	Full access Full access Read only Hidden	
●··ExtCalM ●··ExtCalM ●··ExtCalM ●··ExtCalM		Read only Full access	
i∰⊷ Evaluation i∰⊷ DefaultSettir i∰⊷ Settings	Normal user Access mode for norm	nal users.	
i - Samplelist h i - Samplelist b i - Samplelist fc	Thermo.Imhotep.ExtC	al.View.ExtCalMethodViewStan	dards
 Hornov Samplelist HsoDil RawData Spectra StdAdd TRQuant 	 Accessibility AccessibleDescrit AccessibleName AccessibleRole Appearance BackColor BackgroundImag BackgroundImag BorderStyle Cursor 	Default Control e (none)	
4 III +	Accessibility		

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.



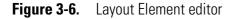
Element Editor



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.

Element editor		
⊕ H ▲	Element: Carbon	
Ē. Li		
⊕ Be ⊕ B	Base	
⊕ C	Atomic number	6
⊕ U ⊕ N	Group	14
	Period	2
⊕ • F	Symbol	C
⊕. Ne	Ionization potentials	
	First ionization potential [eV]	11,261
	Second ionization potential [eV]	24,383
	Misc.	
	Block	P
	Electron affinity [kJ/mol]	121,78
	Electronegativity	2,55
	Relative sensitivity factor	1
	Series	Nichtmetall
ш. К	Visualization	
	Color	127; 127; 127
⊕. Sc		
⊕ - Cr	Atomic number	
	The number of protons in the nucleus.	
🖶 Fe 🦳		
- n - Co		



* To open 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





- 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 Configurator to open Configurator.



- 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.

Add isotope	—
Add an isotope to Fl	luorine
Mass:]
OK	Cancel

Figure 3-7. Element editor - add isotope

5. Enter the **Mass** of the isotope and click **OK** 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 Configurator to open Configurator.



- 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.

Element editor			
⊖•H ▲	Isotope: 3 Helium		
2H 3H	<pre> 2↓ □ </pre>		
⊡ He	Base		
	Abundance [%]	0,000138	
4He	Atomic number	2	
	Identifier	3He	
	Is default	False	×
⊡ · B	Mass [amu]	3,016029297	
- 10B	Mass number [amu]	3	
11B	Symbol	He	
⊕ F			
⊕ · Ne			
⊕ Na			
⊕ · A			
⊕ Si			
⊕ P			
⊕∽ S			
	la dafa da		
	Is default	atona fartha alamant	
	True if the isotope is a default is	stope for the element.	

Figure 3-8. Default isotope properties

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

7. Click \square 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.

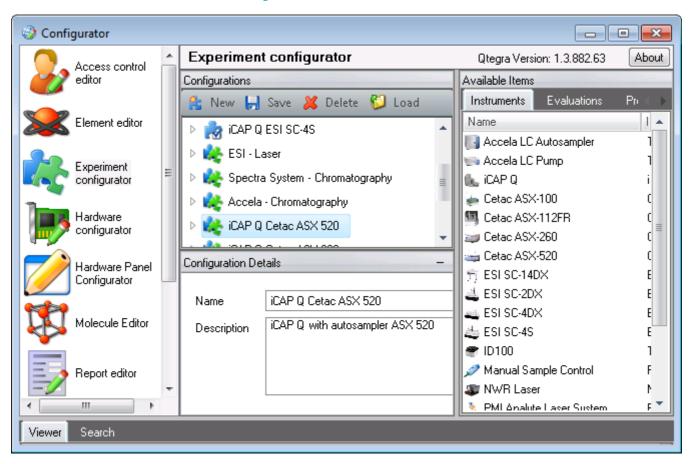


Figure 3-9. Layout Experiment Configurator

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

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

Table 3-3. Experiment configurator commands

* To open Experiment configurator

Click ^{Configurator} to open **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 Configurator to open Configurator.



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

Configurations		
😤 New 📙	Save 💥 Delete ઇ Load	
👂 🎎 Accela -	Chromatography	*
🖻 🎎 icap q (Cetac ASX 520	
🖻 🌺 icap q (Cetac ASX 260	
🕨 🎎 icap q i	ManualSampling	
🎎 New Exp	periment Configuration	=
		•
Configuration Deta	ails	-
		_
Name	New Experiment Configuration	
Description	Description]

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**.

Available Items	3		
Instruments	Evaluations F	Preset Configurations	
Name		Description	
💷 Cetac AS>	<-112FR	Cetac ASX-112FR Autosampler	
j Cetac AS>	<-260	Cetac ASX-260 Autosampler	
🚋 Cetac AS>	<-520	Cetac ASX-520 Autosampler	
📆 ESI SC-14	DХ	ESI SC-14DX Autosampler	
🚢 ESI SC-2D	X	ESI SC-2DX Autosampler	
🛋 ESI SC-4D	X	ESI SC-4DX Autosampler	
🕹 ESI SC-4S	;	ESI SC-4S Autosampler	
൙ ID100		Thermo ID100 Autodilutor	
🥖 Manual Sa	ample Control	Provides prompts for the user	
💵 NWR Las	er	New Wave Research Laser	
🚴 PMI Analy	te Laser System	Photon Machines Analyte Las	
🧎 PMI Fusio	n Laser System	Photon Machines Fusion Lase	
📑 SpectraS'	YSTEM® LC Autos	amp Thermo Scientific SpectraSYS	
🌓 SpectraSY	/STEM® LC Pump	Thermo Scientific SpectraSYS	
📑 TraceGC		Trace Gas Chromatograph	-

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**.

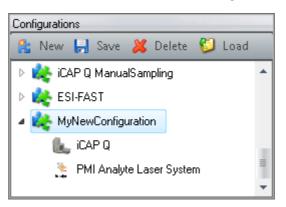
7. Drag and drop **iCAP Q** from the tab **Instruments** to your new Configuration.

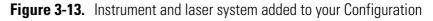
Configurations			ailable Items				
😤 New 样	Delete 🚆	In	struments	Evaluatio	ns	Prese 🧃	►
🗼 Accela	- Chromatogr	Na	ame		Descr	iption	*
	Cetac ASX 5	1	Accela LC	Pump	Them	no Ac	
		h	icap q		iCAP	Q Ma	
icap Q	Cetac ASX 2	🍉	Cetac AS>	<-100	Cetac	: ASX	
🛛 🎎 icap q	ManualSamp	53	Cetac AS>	<-112FR	Cetac	: ASX	
💒 ESI-FAS	ST 🔳		⊂Cetac AS≻	<-260	Cetac	: ASX	
		1	⊨Cetac AS≻	(-520	Cetac	: ASX	
S MyNew	Configuration		ESI SC-14	DX	ESI S	SC-14	=
Configuration Det	ails + -	4	ESI SC-2D	X	ESI S	SC-2D	
			ESI SC-4D	X	ESI S	SC-4D	
Name	MyNewConfigurati	14	ESI SC-4S		ESI S	SC-4S	
	iCAP Q with Laser		ID100		Them	no ID1	
Description	ICAI Q MULLASEI		Manual S	ample Co…	Provid	des pr	
			NWR Lase	er	New ¹	Wave	
			PMI Analy	ite Laser	Photo	in Ma.	
			PMI Fusio	n Laser S	Photo	n Ma.	
		1 27	<u></u>	VOTEMA	т		•

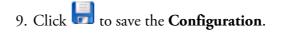
Drop when • is shown, see Figure 3-12.

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.







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 ^{Configurator} to open **Configurator**.



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

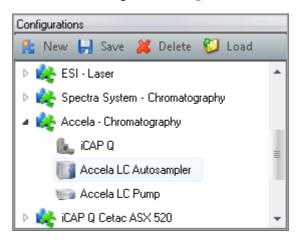


Figure 3-14. Right-click Instrument to edit settings

4. Click	🕐 Edit settings	to open the Settings
	w, see Figure 3-15.	to open the octaings

0.	Settings	×
iCA	PQ Accela LC Autosampler	Accela LC Pump
	Loop Size [µl]	10 🔺
	Stack Number	1
	Syringe Size [µl]	250
	Vial Bottom Sensing	Off
4	Input	
	Inject Hold Release Active I	Selected
	Pump Ready Active High	Selected
4	Output	
	Autosampler Ready Active I	Cleared
	Gradient Start Active High	Cleared
Autosampler Ready Active High This sets the active level of the AS Ready line, which indicates that the autosampler is ready to start an injection.		
Fa	ctory Defaults	OK Cancel

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



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

🗘 Settings	E
iCAP Q Accela LC Autosampler Acce	la LC Pump
⊿ General	
Pump Model	Accela LC 📃 🔍
Serial Number	None
A High Pressure Mode	Accela LC
Compression Correction Factor [%]	Accela 600
Pre-Compression Attenuation [%]	Accela 1250
Low Pressure Mode	
Compression Correction Factor [%]	106
Pre-Compression Attenuation [%]	25
Pump Model Select the appropriate pump model.	
Factory Defaults	OK Cancel

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

8. Select an item from the list.

9. Click	ОК	
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 ^{Configurator} to open **Configurator**.



3. Click while 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 ٠



1. Click Configurator to open Configurator.



- 3. In the list of **Configurations**, right-click the Configuration you wish to add to the list of Preset Configurations.
- Add to preset configuration Rename 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 Configurator to open Configurator.



- Experiment Configurator. 2. Click
- 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.

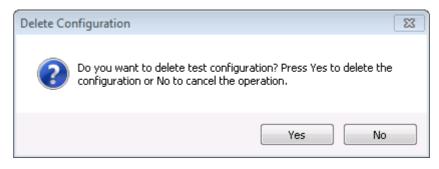
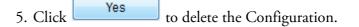


Figure 3-17. Delete Configuration dialog



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. \blacktriangle

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

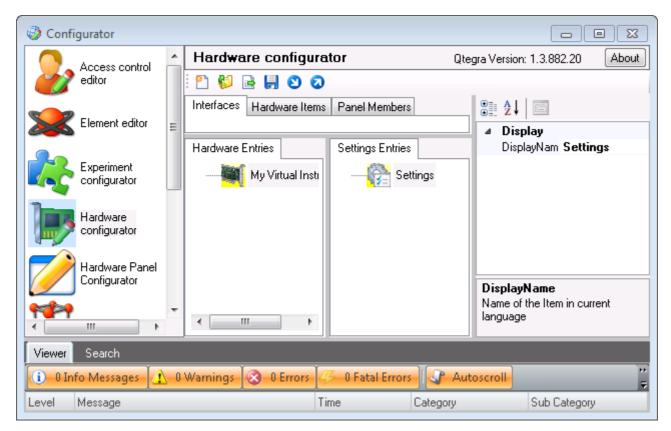


Figure 3-18. Layout Hardware configurator

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.
\odot	To import settings.
	To export settings.

* To open 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.

Hardware Panel Configurator	Qtegra Version: 1.3.882.20 About
🌮 🗳 🔒 🎒 🛛 Z 🛶 🕂 💼 💼 🖽 📾	і ⊫ ╡ ज़ ≞ Ⅲ ॴ 🕺 🔊 🔊
Graphical View Preview	Configurations Script Pool
	Panel configuration iCAP Q ESI SC-4S 🗸
	System configuration iCAP Q ESI SC-4S
	Virtual Instruments
	Name Database
	iCAP Q _Application Data\PluginData\Brigic
	Properties Object Pool Resources Undo Group
18-	
	E Image Text
	E Image Text
8-	Image Switch Dual Range Slider
	-

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

Table 3-5.	Fable 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



TTO D

1. Click ^{Configurator} to open **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.

Configurator				
Hardware	Molecule Editor	Qtegra Ve	ersion: 1.3.882.2	0 About
configurator	🛃 Save			
Hardware Panel Configurator	Enter elements seperated by '.' or choose elements from periodic table.	н		
	Clear	LI Be		
Molecule Editor	Double Charged	Na Mg		
		к са	SC TI V	Cr Mi Fe
Report editor	User defined symbols and masses.	Rb Sr	Y Zr Nb	MO TO RU
Script Editor	Symbol Mass	Cs Ba	La Hf Ta	W Re Os
C#	0.0000 Add	Fr Ra	Ac	
Settings			Ce Pr	Nd Pm Sm
	Polyatomics Symbol		Mass	Abundar
Standard editor	🕸 O.H			
<				•
Viewer Search				
🕕 0 Info Messages 🚺	Warnings 🐼 0 Errors 💯 0 Fatal Errors 🛛 🕼 Autoscr	roll 🗱 Dele	ete selected rov	avs F
Level Message	Time Category		Sub Categor	

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 Configurator to open Configurator.



- 2. Click **Molecule Editor**.
- To create molecules



1. Click Configurator to open Configurator.



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.

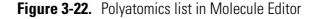
Enter elements seperated by '.' or choose elements from periodic table.		
H.0.0.0	Clear	
Double Charged	Add	

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 Add 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.

Polyatomics		Symbol	Mass	Abundance	
🗱 Ba.O		🗶 1H.160.160.160	48.9926	99.2728	
🇊 Ba++		🗶 2H.160.160.160	49.9988	0.0149	
🇊 Ce++		🗶 3H.160.160.160	51.0007	0.0000	
🗱 CI.O	=	🗶 1H.170.160.160	49.9968	0.0378	
🐯 Bkg		🗶 2H.170.160.160	51.0031	0.0000	
🗱 Other		🔉 3H.170.160.160	52.0050	0.0000	
0.0.0.H 🐮	•	🗶 1H.180.160.160	50.9968	0.1990	
 • 		🛥 2H 180 160 160	52 0031	0 0000	•



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

User defined symbols and masses.			
Symbol	Mass		
	0.0000	Add	

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

11. Click \square to save the changes in the database.

Delete

Configurator Report Editor

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.

		Qtegra Version: 1.3.882.32 About
: 記 📂 🖬 🛤		
i 🔍 🔍 100% -	- ∲ ▶ ⊴ 其 拱	1 5 6 1 1
Report name:		, 📄 Report 🔺
Unnamed report	= 🔁 pageHeader	🖌 🔤 pageHeader 👘
101		groupHeader1
····· report01.rpx		detail1
	= 😑 groupHeader1	pageFooter
	-	⊕ ⊕ Fields
	= 🖂 🗊 detail1	Paramatere
ActiveReports 6	:	
A Label	-	Appearance
■ TextBox	-	ShowParameti True
-	-	Watermark (none)
CheckBox	- 1	WatermarkAlic Center
🗐 RichTextBox	-	WatermarkSizi Clip
🗖 Shape	-	A Behavior
Picture	-	MaxPages 0
/ Line	-	PrintWidth 6.5
	-	ScriptLanguag C# 👻
💾 PageBreak	= 🔄 groupFooter1	Edit Data Source
Barcode		
SubReport		 Appearance
🥭 OleObject 🖳 🖃	Designer 🗇 Script 🔍 Preview	-
Current Selection: A		

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



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

✤ To open Report editor



1. Click Configurator to open Configurator.



- 2. Click **Report editor**.
- ✤ To create a new report template



1. Click ^{Configurator} to open **Configurator**.



- 3. Click 1 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 Configurator to open Configurator.



- 🗾 Report editor.
- 3. Click 🗁 and browse for the report file.
- 4. Select the report file you wish to edit.



- 6. Edit the file.
- 7. Click \blacksquare 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.

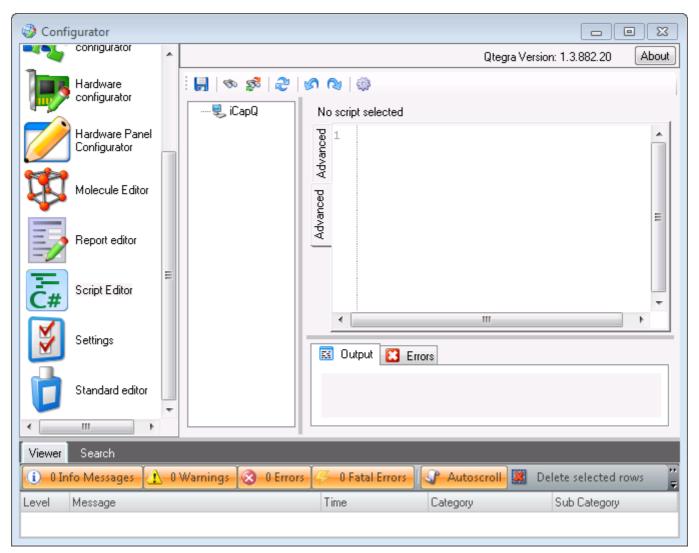


Figure 3-25. Layout Script Editor

* To open Script Editor



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).

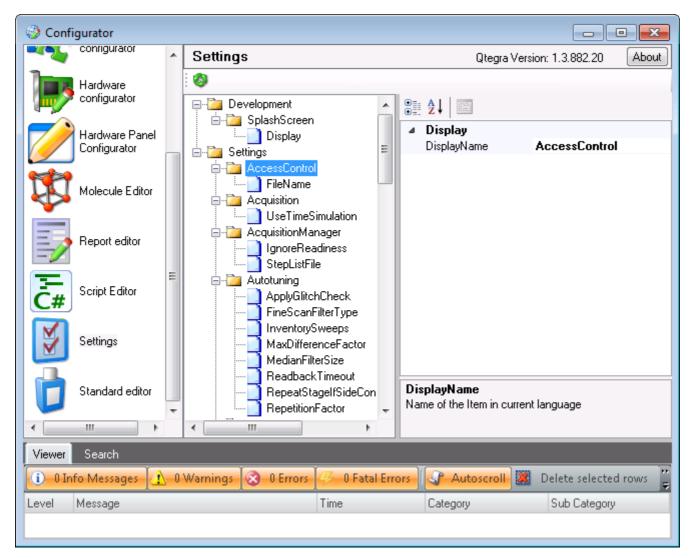


Figure 3-26. Layout Settings

3-34

To open Settings

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.

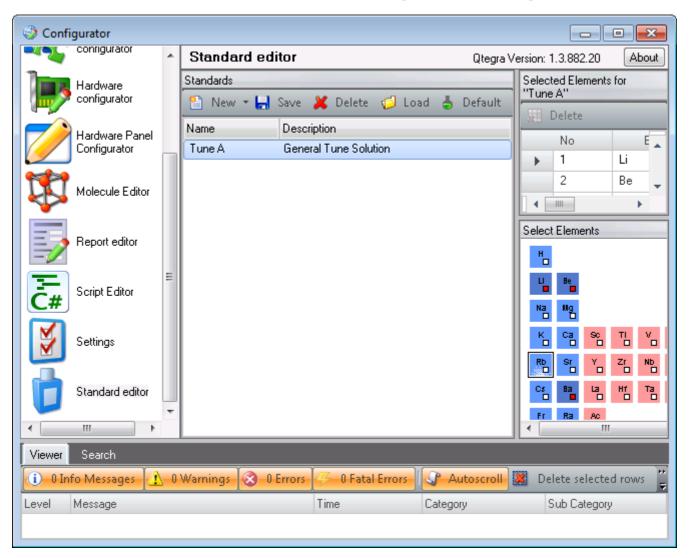


Figure 3-27. Layout Standard editor

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

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

Table 3-7.Standard editor commands

✤ To open Standard editor



1. Click ^{Configurator} to open **Configurator**.



- 2. Click **Standard editor**.
- ✤ To load all standards from the standard database



1. Click ^{Configurator} to open **Configurator**.



Standard editor.



All standards are loaded from the database.

* To save a standard to the standard database



1. Click ^{Configurator} to open **Configurator**.



- 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 ^{Configurator} to open **Configurator**.



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



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







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



2. Click 5 Standard editor .	
3. Click to open the Set Defa Figure 3-29.	ult Concentration window, see
Set Default Concentration	×
Default Concentration :	10 ppb 🔻

Figure 3-29. Set Default Concentration window

- 4. Change the default concentration and unit as required.
- 0K 5. Click to exit the window.

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

0K

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



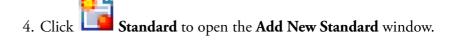
1. Click ^{Configurator} to open **Configurator**.

Cancel



Standard editor										
Stan	dards			_						
2	New 🝷	H	Save	9	Defaul	t				
2	Standard									
2		Internal Standard								
8	Isotop	New Standard								
Create new Standard						P				

Figure 3-30. Creating a new standard



- 5. Click we 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.

- 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
- 9. To remove the element, click the respective element in the periodic table again.
- 10. Repeat until all elements have been added.

11. Click \blacksquare 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 Configurator to open Configurator. 2. Click **Standard editor**. 🎦 New 3. Click The drop-down menu opens, see Figure 3-31. Standard editor Standards New - 🔜 Save 占 Default 2 Standard **Internal Standard** 2 Isotope Dilation New Internal Standard Create new Internal Standard

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.

- 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 ^{Configurator} to open **Configurator**.
- 2. Click **Standard editor**.
- 3. Click 💾 New 🔻

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

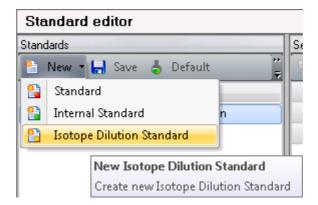


Figure 3-32. Creating a new standard

- 4. Click **Isotope Dilution Standard** to open the **Add New Standard** window.
- 5. Enter the Standard Name and a Standard Description.
- 6. Click 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.

- 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

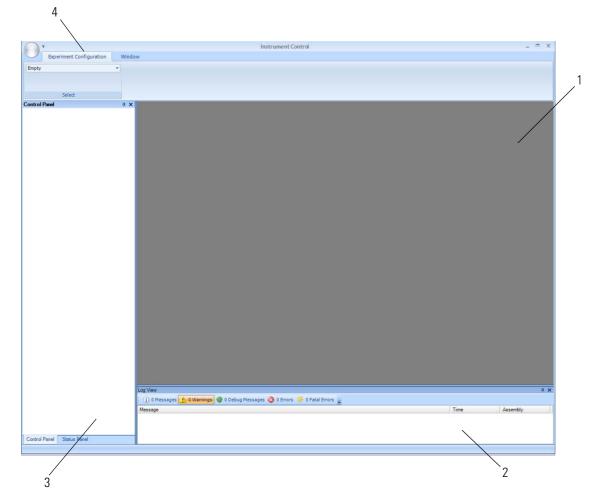


1. Click Control to open Instrument Control.

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



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 Control 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.

-	Instrument Control 🛛 🗕 🗖 🗙					
Experiment Confi	guration iCAP Q Window					
🚱 Base 🛛 Blue	Layout Default About Qtegra Add this Layout to favourites					
Select Blend 🔻	Show Quick Access Toolbar Below the Ribbon					
Palette	Mi <u>n</u> imize the Ribbon					

Figure 4-2. Window ribbon of Instrument Control tool

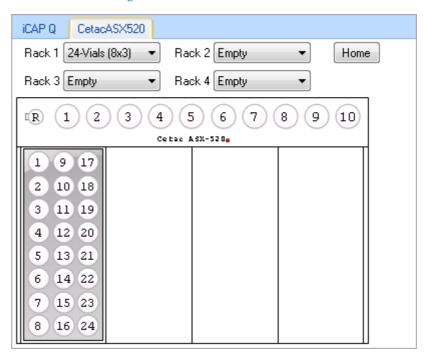
4. Select Minimize the Ribbon.

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.





* To display the data view region of an instrument component



- 1. Click Control 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.

	Ir	nstrument	t Control					_ = x
Experiment Configu	ration iCAP Q	Wind	ow					
On Off Run Control	Select STD - Select STD - Edit S Apply Tune Settings Measurement mode		 Show Analog Spectrum Normal Display 			•	Wizards	Views
Control Panel	ESI_SC4S ESI FAS	Т						
Major	Molecules							
High Voltage Disable E E Be Hard Soft Extra					А	CN BB SiP BB	O F E CI	He Ne He Ar
Major K Ca	Sc Ti ∨ Cr	Mn Fe		Cu Zr		Ge As	Se Bi	
Minor Rb Sr	Y Zr Nb Mo		u Rh Pd		d In	Sn Sb ⊞⊞ mo	Te I	Xe
Torch Position Cs Ba	La Hf Ta W	Re 0	s Ir Pt	Au H	9 TI	Pb Bi	Po At	Rn 👻
CCT Enabled	d 🛆 Identifier	A Dwe	ll time (s)	Channels	Spacing	r (u) F	Resolution	Cr 🔺
RF Generator	🗸 88Sr	0.01	1		0.1	N	ormal	0, 🔻
Vacuum			1111					•
Valves Add	Analyte							
Mass Calibrat Analyte T	able Formula Table							
Mass Calibrat Analytes	Data Display							
🏂 🤧 🍹 🗛	ntensities							
Contr Statu Average I	ntensities							
Log View								
								.::

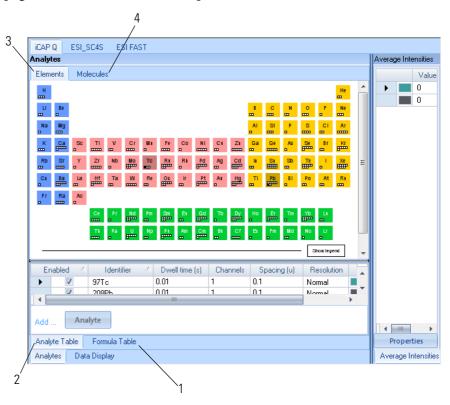
Figure 4-4. Instrument Control with periodic table in the data view region

* To display the iCAP Q settings view region

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.

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 Control 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

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.

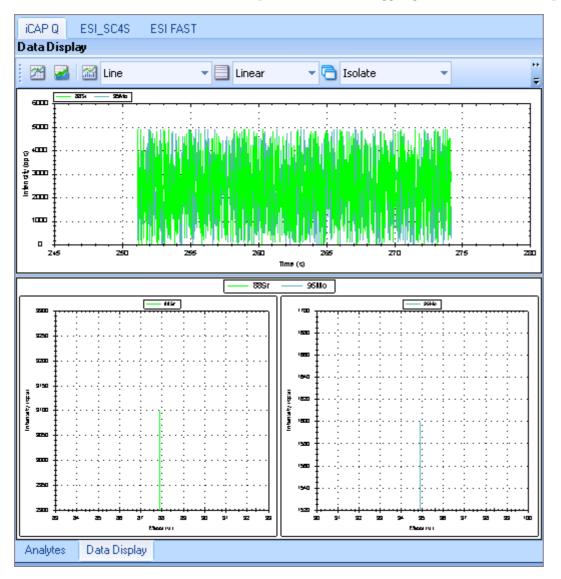


Figure 4-6. iCAP Q tab Data Display showing spectrum and chromatogram

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

lcon	Description
2	Button to toggle the chromatogram window.
	Button to toggle the spectrum window.
Line	Options for the presentation of data series display within spectrum window.
Point Stick	
Linear Linear Linear	Options for the scale of data series display in spectrum window.
Isolate None Isolate Difference	Options for the segmentation strategy of data series in spectrum window.
None	Options for the stacking strategy of data series in chromatogram window.

Table 4-1.	Data display options
------------	----------------------

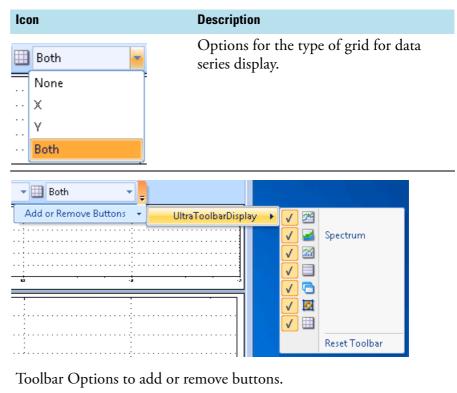


Table 4-1.Data display options

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 Control 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.

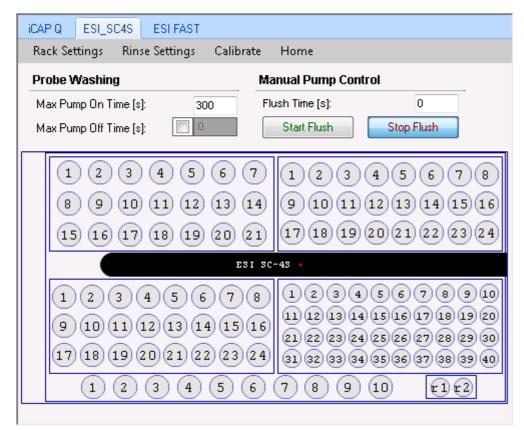


Figure 4-7. Instrument Control with integrated autosampler tab showing

* To open the peripheral tab



- 1. Click Control 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.

\bigcirc	⇒ Instrument	Control	- = x
\bigcirc	Experiment Configuration	Window	
iCAP-	Q with ESI SC-4S 👻		
	Select		



✤ To load a Configuration



- 1. Click Control to open Instrument Control.
- 2. Select the Experiment Configuration ribbon tab.
- 3. In the group **Select**, click it 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.

-	Ŧ		Instrum	ent Control				_ = X
0	Experiment Configur	ration iCAP Q	Window	1				
	👝 🕨 Run	Select STD	· •	🔕 🔤 Show	Analog			
On	Off International Internationa	🧭 Edit 🚯 Apply Tune Se	ttings	Spectrum	Normal	Ŧ	Wizards	Views
	Control	Measurement	mode		Display			

Figure 4-9. The iCAP Q tab

✤ To open the iCAP Q ribbon



- 1. Click Control 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. Con	ntrol buttons for il	CAP Q instrument
----------------	----------------------	------------------

lcon	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 Control 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.

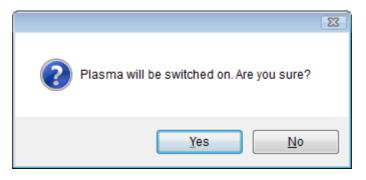


Figure 4-11. Confirm switching on plasma



The plasma is switched on.

* To start data acquisition in the real-time display



- 1. Click Control 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 Control 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 Control 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

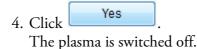


- 1. Click Control to open Instrument Control.
- 2. In the data view region, select the **iCAP Q** tab. The ribbon **iCAP Q** is activated.

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

		83
?	Plasma will be switched off. Are you sure?	
	Yes No	





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).

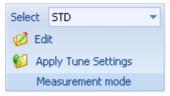


Figure 4-13. Measurement mode group of the iCAP Q ribbon

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.

ltem	Settings	Description	
	ССТ	The CCT measurement mode pressurizes the cell with gas which may lead to a chemical reaction of the generated ions.	
Select	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.	
1	Edit	Displays Measurement Mode settings in the data view region.	
		Measurement Mode settings can be viewed and edited in the data view region.	
6	Apply Tune Settings	Saves tune settings modified in the Control Panel to the current measurement mode.	

Table 4-3. Buttons of Measurement mode group

* To load a Measurement mode into Instrument Control



- 1. Click 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 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 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 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 September 2015 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.

iCAP Q ESI_ easurement M	SC4S ESIFAST odes				
Measurement n	node: STD	¥	Add new mode	Delet	te selected mode
Added stabiliz	zation time [s]:	10.00	Excluded Ranges:	Begin	End
Source autob	une configuration: 🖡	ligh Matrix	-	▶ 0	4.59
Jource auton		ngri maux		11.41	22.59
				27.41	28.59
🔽 Master in	source tune group			29.41	30.59
				31.41	32.59
				33.41	38.59
				39.41	42.59
				79.41	80.59
				EE 41	EC EO
Current tune se)ate	tting: STD CCT Entry Lens	Angular Deflection	Deflection Entry Lens	Extraction L	ens 1 Polarity
3/2/2012 9:07	0.00	-336.90	0.00	0	
/2/2012 9:05			0.00	0	
2/15/2012 10:	0.00	-250.00	0.00	0	•
Analytes Data	a Display Measur	ement Modes			



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



- 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 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 *i* **Edit**. A new tab **Measurement Modes** opens in the data view region.
- 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.

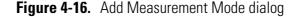
* To add a new Measurement mode in the Edit mode



- 1. Click 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 **¹⁰ Edit**. A new tab **Measurement Modes** opens in the data view region.
- 4. Click Add new mode

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

Add Measurement Mode		
Name for the new measurement mode:		
C	ОК	Cancel



- 5. Enter a Name for the new measurement mode.
- 6. Click

The new measurement mode is added to the list.

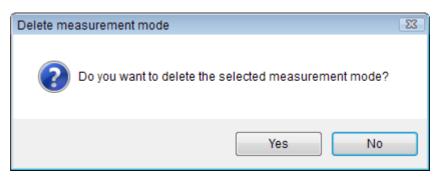
* To delete a new Measurement mode in the Edit mode

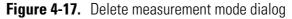


- 1. Click Control to open Instrument Control.
- 2. In the data view region, select the **iCAP Q** tab. The ribbon **iCAP Q** is activated.
- 3. In the group **Measurement mode**, click *i* **Edit**. A new tab **Measurement Modes** opens in the data view region.
- Select the mode you wish to delete from 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.





6. Click	Yes
U. CIICK	

The selected measurement mode is deleted from the list.

✤ To close the Edit mode



1. Click 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 ^{CEdit}. 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

ltem	Meaning	Description	
٩	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.	
24	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.	
9 0 0 9 0 0 9	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.	
	Normal	Sets mode in the iCAP Q tab Data Display to Normal. Each scan is shown individually.	
Spectrum	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 Control 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 Control 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.
--

lcon	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.
J.	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.

Table 4-3. Buttons of wizard group	Table 4-5.	Buttons of Wizard group
------------------------------------	------------	-------------------------

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 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 **Wizard** group, click **Report**.

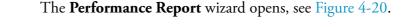




Figure 4-20. Welcome to the Performance Report Wizard

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

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

Performance Report Wizard	
Select an Performance report Select the Performance report that is to be edited from the list b	elow.
Available sequences:	Description:
🚰 ССТ	Performance report for standard mode.
E CCTS	
F KED	
F KEDS	
STDS	
	· · · · · · · · · · · · · · · · · · ·
	< Back Next > Cancel
Analytes Data Display Performance Report Wizard	

Figure 4-21. Selecting Performance Report

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

Elemer	nts	Molecu	iles																
	н																	He	
	Li ••	Be											<mark>в</mark>	с ш	N E	0	F	Ne	
	Na	Mg											A -	Si	P	s 	CI B	Ar	
	к	Ca	Sc 🛛	т 	×	Cr	Mn =	Fe	Co	Ni	Cu B	Zn	Ga E	Ge	As =	Se Brrrr	Br ===	Kr Beener	
	Rb B	Sr	Y	<u>.</u>	Nb	Mo	To	Ru	Rh	Pd	Ag	Ed	in ••	Sn ⊞⊞⊞	sb 	Te =====	_ _	Xe =====	
	Cs =	Ba	la B	Hf	та		Re	Os	lr B	Pt	Au	Hg	п 	в	Bi	Po E	At B	Rn	
	Fr	Ra	Ac																
				Ce	Pr -	Nd	Pm	Sm	Bu .	Gd	ъ	Dy	Ho	. 6	Tm -	Yb	ւս 		
				Th	Pa -		Np	Pu	Am .	Cm	Bk	Cf	в.	Fm.	Md	No	ي ا		
																— [Show leg	je nd	

Figure 4-22. Selecting Analytes in the periodic table

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

Performance Report Wiz	ard				
Select Analytes					
Use this page to select	the analyte	es that the Performance report	will report on		
Elements Molecules					
Polyatomics		Symbol	Mass	Abundance	
🗱 O.H					
🗱 Ar.Cl	≡				
15 Ce.O					
100 V.O					
🗱 U.O.O 🗱 Ba.O					
NPF D	-				
	•				
Matrix					
Ar 🗐					
□ □ □					
I III N					
С					
Н					
□ □ □.H					
		<u> </u>			
			< Ba	ack Next >	Cancel
Analytes Data Display	Perfor	nance Report Wizard [STD]			

Figure 4-23. Selecting molecules

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.

Selected analy	tes:	Defined ratios:
Analyte	Mass	() 137Ba++/137Ba
Bkg4.5	4.5	(J) 140Ce.160/140Ce
7Li	7.016005	
59Co	58.9332	
137Ba++	68.45291	
115In	114.9039	
137Ba	136.9058	
140Ce	139.9054	
140Ce.160	155.9004	
Bkg220.5	220.5	
238U	238.0508	

Figure 4-24. Defining ratios for the Analytes

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

Performance Report Wizard							
Define tests Use this page t	Use this page to define the tests to perform to validate if the instrument has been tuned correctly						
Runs: 5	5 🚖 Sweeps: 6	io 🚖	Duration: 5m 0	s			
	Analyte	Dwell[s]	Stability [%]	Condition	Limit		
🕨 🕨 Bkg	(g4.5	0.1		Less than	3		
7Li	i	0.1	2	Greater than	40000		
590	ICo	0.1	2	Greater than	80000		
137	37Ba++	0.1		Not used		=	
115	5In	0.1	2	Greater than	200000		
137	78a	0.1		Not used			
140	0Ce	0.1		Not used			
140	0Ce.160	0.1		Not used			
Bkg	:g220.5	0.1		Less than	1	_	
			-	_ ·		Ť	
				<pre></pre>		Cancel	
Analytes Data	Display Performance Rep	ort Wizard [ST	D]				

Figure 4-25. Defining tests

15. Define the mass calibration tests, see Figure 4-20	15. I	Define the	mass	calibration	tests,	see	Figure	4-26
--	-------	------------	------	-------------	--------	-----	--------	------

Perfo	ormano	e Report Wizard				
		ss calibration to				
L	Jse this	page to define the	e tests to p	erform to validate the acc	curacy of the instrument mass ca	libration.
	_	2		B () ()	0.050	
	Sweep	is: 3	÷	Point spacing:	0.050 🚖 Duration: (Jm 36s
	Dwell [s] 0.1		Measure width [%]	5 🚔	
				I		
		Analyte	Use	Max. error [u]	Min. peakwidth [u]	Max. peakwidth [u]
	•	Bkg4.5		0.1	0.65	0.85
		7Li	V	0.1	0.65	0.85
		59Co	\checkmark	0.1	0.65	0.85
		115ln	1	0.1	0.65	0.85
		Bkg220.5		0.1	0.65	0.85
		238U	~	0.1	0.65	0.85
				,	'	
					< Back	Next > Cancel
And	lytes	Data Display	Performe	nce Report Wizard (STD)		
Anal	iytes	Data Display	Ferrormal	ice neport wizara (STD)		

Figure 4-26. Defining mass calibration tests

17. Select a **Performance Report** from the list.

For **Name**, you can also enter a new name for the report, see Figure 4-27.

	erformance report existing Performance report from t	he list if you want to overwrite it or enter a new name in the Name field to create a new
Name:	NewPerformanceReport	Description:
	TS D	
s⊤ s⊤ s⊺ s⊺	D	Solution required:
Analytes D	9ata Display Performance Re	Cancel Kort Cancel Cort Performance Report Wizard [STD]

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.

Performance Report Wiza	rd
	Completing the Performance report editor wizard.
ThermoFisher	The Performance report has been successfully saved and is ready to use.
	< Back Finish
Analytes Data Display	Performance Report Wizard [STD]

- Figure 4-28. Completing Performance Report wizard
 - To create a new Performance Report with the Performance Report Wizard



- Instrument 1. Click 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 **Wizard** group, click **Report**. 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.

Select	Performance Report Wizard Select Analytes Use this page to select the analytes that the Performance report will report on																		
					aiytes			imance											
Elemen	its H	Molecu	lles															He	
		-															-		
	نا •••	Be											в —	с —	N E	0 	-	Ne ====	
	Na	Mg 											A -	Si	P	s 	CI B	Ar	
	К	Ca	Sc.	Ti	×	Cr	Mn	Fe	Co -	Ni	Cu		Ga 🚥	Ge	As •	Se E	Br 	Kr Beener	
	Rb 	Sr	Y	<u>ت</u>	Nb	Mo	To	Ru	Rh	Pd	Ag B	_Cd	ln -	Sn ⊞⊞	Sb 	Te	_ I	Xe ====	
	Cs •	Ba	La ED	Hf	Ta E	w	Re	Os	lr B	Pt	Au	Hg	п 	РЬ	Bi	Po B	At B	Rn	
	Fr	Ra	Ac																
				Ce	Pr	Nd	Pm	Sm	Eu ==	Gd	ъ	Dy	Ho	. Br 	Tm	УЬ	Lu 		
				Th	Pa		Np	Pu	Am	Cm	Bk	Cf	B	Fm	Md	No	_ lr		
																— [Show leg	jend	
													< Ba	ck		Next >			Cancel
Analyte	s E) ata Di	splay	Per	rforma	nce Re	port W	/izard											

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

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

	-	nat the Performance report wi	ill report on		
Elements Molecules Polyatomics		ymbol	Mass	Abundance	
I Olyacomics		🗽 130Ba.160	145.9012	0.1057	
St Ar.Cl		🛣 132Ba.160	147.9000	0.1007	
Si Ce.O		🛣 134Ba.160	149.8994	2.4112	
5. U.O		🗶 135Ba.160	150.9006	6.5763	
3 U.O.O		🗶 136Ba.160	151.8995	7.8353	
Ba.O		🗶 137Ba.160	152.9007	11.2033	=
de n	· · ·	🗶 138Ba.160	153.9002	71.5294	=
•		🕱 130Ba.170	146.9054	0.0000	
Matrix		😹 132Ba.170	148.9042	0.0000	
Ar		😹 134Ba.170	150.9036	0.0009	
0		😹 135Ba.170	151.9048	0.0025	
N N		😹 136Ba.170	152.9037	0.0030	
ГС		🗶 137Ba.170	153.9049	0.0043	
Η		🗶 138Ba.170	154.9044	0.0272	
— 0.H		🗶 130Ba.180	147.9054	0.0002	
		🗼 132Ba.180	149.9042	0.0002	
			< Back	Next >	Cancel

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

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

Selected analyte	es:	Defined ratios:
Analyte	Mass	(1) 137Ba++/137Ba
Bkg4.5	4.5	(J) 140Ce.16O/140Ce
7Li	7.016005	
59Co	58.9332	
137Ba++	68.45291	
115In	114.9039	
137Ba	136.9058	
140Ce	139.9054	
140Ce.16O	155.9004	
Bkg220.5	220.5	
238U	238.0508	

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

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

Define	Performance Report Wizard Define tests									
Use	Use this page to define the tests to perform to validate if the instrument has been tuned correctly									
	Runs	: 1 🚔	Sweeps: 100	Duration: Om	Os					
		Analyte	Dwell[s]	Stability [%]	Condition	Limit				
		7Li	0.1		Not used					
	•	59Co	0.1		Not used 🔤					
		115ln	0.1		Not used					
		138Ba	0.1		Greater than					
		140Ce	0.1		Less than					
		238U	0.1		Not used					
					< Back Next >	Cancel				
Analyte	es D) ata Display	Performance Report Wi	zard						

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

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

Performan	ce Report Wiza	nd							
	Define mass calibration tests Use this page to define the tests to perform to validate the accuracy of the instrument mass calibration.								
030 (1).	s page to define			accuracy of the instan					
Sweep	os: 10	* *	Point spacing:	0.050 🚖	Duration:	Om Os			
,									
Dwell	[s] 0.1		Measure width	[%] 5 🚔					
	Analyte	Use	Max. error [u]	Min. peakwidt	h ful	Max. peakwidth [u]			
•	59Co		0.1	0.65	n [a]	0.85			
			·						
				ſ	< Back	Next > Cancel			
Analytes	Data Display	Perfo	rmance Report Wizard						
Analytes	Data Display	Fello	mance report wizalu						

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.

Performance Report Wizard		
Save the Performance report Select an existing Performance repo Performance report.	rt from the list if you want to ov	verwrite it or enter a new name in the Name field to create a new
		Description:
Name: Report1		*
CCT quick 0.95amu CCT quick CCT quick KED quick 0.95amu KED quick bkg with Li KED quick bkg KED quick with Li KED quick KED quick KED STD quick bkg STD quick bkg		Solution required:
		<pre></pre>
Analytes Data Display Performa	nce Report Wizard	

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.

Performance Report Wizard							
	Completing the Performance report editor wizard.						
ThermoFisher	The Performance report has been successfully saved and is ready to use.						
	< Back Finish						
Analytes Data Display	Performance Report Wizard						

Figure 4-36. Completing the Performance Report wizard

✤ To run an existing Performance Report with the Performance Report Wizard



- Instrument 1. Click 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 **Wizard** group, click **Report**. 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 R	eport, see	Figure	4-38.
----------------------------------	------------	--------	-------

Performance Report Wizar	1	
Select an Performance r		
Select the Performance re	eport that is to be run from the lis	t below.
Available sequences:		Description:
🚰 CCT 🛛 k 0.95amu		A
CCTS k		
KED		
F KEDS k 0.95amu		
STDS		-
		-
,		
		<pre></pre>
Analytes Data Display	Performance Report Wizard	

Figure 4-38. Selecting Performance Report

		Т	Click Next . The perform Figure 4-39.	nance report	t requires the	samples to be	placed, see
Performance R		d					
Load the sam	ple						
The required	d solution is:	probe into the solution ar 13 and 0.5% HCl.	nd select ''Nex	t" to start the d	ata acquisition.		
					< Back	Next >	Cancel
Analytes Da	ta Display	Performance Report V	/izard [CCT]				

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.

Performance Report Wizard	
Acquisition status	
This page shows the progress of the data acquisition.	
Acquisition status	
Setting up for mass calibration verification	
4 Mass calibration verification scan started	
Sweep completed: 1/3	
Sweep completed: 2/3	
Sweep completed: 3/3	
Found a peak for mass 7Li; Mass Difference: 0.02459 amu; Width: 0.74 amu	
Found a peak for mass 59Co; Mass Difference: 0.00441 amu; Width: 0.71 amu	
Found a peak for mass 115ln; Mass Difference: 0.00873 amu; Width: 0.75 amu	
Found a peak for mass 238U; Mass Difference: 0.01795 amu; Width: 0.79 amu	
The mass calibration verification has passed	
Setting up for performance verification	
Performance verification scan started. Run 1 of 5	
Sweep completed: 1/60	
Sweep completed: 2/60	
Sweep completed: 3/60	
< Back Next > Cance	
Analytes Data Display Performance Report Wizard [STD]	

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.

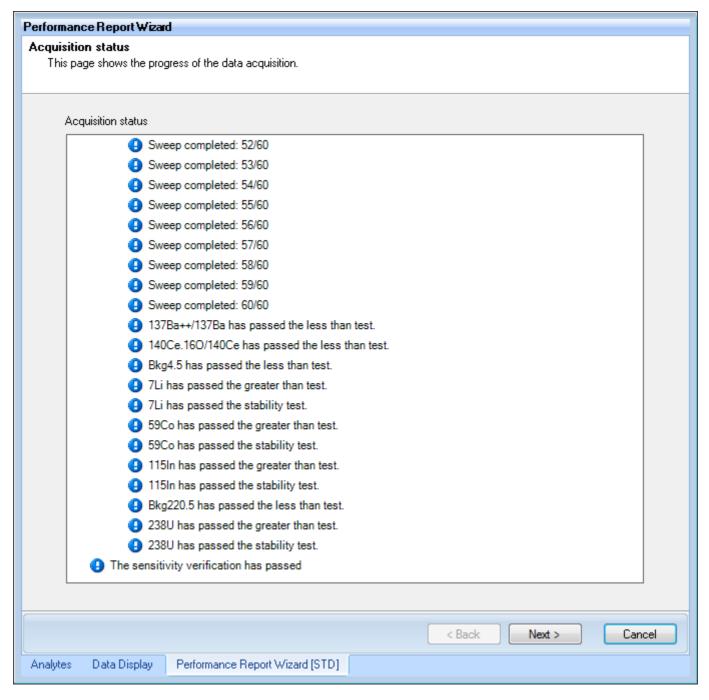


Figure 4-41. Acquisition completed for the Performance Report Wizard

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

Performance Report Wizard							
	Completing the Performance report run wizard.						
ThermoEisher	The Performance report tests have been successfully executed.						
ThermoFisher SCIENTIFIC	Open Report						
	< Back Finish						
Analytes Data Display	Performance Report Wizard [STD]						

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 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 **Wizard** group, click **Report**. 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.

Performance Report Wizard	ł		
Load the sample			
Please place the sample The required solution is: 1 ppb Tune B in 2% HNO	probe into the solution and select "Next 13 and 0.5% HCI.	t" to start the data acquisition.	
		< Back Next >	Cancel
Analytes Data Display	Performance Report Wizard [CCT]		

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.

Performance Report Wizard
Acquisition status
This page shows the progress of the data acquisition.
Acquisition status
Setting up for mass calibration verification
Mass calibration verification scan started
Sweep completed: 1/3
Sweep completed: 2/3
Sweep completed: 3/3
Found a peak for mass 7Li; Mass Difference: 0.02433 amu; Width: 0.74 amu
Found a peak for mass 59Co; Mass Difference: 0.00394 amu; Width: 0.71 amu
Found a peak for mass 115ln; Mass Difference: 0.00594 amu; Width: 0.74 amu
Found a peak for mass 238U; Mass Difference: 0.01059 amu; Width: 0.78 amu
Intermass calibration verification has passed
Setting up for performance verification
Performance verification scan started. Run 1 of 5
Sweep completed: 1/60
Sweep completed: 2/60
Sweep completed: 3/60
< Back Next > Cancel
Analytes Data Display Performance Report Wizard [STD]

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.

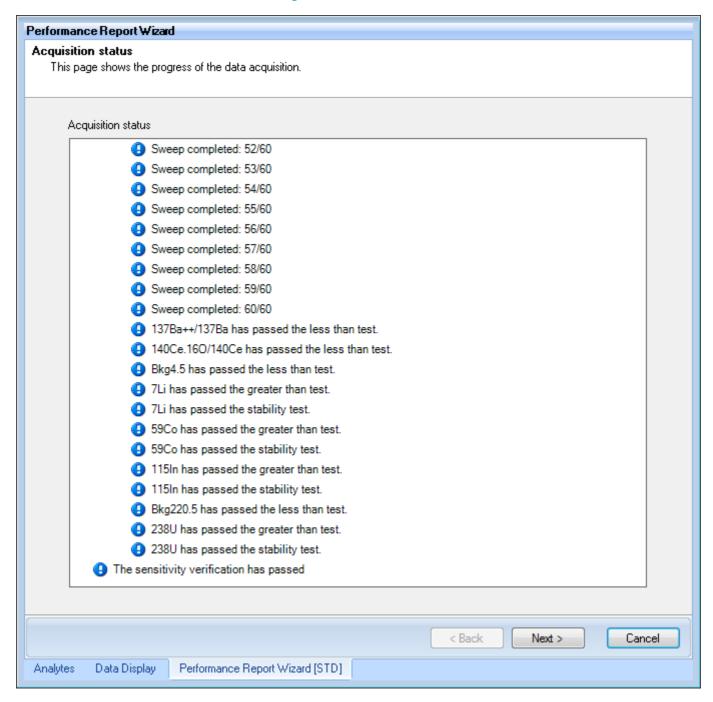


Figure 4-46. Acquisition completed for the Performance Report Wizard

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

Autotune

3. In the **Wizard** group, click (arrow next to or below Autotune) to open the drop-down menu, see Figure 4-48.

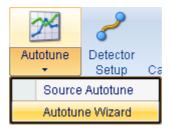


Figure 4-48. Autotune drop-down menu

4. Click Autotune Wizard.

The Autotune wizard opens, see Figure 4-49.

Autotune Wizard						
	Welcome to the Autotune Wizard					
	This wizard will guide you through creating, editing or running an autotune sequence					
	Please select one of the following options:					
	Edit an existing Autotune sequence					
	This option allows you to edit a previously created Autotune sequence					
	Create a new Autotune sequence					
	This option allows you to create an new Autotune sequence					
	Run an existing Autotune sequence					
	This option allows you to start an Autotune sequence					
	Run Autotune sequence from active Measurement mode					
	This option allows you to start the Autotune sequence of the active Measurement mode					
Thermo Fisher						
	< Back Next > Cancel					
Analytes Data Display	Autotune Wizard					

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.

Autotune Wizard	
Select an autotune sequence	
Select the autotune sequence that is to be edited from t	he list below.
Available sequences:	Description:
🚰 ССТ	STD default values. Use this script as template for STD autotunes.
🚰 KED	
SourceTune High Matrix	
SourceTune High Sensitivity STD	
	_
	< Back Next > Cancel
Analytes Data Display Autotune Wizard	

Figure 4-50. Select Autotune sequence in Autotune wizard

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

Control	Use Default	Autotune	Default	Min	Max	Coarse Step
Plasma Power		V	1300	600	2000	10
Cool Flow		V	14	10	20	0.1
Auxilliary Flow		V	0.8	0.5	1.2	0.1
Nebulizer Flow		V	0.8	0.6	1	0.01
Torch Horizontal Posi			0	-1.5	1.5	0.02
Torch Vertical Positio			0	-1.5	1.5	0.02
Sampling Depth			6	4	8	0.1
Extraction Lens 1 Po			4	2	8	0.05
Extraction Lens 1 Ne			-200	-500	-50	1
Extraction Lens 2			-180	-300	-100	0.5
Deflection Entry Lens			-30	-35	-15	1
CCT Focus Lens			3	-5	8	0.2
CCT Entry Lens			-80	-250	-50	1
CCT Bias			-2	-6	2	0.1
CCT Exit Lens			-200	-250	-50	1
Focus Lens			21	10	30	0.2

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

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

Autotune V	Vizard									
Select Ar Use this	alytes s page to select (the analytes tha	at the Autotun	e sequ	ience	is to u	ise t	o tune the instru	ment.	
Elements	Molecules							Analyte	Dwell time	
							He D	115In 7Li	0.1 0.1	
LI Be						8	e B	59Co	0.1	
Na Mg						AL	SI	238U	0.1	
• •	SC TI V		e Co NI	C.	Zı	Ga Ga	Ge			
Rb Sr	Y Zr Nb					_h	sı IIII			
Cs 👪		W Re C	is ir Pt		Hg	TI B	₽₽			
Fr Ra	AC									
	Ce Pr	Nd Pm S	m El Gd	ъ	Dy.	Но	Er			
	Ti Pa		Am Cm	BK 	C1	8	Fit •			
					Sho	vlegend				
•		III			_		÷.			
								< Back	Next >	Cancel
Analytes	Data Display	Autotune W	izard [STD]							

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

13. Define ratios, see Figure 4-53.

Autotune Wizard	I					
Define ratios						
Use this page	e to define the ratios t	hat the Autotune	sequence is to use to	o tune the instrume	nt.	
Selected a	nalytes:		Define	d ratios:		
Analyte	Mass					
115ln	114.9039					
97Tc	96.9064					
193lr	192.9629					
120Sn	119.9022					
				< Back	Next >	Cancel
Analytes Data	a Display Autotur	e Wizard [STD]				

Figure 4-53. Define ratios in Autotune wizard

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

totune Wiza efine condi Use this pa <u>o</u>		onditions (o achieve t	o pa	uss this stage	e of the A	utotune sequen	ce.		
Stage name	Cond1						🔲 Use	Old Style	Page: 1	
Fine Scan Sweeps:	1	Coars Swee	e Scan eps:	10	¢	🕅 F	letune Fine	Scan Ra	inge Percentage [%]	70
Autotune	Control	Divisor	Filter Size		Analyte		Condition		Limit	1
V	Plasma Power	20	3		115In		Maximize	-	10000	
V	Cool Flow	20	3		ł		Not used			
V	Auxilliary Flow	20	3				Greater than			
V	Nebulizer Flow	20	3				Less than			
							Maximize			
						,	Minimize			
									,	
			•							
							< Back	Ne	xt > Canc	el
				_						

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.

Autotune Wizard						
Save the Autoto Select an exist new Autotune	ing Autotune sequence	from the list if you v	vant to overwrite it	or enter a new name	e in the Name fie	eld to create a
			Description:			
	New autotune sequend Tune High Matrix Tune High Sensitivity		Solution requ	red:		•
		•		< Back	Next >	Cancel
Analytes Data	Display Autotune W	/izard [STD]				

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

Autotune Wizard	
	Completing the Autotune sequence editor wizard
ThermoFisher	The autotune sequence has been successfully saved and is ready to use.
Analytes Data Display	< Back Finish Autotune Wizard [STD]

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.

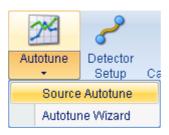
* To run the Source Autotune Wizard

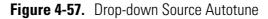


- 1. Click Control to open Instrument Control.
- 2. In the data view region, select the **iCAP Q** tab. The ribbon **iCAP Q** is activated.

Autotune

3. In the **Wizard** group, click (arrow next to or below Autotune) to open the drop-down menu, see Figure 4-57.





You can also directly click it o open the Source Autotune wizard.

4. Click **Source Autotune**.

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

Autotune Wizard [SourceTune High Matrix 1550W]
Load the sample.
Please place the sample probe into the solution and select "Next" to start the data acquisition.
The required solution is:
< Back Next > Cancel
Analytes Data Display Autotune Wizard [SourceTune High Matrix]

Figure 4-58. Start Source Autotune wizard

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

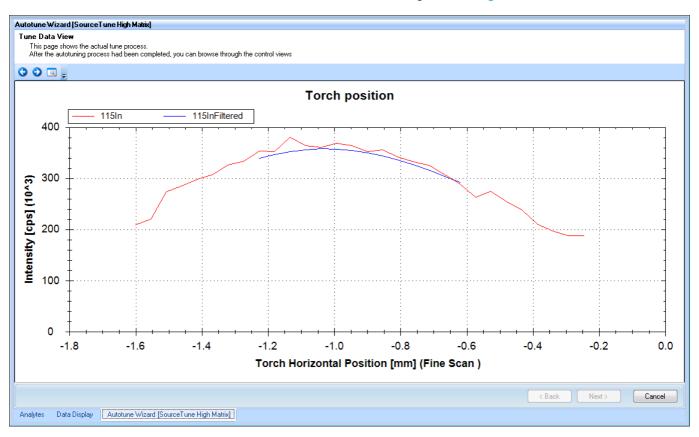
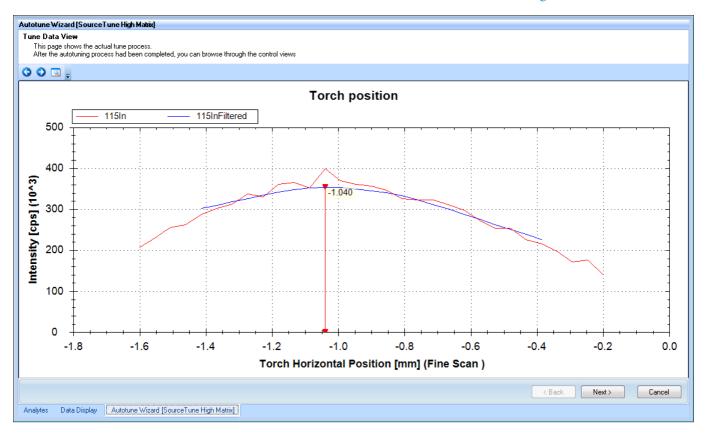


Figure 4-59. Tune Data View Source Autotune wizard



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

Figure 4-60. Tune Data View Source Autotune wizard

The Acquisition Status window opens, see Figure 4-61.

Autotune Wizard [SourceTune High Matrix]
Acquisition status
This page shows the progress of the data acquisition.
Acquisition status
Stage finished
▲ ④ Starting Stage: CCT Focus Lens
Details
Stage finished
Starting Stage: Nebulizer (1.9 % CeO)
Details
Stage finished
▲ ④ Starting Stage: Extraction Lens 2 @ final Plasma Temperature
▷ 🕒 Details
Stage finished
Starting Stage: CCT Focus Lens @ final Plasma Temperature
▷ 🕒 Details
Stage finished
A 🕘 Summary:
Analyte 115In: Original Intensity 345340 cps, Tuned Intensity 345667 cps, Increased by: 327 cps
Analyte 140Ce: Original Intensity 386474 cps, Tuned Intensity 328177 cps, Decreased by: 58296 cps
Analyte 140Ce.16O: Original Intensity 11724 cps, Tuned Intensity 5579 cps, Decreased by: 6144 cps
Analyte 7Li: Original Intensity 91953 cps, Tuned Intensity 85188 cps, Decreased by: 6765 cps
Analyte 59Co: Original Intensity 180585 cps, Tuned Intensity 177540 cps, Decreased by: 3045 cps
Analyte 238U: Original Intensity 490254 cps, Tuned Intensity 470304 cps, Decreased by: 19950 cps
Ratio 140Ce.16O/140Ce: Original Value 0.0303, Tuned Value 0.017, Decreased by: 0.0133
Autotuning completed.
< Back Next > Cancel
Analytes Data Display Autotune Wizard [SourceTune High Matrix]

Figure 4-61. Acquisition Status Source Autotune wizard

The Acquisition Status window opens, see Figure 4-62.

Autotune Wizard [Source	Tune High Matrix]
	Completing the Autotune sequence run wizard
at the state	The autotune sequence has not been executed successfully
Thorma Eicher	 Do you want to save the result in the Measuremode STD? ● Yes ● No
Thermo Fisher SCIENTIFIC	🔲 Open Report
	< Back Finish
Analytes Data Display	Autotune Wizard [SourceTune High Matrix]

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

Detector Setup Wizard						
	Welcome to the Detector Setup Wizard					
	This wizard guides you through the steps necessary to set up the detector. It adjusts the detector voltages to provide the optimum performance from the detector.					
	 Detector Cross Calibration Detector HV Setup and Cross Calibration Detector Setup after analyzer was opened 					
ThermoFisher SCIENTIFIC	Install new Detector					
Analytes Data Display	< Back Next > Cancel Detector Setup Wizard					

Figure 4-63. Welcome to the Detector Setup Wizard

5. Select Detector Cross Calibration.

The periodic table window opens, see Figure 4-64.

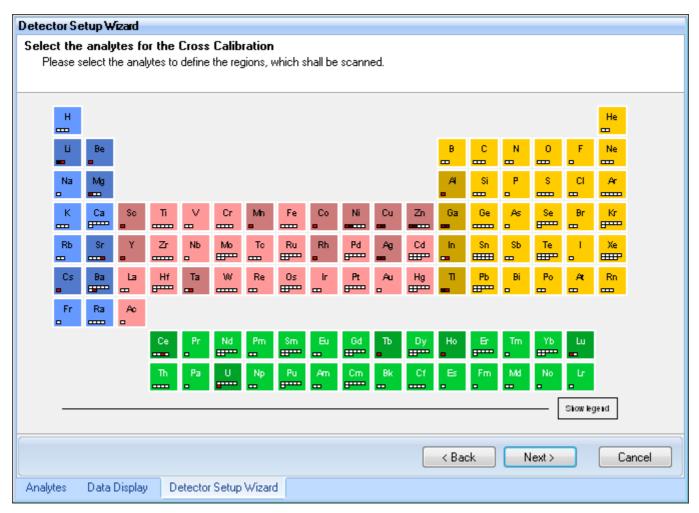


Figure 4-64. Select analytes for Detector Setup Wizard

7. Select your analytes.

The Load the Sample window opens, see Figure 4-65.

Detector S	etup Wizard					
Load the	Sample.					
Place t	he sample probe i	nto the solution and select	"Next" to start the sample u	ptake delay.		
				< Back	Next >	Cancel
Analytes	Data Display	Detector Setup Wizard				

Figure 4-65. Load sample for Detector Setup Wizard

9. Place the probe into the setup solution.

The Waiting for sample uptake window opens, see Figure 4-66.

Detector S	etup Wizard					
	or sample uptal ige shows the amo	ce. ount of time left before the a	acquisition srarts.			
Ŵ	visard will automati	cally move to the next pag	/hen the timer has completed e. delay has finisched then press			
U	Jptake Delay				Pause	
Í					Continue	
			(< Back	Next >	Cancel
Analytes	Data Display	Detector Setup Wizard				

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.

Detector S	etup Wizard				
	ffset Determina				
The and	alog offset is now	measured.			
🕘 Ana	log baseline deter	rmination started!			
			K Back	Next >	Cancel
Analytes	Data Display	Detector Setup Wizard			

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

The Cross Calibration starts, see Figure 4-68.

Detector S	etup Wizard 👘				
Cross Cal					
Shows	the progress of th	e cross calibration			
🕒 Starti	ng Cross Calibratio	on			
			< Back	Next >	Cancel
Analytes	Data Display	Detector Setup Wizard			

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

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

Detector Setup Wizard						
Cross Cal						
Shows	the progress of th	e cross calibration				
Starti	ng Cross Calibra	tion				
Sweep 1/10 completed.						
	Sweep 2/10 completed.					
<u> </u>						
				< Back	Next >	Cancel
Analytes	Data Display	Detector Setup Wizard				

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.

Detector Setup Wizard							
Shows a summery of all messages generated by the detector voltage setup.							
Analog baseline determination started!	Average cross calibration factor of 108989.79 for mass: 140; rsd: 3.46; channels: 33						
Confidence interval(95%) analog baseline: 0.001949 RSD at 1.0 Mcps	Average cross calibration factor of 116677.18 for mass: 159; rsd: 2.61; channels: 40						
Analog baseline determination finished!	Average cross calibration factor of 117034.45 for mass: 165; rsd: 2.52; channels: 38						
Starting Cross Calibration	Average cross calibration factor of 118472.92 for mass: 181; rsd: 2.66; channels: 22						
Sweep 1/10 completed.	Average cross calibration factor of 129604.58 for mass: 205; rsd: 3.02; channels: 34						
Sweep 2/10 completed.	Average cross calibration factor of 125447.52 for mass: 238; rsd: 2.31; channels: 38						
Sweep 3/10 completed.	Cross calibration successfully completed.						
Sweep 4/10 completed.							
Sweep 5/10 completed.							
Sweep 6/10 completed.							
Sweep 7/10 completed.							
Sweep 8/10 completed.							
Sweep 9/10 completed.							
Sweep 10/10 completed.							
Average cross calibration factor of 58472.68 for mass: 7; rsd: 4.06; channels: 37							
Average cross calibration factor of 61166.45 for mass: 9; rsd: 2.61; channels: 40							
Average cross calibration factor of 65081.69 for mass: 24; rsd: 2.67; channels: 39							
Average cross calibration factor of 68480.73 for mass: 27; rsd: 1.75; channels: 36							
Average cross calibration factor of 74676.96 for mass: 45; rsd: 2.21; channels: 40							
Average cross calibration factor of 84991.42 for mass: 55; rsd: 2.92; channels: 40							
Average cross calibration factor of 94923.08 for mass: 58; rsd: 2.56; channels: 40							
Average cross calibration factor of 92441.21 for mass: 59; rsd: 2.18; channels: 40							
Average cross calibration factor of 98724.65 for mass: 63; rsd: 2.75; channels: 39							
Average cross calibration factor of 97614.35 for mass: 64; rsd: 2.22; channels: 39							
Average cross calibration factor of 101336.28 for mass: 65; rsd: 3.73; channels: 21							
Average cross calibration factor of 99814.48 for mass: 66; rsd: 3.03; channels: 37							
Average cross calibration factor of 96159.27 for mass: 69; rsd: 3.32; channels: 39							
Average cross calibration factor of 98302.69 for mass: 71; rsd: 2.70; channels: 40							
Average cross calibration factor of 97042.03 for mass: 88; rsd: 2.97; channels: 40							
Average cross calibration factor of 95959.57 for mass: 89; rsd: 3.54; channels: 39							
Average cross calibration factor of 104387.43 for mass: 103; rsd: 3.06; channels: 33							
Average cross calibration factor of 111908.60 for mass: 115; rsd: 3.33; channels: 36							
Average cross calibration factor of 113994.42 for mass: 133; rsd: 3.32; channels: 32							
Average cross calibration factor of 114251.15 for mass: 138; rsd: 2.71; channels: 39							
	< Back Next > Cancel						
Analytes Data Display Detector Setup Wizard							
Anaytos Data Display Detector Jetup Wizard							

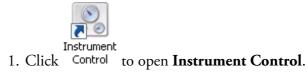
Figure 4-70. Detector Setup summary in wizard

14. Click Next, see Figure 4-71.

Detector Setup Wizard							
Summery							
Shows a summery of all messages generated by the detector voltage setup.							
Analog baseline determination started!	Average cross calibration factor of 108989.79 for mass: 140; rsd: 3.46; channels: 33						
Confidence interval (95%) analog baseline: 0.001949 RSD at 1.0 Mcps	Average cross calibration factor of 116677.18 for mass: 159; rsd: 2.61; channels: 40						
Analog baseline determination finished!	Average cross calibration factor of 117034.45 for mass: 165; rsd: 2.52; channels: 38						
Starting Cross Calibration	Average cross calibration factor of 118472.92 for mass: 181; rsd: 2.66; channels: 22						
Sweep 1/10 completed.	Average cross calibration factor of 129604.58 for mass: 205; rsd: 3.02; channels: 34						
Sweep 2/10 completed. Sweep 3/10 completed.	Average cross calibration factor of 125447.52 for mass: 238; rsd: 2.31; channels: 38 Cross calibration successfully completed.						
	Cross calibration successfully completed.						
Sweep 4/10 completed. Sweep 5/10 completed.							
Sweep 5/10 completed.							
Sweep 6/10 completed.							
Sweep 8/10 completed.							
Sweep 9/10 completed.							
Sweep 10/10 completed.							
Average cross calibration factor of 58472.68 for mass: 7; rsd: 4.06; channels: 37							
Average cross calibration factor of 61166.45 for mass: 9; rsd: 2.61; channels: 40							
Average cross calibration factor of 65081.69 for mass: 24; rsd: 2.67; channels: 39							
Average cross calibration factor of 68480.73 for mass: 27, rsd: 1.75; channels: 36							
Average cross calibration factor of 74676.96 for mass: 45; rsd: 2.21; channels: 40							
Average cross calibration factor of 84991.42 for mass: 40, 150: 2.21; channels: 40							
Average cross calibration factor of 94923.08 for mass: 58; rsd: 2.56; channels: 40							
Average cross calibration factor of 92441.21 for mass: 59; rsd: 2.18; channels: 40							
Average cross calibration factor of 98724.65 for mass: 63; rsd: 2.75; channels: 39							
Average cross calibration factor of 97614.35 for mass: 64; rsd: 2.22; channels: 39							
Average cross calibration factor of 101336.28 for mass: 65; rsd: 3.73; channels: 21							
Average cross calibration factor of 99814.48 for mass: 66; rsd: 3.03; channels: 37							
Average cross calibration factor of 96159.27 for mass: 69; rsd: 3.32; channels: 39							
Average cross calibration factor of 98302.69 for mass: 71; rsd: 2.70; channels: 40							
Average cross calibration factor of 97042.03 for mass: 88; rsd: 2.97; channels: 40							
Average cross calibration factor of 95959.57 for mass: 89: rsd: 3.54: channels: 39							
Average cross calibration factor of 50595.07 for mass: 89, rsd: 3.04; channels: 39							
Average cross calibration factor of 111908.60 for mass: 105, rsd: 3.30; channels: 36							
Average cross calibration factor of 113994.42 for mass: 133; rsd: 3.32; channels: 32							
Average cross calibration factor of 114251.15 for mass: 135, 136, 2.71; channels: 32							
	< Back Finish						
Analytes Data Display Detector Setup Wizard							
Analytes Data Display Detector Setup Wizdru							

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



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

Detector Setup Wizard					
	Welcome to the Detector Setup Wizard				
	This wizard guides you through the steps necessary to set up the detector. It adjusts the detector voltages to provide the optimum performance from the detector.				
	Detector Cross Calibration				
	Oetector HV Setup and Cross Calibration				
	Detector Setup after analyzer was opened				
	Install new Detector				
ThermoFisher SCIENTIFIC					
	< Back Next > Cancel				
Analytes Data Display	Detector Setup Wizard				

Figure 4-72. Welcome to the Detector Setup Wizard

5. Select Detector HV Setup and Cross Calibration.

The periodic table window opens, see Figure 4-73.

	etector Setup Wizard Select the analytes for the Cross Calibration															
Ple	Please select the analytes to define the regions, which shall be scanned.															
Н																
Li	Be											в	С	N	0	F
Na	■ Mg											AI	Si	P	s	
ĸ	Ca Brrrrr	Sc	Ti	V	Cr	Mn •	Fe	Co	Ni	Cu	Zn	Ga	Ge	As =	Se	Br
Rb	Sr	Y	Zr	Nb	Mo	TC	Ru	Rh ■	Pd	Ag	Cd	ln •••	Sn ⊞⊞	Sb 	Te	
Cs ■	Ba	La	Hf	Ta		Re	Os	lr 	Pt	Au	Hg	TI	Pb	Bi	Po ==	At
Fr	Ra	Ac														
			Ce	Pr -	Nd	Pm.	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm ■	Yb	Lu
Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr																
	Show legend															
										<	Back		Next >		Car	ncel
Analyti	es D	ata Dis	play	Detecto	or Setup	Wizard										

Figure 4-73. Select analytes for Detector Setup Wizard

7. Select your analytes.

The Load the Sample window opens, see Figure 4-74.

Detector S	etup Wizard		
Load the			
	he sample probe i	into the solution and select	ct "Next" to start the sample uptake delay.
i lace (ne sample probe	into the solution and select	, Next to start the sample uptake delay.
			<pre> Back Next > Cancel</pre>
Analytes	Data Display	Detector Setup Wizard	

Figure 4-74. Load sample for Detector Setup Wizard

9. Place the probe into the setup solution.

The Waiting for sample uptake window opens, see Figure 4-75.

Detector Setup Wizard	
Waiting for sample uptake. This page shows the amount of time left before the acquisition srarts.	
Waiting for the sample to reach the plasma. When the timer has completed the acquisitio wisard will automatically move to the next page. If you want to start the acquisition before this delay has finisched then press the 'Next' bu	
Uptake Delay	Pause Continue
Analytes Data Display Detector Setup Wizard	Next > Cancel

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.

Detector Setup Wizard		
Analog Offset Determina		
The analog offset is now	measured.	
Analog baseline deter	rmination started!	
	K Back	Vext > Cancel
Analytes Data Display	Detector Setup Wizard	

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.

Acquisition	status	
•	Pulse counting voltage = 1300V	-
0	Peak at mass 114.904 is valid for the plateau calculation	
0	Peak at mass 132.905 is valid for the plateau calculation	
9	Peak at mass 136.000 is valid for the plateau calculation	
0	Peak at mass 137.000 is valid for the plateau calculation	
0	Peak at mass 137.905 is valid for the plateau calculation	
0	Peak at mass 139.905 is valid for the plateau calculation	
0	Peak at mass 142.000 is valid for the plateau calculation	
9	0 peaks are on the plateau	
0	Pulse counting voltage = 1400V	
6	Peak at mass 114.904 is valid for the plateau calculation	
9	Peak at mass 132.905 is valid for the plateau calculation	
9	Peak at mass 135.000 is valid for the plateau calculation	
9	Peak at mass 136.000 is valid for the plateau calculation	
9	Peak at mass 137.000 is valid for the plateau calculation	
9	Peak at mass 137.905 is valid for the plateau calculation	
9	Peak at mass 139.905 is valid for the plateau calculation	
9	Peak at mass 142.000 is valid for the plateau calculation	
9	6 peaks are on the plateau	
📔 🔁 Tu	ining XCal factor	=
9	Mass 102.906 : Factor 93396 : RSD 3.196	
9	Mass 109.000 : Factor 101772 : RSD 2.783	
9	Mass 114.904 : Factor 100050 : RSD 3.734	
(1	Mass 132.905 : Factor 102075 : RSD 2.521	
(1	Mass 137.905 : Factor 101757 : RSD 2.882	
(1	Mass 139.905 : Factor 98299 : RSD 3.011	
(1	Mass 106.905 : Factor 102013 : RSD 2.268	
9	XCal Factor error = -0.001	
📔 🕒 Fi	ne plateau search (25V steps)	
6	Pulse counting voltage = 1175V	-
		_

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.

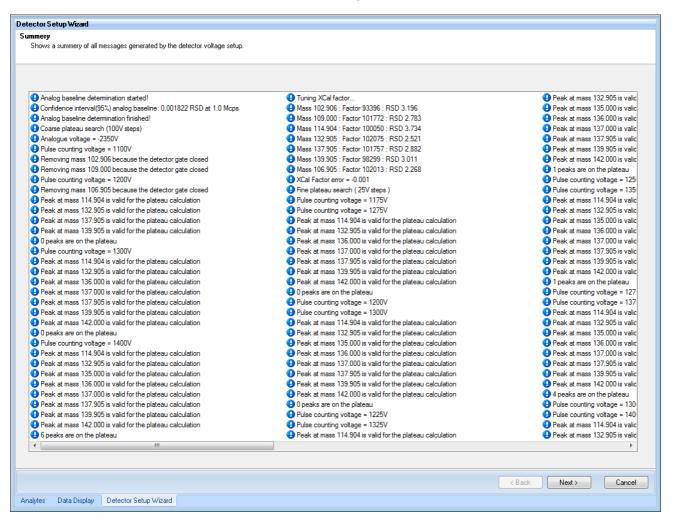


Figure 4-78. Summary of detector HV setup and cross calibration

13. Click Next.

Detector Setup Wizard	
ThermoFisher	The detector voltages have been set. The instrument is now ready to use.
	< Back Finish
Analytes Data Display	Detector Setup Wizard

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

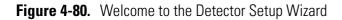


- 1. Click Control to open Instrument Control.
- 2. Be sure to change to STD/STDS mode before starting the wizard.
- 3. In the data view region, select the **iCAP Q** tab. The ribbon **iCAP Q** is activated.



- 4. In the **Wizard** group, click Setup.
 - The Detector Setup Wizard opens, see Figure 4-80.

Detector Setup Wizard								
	Welcome to the Detector Setup Wizard							
	This wizard guides you through the steps necessary to set up the detector. It adjusts the detector voltages to provide the optimum performance from the detector.							
	Detector Cross Calibration							
	Detector HV Setup and Cross Calibration							
	Detector Setup after analyzer was opened							
	Install new Detector							
ThermoFisher SCIENTIFIC								
	< Back Next > Cancel							
Analytes Data Display	Detector Setup Wizard							



5. Select Detector Setup after analyzer was opened.

The periodic table window opens, see Figure 4-81.

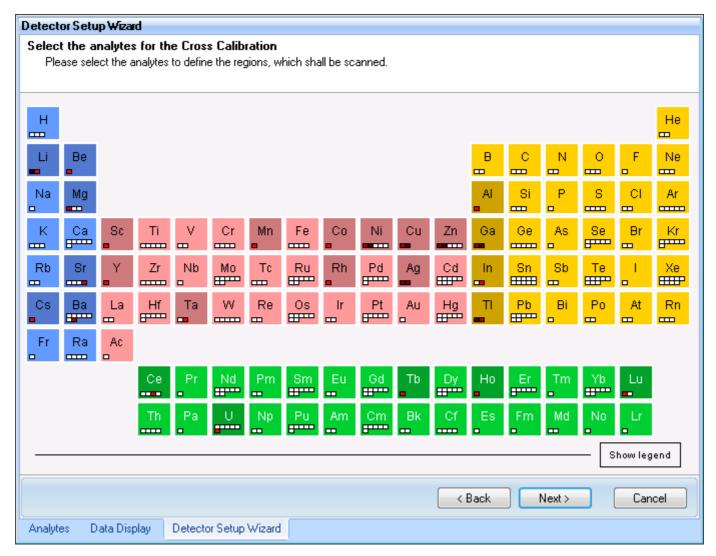


Figure 4-81. Select analytes for Detector Setup Wizard

7. Select your analytes.

The Load the Sample window opens, see Figure 4-82.

Detector S	etup Wizard				
Load the					
Place t	he sample probe i	nto the solution and select	"Next" to start the same	ole uptake delay.	
	··· · · · · · · · · · · · · · ·				
				< Back Next >	Cancel
Analytes	Data Display	Detector Setup Wizard			

Figure 4-82. Load sample for Detector Setup Wizard

9. Place the probe into the setup solution.

The Waiting for sample uptake window opens, see Figure 4-83.

Detector Setup Wizard		
Waiting for sample upta	ke.	
This page shows the amo	ount of time left before the	acquisition starts.
Waiting for the sam wizard will automat	ple to reach the plasma. W ically move to the next pag	When the timer has completed the acquisition will start and this ge.
If you want to start	the acquisition before this	delay has finisched then press the 'Next' button.
-		
Uptake Delay		David
		Pause
		Continue
		K Back Next > Cancel
Analytes Data Display	Detector Setup Wizard	

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.

Detector 9	Setup Wizard				
	Offset Determina				
Thea	analog offset is now	measured.			
A Comparison of the second	nalog baseline deter	mination started!			
			< Back	Next >	Cancel
Analytes	Data Display	Detector Setup Wizard			

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.

Detector Se	tup Wizard				
Counting	Threshold Dete	ermination			
The va	alue for the Countin	g Amplifier Discriminator vo	oltage is now determined.		
		threshold determination m			
	anse tune started.	shold determination started	J.		
	arse tune finished.				
	e tune started.				
_		CPS. Setting 0.78750000	0000005 V.		
	_	_			
				K Back N	lext > Cancel
Analuteo	Data Display	Detector Setup Wigard			
Analytes	Data Display	Detector Setup Wizard			

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.

Detector Setup Wizard	
Acquisition status This page shows the progress of the data acquisition.	
Acquisition status	
Coarse plateau search (100V steps)	
Analogue voltage = -2012.5V	
Pulse counting voltage = 1137.5V	
Pulse counting voltage = 1237.5V	
Pulse counting voltage = 1337.5V	
Peak at mass 102.906 is valid for the plateau calculation	
Peak at mass 114.904 is valid for the plateau calculation	
Peak at mass 132.905 is valid for the plateau calculation	
Peak at mass 137.905 is valid for the plateau calculation	
Peak at mass 139.905 is valid for the plateau calculation	
O peaks are on the plateau	
Pulse counting voltage = 1437.5V	
Peak at mass 102.906 is valid for the plateau calculation	
Peak at mass 106.905 is valid for the plateau calculation	
Peak at mass 109.000 is valid for the plateau calculation	
Peak at mass 114.904 is valid for the plateau calculation	
Peak at mass 132.905 is valid for the plateau calculation	
Peak at mass 137.905 is valid for the plateau calculation	
Peak at mass 139.905 is valid for the plateau calculation	
O peaks are on the plateau	
Pulse counting voltage = 1537.5V	
Peak at mass 102.906 is valid for the plateau calculation	
Peak at mass 106.905 is valid for the plateau calculation	
Peak at mass 109.000 is valid for the plateau calculation	
Peak at mass 114.904 is valid for the plateau calculation	
Peak at mass 132.905 is valid for the plateau calculation	
Peak at mass 137.905 is valid for the plateau calculation	
< Back Next > Cance	
Analytes Data Display Detector Setup Wizard	

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.

Detector Se	tup Wizard					
Counting Gate Level Setup						
The va	ue for the Countin	ng Gate Level Voltage is no	ow determined.			
O Cou	nting Gate Level	Satura atartad				
	Inting Gate Level	Setup statted.				
				< Back	Next >	Cancel
Analytes	Data Display	Detector Setup Wizard				

Figure 4-87. Counting gate level setup

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

Detector Setup Wizard				
Cross Calibration				
Shows the progress of the cross calibration				
Starting Cross Calibration				
Sweep 1/3 completed.				
Sweep 2/3 completed.				
Sweep 3/3 completed.				
Average cross calibration factor of 60560.57 for mass: 7; rsd: 6.10; channels: 61				
Average cross calibration factor of 64600.99 for mass: 9; rsd: 6.47; channels: 62				
Average cross calibration factor of 68359.39 for mass: 24; rsd: 5.56; channels: 64				
Average cross calibration factor of 72515.45 for mass: 27; rsd: 4.76; channels: 65				
Average cross calibration factor of 75231.97 for mass: 45; rsd: 5.30; channels: 68				
Average cross calibration factor of 91963.24 for mass: 58; rsd: 3.95; channels: 68				
Average cross calibration factor of 90568.29 for mass: 59; rsd: 4.17; channels: 65				
Average cross calibration factor of 93057.13 for mass: 60; rsd: 5.59; channels: 62				
Average cross calibration factor of 95228.55 for mass: 63; rsd: 5.22; channels: 64				
Average cross calibration factor of 94786.73 for mass: 64; rsd: 6.00; channels: 58				
Average cross calibration factor of 96246.85 for mass: 65; rsd: 5.32; channels: 40				
Insufficiant number of channels for mass 66Zn. 5 channels found.				
Average cross calibration factor of 93731.13 for mass: 69; rsd: 5.14; channels: 67				
Average cross calibration factor of 95605.49 for mass: 71; rsd: 4.79; channels: 62				
Average cross calibration factor of 93867.96 for mass: 88; rsd: 4.35; channels: 65				
Average cross calibration factor of 92039.81 for mass: 89; rsd: 5.33; channels: 63				
Average cross calibration factor of 99233.01 for mass: 103; rsd: 5.17; channels: 60				
Average cross calibration factor of 104048.81 for mass: 107; rsd: 5.86; channels: 55				
Average cross calibration factor of 104870.53 for mass: 109; rsd: 6.95; channels: 54				
Average cross calibration factor of 104312.43 for mass: 115; rsd: 3.84; channels: 61				
Average cross calibration factor of 103863.28 for mass: 133; rsd: 4.55; channels: 59				
Average cross calibration factor of 102904.78 for mass: 138; rsd: 4.49; channels: 60				
Average cross calibration factor of 99849.13 for mass: 140; rsd: 4.01; channels: 61				
Average cross calibration factor of 104495.36 for mass: 159; rsd: 3.01; channels: 63				
Average cross calibration factor of 107634.75 for mass: 165; rsd: 3.60; channels: 62				
Average cross calibration factor of 106083.78 for mass: 181; rsd: 4.48; channels: 62				
Average cross calibration factor of 109545.34 for mass: 203; rsd: 7.20; channels: 23				
Average cross calibration factor of 113816.85 for mass: 205; rsd: 4.23; channels: 59				
Average cross calibration factor of 111153.52 for mass: 238; rsd: 4.21; channels: 62				
Cross calibration successfully completed.				
< Back Next > Cancel				
Analytes Data Display Detector Setup Wizard				

Figure 4-88. Cross calibration progress of detector setup

The summary is shown, see Figure 4-89.

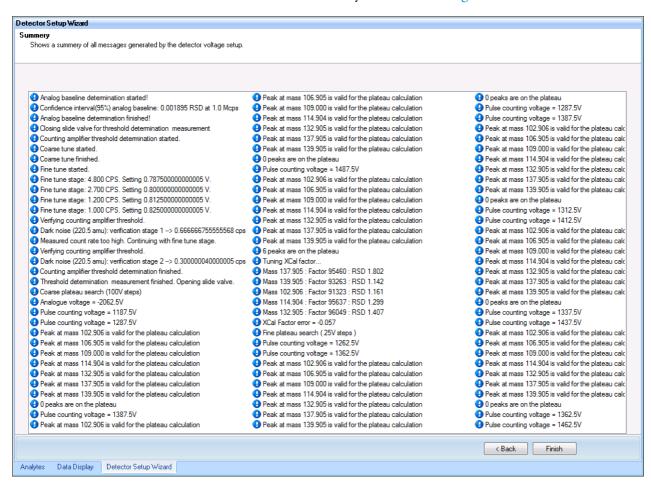


Figure 4-89. Summary of detector setup

Detector Setup Wizard	
ThermoFisher	The detector voltages have been set. The instrument is now ready to use.
	< Back Finish
Analytes Data Display	Detector Setup Wizard

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

Mass Calibration Wizard			
	Welcome to the Mass Calibration Wizard.		
	This wizard guides you through the steps necessary to set a mass calibration.		
Thermo Fisher SCIENTIFIC			
	< Back Next > Cancel		
Analytes Data Display	Mass Calibration Wizard		

Figure 4-91. Welcome to the Mass Calibration wizard

The Coarse Mass Calibration window opens, see Figure 4-92.

Mass Calibration Wizard		
Coarse Mass Calibration Do you want to execute a	a coarse mass calibration first?	
🔲 Execute a Coarse M	1ass Calibration first	
	< Back Next > Cancel	
Analytes Data Display	Mass Calibration Wizard	

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.

Mass Calibration Wizard				
Coarse Mass Calibration				
Do you want to execute a coarse mass calibration first?				
📝 Execute a Coar	e Mass Calibration first			
📃 Load Tune Sett	ngs			
Autotune sequence	•			
	< Back Next > Cancel			
Analytes Data Displa	Mass Calibration Wizard			

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.

Mass Calibration Wizard			
Coarse Mass Calibration			
Do you want to execute a coarse mass calibration first?			
Execute a Coarse Mass Calibration first			
🔽 Load Tune Settings			
Autotune sequence			
K Back Next > Cancel			
Analytes Data Display Mass Calibration Wizard			

Figure 4-94. Tune setting selected Mass Calibration wizard

The Load the Sample window opens, see Figure 4-95.

Mass Calibration V	izard
Load the Sample	
Place the samp	e probe into the solution and select ''Next'' to start the sample uptake delay.
	< Back Next > Cancel
Analytes Data [splay Mass Calibration Wizard

Figure 4-95. Load Sample in Mass Calibration wizard

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

Mass Calibration Wizard				
Waiting for sample uptake. This page shows the amount of time left before the acquisition starts.				
wizard w	ill automatically m	ove to the next page.	imer has completed the acquis finisched then press the 'Next	
Uptake I	Delay			Pause Continue
Analytes	Data Display	Mass Calibration Wizard	< Back Next >	Cancel

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.
- 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.

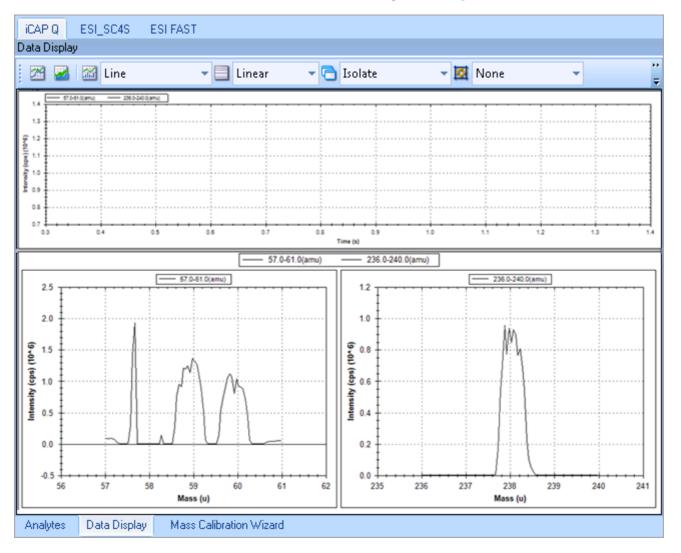


Figure 4-97. Data Display of mass calibration

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

lass Calibration Wizard				
Acquisition status				
This page shows the progress of the data acquisition.				
Trying to find peak 115In				
Peak 115In found at mass 114.902162030287				
Optimizing peak width with DCDacOffset, iteration 3				
O Trying to find peak 115In				
Peak 115In found at mass 114.902723407847				
PeakWidth: 0.405333953623781 for Mass 114.902723407847; Requested PeakWidth: 0.375				
Peak width not within tolerance of 0.02				
Setting DCDacOffset to -51.2975064463635				
I Trying to find peak 115In				
Peak 115In found at mass 114.912037729764				
PeakWidth: 0.376443092832631 for Mass 114.912037729764; Requested PeakWidth: 0.375				
Optimizing peak position with RFDacOffset, iteration 3				
Trying to find peak 115In				
Peak 115In found at mass 114.913616492257				
M Fine Mass Calibration completed (High Resolution)!				
< Back Next > Cancel				
Analytes Data Display Mass Calibration Wizard				

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.

Mass Calibration Wizard		
	Completing the Mass Calibration wizard	
ThermoFisher SCIENTIFIC	Show Mass Calibration	
	< Back Finish	
Analytes Data Display	Mass Calibration Wizard	

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.

lcon	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.
24	Autotune Report	Opens the Autotune Report tab in the data view region. Recorded Autotune reports can be viewed, exported or printed.
S	Detector Setup Report	Opens the Detector Report tab in the data view region. Shows the results of the detector setup.
С.	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.

Table 4-6.	Buttons of Views group
------------	------------------------

* To view Readback Plot



- 1. Click 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 Views group, click **Readback Plot**.

The **Readback Plot** tab opens in the data view region, see Figure 4-101.

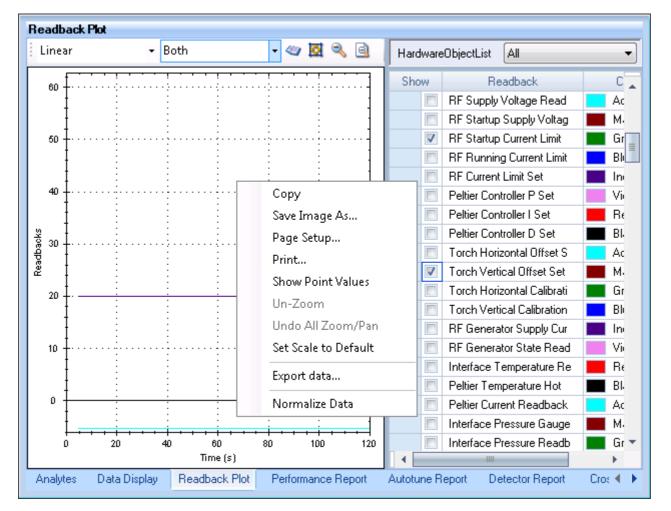


Figure 4-101. Readback Plot in data view region

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

137Ba			0.1		Passed	
	Stability Test	Limit:	0	Result: 0.0 %		
	Sensitivity Test		3,613.0		0.0	
137Ba++			0.1		Passed	
	Stability Test	Limit:	0	Result: 0.0 %		
	Sensitivity Test		92.0		0.0	
137Ba++,	/137Ba		0.1		Passed	
	Stability Test	Limit:	0	Result: 0.0 %		
	Sensitivity Test		0.0254	Less than	0.06	
140Ce			0.1		Passed	
	Stability Test	Limit:	0	Result: 0.0 %		
	Sensitivity Test		79,397.0		0.0	
140Ce.16	60		0.1		Passed	
	Stability Test	Limit:	0	Result: 0.0 %		
	Sensitivity Test		219.0		0.0	

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 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 **Views** group, click **Autotune Report**.

The Autotune Report tab opens in the data view region, see Figure 4-103.

🔄 Content 🔌 Exp	port 🗊 Print 🛛 🛅 Copy	🐻 Find	View Single Page	-	Zoom 🔍 🔍 100 %	👻 🔶 Previous	🔿 Next
Report Name Autotu	ne-SourceTune High Matrix-2	20120225-134	132585.xml	-			
	Autotune Report: Instrument: Operator: Sequence: Serial Number: Solution: Summary	iCAP (MP1-P Source Undefi	C\MP1 Tune High Matrix				
	The autotuning was suc		Intensity [cps]		uned Intensity [cps]	-	
	115In	137797	i intensity [cps]			-	
	140Ce	169635			45826	-	
	140Ce.16O	5248			644	-	
	7Li	25229			4318	-	
	59Co	49132			6447	-	
	238U	195152			40647	-	
	140Ce.16O/140Ce	0.0309		0.	.0181	-	
	Control Changes					_	
	Control		Original Value		Tuned Value	-	-
Analytes Data Display	Autotune_Report						

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 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 **Views** group, click **Content of Content of Content of Content**

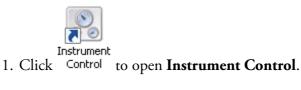
The **Detector Setup Report** tab opens in the data view region, see Figure 4-104.

ICAP Q Detector Report				
7	oort 🌀 Print	🞒 Copy 😹 Find View	Single Page	-
Report Name Detecto	orSetup-20120404	-173513218.xml		•
Detector Typ Detector Se	iCA Gerial Number: Und pe: DM4	2-04-04 17:35 P Q efined 440 Standard 24 - 1		
		Counting Voltage		
1310 -	Counting Voltage			1
1300 -				
1290 -	1			
8 1280 ·				
5 1270 ·	-			
1260				
Analytes — Data Display	Detector Report			

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

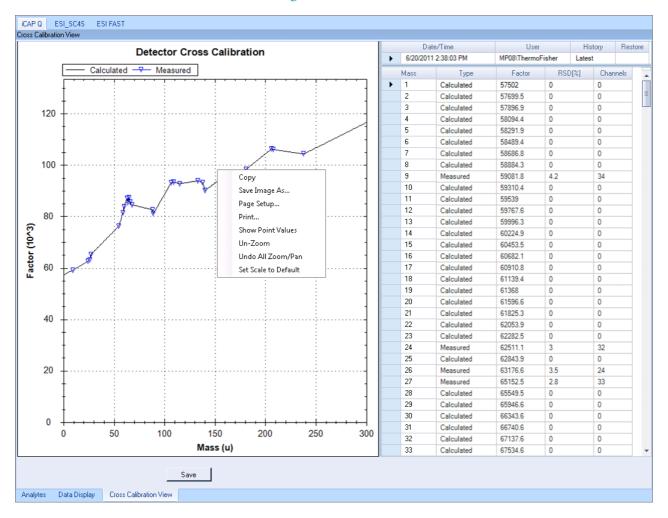
The toolbar of the report offers options, for example, to view the report, or print or export data.

* To view Cross Calibration result



- 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.





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 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 Views group,	1. 1	16	0.111	
3. In the Views group,	click	Mass	Calibration.	

The **Mass Calibration View** tab opens in the data view region, see Figure 4-106.

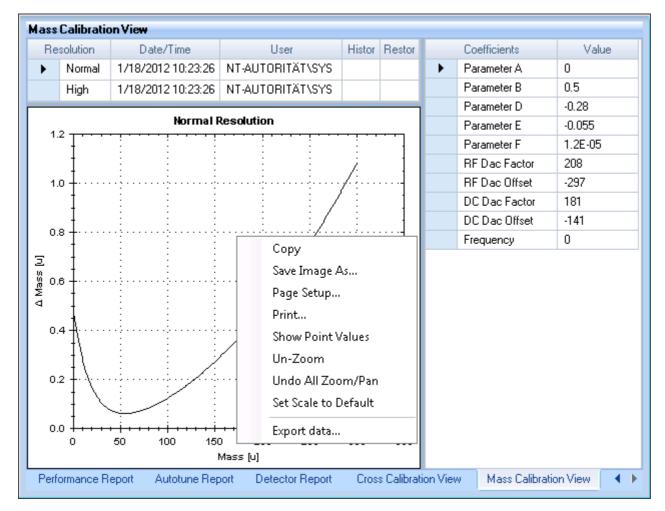


Figure 4-106. Mass Calibration View tab in data view region

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.

	Instrument Control		_ = X
Experiment Configurati	on iCAP Q Window		
🚱 Base 🛛 Blue 👻	Layout Default Add this Layout to favourites	About Qtegra	
Select Blend 💌	😫 Remove Layouts		
Palette	Layout	Help	

Figure 4-107. Window tab

✤ To select the layout



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



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

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

🖳 Enter Name For Layout	8
MyLayout	
OK Cancel	
	н

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

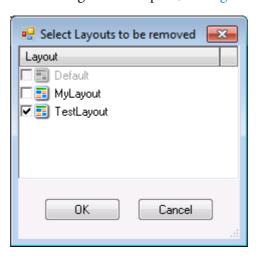


Figure 4-109. Select Layouts to be removed dialog

- 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 Control 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 it 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 Control 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 OK to close the window.

Control Panel

Control Panel iCAP Q			
Major			
High Voltage Disable	Enable		
Extraction Lens	I Positive [V]		 Hard Soft -2.375
CCT Focus Lens	[V]		12.25
Angular Deflection	on [V]	Ϋ́	
CCT Bias [V]			√ 35.00
CCT Mass [V]			0.0
L Focus Lens [V]			×
			35.00
Major			
Minor			
Torch Position			
Gas Flow			
		2222	*****
Control Panel	Status 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 Control 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 Control 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.

Show <u>M</u> ore Buttons	
Show <u>F</u> ewer Buttons	
Navigation Pane Options	
Add or Remove Buttons	►
	Show <u>F</u> ewer Buttons Navigation Pane Options

Figure 4-111. Selecting Navigation Pane Options

4. Click Navigation Pane Options.

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

Navigation Pane Options	— ×
Display buttons in this order	
 Minor Torch Position Gas Flow CCT RF Generator III 	Move Up Move Down
ОК	Cancel

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 to confirm your selection and close the window.
- ✤ To add or remove pages



- 1. Click Control 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.

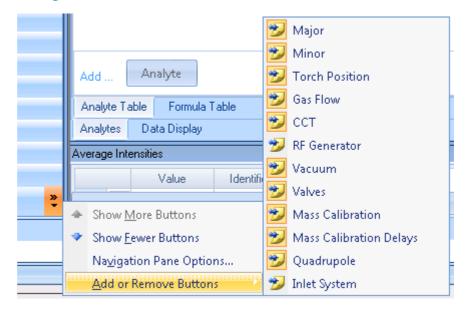


Figure 4-114. Selecting the Control Panel pages to be displayed

- 5. Click a deactivated ²² page to activate the display. The selection menu closes and the page is added to the display.
- 6. Click an activated ²² 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.

icap q
Major
High Voltage Disable Enable
Extraction Lens 1 Positive [V]
CCT Focus Lens [V]
Angular Deflection [V]
CCT Bias [V]
CCT Mass [V]
Focus Lens [V]
Pole Bias [V]
Analog Intensity Readback [V]
Extraction Lens 2 [V]

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
	running paramotoro	or the major page

Table 4-7. Turning parameters of	n 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.

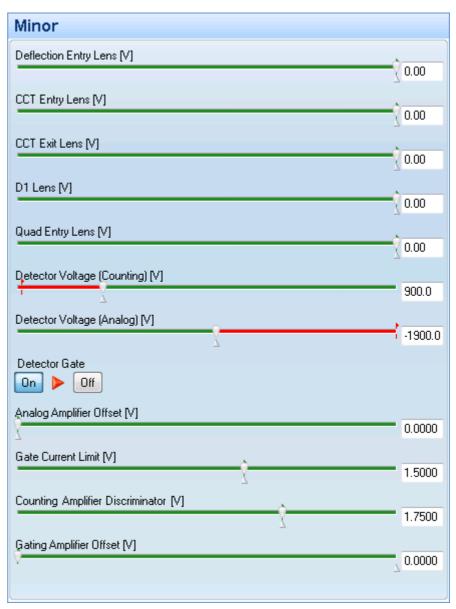


Figure 4-116. Tuning page Minor

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.

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	
Analog Amplifier Offset [V]	- - Amplifier and offset values of the ion
Gate Current Limit [V]	detection unit.
Counting Amplifier Discriminator [V]	-
Gating Amplifier Offset [V]	Voltage of amplifier offset.

Table 4-8.Tuning parameters of the Minor page

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.

Torch Position
Torch Horizontal Position [mm]
0.01
Torch Vertical Position [mm]
7
Sampling Depth [mm]
X Motor Moving Stopped
Y Motor Moving Stopped
Z Motor Moving Stopped

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.

Gas Flow	
Cool Flow [I/min]	
7	0.000
Auxilliary Flow [I/min]	
Σ.	0.0000
Nebulizer Flow [I/min]	
	0.0000
Argon Supply	
Additional Gas 1 Pressure Switch	
Additional Shut-Off Valve 1	
Additional Gas Flow 1 [%]	
7	0.00

Figure 4-118. Tuning page Gas Flow

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

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.

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.

Tuble I for Tulling parameters of the day new page	Table 4-10.	Tuning parameters of the Gas Flow page
--	-------------	--

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.

сст	
Penning Pressure [mbar]	·· 2.000e-009
CCT1 Valve On Off	
CCT1 Flow [ml/min]	0.000
CCT1 Flush Valve	
CCT2 Valve	
CCT2 Flow [ml/min]	0.000
CCT2 Flush Valve	

Figure 4-119. Tuning page CCT

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

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.

Table 4-11.Tuning parameters of the CCT page

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.

RF Generator	
Plasma Power [W]	
<u>Zi</u>	0.0
RF Generator Supply Voltage [V]	0.00
RF Generator Supply Current [A]	0.00
	0.00
Plasma Power [W]	
	0.00
RF Generator State	0.00
RF Ignite	
On > Off	
Door Lock	
Open 🕨 Closed	
FET Temp	
RF Supply Power	
Ok Error	
Interface Temperature [°C]	
	90.00
Plasma Cooling Water Flow [I/min]	0.00

Figure 4-120. Tuning page RF Generator

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

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.

•••	
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.

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

Vacuum

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

Vacuum	
Pirani Pressure (mbar)	00e-003
Analyzer Pressure	
Penning Pressure [mbar]	00e-009
Vacuum System	
Turbo Pump Supply Current [A]	0.00
	0.00
Turbo Pump Speed [Hz]	0.00

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.

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.

Table 4-13.	Tuning parameters of the Vacuu	im page
	ranning parametere er ine vaeda	iiii pago

Valves

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

Valves
Slide Valve Open
Slide Valve Closed
Pirani Pressure (mbar) Penning Pressure (mbar)
Expansion Valve Open Close
Slide Valve Open Close
Backing Valve Open Close
Main Water Valve Open Close
Plasma Cooling Water Valve Open Close
Water Level Error
Inlet Fan Speed (rpm)
Outlet Fan Speed (rpm) Outlet Fan Speed (rpm) Outlet Fan Speed (rpm) Outlet Fan Speed (rpm)
External Fan Speed (rpm)

Figure 4-122. Tuning page Valves

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

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.

Table 4-14.Tuning parameters of the Valves page

Mass Calibration

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

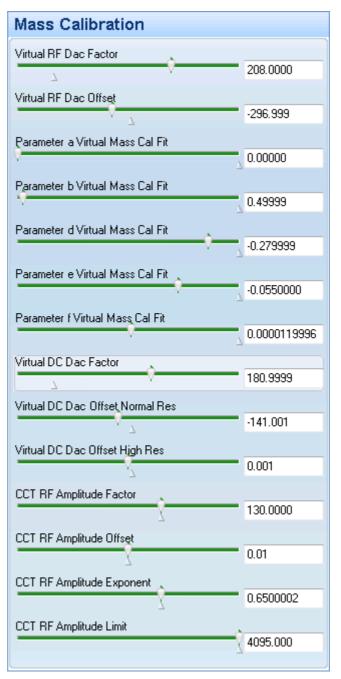


Figure 4-123. Tuning page Mass Calibration

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 <i>a</i> of virtual mass calibration fit.
Parameter b Virtual Mass Cal Fit	Parameter <i>b</i> of virtual mass calibration fit.
Parameter c Virtual Mass Cal Fit	Parameter <i>c</i> of virtual mass calibration fit.
Parameter d Virtual Mass Cal Fit	Parameter <i>d</i> of virtual mass calibration fit.
Parameter e Virtual Mass Cal Fit	Parameter <i>e</i> 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.

Mass Calibration Delays	
Delay after RF to lower Mass	
7	15000.00
Delay after DC to lower Mass	
	2000.000
Delay after DC to higher Mass	
<u> </u>	1000.005
Delay after RF to higher Mass	
<u> </u>	0.000

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.

Quadrupole	
negative Quad RF DC Offset [V]	
	0.00
positive Quad RF DC Offset [V]	0.00
Quad RF Amplitude [V]	
Z	0.00
Quad RF DC Offset [V]	
ν Δ	0.000
Tune Quad RF Resonance	
Start > Stop	
Quad RF Frequency (MHz)	

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	Б
Tune Quad for Resonance	For service or maintenance operation only.
Tune Quad fer fæsonance	

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.

Inlet System	
Exhaust Flow [mbar]	0.01
Peristaltic Pump Enable Disable	
Peristaltic Pump CCW	
Peristaltic Pump Turbo	
Peristaltic Pump Speed [rpm]	0.0
Enable Spray Chamber Cooling	
Spray Chamber Temperature [°C]	
Ž	-20.92
Peltier Temperature Hot Side [*C]	
Spray Chamber Temperature Cold Side [*C]	90.00
Spray chamber reinperature cold side [c]	20.00
Peltier Current [A]	0.00
Peltier Voltage [V]	0.00
	0.00

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.

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.

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

Status Panel

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

Status Panel			.
icap q			
Script List			
i 🔛 🕨 🔳 🖇	🏂 🎘 🍕	2	
Script Name		State	
🦨 DefaultScript.	CS	Init	
•			•
Control Panel	Status Pa	inel 👘	

Figure 4-127. Control Panel

* To open Status Panel



- 1. Click 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 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.

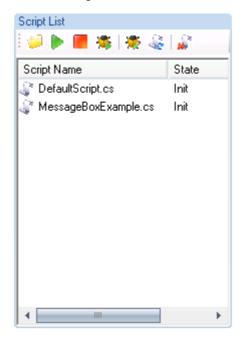
Image: Second state Image: Second st	 Scripts 	• •	Search Scripts	×
Organize 🔻 New folder				0
Name	Date modified	Туре	Size	
DefaultScript.cs	25.05.2012 10:08	CS File	8 KB	
GuidosTestScript1.cs	25.05.2012 10:08	CS File	1 KB	
HWScriptExample.cs	25.05.2012 10:08	CS File	1 KB	
📄 Inlet System-Prepare Exampl	25.05.2012 10:08	CS File	7 KB	
MessageBoxExample.cs	25.05.2012 10:08	CS File	1 KB	
File name:		•	C# files (*.cs) Open Cancel	•

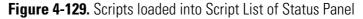
Figure 4-128. Dialog to open scripts

4. Select the script you wish to open.



The script is loaded into the Status Panel, see Figure 4-129.





✤ To run a script



- 1. Click 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 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 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 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 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 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 Control 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.

🖳 _Application Data\Scripts\MessageBoxExample.cs 🏹 🧒 1 ٠ public class MessageBoxExample 2 { public void Main() 4 5 { string result = MessageBox.Show("Just press any button.", 6 7 Ξ if(result == "Yes") 9 ł MessageBox.Show("You have pressed Yes.", "MessageBoxE 10 11 else if(result == "No") 12 13 ł MessageBox.Show("You have pressed No."); 14 15 else if (result == "Cancel") 16 17 ł MessageBox.Show("You have pressed Cancel.", "MessageF 18 19 } 20 } } 21 ٠ Ш b Info •) Current State: Init

Figure 4-130. Script Editor

5. Edit your script.



7. Click . The script editor closes.

* To remove a script from the Script List



- 1. Click 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 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.

LogV	iew				
Viewer Search					
i	7 In	fo Messages 🚺 0 Warnings	🛞 0 Erro	ors	₽ ₹
Level		Message	Time	Categ	4
	(Detector Voltage (Analog) Set set to -1900.	4/13/201	Contr	J Autoscroll
	 Communications with the iCAP Q instrument has been established! 		4/13/201	Contr	
					•

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 Control to open Instrument Control.
- 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.

Instrument Control Log View Region

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

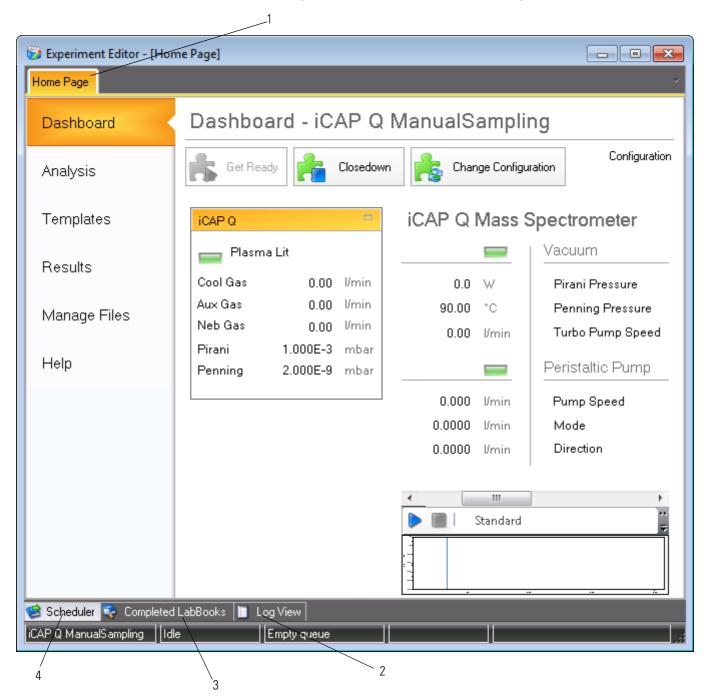
- User Interface of the Experiment Editor Tool
- Dashboard Page of Experiment Editor
- Analysis Page
- Templates Page
- Results Page
- Manage Files Page
- Help Page
- Scheduler
- Completed LabBooks
- Log View Region
- To open the Experiment Editor tool



1. Click Editor 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

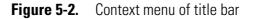


1. Click Editor to open Experiment Editor.

2. Right-click the **Scheduler, Log View** or **Completed LabBooks** title bar or tab.

The context menu opens, see Figure 5-2.





- 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.

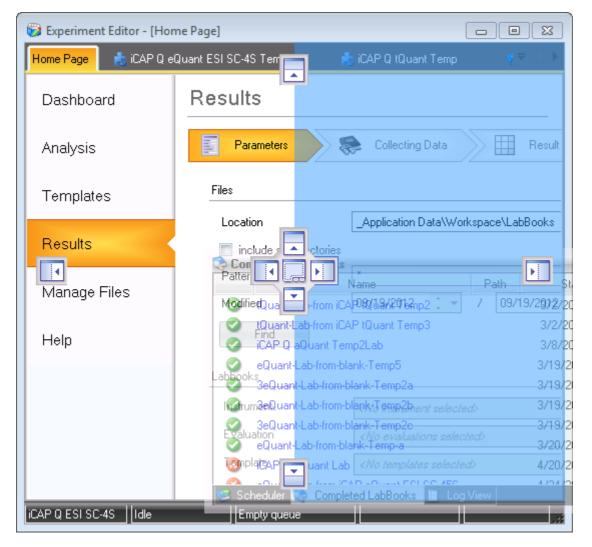


Figure 5-3. Moving Completed LabBooks

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.



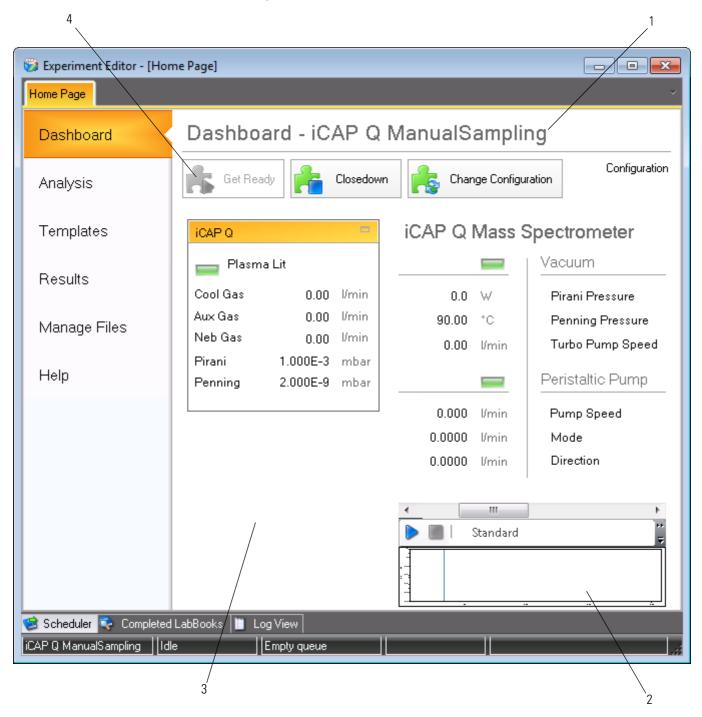
Figure 5-4. Position indicator to move tab

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.

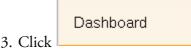
The main part (**3** in Figure 5-5) of the Dashboard page presents an overview of all main settings of the iCAP Q system.

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



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 Editor to open Experiment Editor.

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



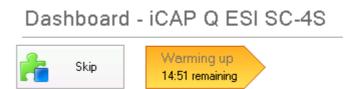
The Get Ready window opens, see Figure 5-6.

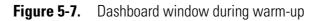
Get Ready								
icap q esi s								
iCAP Q mit autosar	npler E	SI SC-4S						
The following Options are av iCAP Q	ailable	:						
📃 Use Manual Sampling								
Measurement Modes:	ST) - High M	atrix					
	🔽 s	TD						=
		CT						
	🗖 К							
	STE	DS - Hiah S	ensitivity —					Ŧ
ESI SC-4S								
Timings:	Wash	time (s)	30	U	ptake time (s)	30)	
Sample positions:			uning		Rack		Vial	
	+	Performan	ice report		Standard		1	
		Autotune			Standard		1	
		Mass calib	oration		Standard		1	
📝 Warm up 🛛 15 🛛 Mi	inutes				OK		Cancel	

Figure 5-6. Get Ready window

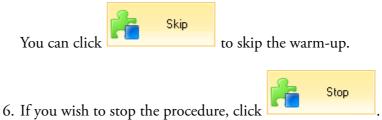
- 4. Select a Measurement Mode.
- 5. Click

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





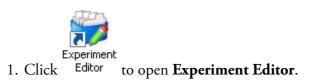
After warm-up, the performance report is started.



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



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



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

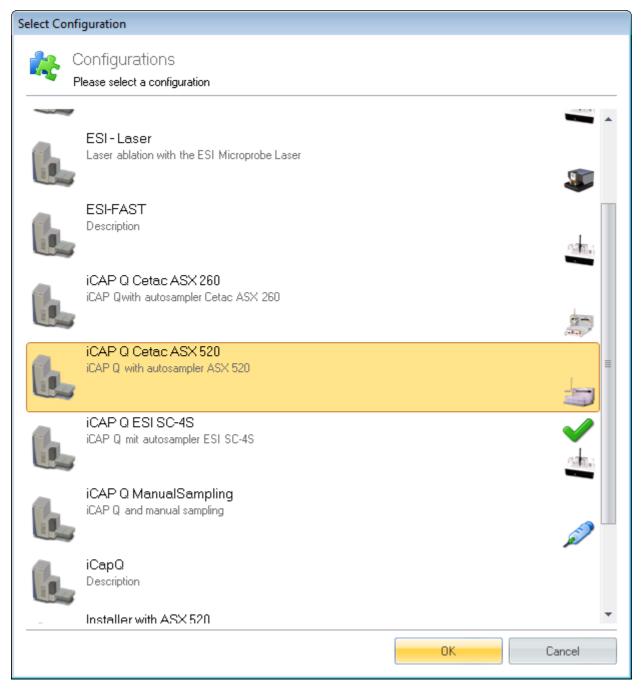


1. Click Editor to open Experiment Editor.

2. On the **Home Page**, click **Dashboard**. The **Dashboard** page of Experiment Editor opens. 3. Click Change Configuration

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

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





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 Editor 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.

iCAP Q	•	iCAP Q Mass S	pectromete	er			
Plas	ma Lit	Plasma / RF			Vacuum		Interlocks
Cool Gas Aux Gas Neb Gas Pirani Penning	13.92 //min 0.80 //min 0.87 //min 1.810E+0 mbar 3.943E-7 mbar	Forward Power Interface Temp Cooling Water Flow Gas Flow Cool Gas Flow	3.41	°C	Pirani Pressure Penning Pressure Turbo Pump Speed Peristaltic Pump Pump Speed	1.810E+0 mba 3.943E-7 mba 998.98 Hz 40.0 rpm	Interface Temperature Error Low Water Flow Hardware Lock Open Water Valve Closed Low Argon Pressure
ESI_SC4S Conn Fast	nected	Auxilliary Gas Flow Nebulizer Gas Flow	0.7962 0.8724	l/min l/min	Mode Direction	Normal Clockwise	Low Cool Gas Flow Low Exhaust Flow Plasma Lit Sensor Error
Valve 1 Valve 2 Pump Rack Vial	Load Load Off Standard 8	Standard	Select a standard		Mode Select a mode		· · · · · · · · · · · · · · · · · · ·
		(1000) 1000 1000 1000					
		0 14	•		11:00		12:00

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 Editor 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.

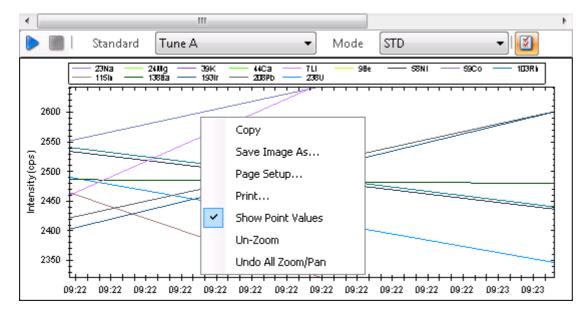


Figure 5-10. Real-time display on Dashboard

- 6. Click lostop 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 is 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.

🔯 Experiment Editor - [Ho	me Page]		• •
Home Page 🛛 🛸 tQuant-L	ab-from iCAP tQuan	t Temp 🥦 eQuant-Lab-from-blank-Temp5 - [Completed]	~
Dashboard	Analysis	3	
Analysis		te LabBook a new LabBook based on an existing Template or LabBook	Re: Oper
Templates	Name	eQuant-Lab-from-existLab	
Results	Location	LabBooks	
Manage Files Help	Tem Sam CSV Map	name	
	🔘 Create	Book Name EQuant-Lab-from-blank-Temlab e a new LabBook from a blank Template uation eQuant v	
		Create LabBook an existing LabBook	
		Open	-
199	•	III	P.
Log View Viewer Search			д
	📚 Completed Lat		
iCapQ Idle			

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

3. Below 🏷, click	Open
	1.0.1.1

The Browse for LabBook window opens, see Figure 5-12.

📚 Browse for LabBook		×
🔾 🗢 🕤 My LabBook	Ine Number	-
📁 Create New Folder 🔳 V	ïewys 🔻	
🕤 LabBooks	Name	Template 💌 🔺
	😪 QA-QC-DUP	QA-QC_1
	😪 rQuant	IVA-Test
	📚 tQuant-Lab-from iCAP tQuant Te	iCAP Q tQuant Temp
	😪 tQuant-Lab-from iCAP tQuant Te	iCAP Q tQuant Temp
	😪 tQuant-Lab-from iCAP tQuant Te	iCAP Q tQuant Temp
	😪 iCAP Q tQuant Spectra LabBook	iCAP Q tQuant Spectra
	😪 iCAP Q ESI SC-4S tQuant TempL.	. iCAP Q ESI SC-4S tQuant
	iCAP Q ESI SC-4S tQuant TempL.	. iCAP Q ESI SC-4S tQuant 💌
	•	•
Filename : tQuant-Lab-from iC	AP tQuant Temp.imexp	LabBook files (*.imexp) 🔹
		OK Cancel

Figure 5-12. Browse for LabBook window

4. Select a LabBook.

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

* To open a Recent LabBook



- 1. Click Editor 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.

😼 Experiment Editor - [Ho	me Page]	
Home Page 🛛 😒 tQuant-L	.ab-from iCAP tQuant Temp	🛸 eQuant-Lab-from-blank-Temp5 💡 [Com] 🗮 💷 🕨
Dashboard		▲
Analysis		Recent LabBooks Open a recent LabBook
Templates		eQuant-Lab-from-blank-Temp5 _Application Data\Workspace\LabBooks
Results		tQuant-Lab-from iCAP tQuant Temp _Application Data\Workspace\LabBooks
Manage Files		eQuant-Lab-from-blank-Temlab _Application Data\Workspace\LabBooks
Help		eQuant-Lab-from-blank-Temp _Application Data\Workspace\LabBooks
		iCAP Q aQunat TempLab3 _Application Data\Workspace\LabBooks
	¥	eQuant-Lab-from-blank-Temp2 _Application Data\Workspace\LabBooks
	✓ …	tQuant-Lab-from iCAP tQuant Temp2 Application Data\Workspace\LabBooks
🗋 Log View		4
Viewer Search		
Scheduler 📋 Log View		
iCapQ Idle	Empty queue	

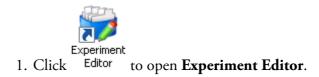
Figure 5-13. Recent LabBooks

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



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.

Home Page	
Dashboard	Analysis
Analysis	Create LabBook Create a new LabBook based on an existing Template or LabBook
Templates	Name eQuant Quality Control Lab
Results	Location LabBooks
Manage Files	 O Create a new LabBook from an existing Template ■ Template Name iCAP Q eQuant Quality Control ■
Help	Samples 3 Import from CSV
	Mapping Name
	Create a new LabBook from an existing LabBook
	LabBook Name IQuant-Lab-from iCAP tQuant Temp2
	Create a new LabBook from a blank Template
	Evaluation •
	Create LabBook
	< •

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.

 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 A new	Create LabBook tab opens for the nev	to create the new LabBook. v LabBook.
8.	Metho	od Parameters.	from a blank Template, define the n page 6-15 for details.
9.	Click	Sample List to check	the sample list parameters.
	when created	creating a LabBook. 7	ined by the number of samples selected The Sample List in the LabBook is s defined in "Sample Definition for a
10.		-	o define the data for export. mplate" on page 6-125 for details.
11.	In the LabBo	toolbar of your LabB ook.	Book page, click Book to save your

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 Editor 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 **Save** to save your LabBook.

Deleting a LabBook

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

To delete a LabBook



1. Click Editor 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.

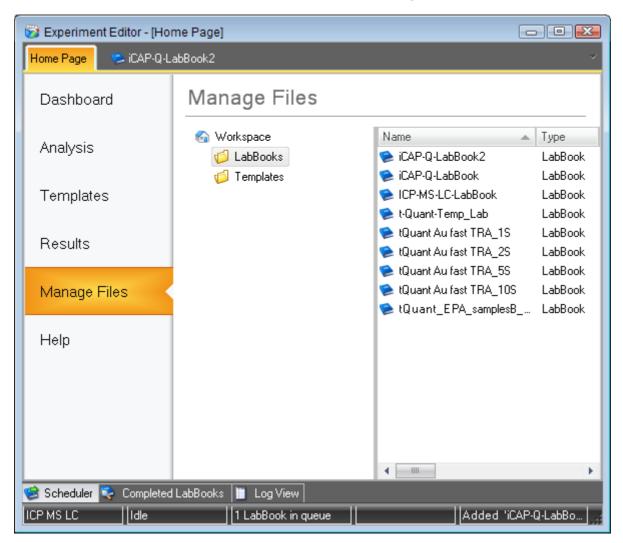


Figure 5-15. Manage Files - LabBooks

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

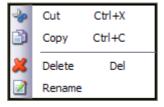


Figure 5-16. Context menu Manage Files

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 Editor 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 Close 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.

🔯 Experiment Editor - [Hor	me Page]	
Home Page 🛛 🛸 tQuant-L	ab-from iCAP tQuant Temp 😪 eQuant-Lab-from-blank-Temp5 - [Completed]	~
Dashboard	Templates	
Analysis	Create Template Create a blank Template, or one based on an existing Template or LabBook	Re: Opei
Templates	Name iCAP Q eQuant Temp2	
Results	Location Templates	R
Manage Files	Create a blank Template Configuration iCapQ	
Help	Use current	R
	Evaluation •	1
	Create a new Template from an existing Template	
	Template Name CAP 0 aQuant Temp	2
	Create a new Template from an existing LabBook	
	LabBook Name	5
	Create Template	
	Open Template Open an existing Template	
	Open	
	<	
🗋 Log View		Ļ
Viewer Search		
Scheduler 🗋 Log View	Completed LabBooks	

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



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



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 Editor 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.

🕵 Browse for Template			×
🕥 🗸 🕤 My Templates 🛛	•		•
📁 Create New Folder 🔳 Views	•		
🕤 Templates	Name	🔺 Туре	Created 🔺
	📩 iCAP Q Accela Chromatography	Template	Wednesda
	📩 iCAP Q aQuant Temp2	Template	Thursday, 🔳
	📩 iCAP Q aQuant Temp3	Template	Thursday,
	📩 iCAP Q aQuant Temp	Template	Tuesday,
	📩 iCAP Q ASX 260	Template	Monday, F
	📩 iCAP Q ASX 520	Template	Thursday,
	📩 iCAP Q eQuant Quality Control	Template	Wednesda
	📩 iCAP Q eQuant Temp4	Template	Tuesday, I 🔻
	•		+
Filename :		Template files (*.i	mtpl) 👻
		ОК	Cancel

Figure 5-18. Browse for Template window

4. Select a Template.

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

✤ To open a Recent Template



- 1. Click 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.

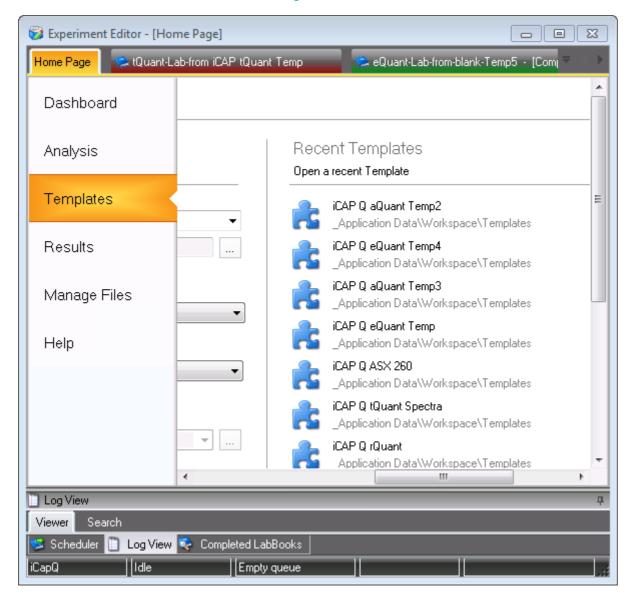


Figure 5-19. Recent Templates

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 Editor 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.

🤯 Experiment Editor - [Hor	me Page]					x
Home Page						~
Dashboard	Templat	es				
Analysis		ite Templa a blank Templ		existing Template or Lab	Book	
Templates	Name	iCAP Q eQua	int Temp		•	
Results	Location	Templates				
Manage Files		e a blank Temp iguration i	late CapQ		•	Ξ
Help			Use current			
	Eva	uation	eQuant		•	
	🔘 Creat	e a new Templa	ate from an existing Templ	ate		
	Tem	plate Name 🛛 🕅	CAP Q aQuant Temp		· · · ·	
		_	ate from an existing LabBo	ok		
	Labi	Book Name			· · · · ·	
					Create Template	-
	•		III		1	E T
😒 Scheduler 📗 Log View	📚 Completed La	Books				
iCapQ Idle	Empty	queue				

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 Template 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 Save 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 Editor 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 **Save** to save your Template.

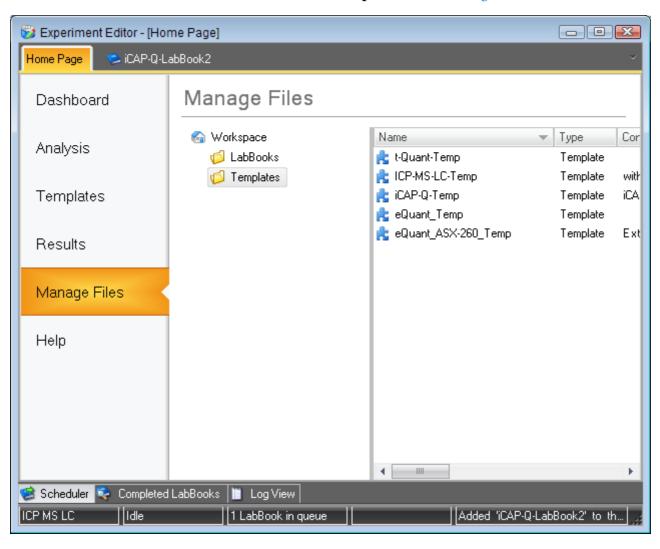
Deleting a Template

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

* To delete a Template



- 1. Click Editor 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.

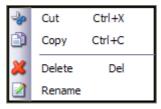


Figure 5-22. Context menu Manage Files

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 Editor 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 Close 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.

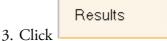
😺 Experiment Editor - [Ho	me Page]	
Home Page 🛛 🛸 tQuant-L	ab-from iCAP tQuant Temp	🛸 eQuant-Lab-from-blank-Temp5 - [Completed] 🛛 🗸 🗸
Dashboard	Results	
Analysis	Parameters	📚 Collecting Data 🔠 Result
Templates	Files	
Results	Location	_Application Data\Workspace\LabBooks
Manage Files	Pattern Modified	× 03/13/2012 - V 03/13/2012 - V
Help	Find	
	Labbooks	
	Instrument	<no instrument="" selected=""></no>
	Evaluation	<no evaluations="" selected=""></no>
	Template	<no selected="" templates=""></no>
	Samples	
	Identifier	
	Comment	
	run query	
🛸 Scheduler 📋 Log View	📚 Completed LabBooks	
iCapQ Idle	Empty queue	

Figure 5-23. Results Page of Experiment Editor

* To open the Result page of Experiment Editor



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



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 Editor 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.

Results	
Parameters	📚 Collecting Data 🛛 🖽 Result
Files	
Location	_Application Data\Workspace\LabBooks 🔹
include subdirectories	
Pattern	×
Modified	03/13/2012 : - / 03/13/2012 : -
Find	

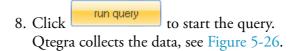
Figure 5-24. Files section in Results page

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.
Labbooks	
Instrument	icap Q 🗸
Evaluation	tQuant 🗸
Template	iCAP Q tQuant Temp 👻

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**.



Results
Parameters Sector Collecting Data Result
Running Query
🜔 tQuant Au fast TRA_10S.imexp: Loading labbook
🜔 tQuant Au fast TRA_2S.imexp: Loading labbook
Q tQuant Au fast TRA_5S.imexp: Loading labbook
🧭 Prepare result: Waiting
Cancel

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

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

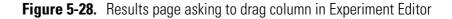
ini.		Parameters			Collecting	g Data	Result							
Row	's				Result									
đ					📑 Ref	resh 🔚 Group B	By 🙇 Pr	esets	PresetR	esults1				-
	•	Name				Sa	mple List		4	175Lu	-12	176Lu		7L
		Survey Conce	entrati		Ivaluatio	Category	Evaluate	Samp	le Type	Value	Unit	Value	Unit	Va
		Survey Conce	entrati		-	Intensity	V	BLK		15	cps	260	cps	
	1	Intensity		≣			V	BLK		164	cps	281	cps	
	1	Intensity aver-	-				V	BLK		12	cps	291	cps	_
	Intensity STD		Ŧ			V	BLK		13	срз	303	cps		
	mns						V	BLK		19	cps	320	cps	
				_		Intensity average	V	BLK		53	cps	291	cps	
Ø				_		Intensity STD	V	BLK		74.1	cps	22.7	cps	
- L	.abb(ook		*		Intensity RSD	V	BLK		141.0	%	7.8	%	
		Name	Merge			Intensity	V	STD		396,669	cps	11,016	cps	
	1	Filename	N			-	V	STD		393,065	CDS	10,916	CDS	
		Instrument					V	STD		394,901	CDS	10,992	CDS	_
	7	Evaluation					V	STD		396,417	CDS	10,966	•	
		Template					V	STD		396,538	CDS	11,047	•	
- 5	amp 🗹	le List Name	Marga			Intensity average	V	STD		395,518	CDS	10,987		
		Label	Merge			Intensity STD	V	STD		1,546.8	CDS	49.8		
		Survey Run				Intensity RSD	V	STD		0.4		0.5	- 1	
		Main Runs				Intensity	V	STD		588,496	CDS	16,222	CDS	_
-	1	Evaluate					V	STD		588,827		16,401	•	

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

- 9. Select the check boxes for the data you wish to display.
- 10. Click is 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.

Result						
🛃 Refresh	🗄 Grou	p By 📩				* -
Drag a colu	mn heade	r here to grou	p by that c	olumn.		
Sample Li	ist					
Comment	Evaluate	Sample Type	Standard	Internal Standard	Diluti	5
mment>	V	STD	STD1	IntSTD1	1	=
mment>	V	STD	STD1	IntSTD1	1	-
mment>	V	STD	STD2		1	
mment>	V	STD	STD2		1	
mment>		STD	STD2		1	
<pre>mment></pre>		STD	STD2		1	*



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

Result	
🙀 Refresh 🥵 Group By	
Standard Z	
+ Standard : (40 items)	
* Standard : STD1 (30 items)	
+ Standard : STD2 (10 items)	
۲. III المراجع	

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.

Resu	lt					_
	Refresh 🔛	Group By			_	17
9	Standard 4					
- St	andard : (40 ite	ems)				*
е	Standard Sample Type	Internal Standard	Dilution Factor	Amount	Final Quan	=
	KNOWN 1	r -	1			
	KNOWN		1			
	KNOWN		1			
	KNOWN		1			
	KNOWN		1			-
4						

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.

4	Presets	PresetRe	esults1			-	•• Ŧ
-12		Sar	mple List			Save	-
Iuatio	Cate	egory	Evaluate	Sample Ty		Save As	
Jant	Intensity		1	BLK			
			V	BLK	×	Delete	
			V	BLK			
			178	DIV	-		



✤ To save result data



- 1. Click 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 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 as to save the results data as new preset. The Save New Preset dialog is displayed, see Figure 5-27.

🖶 Save New P	reset 💽
Name	
Description	Please enter an optional description
	OK Cancel

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.

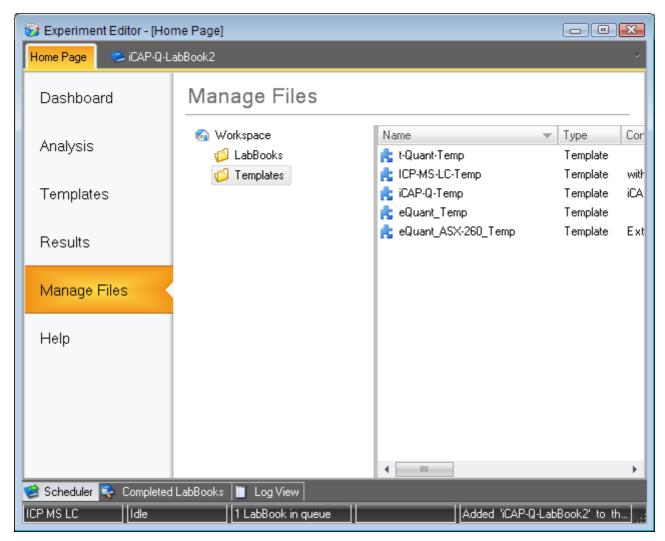


Figure 5-33. Manage Files Page of Experiment Editor

To open the Manage Files page of Experiment Editor *



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

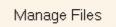


The Manage Files page of Experiment Editor opens.

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



- 1. Click Editor 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 Editor to open Experiment Editor.
- 2. Click the tab Home Page.

Manage Files

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

😼 Experiment Editor - [Ho	me Page]	
Home Page 😒 tQuant-L	ab-from iCAP tQuant Temp	😒 eQuant-Lab-from-blank-Temp5 💡 [Corr 👻 💷 🕨
Dashboard	Manage Files	
Analysis	✓ G Worksp ▷ Ø Lab Collapse	Name LabBooks
Templates	🧔 Ter 🚰 🛛 New Folde	r ja Templates
Results		
Manage Files		
Help		
Scheduler 📔 Log View	Completed LabBooks	

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 Editor 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.

😥 Experiment Editor - [Ho	me Page]	×
Home Page 🛛 🛸 aQuant	🛸 iCAP Q aQuant Temp-manual-Lab2 🥦 iCAP Q aQuant 🔻 🗌	
Dashboard	Manage Files	_
Analysis	Workspace Name LabBor Expand P Q eQuant Lab	•
Templates	Image: Second	
Results	Delete Del PQ tQuant Spectra LabBook	=
Manage Files	 b-iCAP Q Accela Chromatograph New Folder b-iCAP Q Spectra Chromatograph 	
Help	Lab-iCAP-Q-eQuant-manual	*
📚 Completed LabBooks 😒 iCAP Q ESI SC-4S 🛛 Idle	Scheduler 🛄 Log View	

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 Editor 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.

🜍 Experiment Editor - [Ho	me Page]		×
Home Page 🥵 tQuant-L	ab-from iCAP tQuant Temp	🙁 eQuant-Lab-from-blank-Temp5 💡 [Corr 🔻 🕚	►
Dashboard	Manage Files		_
Analysis	 Workspace LabBooks Templates 	Name 🅦 iCAP Q aQuant Temp2Lab	•
Templates	v remplates	eQuant Cut Ctrl+X	
Results		 SeQuar SeQuar Delete Del Rename 	
Manage Files		🛸 eQuant 🛸 eQuant-Lab-from-blank-Temp2	=
Help		 eQuant-Lab-from-blank-Temlab eQuant-Lab-from-blank-Temp 	-
🛸 Scheduler 📋 Log View	📚 Completed LabBooks		
iCapQ Idle	Empty queue		

Figure 5-36. Context menu of file

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

💱 Experiment Editor - [Hor	me Page]	
Home Page 🛛 😒 tQuant-L	ab-from iCAP tQuant Temp	🙁 eQuant-Lab-from-blank-Temp5 🕘 [Corr 🗧 💷 🕨
Dashboard	Manage Files	
Analysis	Workspace	Name
Templates	💋 New Folder 🧭 Templates	
Results		Paste Ctrl+V
Manage Files		📁 New Folder
Help		
😒 Scheduler 📋 Log View	Completed LabBooks	▲
iCapQ Idle	Empty queue	

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 Editor 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.
0		

😼 Experiment Editor - [Ho	me Page]	
Home Page 🛛 😒 tQuant-L	ab-from iCAP tQuant Temp	🛸 eQuant-Lab-from-blank-Temp5 - [Corr 👻 👘
Dashboard	Manage Files	
Analysis	 Workspace LabBooks Templates 	Name A Reference in the Name A Reference in the Name
Templates		eQuant Cut Ctrl+X
Results		 SeQuar Copy <
Manage Files		<pre>eQuantLab-from-blank-Temp2</pre>
Help		 eQuant-Lab-from-blank-Temlab eQuant-Lab-from-blank-Temp
🛸 Scheduler 📋 Log View	😪 Completed LabBooks	
iCapQ Idle	Empty queue	

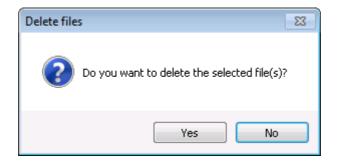
Figure 5-38. Context menu of file

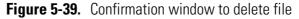
- 5. Select **Copy** from the context menu.
- 6. Select the location for the file.
- 7. Right-click and select **Paste** from the context menu. The file is copied to the selected location.
- * To delete a Template or LabBook file

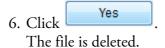


- 1. Click Editor to open Experiment Editor.
- 2. On the **Home Page**, click **Manage Files**. The **Manage Files** page of Experiment Editor opens.
- 3. Select the directory of the file you wish to delete.
- 4. Right-click on the file you wish to delete.

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







* To rename a Template or LabBook file



- 1. Click Editor 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.
--	------------------

😼 Experiment Editor - [Ho	me Page]	
Home Page 🛛 😒 tQuant-L	ab-from iCAP tQuant Temp	🛸 eQuant-Lab-from-blank-Temp5 - [Corr 👻 💷
Dashboard	Manage Files	
Analysis	 Workspace LabBooks Tomoletee 	Name A Reference Augurant Temp2Lab Reference Augurant A
Templates	🧔 Templates	eQuant Cut Ctrl+X
Results		 SeQuar Copy <
Manage Files		eQuant-Lab-from-blank-Temp2
Help		 eQuant-Lab-from-blank-Temlab eQuant-Lab-from-blank-Temp
😒 Scheduler 📋 Log View	📚 Completed LabBooks	
iCapQ Idle	Empty queue	

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.

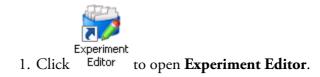
Help Page

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

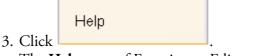
Experiment Editor - [I	Home Page]	
Dashboard	lelp	ŕ
Analysis	Support	Qtegr Qtegra S
Templates Results	Qtegra Help Display help for Qtegra Experiment Editor	This Instr
Manage Files	Getting started	Abc Ven
Help	Informations about new features and searching for ressources that help you to learn working with Qtegra.	S
	How to reach us Please let us know if you need help or if you have idea's on how to improve Qtegra	
	Fools Fools for working with Qtegra	
	Options Customize Qtegra Experimenteditor settings.	
Completed LabBooks	Scheduler D Log View Empty queue	۴.

Figure 5-41. Help Page of Experiment Editor

* To open the Help page of Experiment Editor



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



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



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



4. In the field **Available** on the left, select **Home Page**, see Figure 5-42.

Options	
Available Home Page Scheduler	Home Page Analysis Number of entries in the Labbook Recent List 10 : Clear Template Number of entries in the Template Recent List 10 : Clear
	OK Cancel

Figure 5-42. Home Page settings in Options dialog of Help page

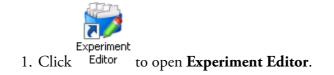
- 5. For **Analysis** on the right, select the number of entries for **LabBook Recent List**.
- 6. From the drop-down list **Clear**, select **All entries** or **Unpinned entries** if you wish to clear the list.
- 7. For **Template** on the right, select the number of entries for **Template Recent List**.
- 8. From the drop-down list **Clear**, select **All entries** or **Unpinned entries** if you wish to clear the list.



Customizing Scheduler Settings

In the **Tools** section on the **Help** page of Experiment Editor, you can define your **Scheduler** settings.

* To customize Scheduler settings



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



4. In the field **Available** on the left, select **Scheduler** to define the settings, see Figure 5-43.

🚱 Options		
Available	Scheduler	
Home Pag	· III · · ·	
Scheduler	Stop	Stop immediately 🔹
		Always ask for stop behaviour
	Suspend	Suspend after the current sample
		Always ask for suspend behaviour
	System Options	
	Closedown	Never closedown
	Export Directory	
	History Entries	50 Clear entries on start of next queue
	Start Queue	V Automatic
		OK Cancel

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.



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



2. Click Scheduler to open the **Scheduler** tab, see Figure 5-44.

Name	😻 Bottom
iCAP Q eQuant TempALab	Remove
	🔀 Remove A

Figure 5-44. Scheduler tool

* To add a LabBook to the Scheduler



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.

😺 Experiment Editor - [3eQuant-Lab-from-blan	ık-Temp2c]
😕 3eQuant-Lab-from-blank-Temp2b 🔸 [Completed]	📚 3eQuant-Lab-from-blank-Temp2c - [Running] 🛛 🗙 📃 🔻 👘
틙 Save 🔀 Close 📄 Run 🗍 Create 🕶	📮 🖻 Recalculate 🛛 👎 Interference
Content	Compound Intensities Graph
 iCAP Q Method Parameters Evaluation Results Compounds Peaks Ratios Concentrations Sample List 	Compound Intensities
	No evaluated data available !
😕 Scheduler	
▶ Run 👖 Suspend 📃 Stop 🌨 Top -	🐟 Up 📎 Down 😻 Bottom 🛛 🔯 Remove 🔉 Remove All 🛛 🚆
Name	
3eQuant-Lab-from-blank-Temp2c	
Scheduler 📔 Log View 🔍 Completed LabBo	boks
iCapQ Running 1 of 1 Lat	

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.

ompleted LabBooks						
N	ame	Path	Started At	Stopped At	Information	
tQuant-Lab-from iC	AP tQuant Temp2		3/2/2012 9:04 AM	3/2/2012 9:04 AM	'tQuant-Lab-from	
tQuant-Lab-from iC	AP tQuant Temp3		3/2/2012 9:25 AM	3/2/2012 9:25 AM	'tQuant-Lab-from	
iCAP Q aQuant Te	mp2Lab		3/8/2012 8:56 AM	3/8/2012 8:57 AM	'iCAP Q aQuant T	
eQuant-Lab-from-b	ank-Temp5		3/19/2012 9:21 AM	3/19/2012 9:21 AM	'eQuant-Lab-from	
3eQuant-Lab-from-	olank-Temp2a		3/19/2012 2:53 PM	3/19/2012 2:54 PM	'3eQuant-Lab-fro	
3eQuant-Lab-from-	olank-Temp2b		3/19/2012 2:55 PM	3/19/2012 2:56 PM	'3eQuant-Lab-fro	
3eQuant-Lab-from-	olank-Temp2c		3/19/2012 2:57 PM	3/19/2012 2:57 PM	'3eQuant-Lab-fro	
eQuant-Lab-from-b	ank-Temp-a		3/20/2012 9:19 AM	3/20/2012 9:20 AM	'eQuant-Lab-from	

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 Editor to open Experiment Editor.
- 2. Click Completed LabBooks 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

		n Experiment Edit open the Log View	tab, see Figure 5-47.
] Log∀ie w			д
Viewer Search			
🕕 0 Info Messages 🔥 0 Warnings 🔞	0 Errors 🛛 🥰 0 Fatal Errors 🛛	🕜 Autoscroll	Delete selected rows 🚆
Level Message	Time	Category	Sub Category
😒 Scheduler 📋 Log View 📚 Completed Lat	Books		

Figure 5-47. Log View in Experiment Editor

Experiment Editor Log View Region

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 Editor 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 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. Change the settings as appropriate.
- 5. Click 📅 to save your Template.
- * To close a Template



- 1. Click 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 in the toolbar to close the Template.

You can also click in the tab of the Template.

✤ To run a Template



- 1. Click 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 create a LabBook to schedule for execution. The **Create LabBook** window opens, see Figure 6-2.

😤 Create LabBook	×
Template Name	iCAP Q aQuant Temp2
Number Of Samples	3 Import from CSV
Mapping	
Sample Data	
LabBook Name	iCAP Q aQuant Temp2Lab
Location	_Application Data\Workspace\LabBooks
	OK Cancel

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

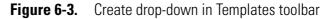


- 1. Click Editor to open Experiment Editor.
- 2. Click the tab **Home Page**.

- 3. Open a Template as described in "Opening a Template" on page 5-22.
- 4. Click Create.

The Create drop-down menu opens, see Figure 6-3.





- 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 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 History window for this Templates opens, see Figure 6-4.

History for iCAP Q eQuant Ter	npA.imtpl			×
Available history entries				
Date		U.	Computer	
4/17/2012 3:35:50 PM		Τ.	VM-TFS01	
4/10/2012 3:38:34 PM		Τ.	VM-TFS01	
4/3/2012 3:52:55 PM		T.	VM-TFS01	
4/3/2012 3:30:04 PM		T.	VM-TFS01	
•	III			- P.
Comment:				
Created				
		_		
Export Audittrail		(Compare Cl	ose

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 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 History dialog for this Templates opens, see Figure 6-4.

History for iCAP Q eQuant Temp	A.imtpl			×
Available history entries				
Date		U.	Computer	
4/17/2012 3:35:50 PM		Τ.	VM-TFS01	
4/10/2012 3:38:34 PM		Τ.	VM-TFS01	
4/3/2012 3:52:55 PM		Τ.	VM-TFS01	
4/3/2012 3:30:04 PM		T.	VM-TFS01	
•				Þ
Comment:				
Created				
Export Audittrail			Compare Clo	se

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.
		dialog opens, see Figure 6-6.

StandardElements StandardElements[0] Concentration DisplayValue 10 10 NormalizedValue 0.01 0.01 UnitDescriptor UnitText ppb ppb UnitType PPB PPB Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements StandardElements StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01			
StandardElements[0] Concentration DisplayValue 10 10 NormalizedValue 0.01 0.01 UnitDescriptor UnitText ppb ppb UnitType PPB PPB Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements IsotopeDilutionElementList StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01	Name	Version 6/28/20	112 Version 6/28/2012.
Concentration DisplayValue 10 10 NormalizedValue 0.01 0.01 UnitDescriptor UnitText ppb ppb UnitType PPB PPB Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements IsotopeDilutionElementList StandardElements IsotopeDilutionElements[0] Concentration DisplayValue 10 NormalizedValue 0.01	-		
DisplayValue 10 10 NormalizedValue 0.01 0.01 UnitDescriptor UnitText ppb ppb UnitType PPB PPB Symbol 24Mg Name IntSTD1 IntSTD1 IntSTD1 UsedForInternalStandard True True True Standards[2] N/A VA VA Description ElemList StandardElements StandardElements StandardElements StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 UnitDescriptor 0.01 0.01			
NormalizedValue 0.01 0.01 UnitDescriptor UnitText ppb ppb UnitType PPB PPB Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements IsotopeDilutionElementList StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01	=		
UnitDescriptor UnitText ppb ppb UnitType PPB PPB Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements IsotopeDilutionElementList StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01		10	10
UnitText ppb ppb UnitType PPB PPB Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements IsotopeDilutionElementList StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01		0.01	0.01
UnitType PPB PPB Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01			
Symbol 24Mg 24Mg Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements IsotopeDilutionElementList StandardElements StandardElements[0] IsotopeDilution DisplayValue 10 NormalizedValue 0.01 UnitDescriptor			
Name IntSTD1 IntSTD1 UsedForInternalStandard True True Standards[2] N/A Description IsotopeDilution StandardElements IsotopeDilutionElementList StandardElements StandardElements StandardElements IsotopeDilution DisplayValue 10 NormalizedValue 0.01 UnitDescriptor			
UsedForInternalStandard True True Standards[2] N/A Description ElemList StandardElements StandardElements[0] StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 UnitDescriptor	-	-	-
Standards[2] N/A Description ElemList StandardElements StandardElements[0] StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 UnitDescriptor			
Description Description ElemList StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 UnitDescriptor			True
LemList StandardElements StandardElementList StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 UnitDescriptor		N/A	
StandardElements StandardElements StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 UnitDescriptor	-		
▲ IsotopeDilutionElementList ▲ StandardElements ▲ StandardElements[0] ▲ Concentration DisplayValue 10 NormalizedValue 0.01 ▲ UnitDescriptor	-		
StandardElements StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 JunitDescriptor			
StandardElements[0] Concentration DisplayValue 10 NormalizedValue 0.01 UnitDescriptor			
✓ Concentration Display∀alue 10 Normalized∀alue 0.01 ✓ UnitDescriptor	-		
Display∀alue 10 Normalized∀alue 0.01 ⊿ UnitDescriptor			
NormalizedValue 0.01 UnitDescriptor	-		10
⊿ UnitDescriptor			
			0.01
	⊿ UnitFest		ррЬ
oncreat ppp	Oniciest		hhn

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 to close the **Comparison** dialog.
- 9. Click **Close** to close the **History** dialog for this Template.
- * To export the audit trail of a Template

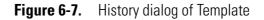


- 1. Click Editor to open Experiment Editor.
 - 2. Click the tab **Home Page**.
 - 3. Open a Template as described in "Opening a Template" on page 5-22.



The History dialog for this Templates opens, see Figure 6-7.

History for iCAP Q eQuant TempA.imtpl		×
Available history entries		
Date	U. Computer	
4/17/2012 3:35:50 PM	T. VM-TFS01	
4/10/2012 3:38:34 PM	T. VM-TFS01	
4/3/2012 3:52:55 PM	T. VM-TFS01	
4/3/2012 3:30:04 PM	T. VM-TFS01	
•		- F
Comment:		
Created		
Export Audittrail	Compare	ose



- 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.

Export Audittrail	pplication Data 🕨 Workspace 🕨 👻 🍫 Search Workspace 🔎
File name: Save as type:	↓ Html files {*.html)
💌 Browse Folders	Save Cancel

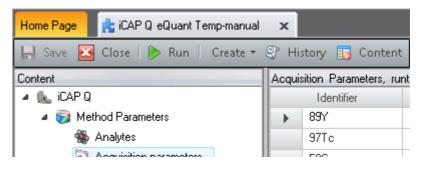
Figure 6-8. History Export Audittrail dialog

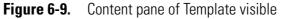
- 7. Click **Browse Folder** if you wish to change the pre-configured location of the file and select the directory.
- 8. Enter a **File name** for the HTML file, and click Save Your standard web browser opens displaying the audit trail information.
- 9. Click **Close** to close the **History** dialog for this Template.
- To hide Content pane



- 1. Click 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.





4. Click Content

The **Content** pane is hidden, see Figure 6-10.

Home	Page 🛛 📩 iCAP (Q eQuant Temp-m	anual 🗙		
	Save 🔀 Close 🖡	▶ Run 📔 Crea	ate 🔻 🎱 H	istory <mark>15 Co</mark> r	ntent
Acquis	ition Parameters, ru	ntime estimation 4	100 millisecor	ids	
	Identifier	Dwell time (s)	Channels	Spacing (u)	Mea
•	89Y	0.01	1	0.1	STD
	97Tc	0.01	1	0.1	STD

Figure 6-10. Content pane of Template hidden

5. Click **Content** to show the **Content** pane again.

Templates

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.

	ate Template e a blank Template, or one based o	n an existing Template or LabBook	
Name	iCAP Q eQuant		
Location	Templates		
Orea	e a blank Template		
Cor	figuration iCapQ		
	Use current		
Eva	luation aQuant		
	None aQuant		
🔘 Crea	e a new Temp <mark>eQuant</mark>		
Ter	nplate Name Raw Data rQuant tQuant		
🔘 Crea	trQuant e a new Tempiate from an existing L	арвоок	
Lab	Book Name	▼	

Figure 6-11. Evaluation types drop-down menu

The main applications for the Evaluations are summarized in Table 6-1.

Evaluation	Description		
aQuant	Created for Standard Addition analysis. In Standard Addition analysi 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.

Analytes Elements Mo	blecules	-						
								He
LI Be			B	C B	N	e B	F	Ne
Na Mg		Uncolored			P	ŝ	ei.	IA.
ж 🚰 🗄	SC TI V Cr Mi Fe	WebElements			As	#	ar Br	etter
Rb Sr		Series			50 9	₽	. I	<mark>₩</mark>
		 Block 			81	Po	at .	R
	Ac	Ionization Poter					_	
	Ce Pr Nd Pm Sm	Electronegativit Electron Affinity			Tm	₩	LI.	
		Individual	,		ud 9	No	יז ני	
		bologe standarda.				- н	de lege	nd
•	p d '	DN.						UDIN.
•		III						•

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.

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.

Table 5-2. Color scheme of periodic table	Table 6-2.	Color scheme of periodic table
--	------------	--------------------------------

To change the color scheme of the periodic table *



- 1. Click 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 **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.

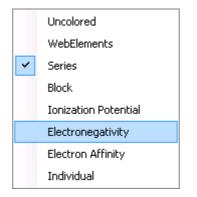


Figure 6-13. Context menu color schemes

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 Otegra

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.

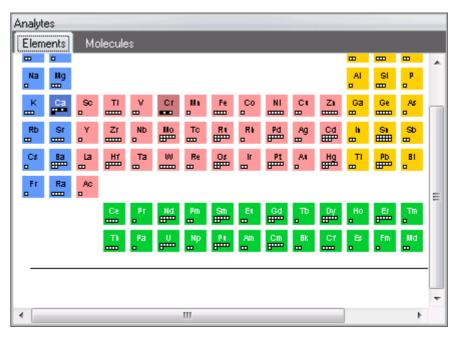


Figure 6-14. Elements page of Analytes

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.

Analytes				
Elements	Molecules			
Polyatomics		Symbol	Mass	Abundance
🐯 O.H	=	🗆 🐲 36Ar.35Cl	70.9364	0.2553
🐯 Ar.Cl		🗆 🗶 37Ar.35Cl	71.9357	0.0000
🐯 Ce.O		🗆 🐲 38Ar.35Cl	72.9316	0.0477
🐯 U.O		🗆 🐲 39Ar.35Cl	73.9312	0.0000
🐮 U.O.O	-	🗆 🐲 40Ar.35Cl	74.9312	75.4669
•	•	🗆 🗶 36Ar.37Cl	72.9334	0.0817
Matrix		🗆 🗶 37Ar.37Cl	73.9327	0.0000
🖵 Ar		🗆 🗶 38Ar.37Cl	74.9286	0.0153
	=	🗆 🗶 39Ar.37Cl	75.9282	0.0000
III N		🗆 🗶 40Ar.37Cl	76.9283	24.1331
С				
Щн	-			
•	•	•	1111	• •

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 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 **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.

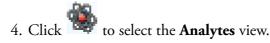
* To select the default isotope of an element (left mouse click)



- 1. Click 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 **Analytes** view.
- 5. Select the Elements page in the Analytes view.
- 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 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.



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.

	Symbol	Mass	Abundance	Interferences						
	40Ca	39.9626	96.94	40Ar(99.600%); 160						
	42Ca	41.9586	0.65	14N + 28Si(91.892%);						
V	43Ca	42.9588	0.14	160 + 27Al(99.762%);						
	44Ca	43.9555	2.09	160 + 1H + 27Al(99.7						
	46Ca	45.9537	0.00	46Ti(8.000%); 1H + 4.						
	48Ca	47.9525	0.19	48Ti(73.800%); 36Ar						
	Select all									

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.

Acquisition Parameters, ru	intime estimation 2	20 seconds 4	150 milliseconds						
Identifier	Dwell time (s)	Channels	Spacing (u)	Measurement mode	Resolution				
44Ca (STD)	0.01	1	0.1	STD	Normal				
88Sr (KED)	0.01	1	0.1	KED	Normal				
93Nb (STD)	0.01	1	0.1	STD	Normal				
59Co (STD)	0.01	1	0.1	STD	Normal				
96Ru (STD)	0.01	1	0.1	STD	Normal				
99Ru (STD)	0.01	1	0.1	STD	Normal	Ţ			
] • [
Advanced Parameters						_			
Number of sweeps:	5	÷			External I	Inpl			
					Digital IN				
Measurement order:	Measurement order: STD KED					Digital IN 2			
						_			
					•	•			

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.

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 \pm 0.4 amu either side of the central channel of the peak (total peak width of 0.8 amu).

Table 6-4.Acquisition Parameters

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 *



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



- Editor to open Experiment Editor. 1. Click
- 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 Interferences in the Toolbar of the Template. The list of interferences and the abundance of the interference on

the isotope opens, see Figure 6-18.

1H + 59Co 59.9410 99.985 40Ar + 20Ne 59.9548 90.148 12C + 48Ti 59.9479 72.988 14N + 46Ti 59.9557 7.971 160 + 44Ca 59.9504 2.081 15N + 45Sc 59.9560 0.366 36Ar + 24Mg 59.9526 0.266 12C + 48Ca 59.9515 0.185 160 + 1H + 43Ca 59.9511 32.590 12Sn++ 59.4517 8.580	iymbol	Mass	Abundance
12C + 48Ti59.947972.98814N + 46Ti59.95577.97116O + 44Ca59.95042.08115N + 45Sc59.95600.36636Ar + 24Mg59.95260.26612C + 48Ca59.95250.18516O + 1H + 43Ca59.95150.135120Sn++59.951132.590	1H + 59Co	59.9410	99.985
14N + 46Ti 59.9557 7.971 16O + 44Ca 59.9504 2.081 15N + 45Sc 59.9560 0.366 36Ar + 24Mg 59.9526 0.266 12C + 48Ca 59.9515 0.135 16O + 1H + 43Ca 59.9511 32.590	🦥 40Ar + 20Ne	59.9548	90.148
160 + 44Ca 59.9504 2.081 15N + 45Sc 59.9560 0.366 36Ar + 24Mg 59.9526 0.266 12C + 48Ca 59.9525 0.185 160 + 1H + 43Ca 59.9515 0.135 12OSn++ 59.9511 32.590	🛃 12C + 48Ti	59.9479	72.988
15N + 45Sc 59.9560 0.366 36Ar + 24Mg 59.9526 0.266 12C + 48Ca 59.9525 0.185 16D + 1H + 43Ca 59.9615 0.135 12OSn++ 59.9511 32.590	🛃 14N + 46Ti	59.9557	7.971
36Ar + 24Mg 59.9526 0.266 12C + 48Ca 59.9525 0.185 16O + 1H + 43Ca 59.9615 0.135 12Osn++ 59.9511 32.590	🛃 160 + 44Ca	59.9504	2.081
I2C + 48Ca 59.9525 0.185 I6O + 1H + 43Ca 59.9615 0.135 I2OSn++ 59.9511 32.590	🛃 15N + 45Sc	59.9560	0.366
a 160 + 1H + 43Ca 59.9615 0.135 a 120Sn++ 59.9511 32.590	🛃 36Ar + 24Mg	59.9526	0.266
a 120Sn++ 59.9511 32.590	🛃 12C + 48Ca	59.9525	0.185
	🛃 160 + 1H + 43Ca	59.9615	0.135
🛃 119Sn++ 59.4517 8.580	🛃 120Sn++	59.9511	32.590
	🛃 119Sn++	59.4517	8.580



6. Click another **Identifier** in the Acquisition Parameters table. The list displays the interferences for the newly selected isotope.



To duplicate rows



- 1. Click 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.

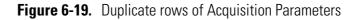


- 4. Click below the Method Parameters to open the **Acquisition Parameters** view in the Template.
- 5. Click the gray field in front of the row or rows you wish to duplicate to select the row or rows.

This way, isotopes in one sample can be defined to be measured with different settings.

Acquis	ition Parar	neters, ru	ntime estimation S	300 millisecor	nds	
	Identifie	r	Dwell time (s)	Channels	Spacing (u)	
	234U (ST	D)	0.01	1	0.1	3
	235U (ST	D)	0.01	1	0.1	:
	236U (ST	D)	0.01	1	0.1	:
	238U (ST	D)	0.01	1	0.1	:
	208Pb (S	TD)	0.01	1	0.1	!
	23N (🙀	Eit colle	to grid	1	0.1	:
-	39K 🚞		-	1	0.1	-
Fit cells						
		Fit cells	; to content			۶.
▲ Advan			to Content			•
		Export				•

6. Right-click on the selected rows. A context menu opens, see Figure 6-19.



* To define Acquisition Parameters



- 1. Click 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 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 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 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.

Export To Excel in the context menu.

6. Select



- 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.

Мо	nitored Analytes							
		Uptake '	Wash					
I	Minimum Delay (s)	30	30					
I	Maximum Delay (s)	300	300					
Δ	Signal Above (cps)	Stability (%F	RSD) Or	n Failure	Dwell Time (s)	Resolution	Wash	Signal Belo
	1000	2	lgi	nore and continue	0.01	Normal	V	1000
	1000	2	lgi	nore and continue	0.01	Normal		1000
	1000	2	lgi	nore and continue	0.01	Normal		1000
•				1111				ŀ
	id a new Mon	itored Analyt	e					

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 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 **Monitor Analytes** view.

* To add an analyte to be monitored



- 1. Click 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 in the list of Method Parameters to open the **Monitor Analytes** view in the Template.
- Define the Minimum Delay [s] and Maximum Delay [s] for Uptake and Wash.
- 6. Click Monitored Analyte 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. ▲

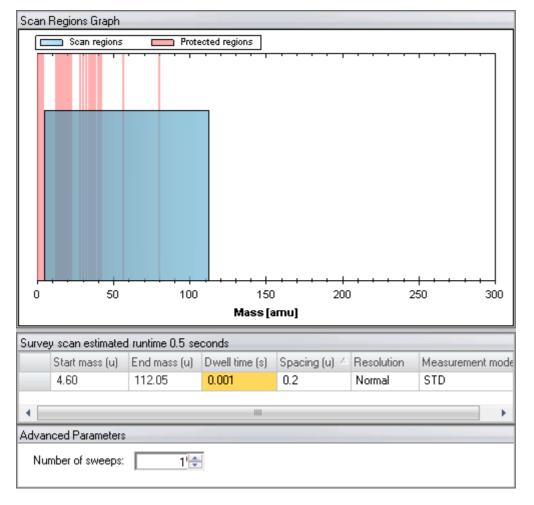
- 8. Define the parameters for this analyte.
- 9. Select the check boxes for **Uptake** and **Wash** to activate monitoring for the analyte.
- 10. For **Signal Above**, select **Ignore and continue** or **Skip this sample** from the drop-down menu **On Failure**.
- 11. For Signal Below, select Ignore 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

	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.
Measuremen mode	nt 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



- Editor to open Experiment Editor. 1. Click
- 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



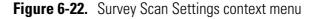
- 1. Click Editor to open Experiment Editor.
- 2. Click the tab **Home Page**.
- 3. Open a Template as described in "Opening a Template" on page 5-22.
- 4. Click in the list of Method Parameters to open the **Survey** scan settings view in the Template.
- 5. Drag the scan region borders in the graphic 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



Editor to open Experiment Editor. 1. Click

- 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.

Add new range
Сору
Save Image As
Page Setup
Print
Un-Zoom
Undo All Zoom/Pan
Set Scale to Default



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.

- 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 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 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. \blacktriangle

Elements selected for analysis in the **Analytes** view are listed in the Interference Correction view, see Figure 6-23.

Interfe	rence Correction			
Identi	fier	Enabled	Correct	ion
	44Ca (KED)			
	88Sr (KED)			
	93Nb (STD)			
	59Co (STD)			
	96Ru (STD)	V	- 1.0477	74 * 95Mo - 0.0544218 * 90Zr
	99Ru (STD)			
	101Ru (STD)			
-	115ln (STD)		- 0.0149	2627 × 1185n
	24Mg (STD)		2	Default interference correction
				Fit cells to grid
				Fit cells to content
				Export to Excel

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 ٠



- 1. Click 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 **Interference correction** view.
- To select analytes for interference correction in Experiment Editor



- 1. Click 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 with 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.

Standards	Select	ed Ele	ments	for "T	[une]	Δ						-			
😬 New 🔻 💥 Delete 🚆	Delete														
Name Desc 💋 Load		No			Elen	nent		Con	centra	ation			Unit		
Tune A Gen 👃 Default		7		Pb				10			ppb				
IntSTD1		8		U				10			ppb				_
		9		Ir				10			ppb				=
	+	10		Bh				10			ppb				-
	Select H U Na K Rb Cs Fr	Be Ng Ca Sr Ba	Sc V La Ac	Ti Zr Hť	V D ND Ta	Cr 0 Mo			Co Ri Ir	NI Pd Pt		Za Cd Hg			N P St B
					_		_	_	_	_	_		_	_	

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	Description		
Concentration	default, the c	Displays the concentration for the element in the standard file. By default, the concentration is set to <i>10</i> . This default can be changed and stored. See "Setting the Default Concentration" on page 6-38.		
		ation for quantification standards is to prepare standards ions that cover the concentration range expected in the		
	analyte which mass and ion	ation for internal standards is to use an internal standard is not present in any of the samples, which has a similar ization potential to the analyte to be corrected and is at a is similar to the expected concentrations of analytes in the		
Unit	default, the u	Displays the concentration unit for the element in the standard file. By default, the unit is set to <i>ppb</i> . This default can be changed and stored. See "Setting the Default Concentration" on page 6-38.		
	The command Table 6-7.	ls of the Standards view of a Template are summarized in		
	Table 6-7. (Commands of the Standards view of a Template		
	Commands	Description		
	2	To create a new standard (for eQuant and trQuant also Internal Standard).		
	×	To delete the selected standard(s).		
	5	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 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 *i* 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 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 *i* to select the **Standards** view.

- 5. Click New to open the **Add New Standard** dialog.
- 6. For eQuant or trQuant Templates, click to open the drop-down menu, see Figure 6-25.

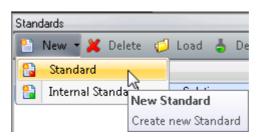


Figure 6-25. Creating a new standard

7. Click **Standard** to open the **Add New Standard** dialog, see Figure 6-26.

Add New Standard		—
Standard Name: Standard Description:		
Create standard from analyt	e list	
		OK Cancel

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 ٠



- Editor to open Experiment Editor. 1. Click
- 2. Click the tab **Home Page**.
- 3. Open a Template as described in "Opening a Template" on page 5-22.



- 4. Click *it* to select the **Standards** view.
- 💾 New 🔻 5. For eQuant or trQuant Templates, click to open the drop-down menu, see Figure 6-25.

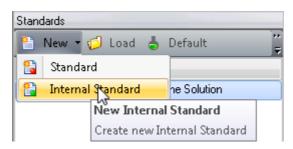


Figure 6-27. Creating a new internal standard

6. Click 📩 Internal Standard to open the Add New Standard dialog, see Figure 6-26.

Add New Standard	X
Standard Name: Standard Description:	
	OK Cancel

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.



- 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 ^{Editor} to open **Experiment Editor**.
- 2. Click the tab **Home Page**.
- 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 *it* to select the **Standards** view.
- 5. Click to open the **Add New Standard** dialog, see Figure 6-26.

Add New Standard		×
Standard Name: Standard Description:		
Create standard from analyte lis		
	OK Cance	1

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 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 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 *ib* 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 OK 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 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 *it* to select the **Standards** view.
- 5. In the **Standards** view, click **befault** to open the **Set Default Concentration** dialog, see Figure 6-30.

Set Default Concentration	×	
Default Concentration :	10 ppm •	
<u> </u>	Cancel	

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 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 *it* 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 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 **W** to select the **Standards** view.
- 5. In the **Standards** view, click the standard to be deleted.
- 6. Click Click to delete the standard.
- 7. Click Yes to confirm the message dialog.
- 8. Click 🗾 to save your Template. The standard is deleted from the Template.

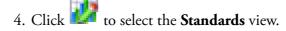
Saving a Standard to the Global Database

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 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.



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.

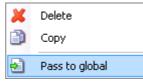


Figure 6-31. Standard context menu

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.

Com	Compounds									
	🗤 Add Compound 📰 Delete 🛛 Internal Standardization									
Con	pound Name	Trace	Auto Detect	Blank	Nor	Retention [s]	Tolerance [s]	Internal Standard	Fit	V
-	AsB	75As (1)	V			67.0000	10.0000	Use as Intern 📷	Linear	N
	DMA	75As (1)	1			87.0000	10.00		Linear	N
	AsIII	75As (1)	1			97.0000	10.00 Use as	Internal Standard	Linear	N
	AsC	75As (1)	V			158.0000	10.0000		Linear	N
	MMA	75As (1)	V			425.0000	10.0000		Linear	N
	AsV	75As (1)	1			670.0000	20.0000		Linear	N
										- F

Figure 6-32. Compounds view for tQuant

The columns that define the properties of the Compounds are listed in Table 6-8.

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	
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
	Experiment 1. Click ^{Editor} to open Experiment Editor .
	2. Click the tab Home Page .
	 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 W to select the Compounds view.
	 To define compounds
	Experiment 1. Click ^{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 I to select the Compounds view in the Template.
	5. Click Add Compound 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 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 **W** to select the **Compounds** view in the Template.
- 5. Click Internal Standardization

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.

Peak Detection			
Smoothing			
Active			
Number of Points :	10		
Number of Passes :	1		
Smoothing Method	Moving Mean 🔹		
Peak Detection			
Selected Integrator :	ICIS 🔹		
ICIS Base Parameters		ICIS Advanced Parameters	
Baseline Window [s] :	10	Minimum Peak Width [s] :	1
Area Noise Factor :	5	Multiplet Resolution [s] :	1
Peak Noise Factor :	10	Area Scan Window :	0
🔲 Constrain Peak Width		Area Tail Extension :	5
Peak Height Percentage :	5	🔲 Calculate Noise as RMS	
Tailing Factor :	1		
Peak Filter			
Minimum Peak Height [cps]:	0		
Minimum Peak Area [cts] :	0		

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 *



- 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.

Be sure to select a Template with the Evaluation tQuant.



4. Click **W** to select the **Peak Detection** view.

To define Smoothing in Peak Detection *



- 1. Click 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 **W** 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 *

Experiment 1. Click 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.



- 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 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 *w* 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.

Peak Detection				
Peak Detection				•
Selected Integrator :	ICIS	•		
ICIS Base Parameters		ICIS Advanced Parameters		_
Baseline Window [s] :	10	Minimum Peak Width [s] :	1	
Area Noise Factor :	5	Multiplet Resolution [s] :	1] =
Peak Noise Factor :	10	Area Scan Window :	0]
🔲 Constrain Peak Width		Area Tail Extension :	5	
Peak Height Percentage :	5	📃 Calculate Noise as RMS		
Tailing Factor :	1]		
				-

Figure 6-34. Peak Detection Integrator ICIS

- For ICIS Base Parameters, enter the value for Baseline Window [s] to review for a local minima.
- 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*.
- 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.
- 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].

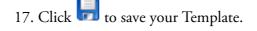
13. Enter the Multiplet Resolution [s].

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.



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 Editor to open Experiment Editor.
- 2. Click the tab Home Page.
- Open a Template as described in "Opening a Template" on page 5-22. Be sure to select a Template with the Evaluation tQuant.

be sure to select a template with the Evaluation (Quant.

4. Click **W** 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.

Peak Detection		
Peak Detection		•
Selected Integrator :	PPD 🔻	=
		•

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 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 *it* 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.

Peak Detection	
Peak Detection	^
Selected Integrator :	Avalon 👻
Avalon Parameters	
Auto Detect Initial Values	
Start Threshold :	10
End Threshold :	5
Area Threshold :	100
PP Resolution :	1
Bunch Factor :	1
Tension :	1
	*

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 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 **W** 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 Genes	sis integrator are displayed, se	e
Figure 6-37.		

ak Detection			
Selected Integrator :	Genesis	•	
Genesis Parameters			
Valley Detection		Baseline Noise Rejection Factor :	2
🔲 Constrain Peak		Percent Largest Peak :	0
Peak Height Percent :	0	SN Threshold :	0
Tailing Factor :	0	Base Signal to Noise Ratio :	0
Expected Peak Half Width :	0	Valley Threshold :	0
🔽 Calculate Noise as RMS		Valley Depth :	0
Base Noise Limit :	0	Peak Signal to Noise Ratio Cut Off :	50
Min Scans in Baseline :	2	Background Update Rate :	0

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.

		ive					
Analyte M	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing	Use for SemiQuant
137Ba 🖇	STD	Yes		Linear	None	Blank	Yes
223Ra 9	STD	Yes		Linear	None	Blank	Yes
223Fr 9	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.

N	0	Element	Isotope 1	Isotope 2	Abundance 1	Abundance 2	Atomic Weight
١.	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



- Editor to open Experiment Editor. 1. Click
- 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 **W** to select the **Parameters** view of the Template.

* To activate and define Internal Standardization for trQuant Template



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

Paramete	ers						
🚺 Inter	nal Standardization ac	tive					
Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing	Use for SemiQuant
71Ga	STD	Yes	· · · · · · · · · · · · · · · · · · ·	Linear	None	Blank	Yes
88Sr	STD			Linear	None	Blank	Yes
93Nb	STD	Use as I	nternal Standard	Linear	None	Blank	Yes
105Pd	STD	Yes	, ,	Linear	None	Blank	Yes
137Ba	STD	Yes		Linear	None	Blank	Yes
223Ra	STD	Yes		Linear	None	Blank	Yes
223Fr	STD	Yes		Linear	None	Blank	Yes
					1		1

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.

Paramete	ers						
🚺 Inter	nal Standardization ac	tive					
Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing	Use for Semi
71Ga	STD	No	Use as Internal Standard	Linear	None	Blank	Yes
88Sr	STD	Yes		Linear	None	Blank	Yes
93Nb	STD	Yes		Linear	None	Blank	Yes
105Pd	STD	Yes		Linear	None	Blank	Yes
137Ba	STD	Yes		Linear	None	Blank	Yes
223Ra	STD	Yes		Linear	None	Blank	Yes
223Fr	STD	Yes		Linear	None	Blank	Yes
•							•

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.

Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing	Use for SemiQuant
71Ga	STD	No	Use as Internal Standard	Linear	None	Blank	Yes
88Sr	STD	Yes		Linear 💌	None	Blank	Yes
93Nb	STD	Yes		Linear	None	Blank	Yes
105Pd	STD	Yes		2nd Order	None 💌	Blank	Yes
137Ba	STD	Yes		Linear	None	Blank	Yes
223Ra	STD	Yes		Linear	None	Blank	Yes
223Fr	STD	Yes		Linear	None	Blank	Yes

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.

Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type		Weighting	Forcing	Use for SemiQuant
71Ga	STD	No	Use as Internal	Linear		None 📷	Blank	Yes
88Sr	STD	Yes		Linear	No	ne	Blank	Yes
93Nb	STD	Yes		Linear	Ab	solute SD	Blank	Yes
105Pd	STD	Yes		Linear	Re	lative SD	Blank	Yes
137Ba	STD	Yes		Linear		None	Blank	Yes
223Ra	STD	Yes		Linear		None	Blank	Yes
223Fr	STD	Yes		Linear		None	Blank	Yes

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.

Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing	Use for SemiQuant
71Ga	STD	No	Use as Internal	Linear	None	Blank 📷	Yes
88Sr	STD	Yes		Linear	None	No	Yes
93Nb	STD	Yes		Linear	None	Zero	Yes
105Pd	STD	Yes		Linear	None	Blank	Yes
137Ba	STD	Yes		Linear	None	Blank	Yes
223Ra	STD	Yes		Linear	None	Blank	Yes
223Fr	STD	Yes		Linear	None	Blank	Yes

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.		

Analyte	Measurement Mode	Quantify	Internal Standard	Fit Type	Weighting	Forcing	Use for SemiQuant
71Ga	STD	No	Use as Internal	Linear	None	Blank	Yes
88Sr	STD	Yes		Linear	None	Blank	No
93Nb	STD	Yes		Linear	None	Blank	Yes
105Pd	STD	Yes		Linear	None	Blank	Yes
137Ba	STD	Yes		Linear	None	Blank	Yes
223Ra	STD	Yes		Linear	None	Blank	Yes
223Fr	STD	Yes		Linear	None	Blank	Yes

Figure 6-45. Parameters for trQuant Template drop-down Use for SemiQuant

- 11. Click 📄 to save your Template.
- * To define isotopes in rQuant Template



- Experiment 1. Click 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 **W** to select the **Parameters** view in the Template.

5. For each eleme	t row, select a value for Isotope 1 from the	
drop-down list	see Figure 6-46.	

Param	eters						
No	Δ.	Element	Isotope 1	Isotope 2	Abundance 1	Abundance 2	Atomic Weight
•	1	Cu	63Cu 🚽	65Cu	69.17	30.83	63.5456
	2	Hf	63Cu	178Hf	0.162	27.297	178.4864
	3	Sn	65Cu	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 6-46. 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.

No	Δ	Element	Isotope 1	Isotope 2	Abundance 1	Abundance 2	Atomic Weight
۲.	1	Cu	63Cu	65Cu 💌	69.17	30.83	63.5456
	2	Hf	174Hf	63Cu	0.162	27.297	178.4864
	3	Sn	114Sn	65Cu	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 6-47. 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.

Blank name Start (s) End (s) Quantify 10.0000 30.0000 10.0000 10.0000 10.0000	Regions					
	Region name		Blank name	Start (s)	End (s)	Quantify
40,0000 00,0000		region1		10.0000	30.0000	
40.0000 80.0000 🛛 🕅	•	region2		40.0000	80.0000	
40.0000 80.0000	Þ					



To open the Regions view ٠



- 1. Click 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 trQuant.



- 4. Click *w* to select the **Regions** view in the Template.
- To add a row to the Regions table ٠



- Editor to open **Experiment Editor**. 1. Click
- 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 **W** to select the **Regions** view in the Template.
- 5. Click Add 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.

Quantific	ation							
_	Quality Control nal Standardization ac	tive						
Analyte	Measurement Mode	Quantify	Internal Standar	d	Fit Type	Weighting	Forcing	Use for
59Co	STD	No	Use as Internal	Standard	Linear	None 👻	Blank	Yes
97Tc	STD	Yes			Linear	None	Blank	Yes
111Cd	STD	Yes			Linear	None	Blank	Yes
185Re	STD	Yes			Linear	None	Blank	Yes
•								×
IS Recov	very	_						
Low warning limit [%]: 80 Low failure limit [%]: 75								
High v	warning limit (%):		120 Hig	gh failure limit [%]	:	125		

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. P	arameters 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
	Experiment 1. Click Editor to open Experiment Editor.
	2. Click the tab Home Page .
	 Open a Template as described in "Opening a Template" on page 5-22. Be sure to select a Template with the Evaluation eQuant or aQuan
	4. Click is to select the Quantification view in the Template.
	 To set the quantification parameters
	Experiment 1. Click 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 W 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.

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.

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).

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.

Table 6-10. Columns of Ratios table

To open the Ratios view ∻



- 1. Click 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 eQuant, aQuant or tQuant.



- 4. Click **W** to select the **Ratios** view in the Template.
- To define isotope ratios (aQuant and eQuant) *



- 1. Click 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 **i** 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.
- 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.

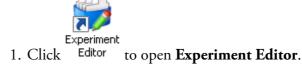
- 9. Click 📙 to save your Template.
- * To define compound ratios (tQuant only)



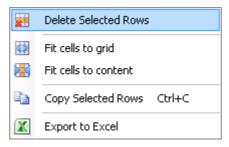
- 1. Click Editor to open Experiment Editor.
- 2. Click the tab Home Page.
- 3. Open a Template as described in "Opening a Template" on page 5-22.
- 4. Click **11** to open the **Ratios** view in the Template.
- 5. Click in a cell in the column **Compound 1** to display the list of available compounds.
- 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.
- Select a compound for column Compound 2. The compound selected in column Compound 2 is the denominator in column Ratio.

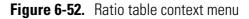
The ratio of both compounds is displayed in the column Ratio.

- 9. Click 📕 to save your Template.
- To delete rows



- 2. Click the tab Home Page.
- 3. Open a Template as described in "Opening a Template" on page 5-22.
- 4. Click **i** 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.





- 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.

Quality Cont	trol Tests	Test details	s for CCB			
🞦 New	🐹 Delete 🗍 🞲 Edit detection limits 🚽	Number of	f analyte failures	to generate	a QC failure	: 1 🚖
Name	Description	Number of	f analyte warning	as to generat	e a QC Eail	ure: 1
Blank 1	ests			go to gonorat	0 4 40 1 4.	
CCB	Continuing Calibration Blank	If this QC I	fails	Ignore and	continue fr	om the next sample
ICB	Initial Calibration Blank					•
МТВ	Memory Test Blank	If this QC I	fails again	Ignore and	continue fr	om the next sample
PRB	Preparation Blank	If this QC I	fails a final time	Ignore and	continue fr	om the next sample
	tion Tests			<u> </u>		•
Calibra	1011 1 Gata	Test Parar	neters			
CCV	Continuing Calibration Verification	Enabled	Analyte	Warn	ing Limit	Failure Limit
ICV	Initial Calibration Verification		59Co (STD)		1	2
LCS	Laboratory Control Standard	V	115ln (STD)		1	2
QCS	Quality Control Standard		7Li (STD)		1	2
Paired	Sample Tests	V	140Ce (STD))	1	2
DUD	5 F .		209Bi (STD)		1	2
DUP	Duplicate	V	238U (STD)		1	2
SER	Serial Dilution					
Spike 1	ests					
LFB	Laboratory Fortified Blank					
M×S	Matrix Spike					
PDS	Post Digestion Spike					
Interna	I Standard Test					
107						
IST	Internal Standard Test					
•	III. •					

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 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 eQuant.

- 4. Select the check box Use Quality Control in Quantification.
- 5. Click **W** to select the **Quality Control** view in the Template.

In Experiment Editor, the Quality Control method parameter of the

eQuant Template offers several types of blank verification, see

Figure 6-54. **Quality Control Tests** Test details for CCB 📔 New Delete Number of analyte failures to generate a QC failure: Ę * Name Description * Number of analyte warnings to generate a QC Failure: 1 -**Blank Tests** If this QC fails Ignore and continue from the next sample CCB Continuing Calibration Blank ICB Initial Calibration Blank If this QC fails again Ignore and continue from the next sample MTB Memory Test Blank = If this QC fails a final time Ignore and continue from the next sample PRB Preparation Blank **Calibration Tests Test Parameters** CCV Enabled Warning Limit Failure Limit Ζ Continuing Calibration Verification Analyte ICV. Initial Calibration Verification 2 7 59Co (STD) 1 LCS 1 1 2 Laboratory Control Standard 115In (STD) 7 2 QCS Quality Control Standard 1 7Li (STD) 2 1 1 Paired Sample Tests 140Ce (STD) 2 1 1 209Bi (STD) DUP Duplicate V 1 2 238U (STD) 111

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.

Blank Verification

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.

Test type	Description	Purpose	Frequency	Limits
ССВ	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.

Quality Cont	rol Tests		Test detail	s for LCS						
🚹 New	🔀 Delete	++ ₹	Number o	f analyte fa	ailures	to gener	ate a QC fai	lure: 1	A V	
Name	Description		Number o	f analute w	varning	s to aen	erate a QC f	Failure: 1	* *	
Blank T	ests									
ССВ	Continuing Calibration Blank		If this QC	fails		Ignore	and continu	e from the next	sample	
ICB	Initial Calibration Blank		If this QC fails again If this QC fails a final time			- (5 ,				
мтв	Memory Test Blank									
PRB	Preparation Blank	=								
Calibra	tion Tests		TID							
			Test Para	1						
CCV	Continuing Calibration Verification		Enabled	Analyte	Low F	Failure	Low Warn	High Warning	High Failure 🔷	
ICV	Initial Calibration Verification			115ln (75	80	120	125	
LCS	Laboratory Control Standard		V	140Ce		75	80	120	125	
QCS	Quality Control Standard		V	209Bi (75	80	120	125	
Paired	Sample Tests		V	238U (75	80	120	125	
			~	59Co (75	80	120	125	
DUP	Duplicate		V	7Li (ST		75	80	120	125	
SER	Serial Dilution									
Spike T	ests									
•	•									

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.

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)

 Table 6-12.
 Quality control calibration tests

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.

Quality Cont	trol Tests		Test detail	s for DUP						
📔 New	🔀 Delete	++ ₹	Number o	f analyte failures	to genera	ate a QC fa	ilure: 1	*		
Name	Description	^	Number o	f analyte warning	gs to gene	erate a QC	Failure: 1	*		
CCV ICV	Continuing Calibration Verification		If this QC	fails	Ignore and continue from the next sample					
LCS	Initial Calibration Verification Laboratory Control Standard		If this QC fails again							
QCS	Quality Control Standard				Ignore and continue from the next sample					
Paired	Sample Tests				<u> </u>					
DUP	Duplicate		Test Para	meters						
SER	Serial Dilution		Enabled	Analyte	Limit	Low Fail	Low Warnin	High W	High F	
Spike Tests				59Co (STD)	100	· · · · ·	80	120	125	
opino i			V	115ln (STD)	100		80	120	125	
LFB	Laboratory Fortified Blank			7Li (STD)	100	75	80	120	125	
MXS	Matrix Spike			140Ce (STD)	100	75	80	120	125	
PDS	Post Digestion Spike			209Bi (STD)	100	75	80	120	125	
	I Standard Test			238U (STD)	100	75	80	120	125	
IST	Internal Standard Test									
٠	IIII •									

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 . 0	uality control	paired sam	ple tests
-----------------------	----------------	------------	-----------

Test type	Description	Purpose	Frequency	Limits
DUP	Duplicate	checks the reproducibility of results by analyzing an unknown sample in duplicate	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

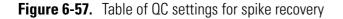
Warning and Failure Limits

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.

Quality Cont	trol Tests		Test deta	ils for LFB					
🔒 New	🔀 Delete	Number	of analyte failure	s to genera	ate a QC fa	ailure: 1	* *		
Name Description Number of analyte warnings to generate a QC Failure: 1								-	
CCV	Continuing Calibration Verif	i	If this QC	fails	lanore a	and contin	ue from the nex	t sample	
ICV	Initial Calibration Verification	·		10.00	[ignore ((admpic	
LCS	Laboratory Control Standard		If this QC	; fails again	Ignore a	and contin	ue from the nex	t sample	
QCS	Quality Control Standard		LEthis OC	fails a final time	and contin	ntinue from the next sample			
Paired	Sample Tests				[Ignore (de nom the new	(sample	
DUP	Duplicate		Test Para	ameters					
SER	Serial Dilution	=	Enabled	Analyte	Qualifier	Low Fail	Low Warning	High Warni	High Fail
Spike T			V	59Co (STD)	100	75	80	120	125
орікої	0000			115ln (STD)	100	75	80	120	125
LFB	Laboratory Fortified Blank		V	7Li (STD)	100	75	80	120	125
MXS	Matrix Spike		V	140Ce (STD	100	75	80	120	125
PDS	Post Digestion Spike			209Bi (STD)	100	75	80	120	125
Interna	l Standard Test	-	V	238U (STD)	100	75	80	120	125
•	IIII •								



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.

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 %

 Table 6-14.
 Quality control spike recovery

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.

Quality Con	trol Tests	Test details for IST							
New Name	Delete	Internal Standard Test enabled							
- Эріке і	C-34.5	Low Warning Limit (%)	80	Low Failure Limit (%)	75				
LFB MXS	Laboratory Fc 🔹 Matrix Spike	High Warning Limit (%)	120	High Failure Limit (%)	125				
PDS	Post Digestion :								
Interna	al Standard Te								
IST	Internal Stanc								

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.

Test details	for CCB						
			nerate a QC failure enerate a QC Failu				
If this QC fa	If this QC fails						times
If this QC fa	ails again	lgno	re and continue fro	om the next sampl	e 🔹	1 韋	times
If this QC fa	If this QC fails a final time Ignore and continue from the next sample -			e •	1 🖨	times	
Test Param	ieters						
Enabled	Analyte		Warning Limit	Failure Limit			
	137Ba		1	2			
	88Sr		1	2			
	90Zr		1	2			
🔽 105Pd			1	2			
	115ln		1	2			

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 0-10. 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.

Table 6-16. Settings for failure rules

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 Editor to open Experiment Editor.
- 2. Click the tab **Home Page**.
- Open a Template as described in "Opening a Template" on page 5-22.
 Be sure to colort a Template for a Owent Evaluation

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 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**.

4. Click **i** to select the **Quality Control** view. On the left, the available **Quality Control Tests** are listed, see

Figure 6-60.

Quality I	Contro	ol Tests				
💾 N	ew	💥 Delete 🛛 📝 Edit detection limits 👘				
Name		Description				
Bla	nk Te	ests				
CCE	3	Continuing Calibration Blank				
ICB		Initial Calibration Blank				
MT	В	Memory Test Blank	=			
PRI	В	Preparation Blank				
Cali	ibrati	ion Tests				
CCN		Continuing Calibration Verification				
ICV		Initial Calibration Verification				
LCS	6	Laboratory Control Standard				
QC	S	Quality Control Standard				
Paired Sample Tests						
DU	Р	Duplicate	_			
CEI	-	Corist Dilution	•			

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 Param	Test Parameters								
Enabled	Analyte	Warning Limit	Failure Limit						
V	59Co (STD)	1	2						
V	115ln (STD)	1	2						
V	7Li (STD)	1	2						
1	140Ce (STD)	1	2						
1	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 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**.

4. Click **W** to select the **Quality Control** view. On the left, the available **Quality Control Tests** are listed, see

Figure 6-62.

Quality Con	trol Tests	
📔 New	🔀 Delete 🛛 🔢 Edit detection limits	
Name	Description	•
Calibra	ition Tests	
CCV	Continuing Calibration Verification	
ICV	Initial Calibration Verification	
LCS	Laboratory Control Standard	1
QCS	Quality Control Standard	1
Paired	Sample Tests	
DUP	Duplicate	=
SER	Serial Dilution	
Spike	lests	
LFB	Laboratory Fortified Blank	
MXS	Matrix Spike	
PDS	Post Digestion Spike	-
•		

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 **T** 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.

	Analyte	Low Failure Limit (%)	Low Warning Limit (%) $ \triangle$	High Warning Limit (%)	High Failure Limit (%)
V 1	115ln (STD)	75	80	120	125
V 1	140Ce (STD)	75	80	120	125
2	209Bi (STD)	75	80	120	125
2	238U (STD)	75	80	120	125
V 5	59Co (STD)	75	80	120	125
7	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 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**.

4. Click *i* to select the **Quality Control** view. On the left, the available **Quality Control Tests** are listed, see

Figure 6-64.

Quality Control Tests							
📔 New	🐹 Delete 🛛 📝 Edit detection limits						
Name	Description	•					
ICV	Initial Calibration Verification						
LCS	Laboratory Control Standard						
QCS	Quality Control Standard						
Paired	Sample Tests						
	Duralianta	•					
DUP SER	Duplicate Serial Dilution						
Spike T	6312						
LFB	Laboratory Fortified Blank						
MXS	Matrix Spike						
PDS	Post Digestion Spike						
Internal Standard Test							
IST	Internal Standard Test						
•							

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 **T** 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 Para	Fest Parameters							
Enabled	Analyte	Limit	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)		
V	59Co (STD)	100	75	80	120	125		
1	115ln (STD)	100	75	80	120	125		
V	7Li (STD)	100	75	80	120	125		
V	140Ce (STD)	100	75	80	120	125		
1	209Bi (STD)	100	75	80	120	125		
V	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 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**.

4. Click to select the **Quality Control** view. On the left, the available **Quality Control Tests** are listed, see Figure 6-66.

Quality Con	trol Tests						
읨 New	🔀 Delete 🛛 👿 Edit detection limits						
Name	Description	*					
ICV	Initial Calibration Verification						
LCS	Laboratory Control Standard						
QCS	Quality Control Standard						
Paired	Sample Tests						
DUP	Duplicate						
SER	Serial Dilution						
Spike	Tests						
LFB	Laboratory Fortified Blank						
MXS	Matrix Spike	= 1					
PDS	Post Digestion Spike						
Internal Standard Test							
IST	Internal Standard Test	•					
•							

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 **T** 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 Para	Fest Parameters									
Enabled	Analyte	Qualifier	Low Failure Limit (%)	Low Warning Limit (%)	High Warning Limit (%)	High Failure Limit (%)				
V	59Co (STD)	100	75	80	120	125				
V	115ln (STD)	100	75	80	120	125				
V	7Li (STD)	100	75	80	120	125				
V	140Ce (STD)	100	75	80	120	125				
V	209Bi (STD)	100	75	80	120	125				
V	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 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**.

4. Click to select the **Quality Control** view. On the left, the available **Quality Control Tests** are listed, see Figure 6-68.

Quality Con	trol Tests				
🖀 New	🐹 Delete 🛛 👿 Edit detection limits				
Name	Description				
ICV	Initial Calibration Verification				
LCS	Laboratory Control Standard				
QCS	Quality Control Standard				
Paired Sample Tests					
DUP	Duplicate				
SER	Serial Dilution				
Spike	l ests				
LFB	Laboratory Fortified Blank				
MXS	Matrix Spike				
PDS	Post Digestion Spike				
Internal Standard Test					
IST	Internal Standard Test				
•					

Figure 6-68. Quality Control Internal Standard Test types

Click the Quality Control Test you wish to define.
 On the right, the corresponding Test details are shown, see Figure 6-69.

est details for IST			
👽 Internal Standard Test enable	ed		
Low Warning Limit (%)	80	Low Failure Limit (%)	75
High Warning Limit (%)	120	High Failure Limit (%)	125



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

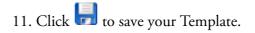
Test Parameters								
Enabled	Analyte	Warning Limit		Failure Limi				
	137Ba		Fil	l down	Ctrl+D			
	88Sr							
	90Zr	1		lup	Ctrl+U			
V	105Pd	2	In	crement fill	Ctrl+N			
	115In	42	Fit	Fit cells to grid				
		8	Fit	Fit cells to content				
		X	E>	Export to Excel				

A context menu opens, see Figure 6-70.



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.



* To create a new quality control test



- 1. Click Editor to open Experiment Editor.
- 2. Click the tab **Home Page**.
- 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 *i* 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 ^{1 New}

A dialog box opens, see Figure 6-71.

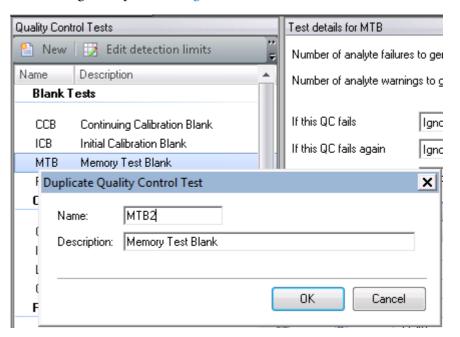


Figure 6-71. Duplicate Quality Control Test window

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 Editor to open Experiment Editor.
- 2. Click the tab **Home Page**.
- 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 **W** 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 Helete

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 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**.

4. Click **W** to select the **Quality Control** view.

5. Click		Edit detection limits
5. Click	82	Edit detection limits

A dialog opens, see Figure 6-72.

Contract	t Require	d Detect	ion Limits		—
🚯 Imp	ort 💋	Export			
Symbol	Concent	ration	Unit		
54Cr		0.000	ppm	-	
137Ba		0.000	ppm	A	
88Sr		0.000	ppb		
90Zr		0.000	ppt	≡	
105Pd		0.000			
115In		0.000	ng/l μg/l		
27AI		0.000	mg/l		
196Pt		0.000	g/l	-	
99Ru		0.000	ppm		
101Ru		0.000	ppm		
95Mo		0.000	ppm		
				Clos	e



- 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	Close	
J. CIICK		•

- 10. Click 📅 to save your Template. The detection limits are saved to the Template.
- ✤ To import an existing analyte list



- 1. Click 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 **W** to select the **Quality Control** view.
- 5. Click Edit detection limits

A dialog opens, see Figure 6-72.

Contract Required Detection Limits								
💕 Import 💋	Export							
Symbol	Concentration	Unit						
54Cr	0.000	ppm						
137Ba	0.000	ppm						
88Sr	0.000	ppm						
90Zr	0.000	ppm						
105Pd	0.000	ppm						
115In	0.000	ppm						
27AI	0.000	ppm						
196Pt	0.000	ppm						
99Ru	0.000	ppm						
101Ru	0.000	ppm						
95Mo	0.000	ppm						
		Close						

Figure 6-73. Contract Required Detection Limits window

6. Click to open the **Import detection limits** dialog, see Figure 6-74.

Import detection limits						8
🔾 🗢 📕 « _Application Da	ata 🕨 Workspace 🕨	- - i + j	Search Wor	kspace		٩
Organize 👻 New folder				-		0
Name	Date modified	Туре	Size			
퉬 LabBooks	21.02.2012 14:17	File folder				
퉬 Templates	23.02.2012 10:43	File folder				
File name:		•	CSV files (*.cs Open		Cancel	• •

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 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 **W** to select the **Quality Control** view.

5. Click Edit detection limits	
A dialog opens, see Figure 6	-75.

Contract Required	Detection Limits	
💕 Import 💕	Export	
Symbol	Concentration	Unit
54Cr	0.000	ppm
137Ba	0.000	ppm
88Sr	0.000	ppm
90Zr	0.000	ppm
105Pd	0.000	ppm
115In	0.000	ppm
27AI	0.000	ppm
196Pt	0.000	ppm
99Ru	0.000	ppm
101Ru	0.000	ppm
95Mo	0.000	ppm
		Close

Figure 6-75. Contract Required Detection Limits window

6. Click **Export** to open the **Export detection limits** dialog, see Figure 6-76.

Export detection limits					×
COO - Market Application D	ata 🕨 Workspace 🕨	+ ⁴ 9	Search Worksp	ace	٩
Organize 🔻 New folder					0
Name	Date modified	Туре	Size		
鷆 LabBooks <u>)</u> Templates	21.02.2012 14:17 23.02.2012 10:43	File folder File folder			
File name: Save as type: CSV files (*.	csv)				•
Hide Folders			Save	Cancel	

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



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

Sample	Defini	tion										
🛄 He	eader										+]
🧾 Bo	ody										=	J
1	r +Þ	Amount	-1	Final Quantity	-12	QC A	ction +=	, QC	Restart	-12	QC Reference 👎	3
9						None						
						None						
			_			None						
•						None						
						None						
•											۱.	
Fc	oter										Ξ	
P	∕ey R	uns 🕫 Main Runs	-12	Comment 🕂	San	nple Type 🗗	Standard 中	QC Action	⊣⊐ QCF	Restart H	□ QC Reference +	2
2		1		<comment></comment>	QC			Non	- 0			
									▲			
								CCB	=			
								CCV L				
								ICB				
								ICV				
								LCS				
								LFB	•		F	

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.

🛄 Fo	oter									=
₽	∕ey Runs +Þ	Main Runs 🕁	Comment 🕂	Sample Type 🕁	Standard 🕁	QC Act	tion +Þ	QC Restart	-12	QC Reference 中
2		1	<comment></comment>	QC	Tune A	CCV		0	•	
								previous QC sample		
•										•

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 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 open a Template with a Configuration including the Cetac ASX-520 autosampler.

		4.	Click 🐸 Cetac A	\SX-520	to open th	e autosampler view, s
			Figure 6-79.			
etac ASX-520						
Time settings		Rack settings		/	Autotune settings	
Wash Time [s]:	30	Rack-1 Type:	24-Vials (8x3)	•	Autotune rack:	Standard 💌
Uptake Time [s]:	30	Rack-2 Type:	Empty	•	Autotune vial:	1
		Rack-3 Type:	Empty	-	Rinse Settings	
		Rack-4 Type:	Empty	•	Rinse Rack:	Rinse Station 🔹
Schematic View					Rinse Vial:	0
IR 1 2	3 4	5 6	7 8 9	10		
		Cetac ASX-520•				
1 9 17 2 10 18 3 11 19 4 12 20 5 13 21 6 14 22						

Figure 6-79. Cetac ASX-520 settings

- 5. Enter the Wash Time [s].
- 6. Enter the Uptake Time [s].
- 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 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 open a Template with a Configuration including the Cetac ASX-260 autosampler.

4. Click Cetac ASX-260 to open the autosampler view, see Figure 6-79.

Cetac ASX-260		
Time settings		Schematic View
Wash Time [s]:	30	[R] (2) (4) (6) (8) (10)
Take up Time [s]:	30	1 3 5 7 9 Cetac ASX-260•
Rack settings		1 8 15
Rack-1 Type:	21-Vials (7x3)	
Rack-2 Type:	Empty -	2 9 16
Autotune settings		3 10 17
Autotune rack:	Standard 👻	4 11 18
Autotune vial:	1	5 12 19
Rinse Settings		6 13 20
Rinse Rack:	Rinse Station 🔹	
Rinse Vial:	0	7 14 21

Figure 6-80. Cetac ASX-260 settings

- 5. Enter the Wash Time [s].
- 6. Enter the Take Up Time [s].
- 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 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 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
4. CIICK	to open the autosampler view, see Figure 6-81

ESI SC-4S						
Analysis settings		End-of-Analysis settings	Rack settings		Autotune settings	
Uptake Time [s]:	30	Additional Wash Time [s]: 0	Rack-1 Type:	Empty 👻	Autotune Rack:	Standard 👻
Wash Time [s]:	30	Wash Complete: Next Labbook 🔹	Rack-2 Type:	Empty 👻	Autotune Vial:	1
Additional Flush [s]:	0		Rack-3 Type:	Empty -		
			Rack-4 Type:	Empty -		
Schematic View						
		ESI SC-4S				
		CF 30 101				

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.

End-of-Analysis settings						
Additional Wash Time [s]:						
Wash Complete:	Next Labbook 🛛 👻					
	Next Labbook					
	Continue Wash Move Home					

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.

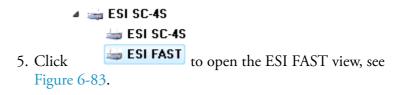
✤ To adjust the ESI FAST settings



- 1. Click 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 open a Template with a Configuration including the ESI autosampler.

4. Click 🚟 ESI SC-4S



File	Basic FAST -	10 Second Load		•	Rinse Settings	Valves / FAST Pump	Peristaltic Pumps
	Event	Action	Parameters	Parameter Units		📝 Max FAST Pump	o Time [s]: 300
×	On Probe Down	Peripump1 On	-60	Speed(rpm)	Valve 1	Valve 2	FAST Pump
	On Probe Down	Load1			Load	Load	Vacuum On
	Probe In Sample	Vacuum On			Inject	Inicot	Vacuum Off
	Probe In Sample	TimerA	10	seconds	Inject	Inject	
	Timer A Expires	Inject1			F .		
	Timer A Expires	Move Rinse			Events Probe in Sample		Actions Vacuum On
	Rinse Completed	Move Next			Rinse Completed		Vacuum Off
	On Rinse	Load1			Move Into Next C On Probe Down	ompleted	Peripump1 On Peripump1 Off
*					On Probe Up On Rinse		Peripump2 On Peripump2 Off
					On Rinse Type2		Load1
					Timer A Expires	E	Inject1
					Timer B Expires		Load2
					Timer C Expires		Inject2
					Timer D Expires		Move Rinse
					Timer E Expires		Move Next Probe Up
					Timer F Expires		Probe Up Probe Down
					Timer G Expires Timer H Expires		Move To(mnv)
					Timer I Expires	-	

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 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 open a Template with a Configuration including the SpectraSystem LC autosampler.

4. Click SpectraSYSTEM® LC Autosampler, see Figure 6-84.

Method Editor						
General		Timed Event Program				
Flush Volume [ul] Needle Height From Bottom [mm] Loop Size [ul] Shutdown Method Sample Viscosity Normal Medium High Injection Type Push Loop	100 0 100	Time [min]	TF1	TF2	TF3	TF4
 Pull Loop Full Loop 						
Tray Heater/Cooler Control						
On Temperature [°C] Column Oven Control	23					
On Temperature [°C]	23					

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 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 open a Template with a Configuration including the SpectraSystem LC pump.

4. Click	📗 SpectraSYSTEM® LC Pump	, see Figure 6-85.

Method Editor											
General		Composition and Flo	w Data					Extern	al Event Program	ı	
Pressure Minimum (Bar)	0	Time [min]	Flow Rate [ml/min]	A [%]	B [%]	C [%]	D [%]		Time [min]	State	
Pressure Maximum (Bar)	17	• 0	0.01	100	0	0	0	•	0		
Equilibration Time (min)	0	*						*			
📃 Shutdown Method											
Solvent Names											
Solvent A								Gradie			
Solvent B											
Solvent C								Profi		Linear	•
Solvent D								Delay	Volume (ml)	0	
Composition and Flow Diagra	am										
120 Flow	Rate [ml/min]	- A [%]	— В [%]	1 .	— c	[%]		– D [%]		0.0	105
Z ¹⁰⁰										0.0	¹⁰³ Ξ
9 80 1										₹ 0.0	101 🛓
10 f					+++++++++++++++++++++++++++++++++++++++		+++++++++++++++++++++++++++++++++++++++			₹ 0.0	103 [u] 101 101 199 [m] 197 1
Bercentage 80 Percentage 40 Percentage 7 20 Percentage										특 특 0.0	197 년
						+ +				[‡] 0.0	095
0.0	0.2	0.4).6 • [min]		0.8		1.0		1.2	

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.
- 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.
- 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 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 open a Template with a Configuration including the Accela LC autosampler.

Templates Peripherals

	4. Click	Accela LC Autosampler, see F	Figure 6-86.
Method Editor			
General		Injection Mode	
Needle Height from Bottom (mm)	2	💿 Partial Loop	
Syringe Speed (µl/sec)	10	Full Loop	
Flush Speed (µl/sec)	2	🔘 No Waste	
Flush Volume (μl)	3000	Loop Loading Speed (µl/sec)	10
Wash Volume (µl)	2000	Tray Heater/Cooler Control	
Flush/Wash Source	Bottle 🔹	🔲 On	
Inject Valve Throw Time (min)	0	Temperature (C)	25
Loop Size (μl)	10	Column Oven Control	
Syringe Size (μl) 🥅 Shutdown	250	🔲 On	
		Temperature (C)	25
Timed Event Program		Bottle/Reservoir Content	
	TF2 TF3 TF4	Reservoir 1	
		Reservoir 2	
本		Reservoir 3	
		Reservoir 4	
		Bottle	

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** $[\mu l]$ (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 **I** to add a row to the **Time Event Program** table.
- 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 Editor to open Experiment Editor.
- 2. Click the tab **Home Page**.
- 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.

6-113

Templates Peripherals

ieneral		Solvent Nam	ies	Gradient Progra
Operating Mode	High Pressure Mode	▼ Name A	Solvent A	Time [m
Start Settings	Manual	▼ Name B	Solvent B	▶ 0
Method Finalizing	Stop at end	👻 Name C	Solvent C	2
Minimum Pressure (psi)	0	Name D	Solvent D	*
Maximum Pressure [psi]	14500			
Pressure Stability [psi]	145			
Stabilization Time Limit [min]	30			
📝 Home Before Run				
iradient Graph				
120 Flow R	ate (µl/min) — 🗕 🗕 A (%)		- B[%]	
120 Flow R	ate (µl/min) ————————————————————————————————————	- -	- B[%]	-⊕ C[%]
100				

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.

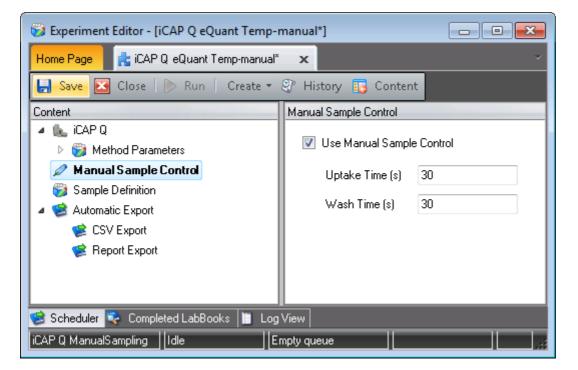


Figure 6-88. Manual Sample Control view in Template

* To define Uptake and Wash Time for manual sampling



- 1. Click 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 open a Template with a Configuration including Manual Sample Control and no other peripheral.

- 4. Click *A* 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.

7	ader Label	-12	Duration [s]	-12	Comme	ant	🗢 Sample	Tupe	-Þ	Standard	-	Dilu
	<ldentifier></ldentifier>	-	3		<comment< td=""><td></td><td></td><td>Type</td><td>1</td><td>Stanuaru</td><td>-</td><td>1</td></comment<>			Type	1	Stanuaru	-	1
▶	<rueriuner></rueriuner>		3		Comment	· ·	UNKNUWN					1
_												
۰ 📃												
Boo	Hu											
000	-,											l l
	-y Interval -¤	L	abel -Þ	Dur	ration [s] -	Þ	Sample Type	-12		Standard -	Þ Diluti	on Fa
		L. Blank	abel 🗗	Dur 3	ration [s] -	⊨ BLK		-Þ		Standard ⊰	⊨ Diluti 1	ſ
7	Interval 🕂		abel +¤		ration [s] -			÷	STD1	Standard ⊰		ſ
7	Interval +⊐ 1	Blank	abel +¤	3	ration [s] -	BLK	l	-		Standard +	1	ſ
7	Interval -⊐ 1 1	Blank STD	abel +Þ	3 3	ration [s] -	BLK STD	 	-12	STD1	Standard ⊀	1 1	on Fa
7	Interval +¤ 1 1 1	Blank STD STD		3 3 3	ration [s] -	BLK STD STD STD	 	- P	STD1 STD1	Standard +	1 1 1	ſ

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.

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 <i>0</i> to <i>100</i> . By default, the number is set to <i>0</i> .
	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 <i>1</i> to <i>1,000,000</i> . By default, the number is set to <i>1</i> .
	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, -		
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	umber/Tray/BlockRack/Tray/Block number of peripheral.	
Vial Number/Vial	Vial number of peripheral.	

 Table 6-18.
 Columns of Sample Definition

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.

Sa	Samplelist							
	2	Label ⊽ ₽	ate ⊽+Þ	Sample Type 🔽 Þ	Standard ⊽+Þ	Dilution Factor 🖓 🕁	Special Blank	Υ+¤
1	•	Blank	V	UNKNOWN		1		-
2		STD	V	STD	STD1	1		
3		STD	V	STD	STD1	1	1: Blank	
4		STD	V	STD	STD1	1	2: STD	
5		STD	V	STD	STD1	1	3: STD 4: STD	=
6		Sample	V	UNKNOWN		1	4: STD 5: STD	
7		water	V	UNKNOWN		1	6: Sample	
8		Blank	V	UNKNOWN		1	7: water	-
9		water	V	UNKNOWN		1		
•	١					•		

Figure 6-90. Sample List view with Special Blank

* To open the Sample Definition view of a Template



- 1. Click 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 **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 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 **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.

Choose Columns	—
Available columns	Show these columns in this order
Name	Name
	Interval
	Label
	Survey Runs
	Main Runs
	Comment
	Sample Type
	Internal Standard
	Standard
	Dilution Factor
	Amount
	Final Quantity
	QC Action
	QC Restart
	QC Reference
	4 ·
	OK Cancel

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.



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 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 **Sample Definition** to open the Sample Definition view of the Template.
- 5. In the Toolbar of the Template, click drop-down menu, see Figure 6-92.





- 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 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.

	ample Definition +						
Bo	dy						Ξ
2	Interval 🕁	Label 🕁	Duration [s] 🗇	Sample Type 🕩	Standard 🕁	Dilution Factor 中	Amount 🕂 🛓
3	1	Blank	3	BLK 🛃		1	
	1	STD	3	UNKNOWN	STD1	1	
	1	STD	3	STD	STD1	1	=
	1	STD	3	BLK	STD1	1	
	1	Sample	3	AVERAGE BLK		1	
	1	water	3	ZERO STD UPDATE CALIB		1	
	1	ni				1	· · · · ·
Footer +							

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.

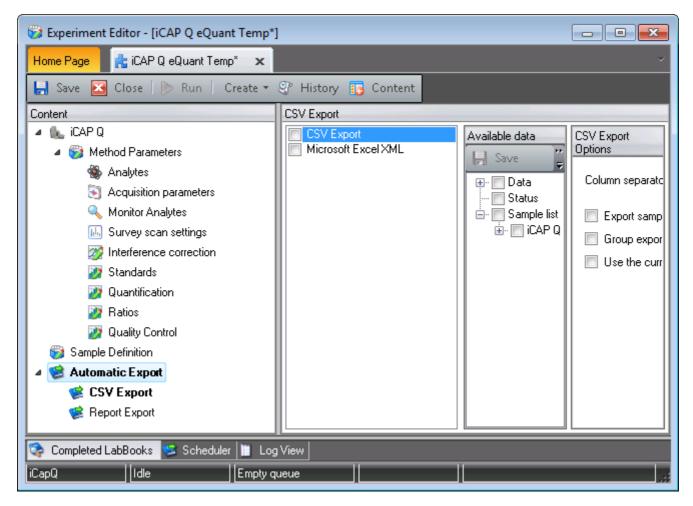


Figure 6-94. Template Automatic Export settings

Upon completion of the LabBook, the data are automatically exported as defined.

* To define automatic export settings



- 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.

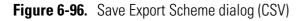
Available data		CSV Export Options
Available data Schemes iCAP Q scheme	▼ ¥ Image: Save as X Image: Save as X Image: Delete X	CSV Export Options Column separator: Semicolon Export sample lines as rows. Group exported blocks. Use the current locale to format numbers.

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.
- 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.

🗟 Save Export S	Scheme	×
Name: Description:	iCAP Q scheme (csv) CSV export	
	Save	el



12. Enter a **Name** and **Description**.



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.

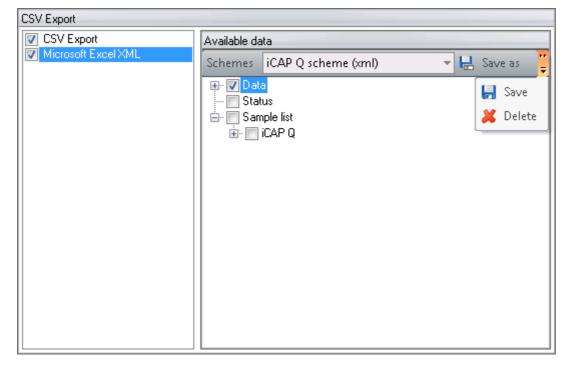
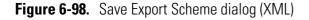


Figure 6-97. Automatic Export, XML settings

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.

🖶 Save Export Se	cheme 🔀
Name:	iCAP Q scheme (xml)
Description:	XML export
	Save Cancel



17. Enter a **Name** and **Description**.



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 Save to save the settings to the Template (or LabBook).
- * To define report export settings



- 1. Click 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 **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.

Report Export						
🚜 Add 📰 Delete						
Ena	abled	Name 🛆	Format			
[1	Calibration report	Portable Document Format (PDF)			
•	1	Chromatogram and compo 🛛 🔫	Portable Document Format (PDF)			
[1	Graph & table report	Portable Document Format (PDF)			
[1	Peak report	Portable Document Format (PDF)			

Figure 6-99. Automatic Export, Report Export active

- 6. Click Add to add a row.
- 7. In the column **Name**, click **I** to open the drop-down menu, see Figure 6-100.

Calibration report				
Chromatogram and compounds report				
Chromatogram and peaks report				
Chromatogram report				
Experiment report				
Graph & table report				
Graph report				
Peak report				
, earlieber.				



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.

Portable Document Format (PDF)					
Rich Text Format (RTF)					
HTML					
Microsoft Excel Worksheet (XLS)					
Tagged Image Format (TIF)					
Plain text					
ActiveReport binary format (RDF)					
The complete XML database					

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 Save 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

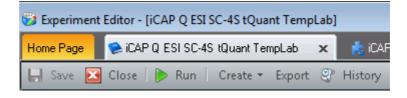


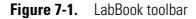
- 1. Click Editor to open Experiment Editor.
- 2. Click the tab Home Page.
- 3. Open a LabBook as described in "Opening a LabBook" on page 5-14.

LabBooks LabBook Toolbar

LabBook Toolbar

In the LabBook tab of Experiment Editor, Qtegra offers buttons to save, close, run or export a LabBook, see Figure 7-1.





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 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. Change the settings as appropriate.
- 5. Click 📅 to save the LabBook.
- ✤ To close a LabBook



- 1. Click 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 in the toolbar to close the LabBook.

You can also click in the tab of the LabBook.

To run a LabBook *



- 1. Click 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 *loc* 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 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 Create.

The Create drop-down menu opens, see Figure 7-2.

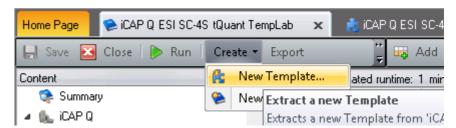


Figure 7-2. Create button in LabBook toolbar

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 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. In the toolbar of the LabBook, click The **Export data** dialog opens, see Figure 7-3.

😥 Export data	
Exporter: Microsoft Excel XML	
Available data	Excel Export Options
Schemes ICAP Q scheme	
🖃 📝 Data 🔛 🔛 Sa 🗄 🐨 🔽 Main Runs	ave Please select a path
Survey Runs	ave as Filename
C Status	
🖻 🖳 Sample list	Open file in Excel after export
i⊡ · □ iCAP Q ⊕ · □ ESI_SC4S	
	Export Cancel

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.

🚽 Save Export S	Scheme	×
Name:	iCAP Q myscheme	
Description:	Enter an optional description	
		Save Cancel

Figure 7-4. Export scheme of LabBook

7. Enter a **Name** and a **Description**.



- 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.



* To view the history of a LabBook



- 1. Click 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 History dialog for this LabBook opens, see Figure 7-5.

History for eQuant.imexp						
Available histo	Available history entries					
Date	User	Co		A		
1/19/2012	MP1	M				
1/19/2012	MP1	М				
1/18/2012	MP1	М				
1/18/2012	MP1	М		T		
Comment:						
E			Company	Close		
Export Auditt	rall		Compare	Ciose		

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 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 History dialog for this LabBook opens, see Figure 7-6.

History f	History for eQuant.imexp					
Availabl	Available history entries					
Date	ι	Jser	Со			-
1/19/2	2012 N	4P1	М			
	2012 N					
	2012 N					
1/18/2	2012 N	4P1	М			-
Commer	it:					
			ſ	C		
Export	t Audittrail			Compare	Clos	se

Figure 7-6. History dialog for LabBooks

5. Press **<Ctrl>** and select the entries you wish to compare.

6. Click to compare the selected entries. The **Comparison** dialog opens, see Figure 7-7.

Comparison		- • ×
Name	Version	Version 🔺
ScanMode	Electric	Electric
Spacing (u)	0.1	0.1 🔳
Tune settings	(null)	(null)
Analytes[1]		
Channels	1	1
Color	.255.86.22.1	.255.86.22.1
Dwell time (s)	0.01	0.01
Enabled	True	True
Identifier	133Cs	133Cs
Measurement mode	STD	STD
Resolution	Normal	Normal
ScanMode	Electric	Electric
Spacing (u)	0.1	0.1
Tune settings	(null)	(null)
Analytes[2]		
Channels	1	1
Color	. 255.76.165	. 255. 76. 165
Dwell time (s)	0.01	0.01
Enabled	True	True
Identifier	181Ta	181Ta 🚽
Show differences only		Close



- 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 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 History dialog for this LabBook opens, see Figure 7-8.

History for eQuant.imexp				
Available history entries				
Date	User	Со		<u>^</u>
1/19/2012	MP1	M		
1/19/2012				
1/18/2012				
1/18/2012	MP1	М		v
Comment:				
Export Audittr	ail		Compare	Close
			compare	

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.

Export Audittrail		
-A_ * _A	pplication Data 🔸 Workspace 🕨 👻 🍫 Search Workspace 🔎	•
File name:]
Save as type:	Html files {*.html)	
💌 Browse Folders	Save Cancel	#

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 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.

Home Page 🛛 😪 iCAP Q eQuant Lab 🛛 🗙							
🔚 Save 🔀 Close 🕪 Run 🛛 Create 🕶	Export	🔮 History 📘	Content				
Content	Acqui	sition Parameters, ru	intime estima				
📚 Summary		Identifier	Dwell time				
👞 iCAP Q	+	43Ca	0.01				
🌍 Method Parameters		46Ca	0.01				
🍓 Analytes		48Ca	0.01				

Figure 7-10. Content pane of LabBook visible

4. Click Content

The **Content** pane is hidden, see Figure 7-11.

Home Page 🛛 😪 iCAP Q eQuant Lab 🛛 🗙							
🔚 Save 🔀 Close 🍺 Run Create 🕶 Export 🍣 History 📻 Content							
Acquisition Parameters, ru	ntime estimation 5	500 millisecor	ids				
Identifier	Dwell time (s)	Channels	Spacing (u)	Measurement			
▶ 43Ca	0.01	1	0.1	STD			

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.

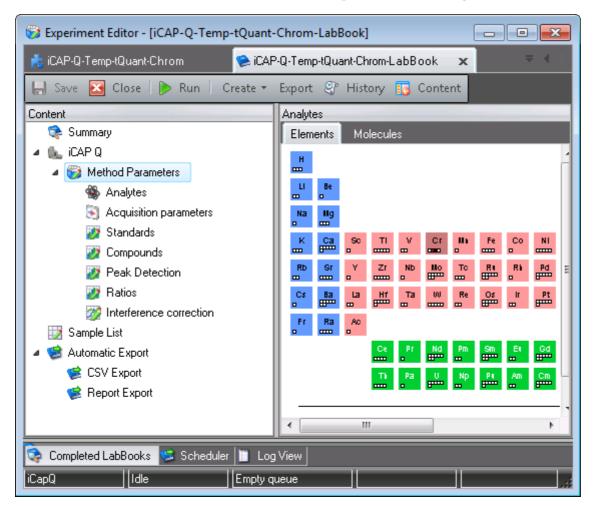


Figure 7-12. LabBook Method Parameters

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.

mary		
Filename: 3eQuant-Lab-	from-blank-Temp4.imexp	
Properties		4
Size	856 KB	
Configuration	iCapQ (Description)	
Instruments	iCAP Q	
Evaluations	eQuant	
Based on template		
Number of samples	9	
Number of results		=
Estimated sample run time	400 milliseconds	
Estimated labbook run time	6 minutes 30 seconds	
Dates		
Created	2/20/2012 11:06:07 AM	
Last modified	2/20/2012 11:06:09 AM	
Started at		
Finished at		
People		
· · · · · · · · · · · · · · · · · · ·	т. ч.	1

Figure 7-13. Summary of LabBook

* To show the summary of a LabBook



- 1. Click 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 Summary 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.

Home Page 🛛 👘 iCAP Q tQuant 🔤 🤇	≥ iCAF	PQt	Quan	Lab 🗙					
📄 Save 🔀 Close 📄 🔈 Run	₩ ╤	a A	dd ୟ	Delete			🔓 Copy 🖞	B Paste	
Content		Sam	plelist	estimated rur	ntime: 10	minutes 26 sec	onds		
🍖 Summary		đ	ž	Label 꼬꾸	St⊽≠	Duration [🖓 🕁	Sample T ⊽+Þ	Standard V	
🔺 👞 icap q		1		blank	Θ	3	BLK		Γ
4 🤯 Method Parameters		2		STD1	0	3	STD	STD1	
🍓 Analytes		3		sample1	0	3	UNKNOWN		
🛐 Acquisition parameters		4	•	sample2	0	3	UNKNOWN		
🐉 Standards	- 11	5		sample3	0	3	UNKNOWN		
🐉 Compounds	- 11	6		blank	0	3	BLK		
👔 Peak Detection	- 11	7		blank	0	3	BLK		
📝 Ratios	- 11	8		STD1	0	3	STD	STD1	
Interference correction	- 11	9		sample1	0	3	UNKNOWN		
🔯 Sample List		10		sample2	0	3	UNKNOWN		
a 🧐 Automatic Export	- 11	11		sample3	0	3	UNKNOWN		
😒 CSV Export	- 11	12		blank	0	3	BLK		
😢 Report Export	- 11	13		blank	0	3	BLK		
	- 11	14		STD1		3	STD	STD1	
	- 11	15		sample1	0	3		5101	
				eample I I		*		×.	
Completed LabBooks 🧏 Scheduler 📗						_			

Figure 7-14. Sample list of LabBook

✤ To view the Sample List



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 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 to add a row below the Sample List.
- * To delete a row to the Sample List



- 1. Click 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 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 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 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.
- Comments 5. Click to show the comment for the selected row. The list of comments opens below the sample list.
- 🎍 Add Comment to add a comment for the selected row. 6. Click The User Comment window opens, see Figure 7-15.

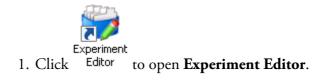
User Comment	×
Enter a comment for sample line 3:	
I	*
	Ψ
	OK Cancel



- 7. Enter your comment.
- 0K 8. Click

The comment is added and the User comment window closes.

To hide comments of the Sample List *



- 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 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.

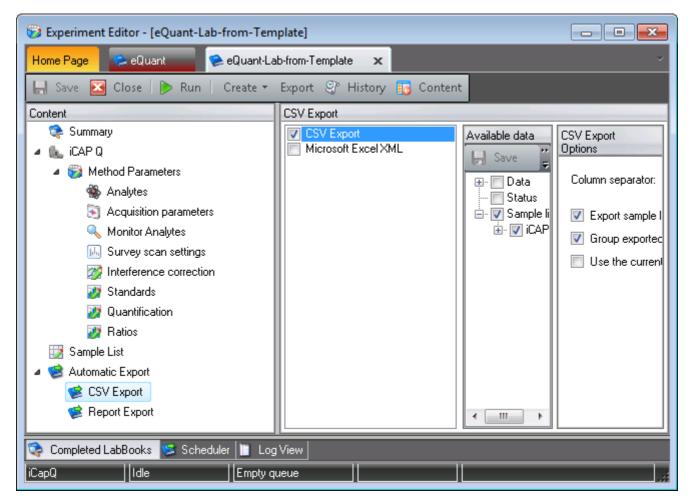


Figure 7-16. LabBook Automatic Export settings

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



✤ To run a LabBook



- 1. Click 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 **v** to schedule the LabBook for execution.

The LabBook is added to the Scheduler and the measurement is started, see Figure 7-17.

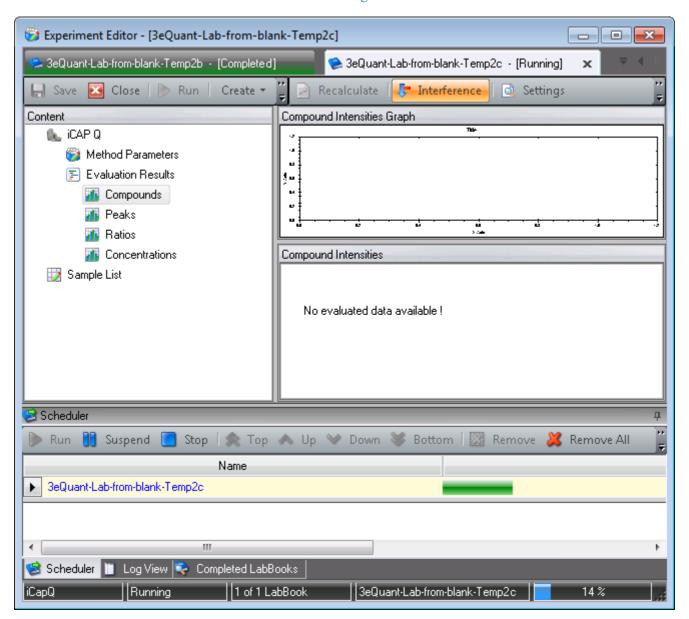


Figure 7-17. Measurement started for scheduled LabBook

The completed LabBook is automatically deleted from the Scheduler and added to **Completed LabBooks**.

5. Click 📚 Completed LabBooks

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



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.

📸 Experiment Editor - [eQuant-Lab-from-blank-Temp2]								
🙁 iCAP Q aQuant Temp2Lab 🦷 🤘	≽ eQuant-Lab-	from-bla	nk-Temp2	×		\equiv 4 \triangleright		
🔚 Save 🔀 Close 📄 Run 🗍 Ci	reate 🔹 📮	📄 Re	calculate		Interference 🛃 Bla	nks-		
Content	Cor	centrati	ons					
📚 Summary		1	No		Time	Sample Type		
🔺 👠 iCAP Q				1	2/17/2012 8:01:49 AM	UNKNOWN		
Method Parameters				2	2/17/2012 8:01:49 AM	STD		
▷ 🕞 Evaluation Results				-	2/17/2012 8:01:53 AM	UNKNOWN		
Instrument State					2/17/2012 8:01:54 AM	UNKNOWN		
 Reports 					2/17/2012 8:01:55 AM	UNKNOWN		
Sample List	i i i			9	2/17/2012 8:01:56 AM	UNKNOWN		
Log Messages								
Signing								
🕨 📃 Query								
						• •		
😪 Completed LabBooks						р		
Name					Path	*		
Q eQuant-Lab-from-blank-Temp2								
📀 tQuant-Lab-from iCAP tQuant Temp						-		
٠ III						E.		
😪 Completed LabBooks 😒 Scheduler	📋 Log View							
iCapQ Idle	Empty queue							

Figure 7-18. Completed LabBook

4. Click **iCAP Q** to show the items added to the LabBook after measurement, see Figure 7-19.

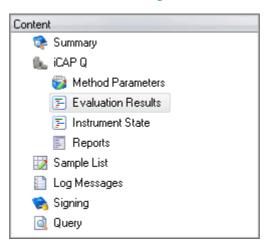


Figure 7-19. Added items of a completed LabBook

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 Editor to open Experiment Editor.
- 2. Click 🗟 Completed LabBooks
- 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 Figure 7-20. to open the **Evaluation Results** view,
- ICAP Q
 ICAP Q



A number of functions that differ according to the evaluation method are available in the toolbar of this view, see Figure 7-21.

🖞 🖻 Recalculate 🛛 🥐 Interference 🖉 Blanks 🖉 Standards 💡								
entrat	tions			Export 💱 History				
P	No	Time	Sample	To Content				
	1	2/17/2012 8:01:49 AM	UNKNOWN					
	2	2/17/2012 8:01:49 AM	STD	😑 Details				
	6	2/17/2012 8:01:53 AM	UNKNOWN	🔒 Hide Thumbnails				
	7	2/17/2012 8:01:54 AM	UNKNOWN	D Suttings				
	8	2/17/2012 8:01:55 AM	UNKNOWN	💁 Settings				
	9	2/17/2012 8:01:56 AM	UNKNOWN	🎛 Column Filter 🝷				

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



- 2. Click 🗣 Completed LabBooks
- In the Completed LabBooks list, click the LabBook you wish to view the result of. The completed LabBook is opened in a new tab.

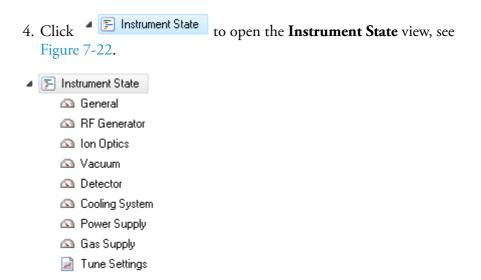


Figure 7-22. Instrument State submenus in completed LabBook

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 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 **Peports** 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 Editor to open Experiment Editor.
- 2. Click the tab **Home Page**.
- 3. Click 📚 Completed LabBooks
- 4. In the **Completed LabBooks** tab, click the LabBook you wish to view.
- 5. Click Log Messages to view the Log Messages of the completed LabBook, see Figure 7-23.

Log N	lessages			_				_
	Logged at 🛛 🖓	Level 🗸	Message	V	Time 🗸	Category 🗸	Sub Category 🗸	
	Line no. 1: BLK	i)	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	i	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	i	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

- 2. Click the tab Home Page.
- 3. Click 🗣 Completed LabBooks
- 4. In the **Completed LabBooks** tab, click the LabBook you wish to view.
- 5. Click Log Messages 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 Editor to open Experiment Editor.
- 2. Click the tab Home Page.
- 3. Click 🗣 Completed LabBooks
- 4. In the **Completed LabBooks** tab, click the LabBook you wish to view.
- 5. Click Log Messages 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.



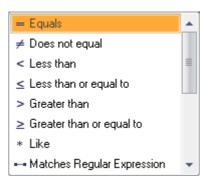


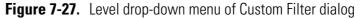
7. Select (**Custom**) from the drop-down menu. The **Custom Filter** dialog opens, see Figure 7-26.

V Custom Filter			
Filter based on	All	•	of the following conditions:
Add	Time		
			OK Cancel



- 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.





- 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.





12. Select an argument from the drop-down menu.



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



- 2. Click 🗟 Completed LabBooks
- 3. In the **Completed LabBooks** tab, click the LabBook you wish to view.

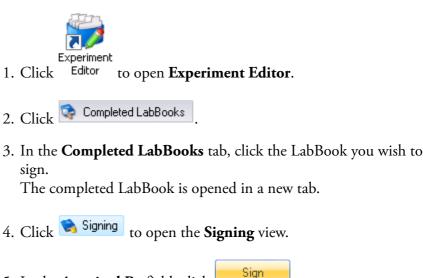
The completed LabBook is opened in a new tab.

4. Click Signing to open the **Signing** view, see Figure 7-29.

ning		
Acquired By:		
Domain	Certificate	
Domain User	Serial No.	
	valid from	
	valid thru	
Sign with different user		Sign
Verified By:		
Domain	Certificate	
Domain User	Serial No.	
	valid from	
	valid thru	

Figure 7-29. Signing in completed LabBook

To sign the LabBook



elect certificate for signature								
Available certificates								
FriendlyName	Owner	HasPrivateKey	Issuer	NotAfter	SerialNumber			
	Ірааре		Ipaape	01/06/2112	78B38034AB4F7D994C7			
					Select Cancel			
					44 444			

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 MicrosoftTM ExcelTM.

NOTICE See also "Results Page" on page 5-30. ▲

* To open the Query view



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 \triangleright Query to open the Query view, see Figure 7-31.

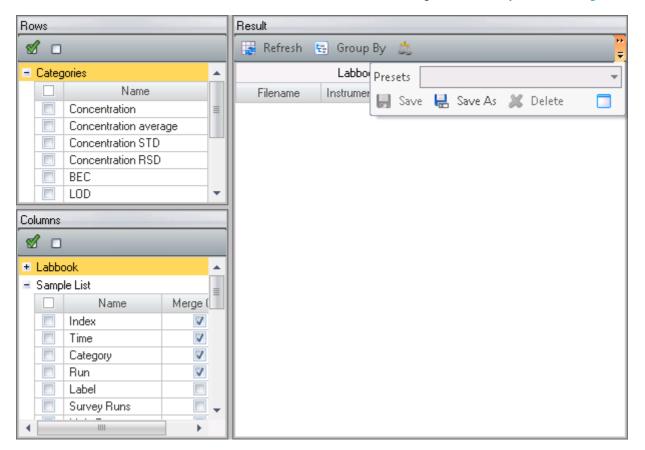


Figure 7-31. Query view in completed LabBook

✤ To place a Query



- 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 \triangleright **Query** 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.

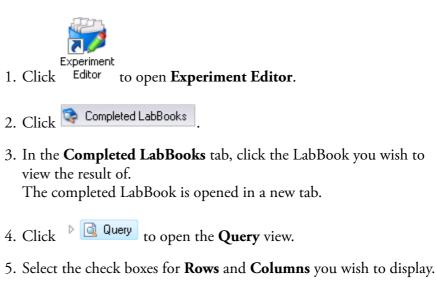
6. In the field **Columns**, select the check boxes for **Labbook**, **Sample** List, and Results you wish to display.

Click *to* select all check boxes.

- Rows Result 🛃 Refresh 🛛 Presets 🐒 🗆 Labbook -12 \checkmark Name * Concentration RSD V Main Runs Index lation Filename V BEC eQuant-Lab-from-blank-Temp 1 2/14/20 1 . 1 LOD 1 V Intensity 1 Intensity average V 1 \checkmark Intensity STD 1 Intensity RSD 1 ÷ 1 Columns 1 1 1 2 2/14/20 1 Labbook . 1 \checkmark Name Merge Cells = 1 \checkmark Filename J 1 V Instrument V 1 1 V Evaluation Template 1 1 Sample List 1 \checkmark Name Merge Cells 1 V Index 1 4
- 7. In the field **Result**, click 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



6. In the field **Result**, click result to display the selected result values.

7. In the **Result** table, right-click to open the context menu, see Figure 7-33.

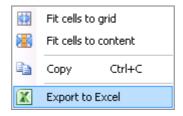


Figure 7-33. Query results context menu

8. Select **Export to Excel** from the context menu. The **Save As** window opens, see Figure 7-34.

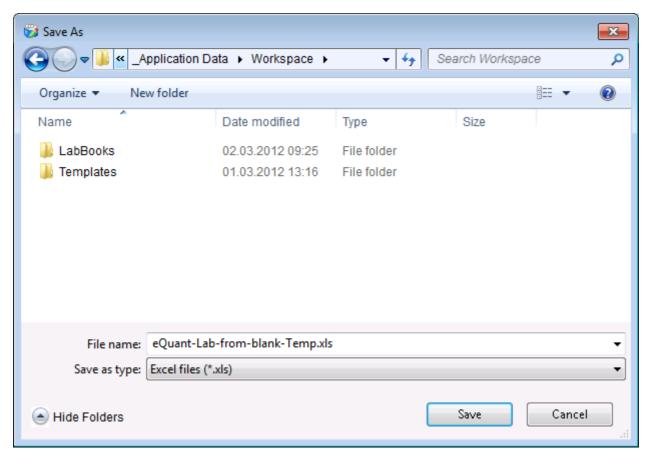


Figure 7-34. Export results window

9. Select a directory and enter a File Name.



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 Editor 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.

Acqui	sition Parameters	, runtime estim	ation 900 r	nilliseconds		
	Identifier	Dwell time (s)	Channels	Spacing (u)	Measurement mode	Resolution
•	232U (STD)	0.01	1	0.1	STD 💌	Normal
	233U (STD)	0.01	1	0.1	CCT	Normal
	234U (STD)	0.01	1	0.1	CCTS	Normal
	235U (STD)	0.01	1	0.1	KED	Normal
	236U (STD)	0.01	1	0.1	KEDS STD	Normal
	238U (STD)	0.01	1	0.1	STDS	Normal
	208Pb (STD)	0.01	1	0.1	ราย	Normal
	23Na (STD)	0.01	1	0.1	STD	Normal
	39K (STD)	0.01	1	0.1	STD	Normal

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 we 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 **W** 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 **i** 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



- 2. Click the tab **Home Page**.
- 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, ESI SC-4S 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 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 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.
- 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.
- 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 Editor 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.

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E	luation	eQuant						

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 **Save** 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 Editor 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 \blacksquare . 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.

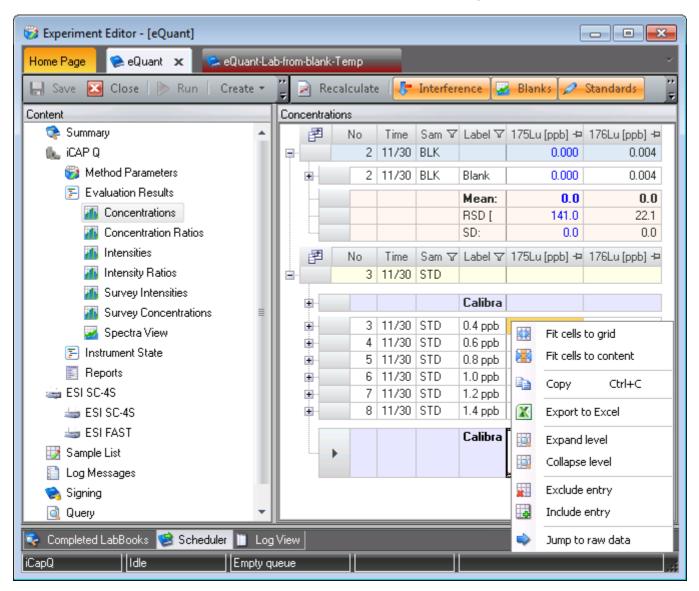


Figure 8-3. Evaluation results Concentrations with context menu

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.

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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 Aximize 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

Add Comment button in the lower right corner of the

Concentrations view.

The toolbar of the Concentrations view includes options to perform a

recalculation with Recalculate, to switch on/off the mathematical interference correction Interference and to switch on/off the use of internal standards Standards. By clicking Blanks 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.

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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.

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👞 iCAP Q	2 1,324,840 38,380	
🜍 Method Parameters	3 1,339,919 38,177	
🗐 Evaluation Results	4 1,341,075 38,227	
The Concentrations	5 1,349,672 38,071	
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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.

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	•					3		82,593	131,1	176	358,	376
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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.

 Table 8-1.
 Intensities calculation strategies

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.

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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.

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📰 Evaluation Results	+			11/30/20		100	542,067	
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Figure 8-9. Evaluation results Survey Intensities

The display is comparable to that of the Intensities view.

Analysis with eQuant Evaluation Results and Data Evaluation

Survey Concentrations

The Evaluation Results **Survey Concentrations** view of the LabBook in Experiment Editor is shown in Figure 8-10.

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Evaluation Results				11/30/2		N/A	
Concentrations			6	11/30/2		N/A	
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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.

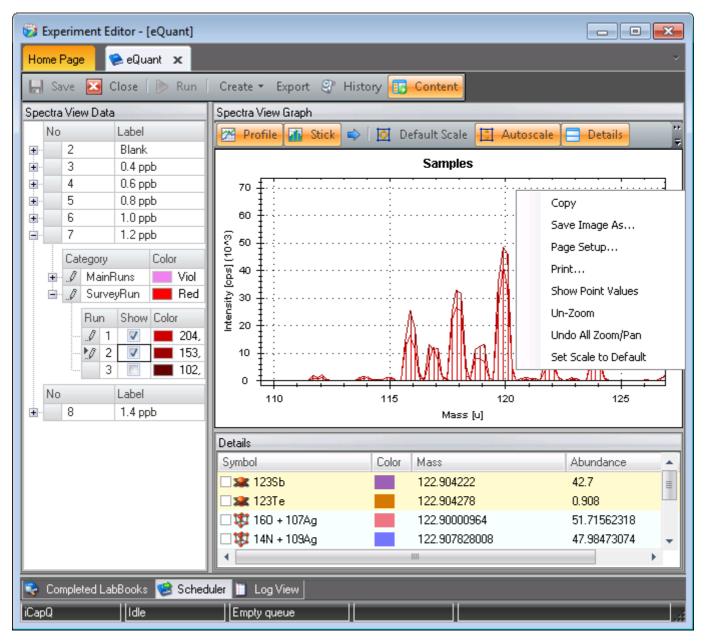


Figure 8-11. Evaluation results Spectra View with context menu

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



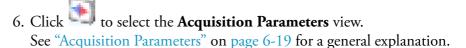
- Editor to open Experiment Editor. 1. Click
- 2. Click the tab **Home Page**.
- 3. Create a Template as described in "Creating a Template" on page 5-24.

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.



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.

Acquis	sition Paramete	rs				
	Identifier	Dwell time (s)	Channels	Spacing (u)	Measurement mode	Resolution
•	14C (CCT)	0.02	1	0.1	сст 💌	Normal
	34S (CCT)	0.02	1	0.1	CCT	Normal
	36S (CCT)	0.02	1	0.1	CCTS	Normal
	14N (CCT)	0.02	1	0.1	KED	Normal
	15N (CCT)	0.02	1	0.1	KEDS STD	Normal
	12C (CCT)	0.02	1	0.1	STDS	Normal
	32S (CCT)	0.02	1	0.1		Normal

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.

External Input Trigger		Level Trigger		Edge Trigger
•	Digital IN 1	None	•	None
	Digital IN 2	None		None
		Low High		



- 12. Click **is** 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 *W* to select the **Compounds** view.

16. Click Add Compound 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 **W** 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 *is* 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 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 the Configuration for your system with iCAP Q, the Evaluation tQuant, and, for example, the LC autosampler and LC pump.

- 4. Click, for example, Accela LC Autosampler to open the LC autosampler view.
- 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 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 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.
- Enter the correct value for column **Duration**. The duration for the measurement should be as long as for the LC method.
- 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 Editor 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.

nalysi			
	ate LabB e a new LabB	UUK look based on an existing Template or LabBook	
Name	tQuant-La	o-from iCAP Spectra Chromatography	
Location	LabBooks		
C		Deals from the station of the second	
	te a new Labi mplate Name	Book from an existing Template	
			•
Sar	mples	100 Import from CSV	
CS/	√ name		*
Maj	pping Name		-
🔘 Crea	te a new Labl	Book from an existing LabBook	
Lab	Book Name	rQuant	*
🔘 Crea	te a new Labi	Book from a blank Template	
Eva	aluation	eQuant	
L *C	2002001	oguain	
			Create LabBook



Creating LabBook for Analysis with tQuant Evaluation

- 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.
- 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.

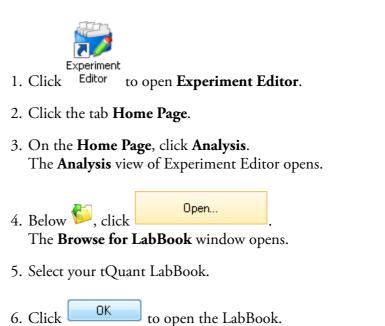
8. Click Create LabBook to create the new LabBook. A new tab opens for the new LabBook.

- 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 **Save** 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



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.

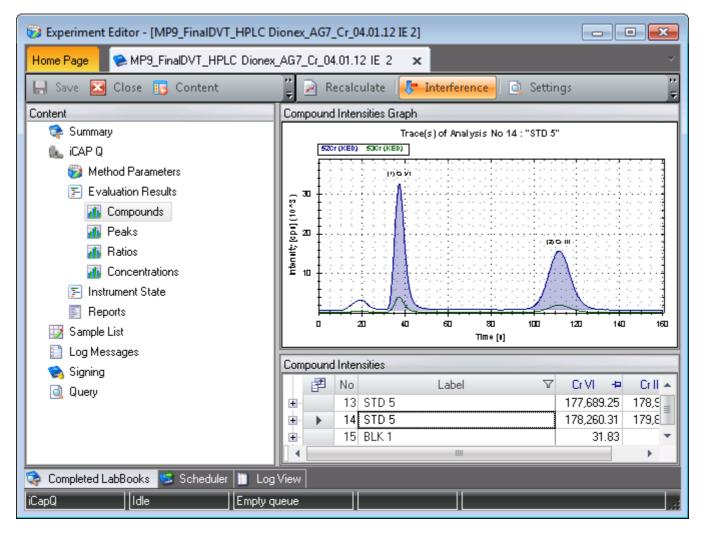


Figure 9-4. Result chromatogram

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.

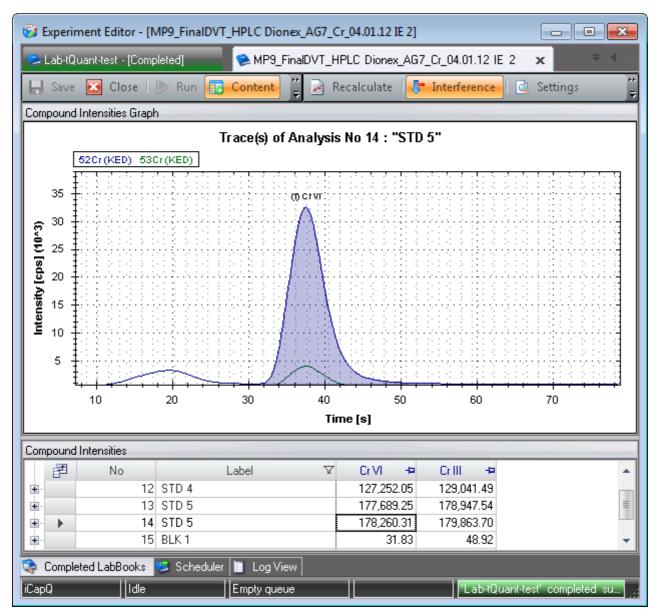


Figure 9-5. Result chromatogram of selected peak

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.

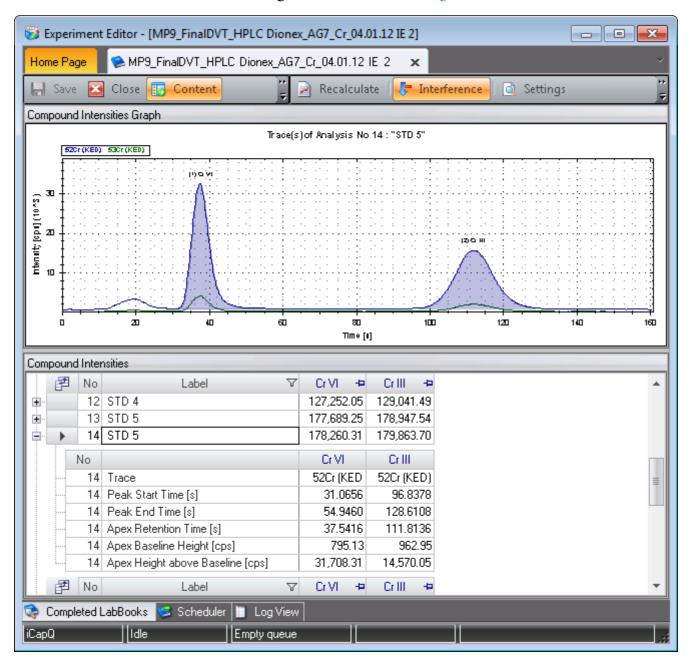
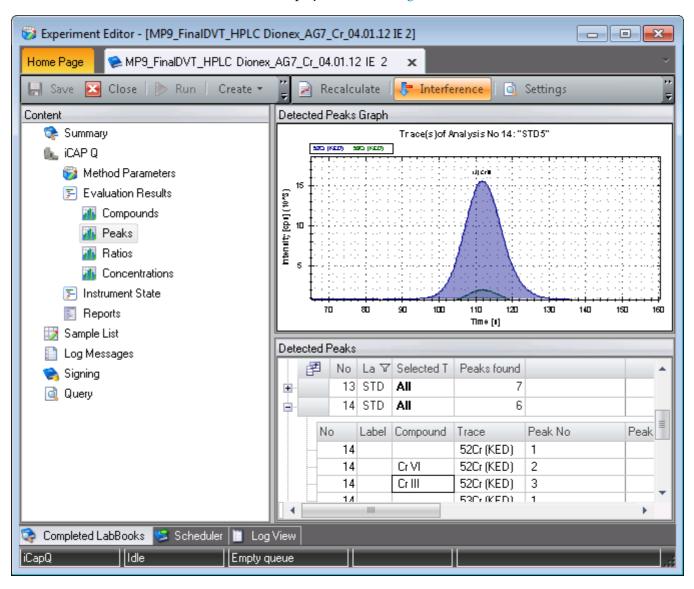


Figure 9-6. Result chromatogram and underlying information

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 Results and Data Evaluation



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.

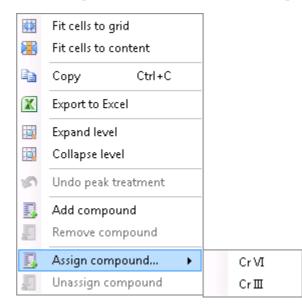


Figure 9-8. Peaks table context menu

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.

		Experiment Editor - [MP9_FinalDVT_HPLC Dionex_AG7_Cr_04.01.12 IE 2*]								
Home Page See MP9_FinalDVT_HPLC Dionex_AG7_Cr_04.01.12 IE 2* ×										
🔚 Save 🔀 Close 🗼 Run 🔞 Content 🛛 🦉 🎅 Recalculate 🔚 Interference 🗔 Settings 👘 🦉										
Content		Peak Ar	ea F	Patios			_			
📚 Summary	*	1 15	١o	Date / Time	Label V	Cr VI / Cr III +				
👞 icap q			4	1/4/2012 10:50:22 AM	BLK 2	0.0620				
👸 Method Parameters			5	1/4/2012 10:55:13 AM	STD 1	0.8628				
🏶 Analytes			6	1/4/2012 11:00:04 AM	STD 1	0.9027				
Acquisition parameters			7	1/4/2012 11:04:55 AM	STD 2	0.9492				
			8	1/4/2012 11:09:46 AM	STD 2	0.9445				
🐉 Standards			9	1/4/2012 11:14:37 AM	STD 3	0.9761				
🐉 Compounds	_		10	1/4/2012 11:19:28 AM	STD 3	0.9507				
😻 Peak Detection	=		11	1/4/2012 11:24:19 AM	STD 4	0.9897	=			
📝 Ratios			12	1/4/2012 11:29:10 AM	STD 4	0.9861				
Interference correction			13	1/4/2012 11:34:02 AM	STD 5	0.9930				
Evaluation Results			14	1/4/2012 11:38:53 AM	STD 5	0.9911				
<u> </u>			15	1/4/2012 11:43:44 AM	BLK 1	0.6506				
			16	1/4/2012 11:48:35 AM	BLK 2	1.4967				
iii Peaks			17	1/4/2012 11:53:26 AM	BLK 2	0.2396				
🚹 Ratios			18	1/4/2012 11:58:17 AM	BLK 2	0.4601				
Concentrations			19	1/4/2012 12:03:08 PM	Water unspiked	376.7616				
🗐 Instrument State			20	1/4/2012 12:07:59 PM	Water unspiked	152.3696				
E Reports			21	1/4/2012 12:12:50 PM	BLK 2	0.4103				
	-		22	1/4/2012 12:17:41 PM	Water spiked	1.9669				
	Log	View								
	Empty qu				1					

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.

Home Page MP9_FinalDVT_HPLC Dionex_AG7_Cr_04.01.12 IE 2 ×								
🔚 Save 🔀 Close ҧ Content 💦 🖳 Recalculate 🕂 Interference 🗔 Settings 🛃 Blanks 🚆								
ontent	Con	centrati	ons					
📚 Summary		E P	No.	Time	Sample T 🔽	Label V	Cr VI [ppt] 🛛 🕫	Cr III [ppt] -
👞 iCAP Q			1	1/4/2	UNKNOW	BLK 1	4.16	-2.8
🜍 Method Parameters			2	1/4/2	BLK		N/A	-2.7
🗐 Evaluation Results			3	1/4/2	AVERAGE		4.16	-2.4
The Compounds			5	1/4/2	STD			
			15	1/4/2		BLK 1	4.31	-2.5
Peaks	•		16	1/4/2	UNKNOW	BLK 2	4.74	-2.4
all Ratios	•		17	1/4/2	UNKNOW	BLK 2	4.28	-2.2
Concentrations			18	1/4/2	UNKNOW	BLK 2	4.31	-2.4
📄 Instrument State	•		19	1/4/2	UNKNOW	Water u	43.17	-2.7
🛐 Reports			20	1/4/2	UNKNOW	Water u	41.77	-2.6
₩ Sample List	•		21	1/4/2	UNKNOW	BLK 2	4.21	-2.6
			22	1/4/2	UNKNOW	Water s	145.23	68.6
	•		23	1/4/2	UNKNOW	Water s	144.20	71.2
🛸 Signing	•		24	1/4/2	UNKNOW	BLK 1	5.59	-2.7
🗟 Query	1		25	1/4/2	UNKNOW	BLK 2	5.15	0.4
			26	1/4/2	UNKNOW	BLK 2	4.30	-2.7
	•		27	1/4/2		Water s	200.29	115.5
			28	1/4/2	UNKNOW	Water s	206.94	121.7

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.

Home Page MP9_FinalDVT_HPLC Dionex_AG7_Cr_04.01.12 IE 2 ×									
🚽 Save 🔀 Close 🚺 Content- 🥛 🖳 Recalculate 🧏 Interference- 🔯 Settings									
Concentrations									
P	No.	Time	Sample Type 🗸	Label V	Cr VI	(ppt) 🕁	Cr III (ppt) 🕫		
	1	1/4/2012 10:3	UNKNOWN	BLK 1		4.16	-2.83		
	2	1/4/2012 10:4	BLK			N/A	-2.79		
	3	1/4/2012 10:4	AVERAGE BLK			4.16	-2.42		
	5	1/4/2012 10:5	STD						
				Calibration Properties					
+				-					
•	5	1/4/2012 10:5	STD	STD 1	48.9	9 (48.3	48.98 (48.9		
+	6	1/4/2012 11:0	STD	STD 1	E0.10				
÷	7	1/4/2012 11:0	STD	STD 2		Fit cel	ls to grid		
÷	8	1/4/2012 11:0	STD	STD 2		Fit cel	ls to content		
•	9	1/4/2012 11:1	STD	STD 3	B	<i>c</i>	Ctrl+C		
+	10	1/4/2012 11:1	STD	STD 3		Сору	Ctri+C		
•	11	1/4/2012 11:2	STD	STD 4		Expor	t to Excel		
•	12	1/4/2012 11:2		STD 4					
•	13	1/4/2012 11:3		STD 5		Expan	id level		
•	14	1/4/2012 11:3	STD	STD 5		Collap	se level		
				Calibrations					
				- and allow		Exclud	le entry		
_		ooks 🥵 Sched	uler 📗 Log View			Includ	e entry		

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.

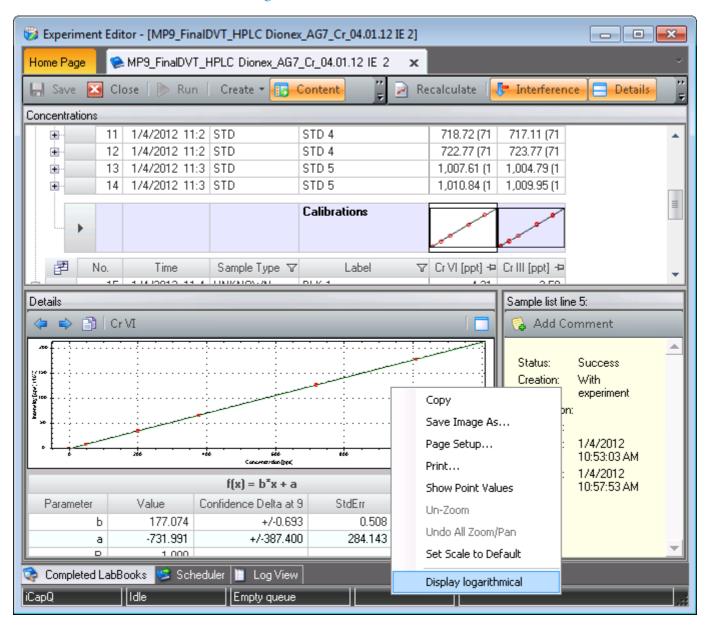


Figure 9-12. Result Concentration view Details

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							
2	Label ∨₽	Status 🖓 🕁	Survey Runs 🖓 🕁	Main Runs 🏹 Þ	Evaluate ⊽+¤	Sample Type	
1	Blank	0	0	1	V	UNKNOWN	
2	STD	Θ	0	1	V	STD	
3	STD	Θ	0	1	V	STD	
4	STD	Θ	0	1	V	STD	
5	STD	Θ	0	1		STD	
6	Sample	Θ	0	1	V	UNKNOWN	
7	water	Θ	0	1	V	UNKNOWN	
8	Blank	0	0	1	V	UNKNOWN	
9	water	0	0	1	V	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.

Acquis	Acquisition Parameters, runtime estimation 40 milliseconds									
Ide	ntifier	Dwell time (s)	ne (s) Channels Spacing (u) Measur		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:

Intensity
$$i = \left(\sum_{k=1}^{channel} i_k\right) / channel$$

- Centroid: Intensity $i = i_k$ with k = channel div 2
- Integral:

Intensity
$$i = \begin{pmatrix} channel \\ \sum_{k=i}^{channel} i_k \end{pmatrix}$$

• 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	Samplelist estimated runtime: 9 minutes 50 seconds								
1	Label ▽무	Status ⊽+=	Surv ⊽ +Þ	Main Runs	\ A b	Evaluate ⊽+¤	Sample Type	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	
1	Blank	0	0	3		V	BLK		
2	STD	0	0	3		V	STD		
3	STD	0	0	3			STD		
4	STD	0	0	3			STD		
5	STD		0	3			STD		
6	Sample		0	3		V	UNKNOWN		
7	water	0	0	3			UNKNOWN		
8	Blank	0	0	3		V	UNKNOWN		
9	water	0	0	3		V	UNKNOWN		
•	1111							•	

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.

Sa	mplelist					
	2	Label ⊽ ₽7 ≠	Sample Type ▽+	Internal Standard 🖓 🕁	Standard ⊽+Þ	Dilution Factor 🖓 🕫 /
1		Blank	UNKNOWN			1
2		STD	STD		STD1	1
3		STD	STD		STD2	1
4		STD	STD		STD3	1
5		STD	STD		STD4	1
6	•	Sample	UNKNOWN	IntSTD 💌		1
7		water	UNKNOWN			1
8		Blank	UNKNOWN	IntSTD		1
9		water	UNKNOWN	IntSTD		1
•	(E State

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.

Quantific	Quantification									
 Use Quality Control Internal Standardization active 										
Analyte	Measurement Mode	Fit Typ 🛆	Quantify	Internal Standard	Weighting	Forcing	Use for 9			
23Na	STD	Linear	No	Use as Internal Standa 🏻 📷	None	Blank	Yes			
24Mg	STD	Linear	Yes		None	Blank	Yes			
39K	STD	Linear	Yes	Use as Internal Standard	None	Blank	Yes			
44Ca	STD	Linear	Yes		None	Blank	Yes			
				•						
•										

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:

$$g_{ISC}$$
 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:

$$i_{Blank_{Isotope}} = \frac{\sum_{j=1}^{i_{Blank_{jIsotope}}} i_{Blank_{jIsotope}}}{\# \text{ blank block lines}}.$$

• 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
	iUPDATECALIB iIsotope
	for a certain concentration c_t is also measured inside one of the samples lines of the preceding standard block
	ist Discoppe.
	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 $\overline{s_t}$ are the reference and averaged target sensitivity in the preceding standard block of each standard isotope, respectively. The sensitivities are calculated using the equations:

$$s_r = \frac{i_{Isotope}^{UPDATECALIB}}{c_{Analyte}^{STD}}$$
$$\overline{s_t} = \frac{i_{Isotope}^{STD}}{c_{Analyte}^{STD}}$$

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.

Option	Description	
Fit Type	Linear	A linear regression curve with
		$f(x) = a_1 x + a_0$
		is calculated given the data points.
	2 nd order	A cubic regression curve with
		$f(x) = a_2 x^2 + a_1 x + a_0$
		will be used.
Forcing	No	Value <i>y</i> for $x = 0$ <i>is</i> 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 $\mathbf{\sigma}_k$ of the analyte over the
		runs in the sample.
	Relative SD	Weight $\omega_k = 1/(\sigma_k/\overline{i_k})$.
		Each point is weighted by the standard deviation σ_k of the analyte over the runs in the sample relative to the mean value $\overline{i_k}$.

 Table 10-2.
 Options for calibration curve calculation

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 $i_{non-standard isotope}$

$$c_{sq} = i_{non-standard \ isotope}/a_i$$
.

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 $\omega_k = 1/(\sigma_k/\overline{i_k})$.
		Each point is weighted by the standard
		deviation σ_k of the analyte over the runs in the sample relative to the mean
		value $\overline{i_k}$.

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.

Standard editor Qtegra Version: 1.3.882.55 About												out		
Standards	Selected Elements for "IsoDilSTD"													
🎦 New 🛪 🔚 Save 🍹	Delete													
🔒 Standard	Element	nt Concentration		Unit	Isotope	1 Isoto	Isotope 2		Abundance 1		Abundance		e2	
📔 Internal Standard	Ru	10		ppb	102Ru	104R	104Ru		31.6		18.7			
🚹 Isotope Dilution Standard —		Ir	10		ppb	193lr	191Ir	1911r		62.7		37.3		
New Isotope Dilution Standard														
Create new Isotope Dilution Standard														
										×.				
	Select Elements													
	Н												He	
	LI Be							8	C	N	0	F	Ne	
	Na Mg							AL	SI D	P	s D	CI	Ar D	
	к са	Sc TI	V Cr	ME - F	Fe Co		ci zi	Ga	Ge	As	8	Br	ĸ	=
	Rb Sr	Y Zr	ND MO	TC F		Pd -	Ag Cd	h D	SI D	Sb_	Te	۱. ا	Xe	
	Cs Ba	la Hí D D	Ta W	Re C)s Ir	Pt .	Al Hg	ТІ	Pb	81	Po	At	R	
	Fr Ra	Ac												
		Ce	Pr Nd	Pm S	in El	Gđ	ть ру	Ho	Er	Tm	Yb III	ц П		
۰ III ا	•				Ţ	11							ł	

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.

Standards	Selected Elements for "IsoDiISTD1"									
🛅 New 💥 Delete 🍟	Delete									
Name De 💋 Load	ntration	Unit	Isotope 1	Isotope 2	Abundance 1	Abundance 2	Atomic Weight			
IsoDilSTD1		ppb	98Mo	96Mo	24.13	16.68	95.9313			
- Derdale		ppb	102Ru	104Ru	31.6	18.7	101.0697			
		ppb	184W	186W	30.67	28.6	183.8489			
		ppb	1920s	1900s	41	26.4	190.2398			
	•						•			
	Select Elements									
	н						<u>^</u>			
	ч	Be				8 <mark>.</mark> C				
	Na	" 9								
	ĸ			Dr Mi Fe		Zi Ga G				
	Rb	sr Y			RI PO Ag		SD Te			
۰	•						۱.			

Figure 10-7. Isotope Dilution Standard in Template



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

$$R_{ATW_{Element}} = \frac{ATW_{Element_{Sample}}}{ATW_{Element_{Sample}}}$$

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. \blacktriangle

Data Evaluation Isotope Dilution

Glossary

This section lists and defines terms used in this manual. It also includes acronyms, metric prefixes, symbols, and abbreviations.

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

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.

В

BEC abbr. for Background Equivalent Concentration (normally in ppt); n=10, depends on the concentration in the blank.

 $BEC = \frac{(blank intensities) \times (concentration of standard)}{(intensity standard - average intensity blank)}$

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.

Е

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).

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.

 $LOD = \frac{(3 \times stdev \text{ of } BLK \text{ intensities}) \times (concentration \text{ of } STD)}{(intensity STD - average intensity BLK)}$

LR abbr. for Low Resolution.

Μ

 \boldsymbol{M}^{\star} molecular ion.

 $\mathbf{M}\mathbf{H}^{*}$ protonated molecular ion.

MS mass spectrometer; mass spectrometry.

m/z mass-to-charge ratio.

0

OD outside diameter.

Ρ

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 μ g/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.

Glossary: WEEE–WEEE

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Thermo Fisher Scientific Inc.

81 Wyman Street P.O. Box 9046 Waltham, Massachussetts 02454-9046 United States

www.thermoscientific.com

