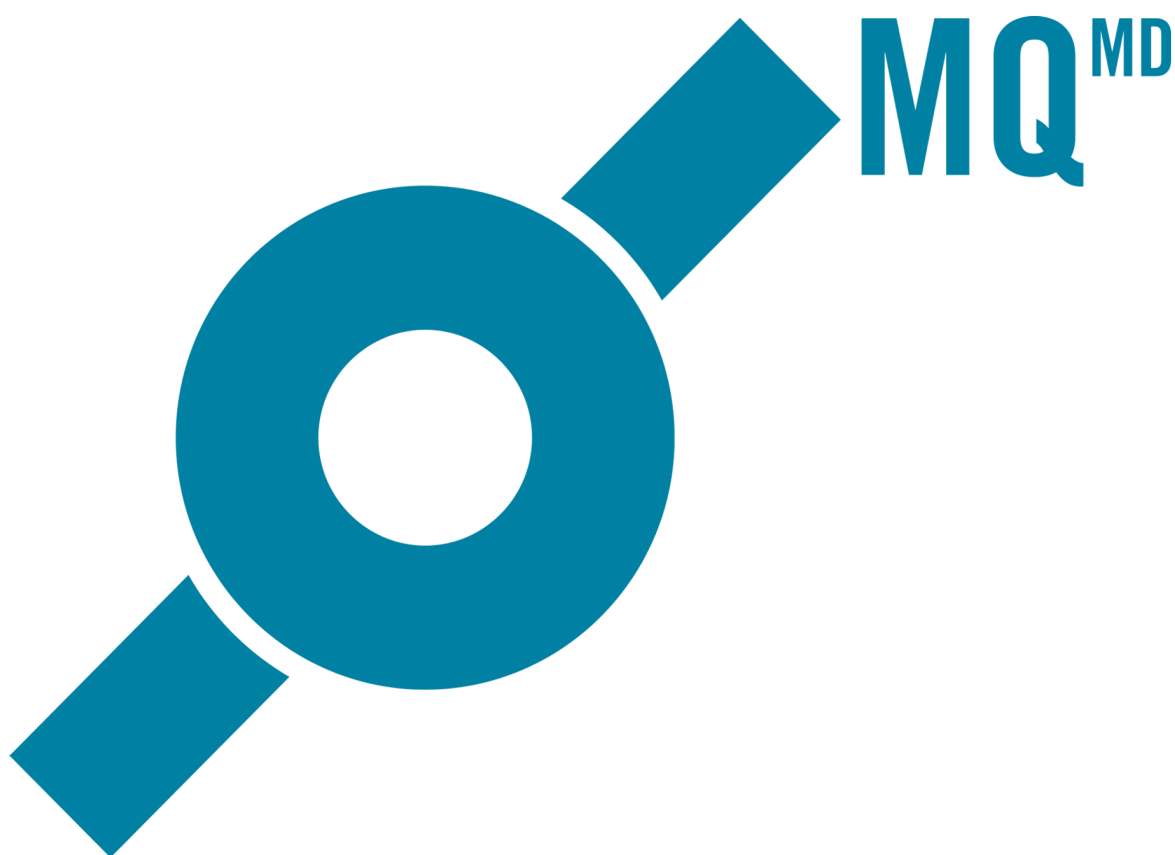

MultiQuant™ MD 3.0.3 Software

User Interface Guide



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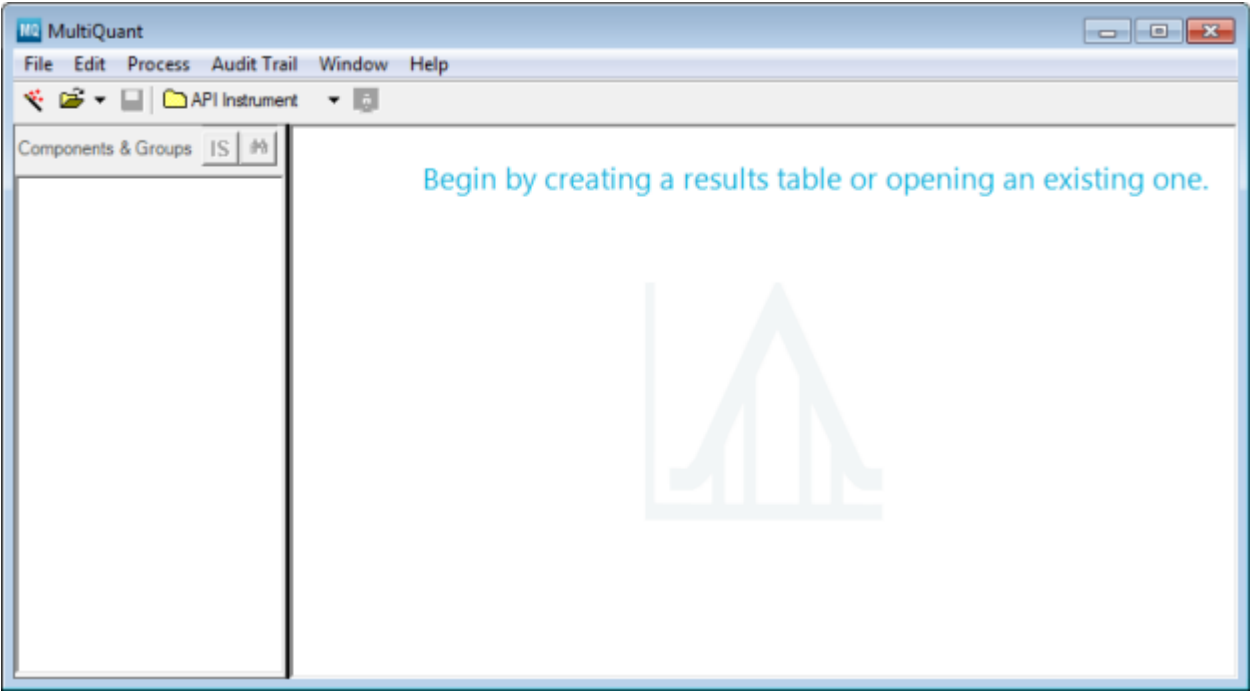
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Main Screen and Menus

1

Figure 1-1 Main Screen



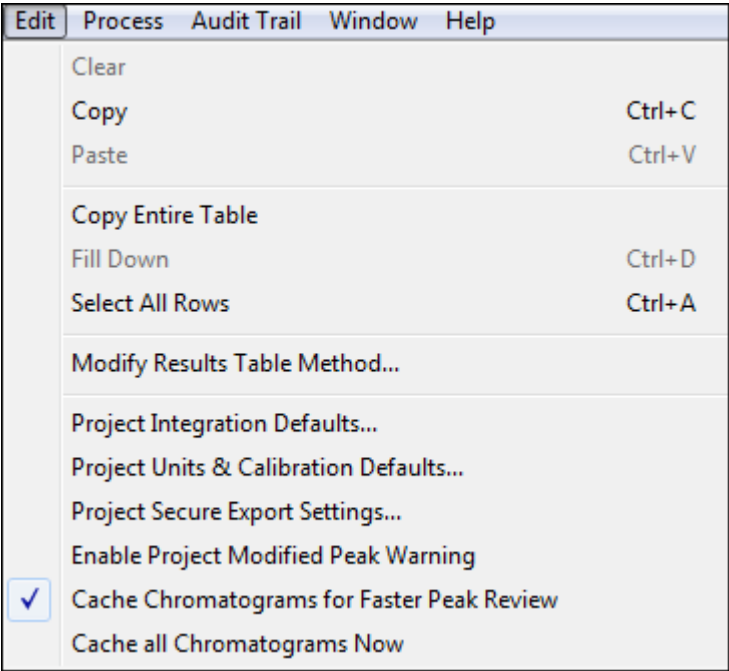
English	Translation
File	
Edit	
Process	
Audit Trail	
Window	
Help	
Begin by creating a results table or opening an existing one.	

Figure 1-2 File Menu

File	Edit	Process	Audit Trail	Window	Help
New Results Table...					Ctrl+N
New Quantitation Method...					
Open Results Table...					Ctrl+O
Open Quantitation Method...					
Save					Ctrl+S
Save As...					
Recent Results Tables					▶
Recent Quantitation Methods					▶
Export					▶
Transfer to LIMS...					Ctrl+L
Export and Save Results Table...					
Create Report and Save Results Table...					Ctrl+R
Exit					

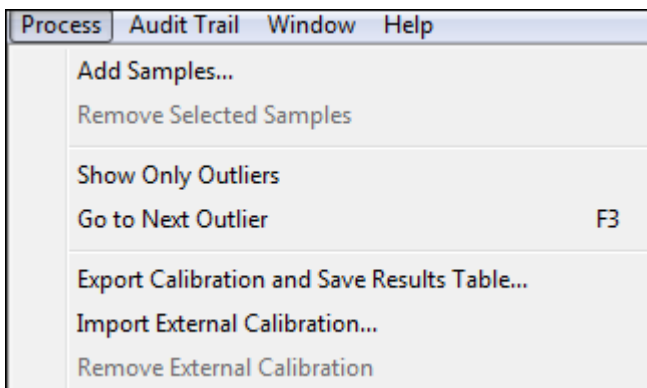
English	Translation
New Results Table	
New Quantitation Method	
Open Results Table	
Open Quantitation Method	
Save	
Save As	
Recent Results Tables	
Recent Quantitation Methods	
Export	
Transfer to LIMS	
Export and Save Results Table	
Create Report and Save Results Table	
Exit	

Figure 1-3 Edit Menu



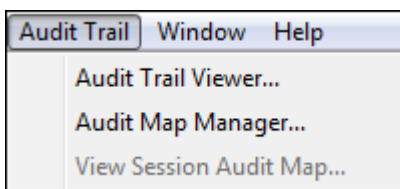
English	Translation
Clear	
Copy	
Paste	
Copy Entire Table	
Fill Down	
Select All Rows	
Modify Results Table Method	
Project Integration Defaults	
Project Units & Calibration Defaults	
Project Secure Export Settings	
Enable Project Modified Peak Warning	
Cache Chromatograms for Faster Peak Review	
Cache all Chromatograms Now	

Figure 1-4 Process Menu



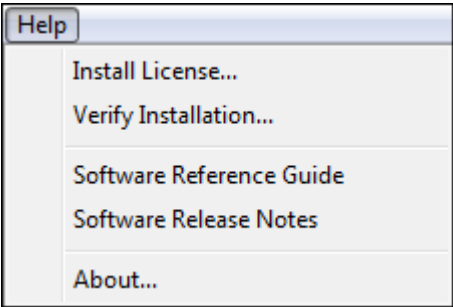
English	Translation
Add Samples	
Remove Selected Samples	
Show Only Outliers	
Go to Next Outlier	
Export Calibration and Save Results Table	
Import External Calibration	
Remove External Calibration	

Figure 1-5 Audit Trail Menu



English	Translation
Audit Trail Viewer	
Audit Map Manager	
View Session Audit Map	

Figure 1-6 Help Menu

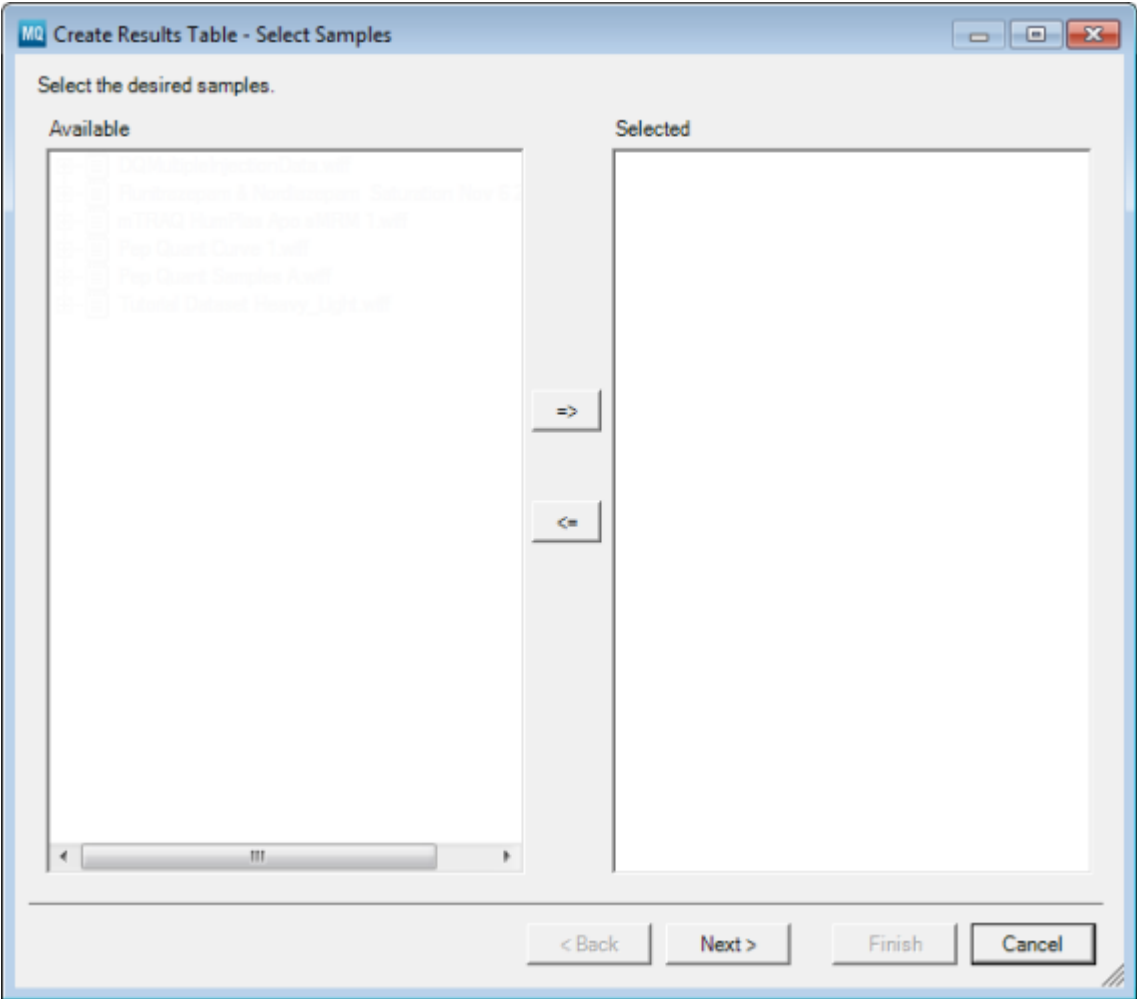


English	Translation
Install License	
Verify Installation	
Software Reference Guide	
Software Release Notes	
About	

Create New Results Table

2

Figure 2-1 Create Results Table - Select Samples

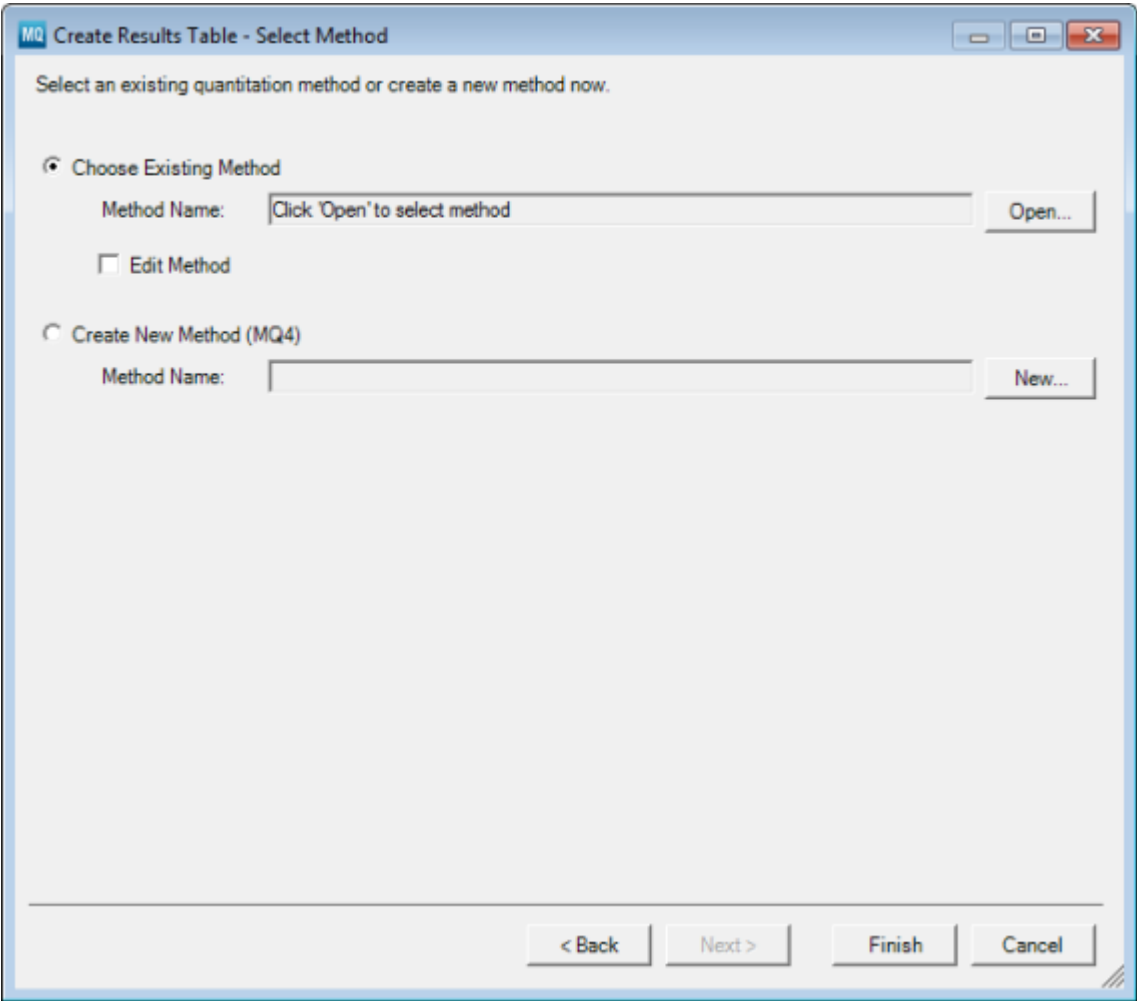


English	Translation
Select the desired samples	
Available	
Selected	

Create New Results Table

English	Translation
Back	
Next	
Finish	
Cancel	

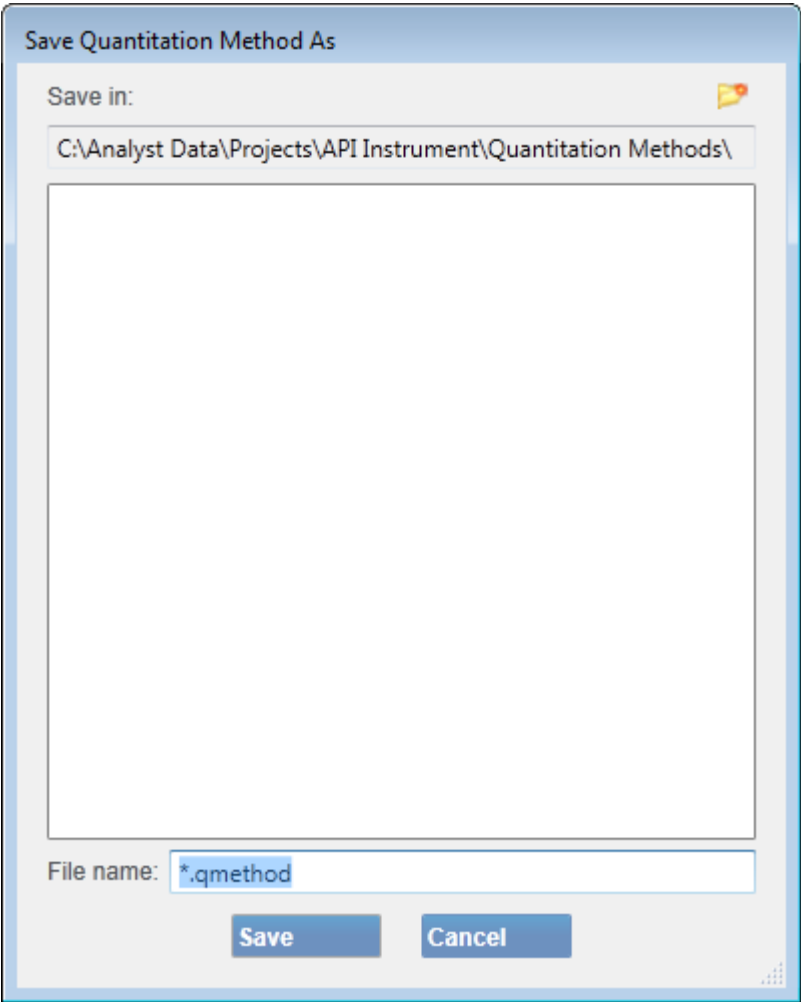
Figure 2-2 Create Results Table - Select Method



Create New Results Table

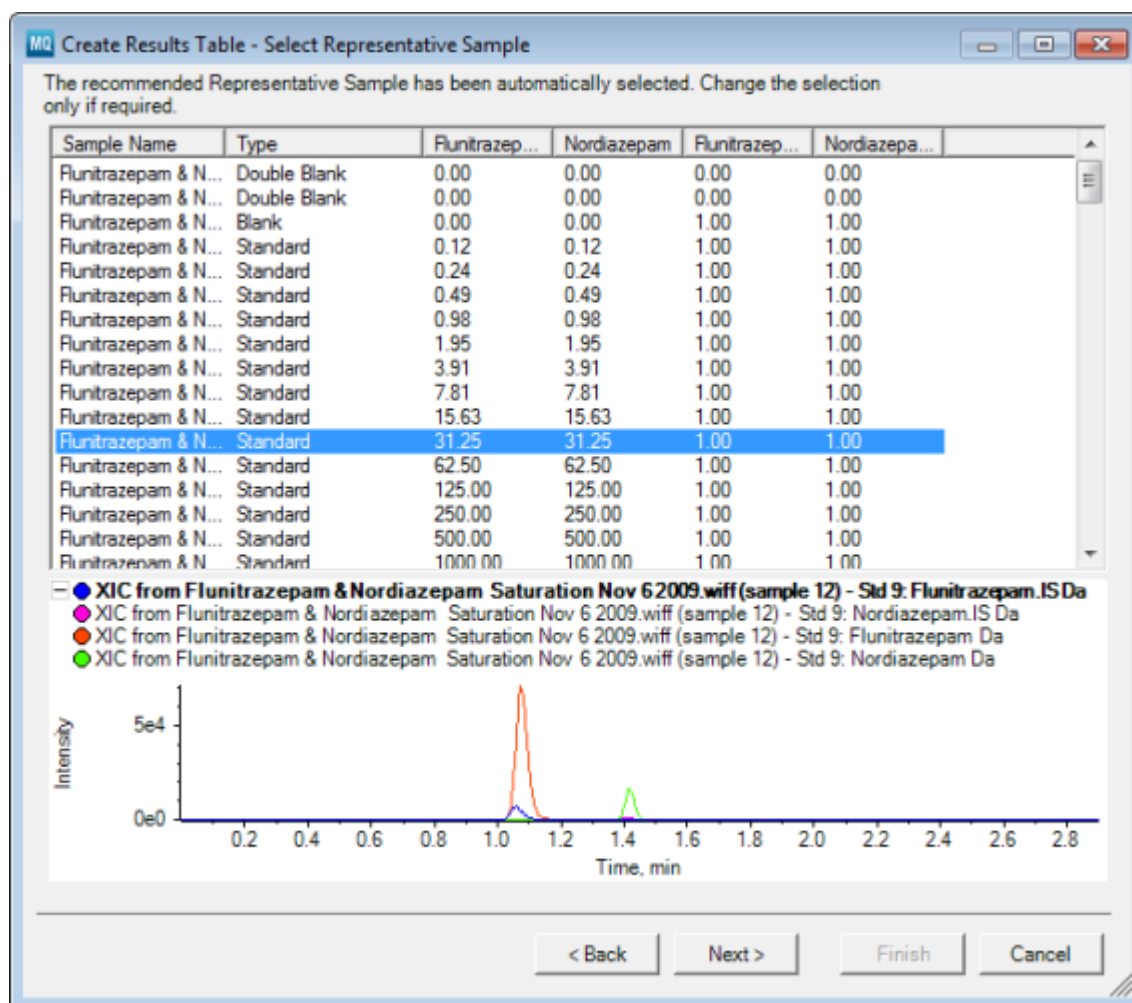
English	Translation
Select an existing quantitation method or create a new method now.	
Choose Existing Method	
Method Name	
Open	
Edit method	
Create New Method	
Method Name	
New	
Back	
Next	
Finish	
Cancel	

Figure 2-3 Save Quantitation Method As



English	Translation
Save in	
File name	
Save	
Cancel	

Figure 2-4 Create Results Table - Select Representative Sample

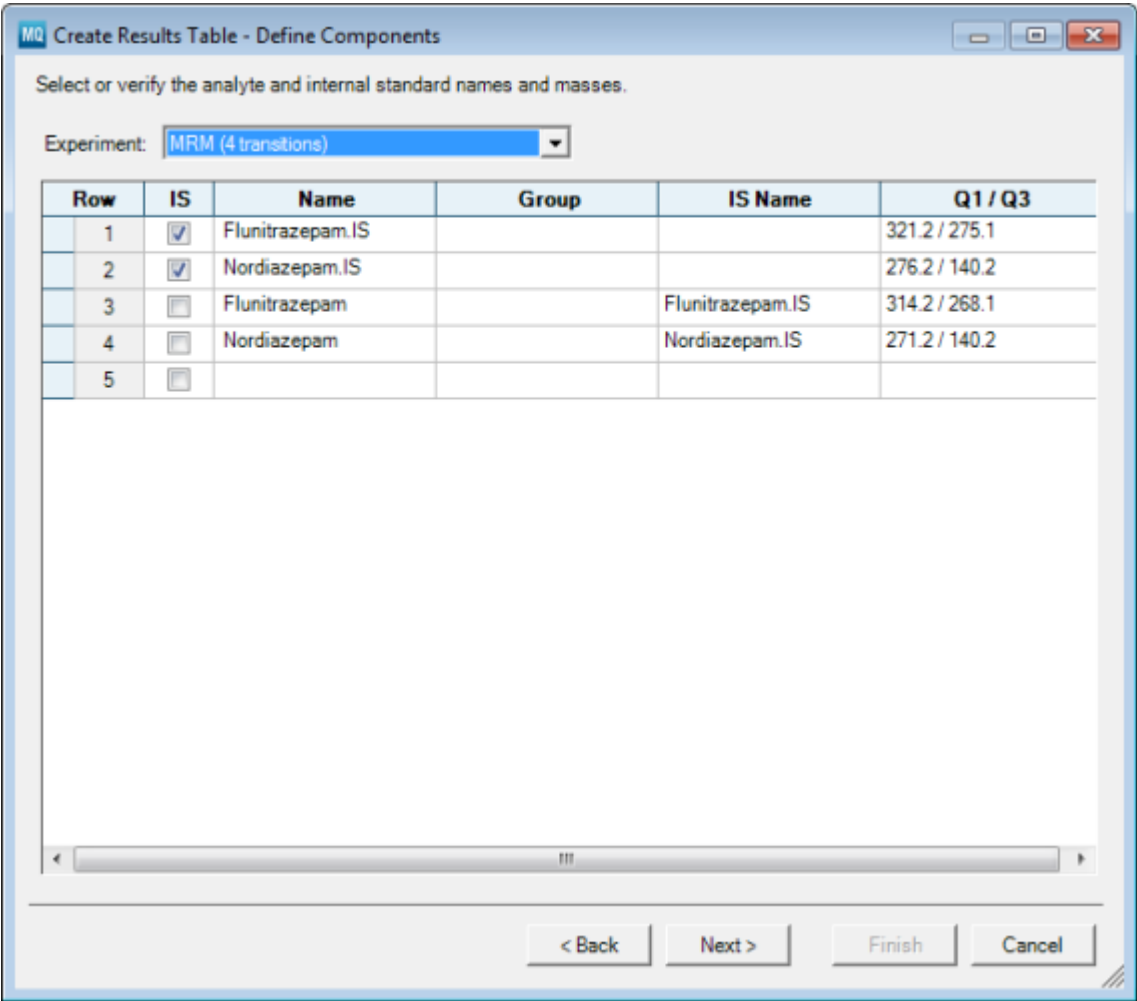


English	Translation
The recommended Representative Sample has been automatically selected. Change the selection only if required.	
Sample Name	
Type	
Back	
Next	

Create New Results Table

English	Translation
Finish	
Cancel	

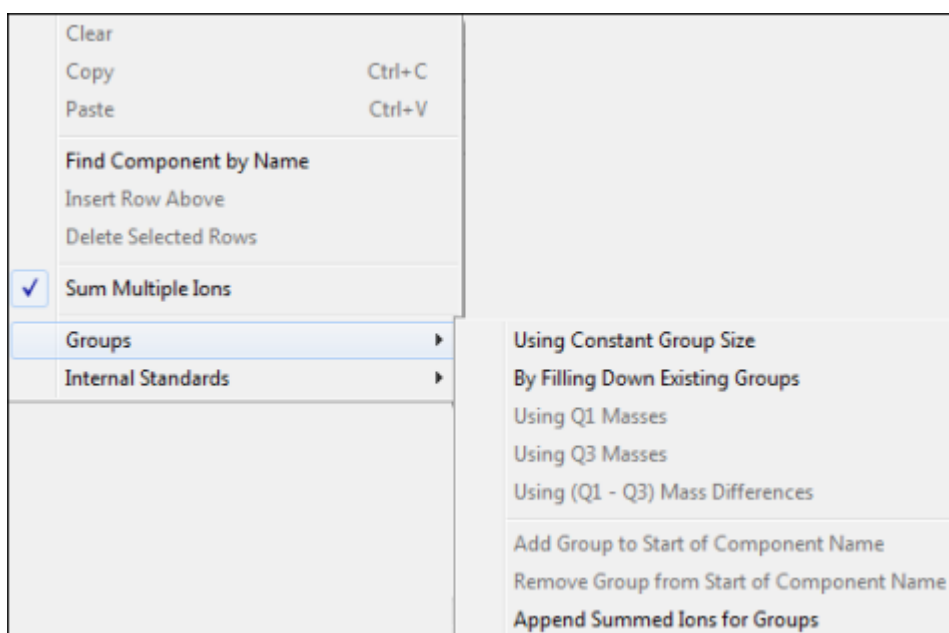
Figure 2-5 Create Results Table - Define Components



English	Translation
Select or verify the analyte and internal standard names and masses.	
Experiment	
Row	

English	Translation
IS (internal standard)	
Name	
Group	
IS Name	
Back	
Next	
Finish	
Cancel	

Figure 2-6 Create Results Table - Define Components Groups Right-Click Menu

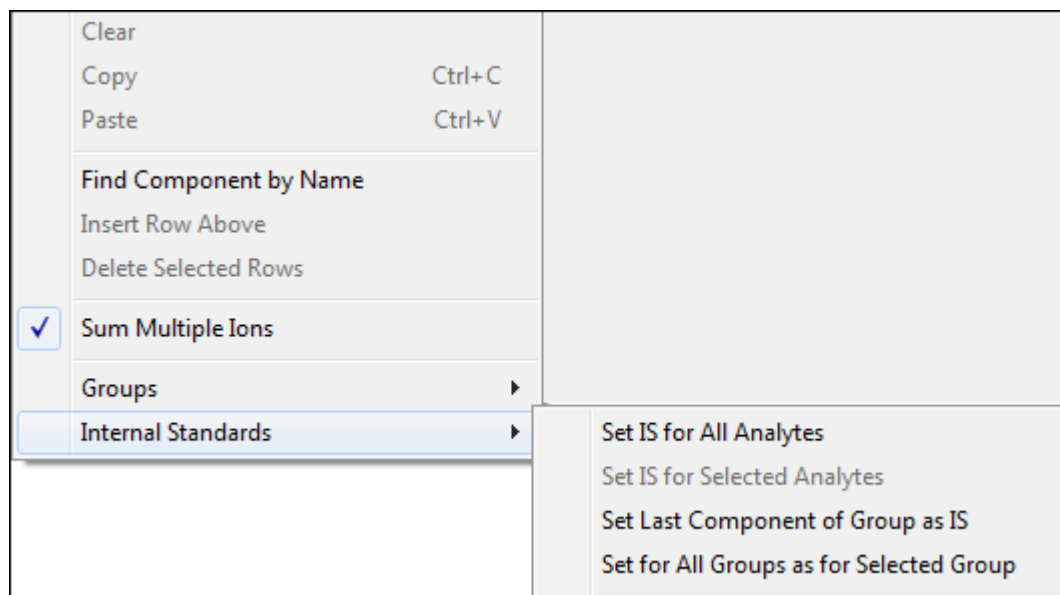


English	Translation
Clear	
Copy	
Paste	
Find Component by Name	
Insert Row Above	

Create New Results Table

English	Translation
Delete Selected Rows	
Sum Multiple Ions	
Groups	
Using Constant Group Size	
By filling Down Existing Groups	
Using Q1 Masses	
Using Q3 Masses	
Using (Q1 - Q3) Mass Differences	
Add Group to Start of Component Name	
Remove Group from Start of Component Name	
Append Summed Ions for Groups	

Figure 2-7 Create Results Table - Define Components Internal Standards Right-Click Menu

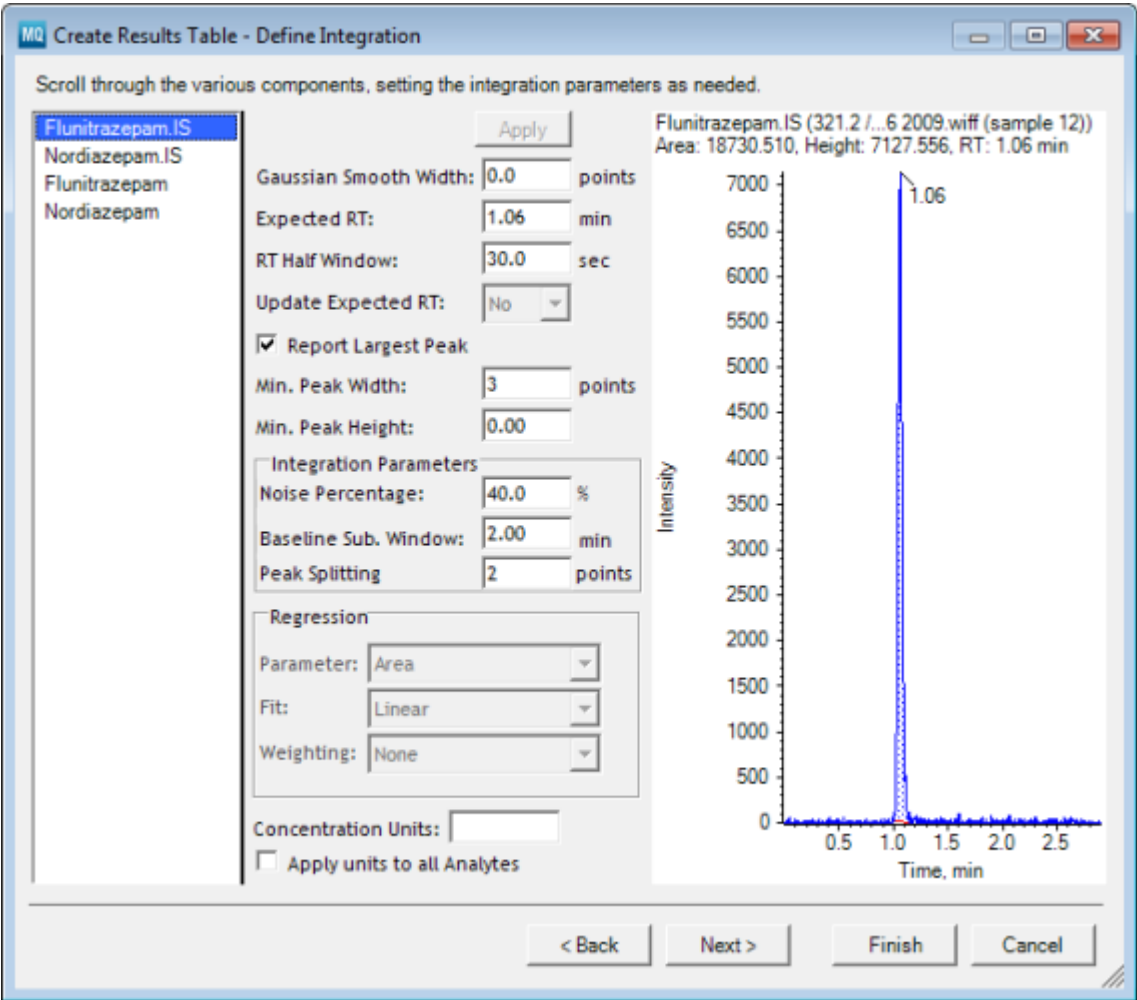


English	Translation
Clear	
Copy	

English	Translation
Paste	
Find Component by Name	
Insert Row Above	
Delete Selected Rows	
Sum Multiple Ions	
Internal Standards	
Set IS for All Analytes	
Set IS for Selected Analytes	
Set Last Component of Group as IS	
Set for All Groups as for Selected Group	

Create New Results Table

Figure 2-8 Create Results Table - Define Integration



English	Translation
Scroll through the various components, setting the integration parameters as needed.	
Gaussian Smooth Width: points	
Expected RT: min	
RT Half Window: sec	
Updated Expected RT: No or Yes	
Report Largest peak	

English	Translation
Min. Peak Width: points	
Min Peak Height:	
Integration Parameters	
Noise Percentage	
Baseline Sub. Window: min	
Peak Splitting: points	
Regression	
Parameter: Area or Height	
Fit: Linear, Linear Through Zero, Mean Response Factor, Quadratic, Power, Wagner, Hill	
Weighting: None, $1/x$, $1/x^2$, $\ln(x)$, $1/y$, $1/y^2$, $\ln(y)$	
Concentration Units	
Apply units to all Analytes	
Back	
Next	
Finish	
Cancel	

Figure 2-9 Create Results Table - Define Integration Right-Click Menu

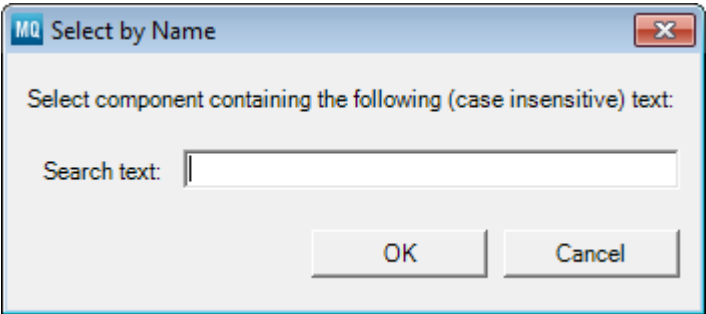
Find Component by Name
Highlight Components with Uncertain RT
Home Graph Axis
Overlay Other Components for Group
Update Retention Times...

English	Translation
Find Component by Name	
Highlight Components with Uncertain RT	
Home Graph Axis	

Create New Results Table

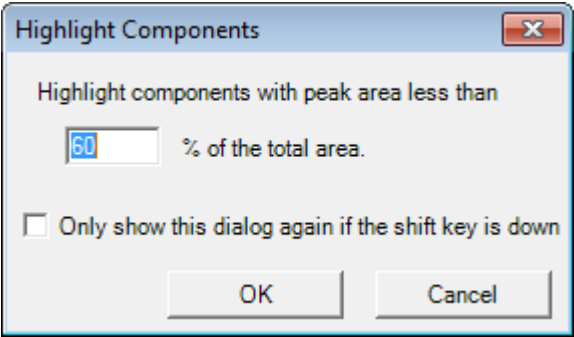
English	Translation
Overlay Other Components for Group	
Update Retention Times	

Figure 2-10 Find Component by Name



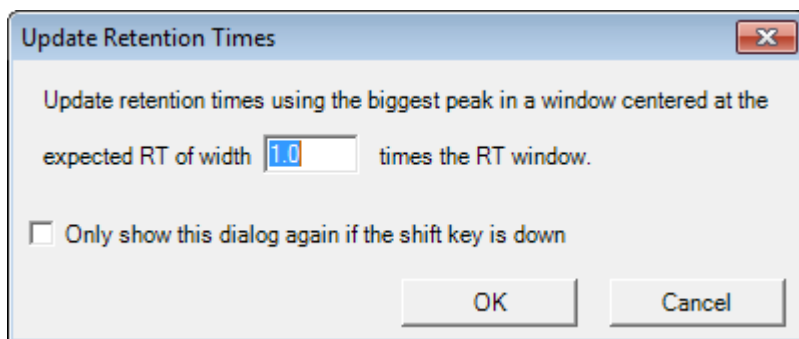
English	Translation
Select component containing the following (case insensitive) text:	
Select text:	
OK	
Cancel	

Figure 2-11 Highlight Components



English	Translation
Highlight components with peak are less than _% of the total area.	
Only show this dialog again if the shift key is down	
OK	
Cancel	

Figure 2-12 Update Retention Times



English	Translation
Update retention times using the biggest peak in a window centered at the expected RT of width _ times the RT window	
Only show this dialog again if the shift key is down	
OK	
Cancel	

Create New Results Table

Figure 2-13 Create Results Table - Outlier Settings

MQ

Create Results Table - Outlier Settings

Set criteria for flagging outliers.

☒ Accuracy for Standards

Max. Accuracy Tolerance for LLOQ (lowest Std): %

Max. Accuracy Tolerance for Stds except LLOQ: %

☒ Accuracy for QCs

Max. Accuracy Tolerance for QC: %

☐ Ion Ratio

☒ Calculated Concentration

Component	Lower Limit of Calculated Concentration	Upper Limit of Calculated Concentration
▶ Flunitrazepam.IS		
Nordiazepam.IS		
Flunitrazepam		
Nordiazepam		

< Back

Next >

Finish

Cancel

English	Translation
Set criteria for flagging outliers.	
Accuracy for Standards	
Max. Accuracy Tolerance for LLOQ (lowest Std)	
Max. Accuracy Tolerance for Stds except LLOQ	
Accuracy for QCs	
Max. Accuracy Tolerance for QC	
Ion Ratio	

English	Translation
Calculated Concentration	
Component	
Lower Limit of Calculated Concentration	
Upper Limit of Calculated Concentration	
Back	
Next	
Finish	
Cancel	

Figure 2-14 Create Results Table - Outlier Settings Right-Click Menu

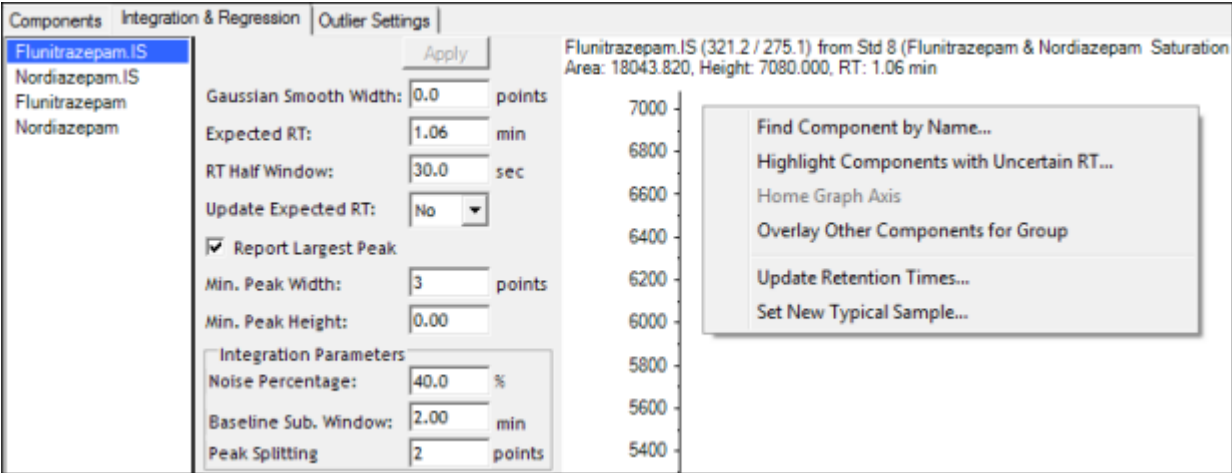
Component	Lower Limit of Calculated Concentration	Upper Limit of Calculated Concentration
► Flunitrazepam.IS		
Nordiazepam.IS		
Flunitrazepam		
Nordiazepam		
<div> Apply to all analytes the Lower Limit of Calc. Concentration Apply to all analytes the Upper Limit of Calc. Concentration </div>		

English	Translation
Apply to all analytes the Lower Limit of Calc. Concentration	
Apply to all analytes the Upper Limit of Calc. Concentration	

New Quantitation Method

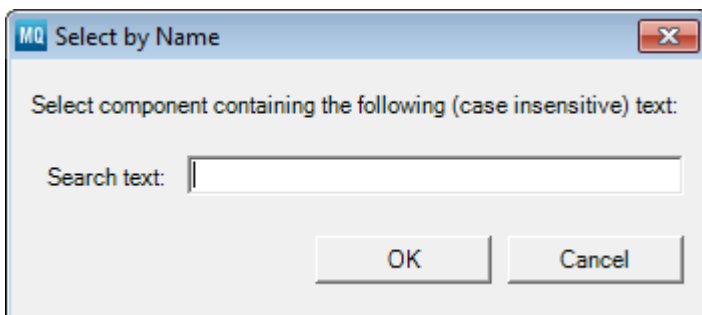
3

Figure 3-1 New Quantitation Method- Integration & Regression Right-Click Menu



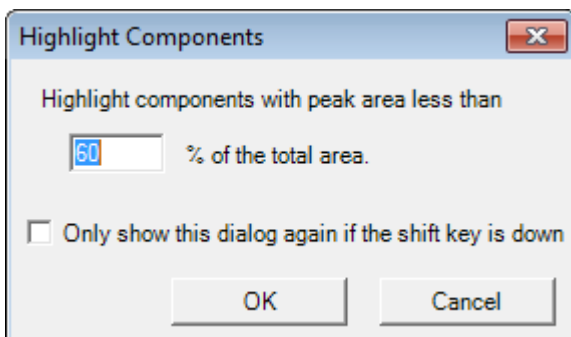
English	Translation
Find Component by Name	
Highlight components with Uncertain RT	
Home Graph Axis	
Overlay Other Components for Group	
Update Retention Times	
Set New Typical Sample	

Figure 3-2 Select by Name



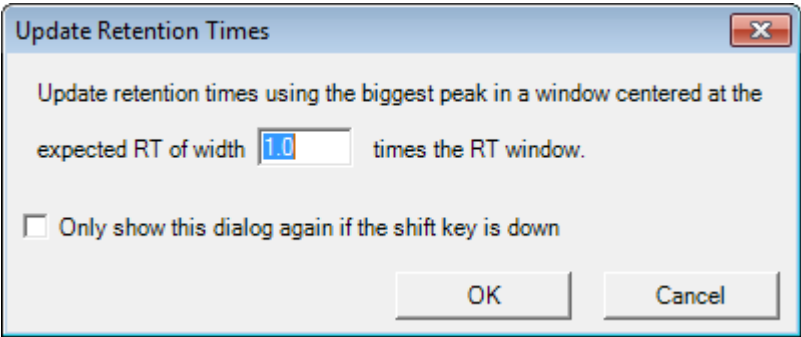
English	Translation
Select component containing the following (case insensitive) text:	
Select text	
OK	
Cancel	

Figure 3-3 Highlight Components



English	Translation
Highlight components with peak area less than _% of the total area.	
Only show this dialog again if the shift key is down	
OK	
Cancel	

Figure 3-4 Update Retention Times

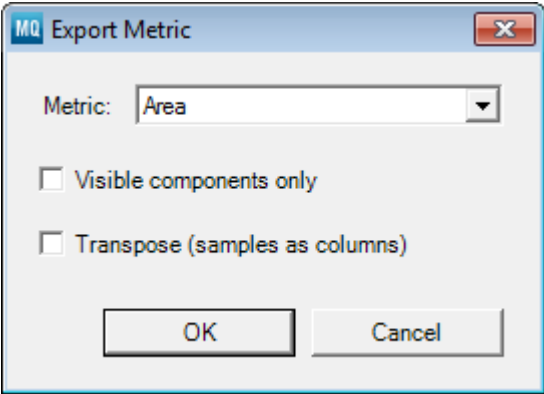


English	Translation
Update retention times using the biggest peak in a window centered at the expected RT of width _ times the RT window	
Only show this dialog again if the shift key is down	
OK	
Cancel	

Export

4

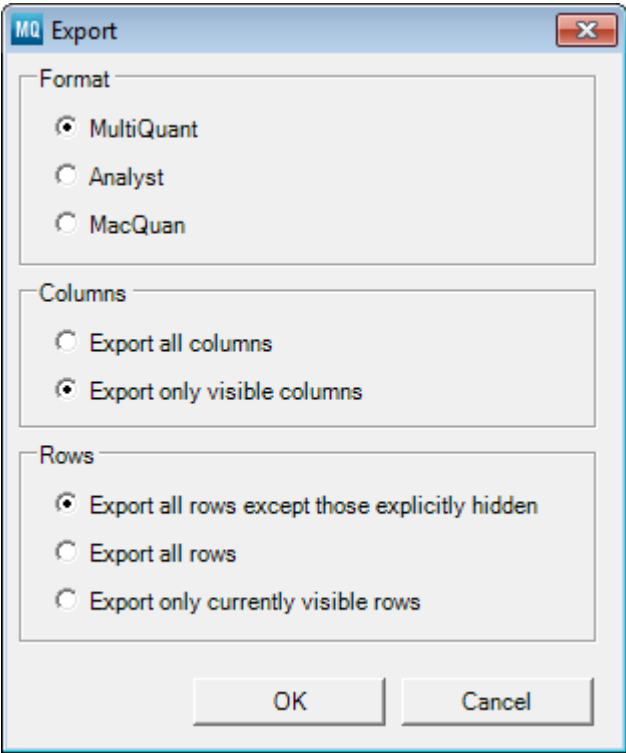
Figure 4-1 Export Metric



English	Translation
Metric: Area, IS Area, Corrected Area, IS Corrected Area, Area Ratio, Height, IS Height, Corrected Height, IS Corrected Height, Height Ratio, Area/Height, IS Area/Height, Corrected Area/Height, IS Corrected Area/Height, Region Height, IS Region Height, Quality, IS Quality, Retention Time, IS Retention Time,	
Only show this dialog again if the shift key is down	
OK	
Cancel	

Export

Figure 4-2 Export and Save Results Table

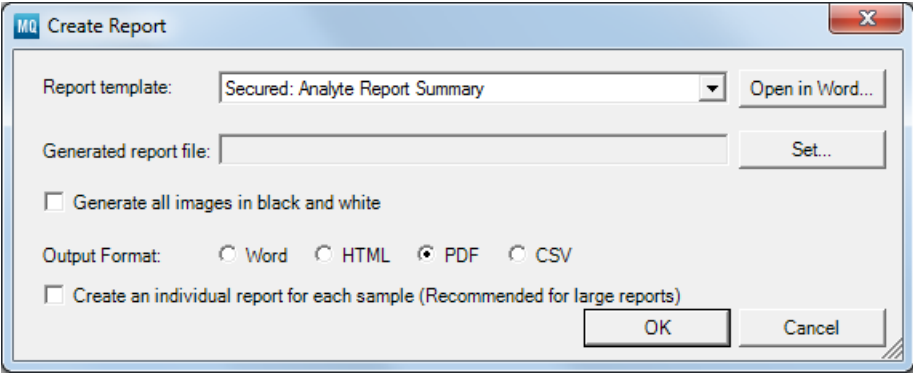


English	Translation
Format: MultiQuant, Analyst, MacQuan	
Columns: Export all columns, Export only visible Columns	
Rows: Export all rows except those explicitly hidden, Export all rows, Export only currently visible rows	
OK	
Cancel	

Create Reports

5

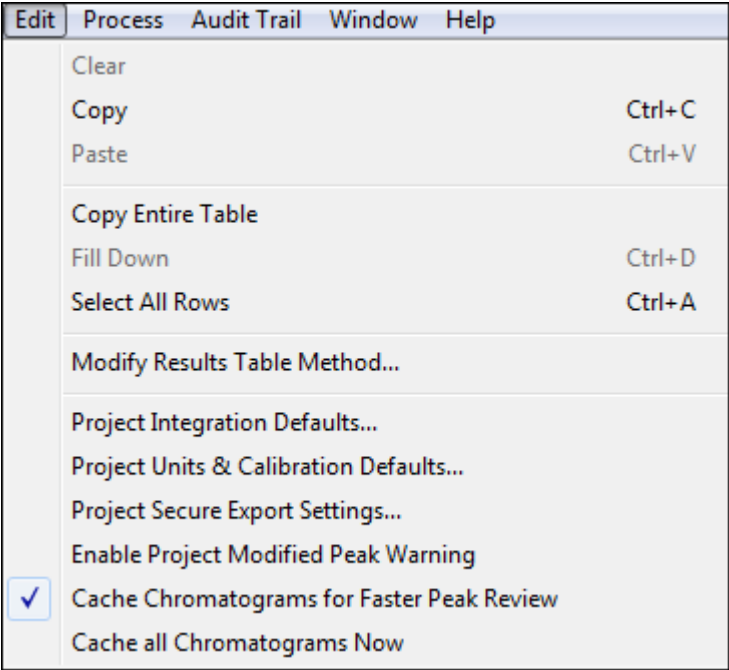
Figure 5-1 Create Report



English	Translation
Report template	
Open in Word	
Generated report file	
Set	
Generate all images in black and white	
Output Format: Word, HTML, PDF, CSV	
Create an individual report for each sample (Recommended for large reports)	
OK	
Cancel	

Edit Menu

Figure 6-1 Edit Menu



English	Translation
Clear	
Copy	
Paste	
Copy Entire Table	
Fill Down	
Select all Rows	
Modify Results Table Method	
Project Integration Defaults	
Project Units & Calibration Defaults	

English	Translation
Project Secure Export Settings	
Enable Project Modified Peak Warning	
Cache Chromatograms for Faster Peak Review	
Cache all Chromatograms Now	

Figure 6-2 Project Integration Defaults (MQ4) Dialog

Integration Defaults

Integration Algorithm: MQ4

Gaussian Smooth Width: 0.0 points

Expected RT: 0.00 min

RT Half Window: 30.0 sec

Update Expected RT: No

☒ Report Largest Peak

Min. Peak Width: 3 points

Min. Peak Height: 0.00

Integration Parameters

Noise Percentage: 40.0 %

Baseline Sub. Window: 2.00 min

Peak Splitting: 2 points

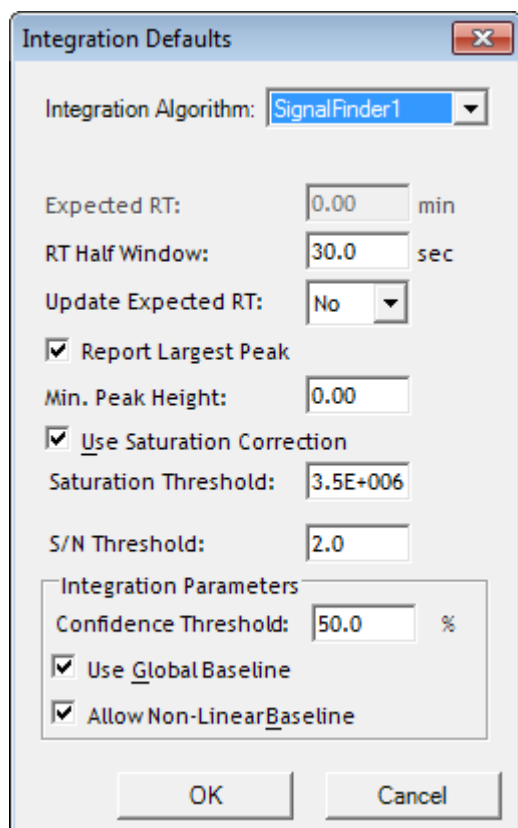
OK Cancel

English	Translation
Integration Algorithm	
Gaussian Smooth Width: points	
Expected RT: min	
RT Half Window: sec	
Updated Expected RT: No, yes	

Edit Menu

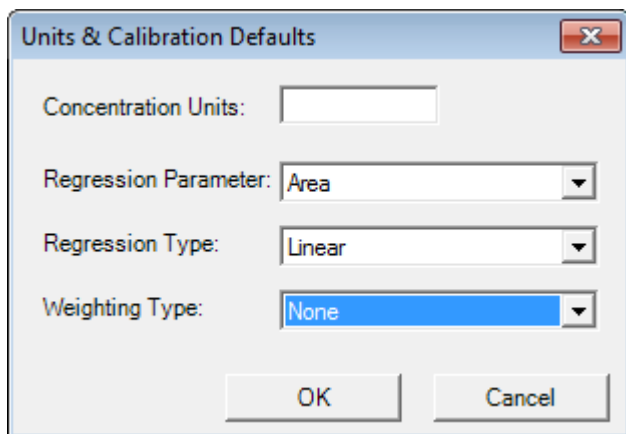
English	Translation
Report Largest Peak	
Min. Peak Width: points	
Min. Peak Height	
Integration Parameters	
Noise Percentage	
Baseline Sub. Window: min	
Peak Splitting: points	
OK	
Cancel	

Figure 6-3 Project Integration Defaults (SignalFinder1) Dialog



English	Translation
Integration Algorithm	
Expected RT: min	
Update Expected RT: No, Yes	
Report Largest Peak	
Min. Peak Height:	
Use Saturation correction	
Saturation Threshold:	
S/N Threshold	
Integration Parameters	
Confidence Threshold	
Use Global Baseline	
Allow Non-Linear Baseline	
OK	
Cancel	

Figure 6-4 Units & Calibration Defaults Dialog

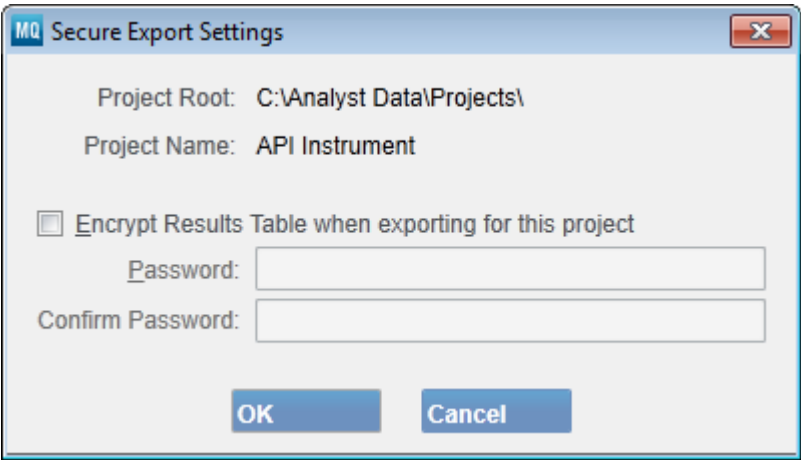


English	Translation
Concentration Units	
Regression Parameter: Area, Height	

Edit Menu

English	Translation
Regression Type: Linear, Linear Through Zero, Mean Response Factor, Quadratic, Power, Wagner, Hill	
Weighting Type: None, 1/x, 1/x ² , ln(x), 1/y, 1/y ² , ln (y)	
OK	
Cancel	

Figure 6-5 Secure Export Settings Dialog

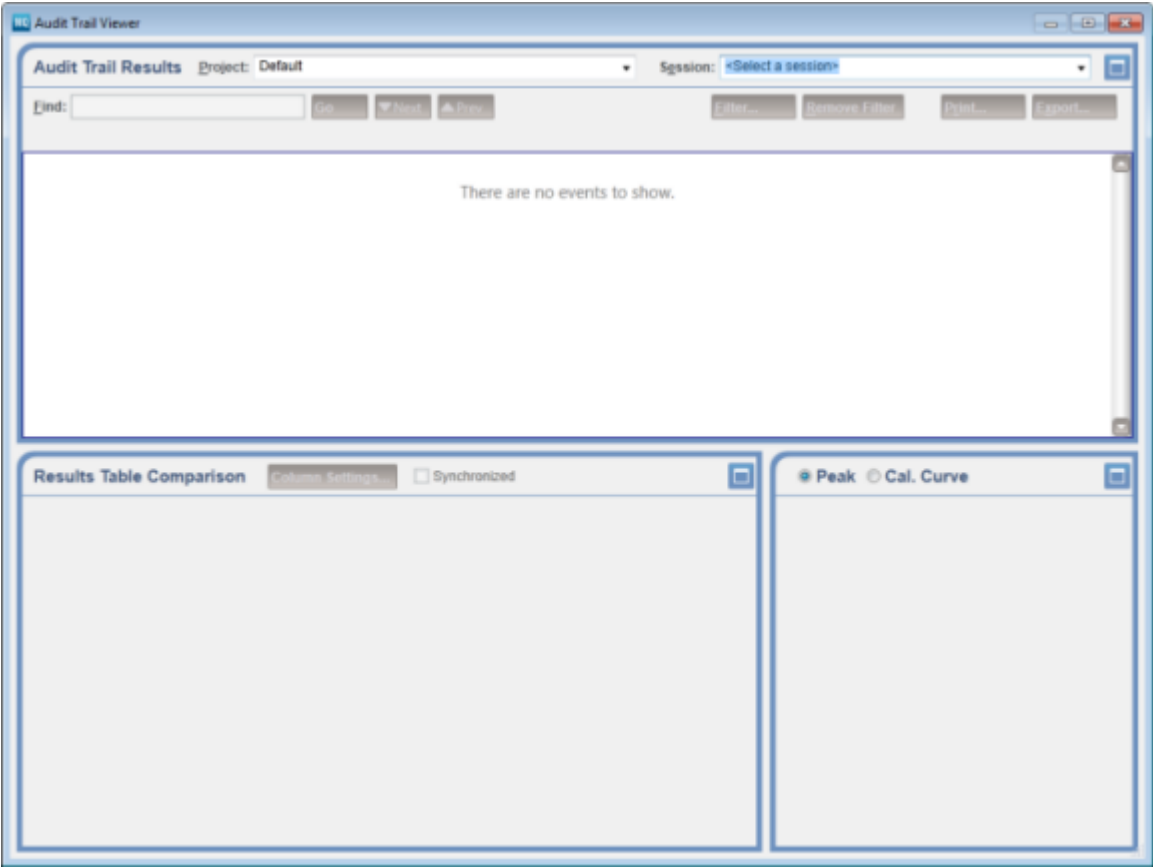


English	Translation
Project Root:	
Project Name:	
Encrypt Results Table when exporting for this project	
Password	
Confirm Password	
OK	
Cancel	

Audit Trail Menu

7

Figure 7-1 Audit Trail Viewer



English	Translation
Audit Trail Results	
Project	
Session	
Find	
Go	
Next	

Audit Trail Menu

English	Translation
Prev	
Filter	
Remove Filter	
Print	
Export	
Results Table Comparison	
Column Settings	
Synchronized	
Peak	
Cal. Curve	

Figure 7-2 Filter Audit Trail Events Dialog

MQ Filter Audit Trail Events

Clear

Find instances where:

Session ☒ is ☐ contains test

And where:

<No filter> ☒ is ☐ contains

And where:

<No filter> ☒ is ☐ contains

And where:

<No filter> ☒ is ☐ contains

☐ **And where time and date are:**

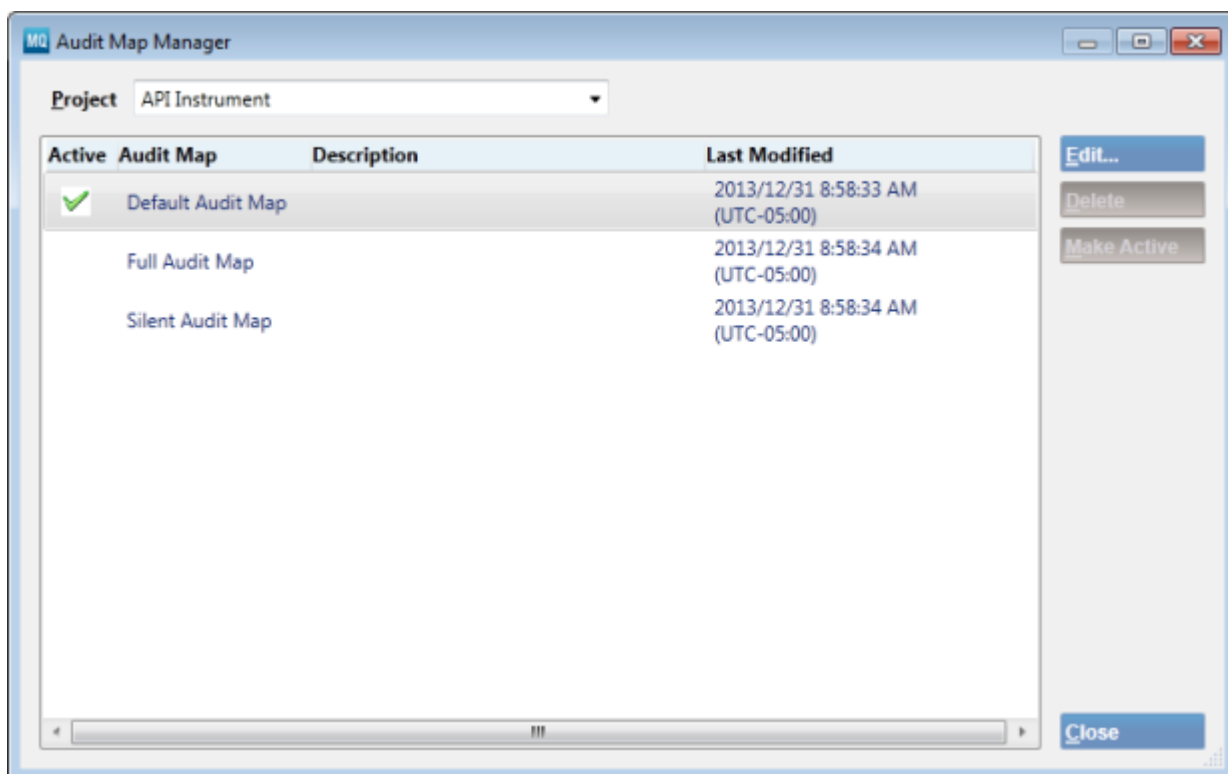
From: 2013/12/31 12:00:00 AM

To: 2013/12/31 11:59:59 PM

OK Cancel

English	Translation
Find instances where (is, contains)	
And where (Description, Sample Name, Full User Name, E-Signature, Reason, No filter)	
And where time and date are	
From	
To	
OK	
Cancel	
Clear	

Figure 7-3 Audit Map Manager Dialog



Audit Trail Menu

English	Translation
Project	
Active	
Audit Map	
Description	
Last Modified	
Edit	
Delete	
Make Active	
Close	

Figure 7-4 Audit Map Editor Dialog

Audit Map Editor

Audit Map: Default Audit Map

Description:

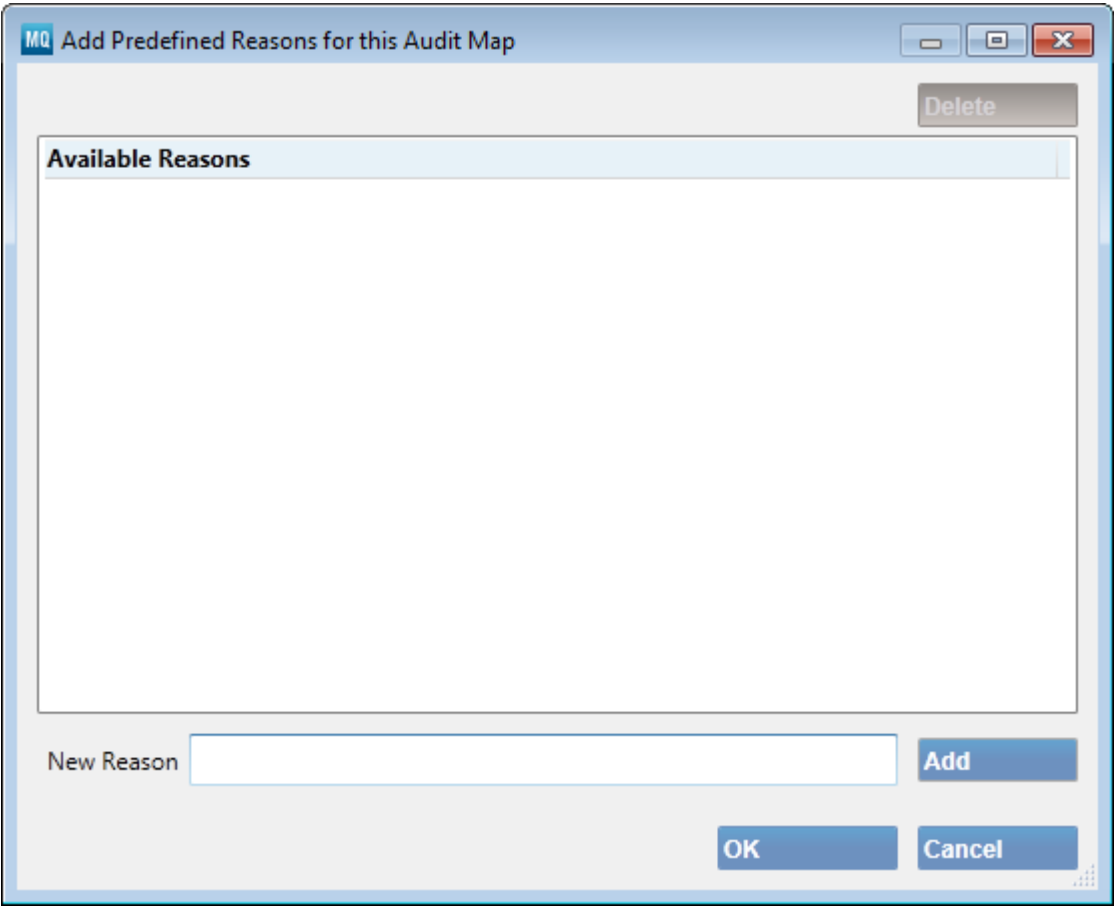
Check Uncheck Add Predefined Reasons...

Event	Audited	Reason Prompt	Predefined Reasons Only	E-Sig	Predefined Reason 1	Predefined Reason 2
New session created	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Session file saved	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Integration parameters changed for sample	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Modify and apply quantitation method	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Actual concentration changed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Sample name changed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Sample type changed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Sample ID changed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Dilution factor changed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Used column changed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Custom columns modified	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Manually integrated	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Clear integration	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Samples added or removed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
External Calibration	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		

Save Save As... Close

English	Translation
Audit Map	
Description	
Check	
Uncheck	
Add Predefined Reasons	
Event	
Audited	
Reason Prompt	
Predefined Reasons Only	
E-Sig	
Predefined Reason 1	
Predefined Reason 2	
New session created	
Session file saved	
Integration parameters changed for sample	
Modify and apply quantitation method	
Actual concentration changed	
Sample name changed	
Sample type changed	
Sample ID changed	
Dilution factor changed	
Used column changed	
Custom columns modified	
Manually integrated	
Clear integration	
Samples added or removed	
External Calibration	
Close	

Figure 7-5 Add Predefined Reasons for this Audit Map Dialog



English	Translation
Delete	
Available Reasons	
New Reason	
Add	
OK	
Cancel	

Revision History

Revision	Reason for Change	Date
A	First release of document.	May 2014
B	Changed AB SCIEX to SCIEX where required. Updated the copyright page. Changed the company logo to SCIEX Diagnostics. Updated the screen shot in Figure 5-1 and the content in the associated table.	June 2017