MultiQuant™ MD 3.0.3 Software

Reference Guide

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Contents

Introduction to the Software 1

This document describes the functionality available in the MultiQuant™ MD software.

Access to the software is based on the role assigned to the user in the Analyst® MD software. Make sure that each user is assigned the correct access to the software.

Only the English version of the following Microsoft operating systems are supported:

- Windows 7 (32-bit and 64-bit) with SP1
- Windows 10

CAUTION: The format for numbers, currencies, dates, and time must be set to English (United States). Setting the format to a different value may result in erroneous data.

MultiQuant™ MD software with audit trail and security features requires the full license and the Analyst® MD software be installed.

The controlled ways to output data from the software are exporting Results Tables, transferring to LIS, and reporting. The other sources of output data such as copying and pasting from Results Tables are not controlled. Users should not use those uncontrolled output methods for regulated purpose.

Note: MultiQuant™ MD software uses the Analyst® MD software screen lock information. No additional setup is required for the MultiQuant™ MD software.

Note: The file and folder structure must be maintained to be able to view chromatograms. If data must be moved, then move the whole project, maintaining the file structure.

Software Help

The software has tool tips and error messages that provide additional information about the software functionality.

- If a field is not available, then move the cursor over the field to display tool tips that explain why the functionality is not available. Additional information includes how to enable the field or which security setting is required to enable the field.
- Error messages include information on the security settings required to use the functionality.

File Types

Table 1-1 Software File Types

File Type	Description
*.qsession	MultiQuant software Results Table. Holds quantitation audit trail data.
*.qmethod	MultiQuant software quantitation method.
*.qmap	MultiQuant software audit map.
*.mqcal	External calibration file.
*.cset	Column settings file.

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File Menu 2

Table 2-1 File Menu Options

Menu Option	Description
New Results Table	Quantitates a data set and then creates a Results Table. Select the data files to process as well as the quantitation method to apply. Refer to Results Table Dialogs on page 43.
New Quantitation Method	An empty quantitation Method Editor is created after the sample is selected. Typically, the user creates a method as part of the New Results Table wizard. However, this command is useful if the user wants to create a method but does not want to immediately apply it to a collection of samples creating a Results Table. • The navigation pane shows the subfolders, wiff files, and samples available in the **Data** folder for the selected project. • Expand individual folders to see any subfolders or wiff files. Expand the wiff file to show the available samples.
Open Results Table	Opens a previously saved Results Table. After selecting the command, a standard **Open** dialog opens. Refer to Results Tables on page 37.
Open Quantitation Method	Opens a previously saved quantitation method. After selecting the command, a standard **Open** dialog opens. Refer to Quantitation Method Editor on page 83.
Save	Used to save the active Results Table or Quantitation Method Editor to a file. If the Results Table or Quantitation Method Editor has never been saved, then the user is prompted for the filename. Otherwise the previous version is overwritten.
Save As	Used to save the active Results Table or Quantitation Method Editor to a new file.
Recent Results Table	Contains submenu items for each recently used Results Table. Select one of the items to open the corresponding file.
Recent Quantitation Methods	Contains submenu items for each recently used quantitation method. Select one of the items to open the corresponding file.

Table 2-1 File Menu Options (continued)

Menu Option	Description
Import	Creates a new quantitation method from a text file. Typically, the user creates a method manually using the New Quantitation Method command (refer to Quantitation Method Editor on page 83) or as part of the process of creating a new Results Table (refer to Results Tables on page 37). This command is useful if the user wants to create or modify a quantitation method. In this case, create a method manually and then use the **Quantitation Method as Text** command.
Export	Contains commands for exporting quantitation methods as .qmethod or .txt files. Refer to Export Submenu on page 11. The controlled ways to output data from the software are exporting Results Tables, transferring to LIMS, and reporting. The other sources of output data, such as copying and pasting from Results Tables, are not controlled. Users should not use those uncontrolled output methods for regulated purposes.
Transfer to LIMS	A LIMS license file is required to activate the feature. Refer to Transfer to LIMS on page 14.
Export and Save Results Table	Exporting Results Tables is one of the controlled methods for data output.
Create Report and Save Results Table	Creates a report in Microsoft Word using the Reporter software. Refer to Reports on page 134. In the event of creating a custom template, the user is responsible for validating the template. The user can edit the number format in the report template editor. If the number format is not specified in the template, then the format in the **Results Table Column Setting** are used in the report.
Exit	Exits the program. The user is prompted to save any unsaved data.

Import a Quantitation Method

1. Click **File > Import > Quantitation Method from Text.**
2. Select the text file.
3. Select a representative sample.

   The Quantitation Method Editor opens.
4. Save the method in the *.qmethod format so that it can be subsequently used to quantitate a new data set.

Export Submenu

The controlled ways to output data from the software are exporting Results Tables, transferring to LIMS, and reporting. The other sources of output data such as copying and pasting from Results Tables are not controlled. Users should not use those uncontrolled output methods for regulated purpose.

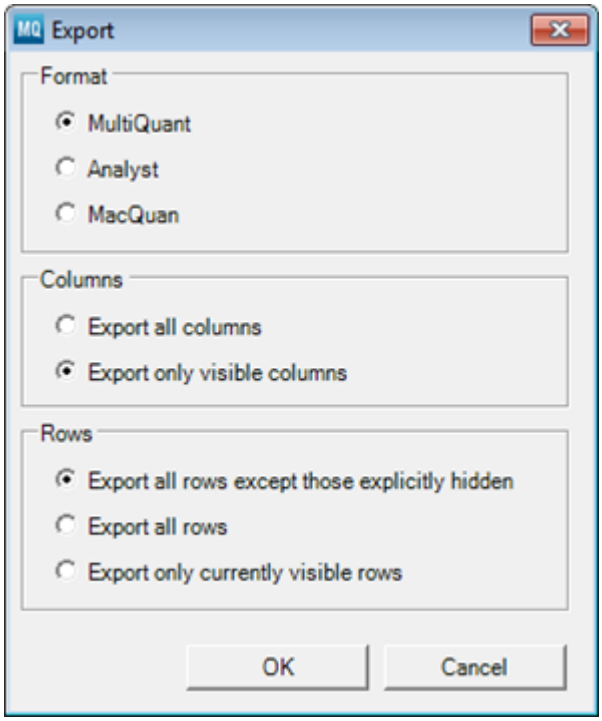
Table 2-2 Export Menu Options

Menu Option	Description
Results Table-Metric	Creates a tab-delimited text file containing the information from the active Results Table. Refer to Export Results Table-Metric on page 13.
Results Table's Quantitation Method as *.qmethod	Exports the quantitation method to a new file. When a Results Table is created, a copy of the quantitation method used to generate the table is saved internally with the table. This is useful if the original quantitation method was deleted or modified and the user wants to apply the original method to a new batch of samples creating a Results Table.
Results Table's Quantitation Method as Text	Exports a copy of that method in a text format. When a Results Table is created, a copy of the quantitation method used to generate the table is saved internally with the table.
Quantitation Method as Text	These files contain a header row and a row for each component (analyte or internal standard). There is a column for the component name, the mass range, each of the integration parameters, and so on. Header rows must not be changed nor should columns be added or deleted if the quantitation method is to be imported into theMultiQuant™ MD software. If the header row for a column that specifies an integration parameter is changed, or the column itself is deleted, the default value as specified in the User Integration Defaults for that integration parameter will be applied for all components. If the header row for any other column is changed or deleted, the method will not be imported. The user should open the method and confirm that all required changes are present in the imported quantitation method. Refer to Table 2-1.

Export Results Tables

Note: The manufacturer assumes no responsibility or contingent liability including indirect or consequential damages, after data has been exported from the software. The Results Table is exported in full precision, regardless of the number format in the column setting.

Figure 2-1 Export Dialog



Label	Description
Format	
MultiQuant	Select to export in full precision. In this format the text file contains a header row that uses the same column names as displayed in the **Results Table**. This is the recommended format to export **Results Tables**.
Analyst	Select to export in the precision defined in the column setting. This format is the same as exported by the Analyst® MD software quantitation **Results Tables**. The difference between this format and the previous format is that the column headers use slightly different names in some cases (to match the Analyst® MD software format) and there are additional header rows for each analyte describing the calibration.
MacQuan	This format is similar to the Analyst® MD software except that the column header names match those used by the MacQuan quantitation package.
Columns	
Export all columns	Select to export all possible fields, including those columns that are currently hidden in the **Results Table**.

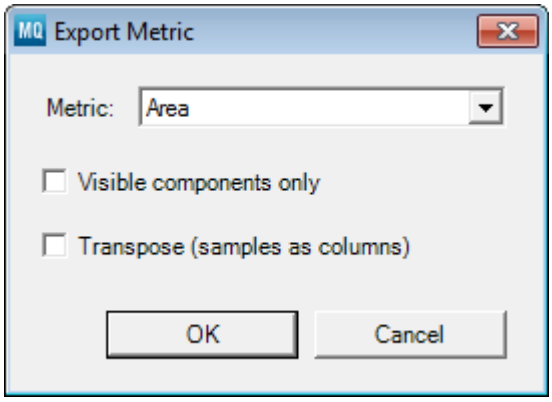
Label	Description
Export only visible columns	Select to export only those columns that are currently shown in the **Results Table**. The user can also select which columns are visible using the **Results Table Column Settings** command. Refer to Results Table Right-Click Menu on page 39.
Rows	
Export all rows except those explicitly hidden	Select to export all rows except those that are hidden due to specific filtering. Refer to Software Icons on page 156. Rows that are hidden due to **Sample Type** filtering or **Component** filtering are exported.
Export all rows	Select to export all rows (that is, all components for all samples).
Export only currently visible rows	Select to export only those rows that are currently displayed in the **Results Table**. Rows that are hidden due to **Sample Type** filtering or **Component** filtering are not included.

Export Results Table-Metric

Note: The manufacturer assumes no responsibility or contingent liability including indirect or consequential damages, after data has been exported from the software. The **Results Table** is exported in full precision, regardless of the number format in the column setting.

Used to create a tab-delimited text file containing the information from the active Results Table.

Figure 2-2 Export Metric Dialog



Label	Description
Metric	Select the field to export. Refer to Results Table Columns on page 54.
Visible components only	If this option is selected, then only those components for which at least one corresponding row is currently visible in the Results Table are exported to the file. If this option is not selected, then information is exported for all components.
Transpose (samples as columns)	If this option is selected, then the resulting file has a column for each sample and a row for each component (analyte or internal standard). If this option is not selected, then there is a column for each component and a row for each sample.

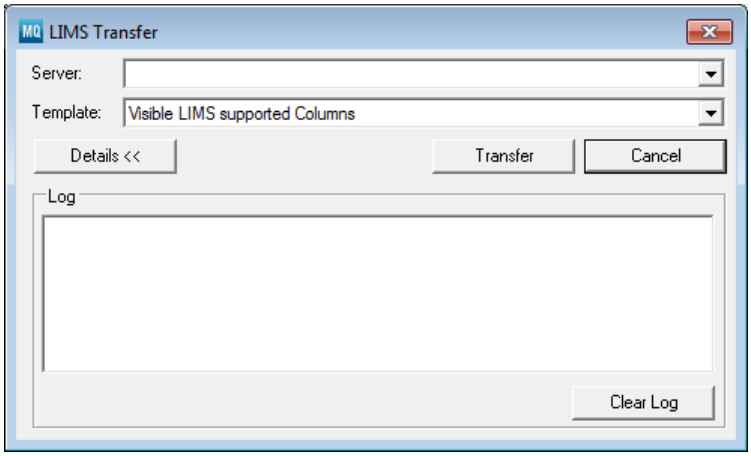
Transfer to LIMS

This command is only available when a Results Table is open. A LIMS license file is required to activate the feature.

The controlled ways to output data from the software are exporting Results Tables, transferring to LIMS, and reporting. The other sources of output data such as copying and pasting from Results Tables are not controlled. Users should not use those uncontrolled output methods for regulated purposes.

1. Click **Help > Install License** to activate a license.

Figure 2-3 LIMS Transfer Dialog



2. Type the server name in the **Server** field in the following format: **http:\\server IP address;port number**.
3. Select a template from the **Template** list.
4. Click **Transfer**.

Edit Menu 3

Table 3-1 Edit Menu Options

Menu Option	Description
Clear	Clears the current selection. This applies when the **Components** tab of the **Quantitation Method Editor** has one or more selected rows.
Copy	When the **Results Table** is active, this command copies the selected portion of the table to the clipboard. When the **Peak Review** or **Calibration** plot is active, a picture of the plot is copied.
Paste	When the **Results Table** is active with an editable selected area, this command pastes cells or columns from the clipboard.
Copy Entire Table	When a **Results Table** or **Statistics Table** is active, this command copies all data to the clipboard. In the case of a **Results Table**, only the currently visible rows and columns are copied.
Fill Down	When the **Results Table** is active with an editable selected area, this command replicates the information in the first selected row to all subsequent selected rows.
Select all Rows	Selects all rows in the currently active **Results Table** or **Statistics Table**. This is useful if the user subsequently wants to apply a command, such as **Copy**, that operates on the selected rows.
Modify Results Table Method	Makes changes to the quantitation method associated with the currently active **Results Table**. This is useful if the user wants to add or remove components. To modify integration parameters only, use the **Update Quantitation Method for Group**. Refer to Peak Review on page 62. When the command is selected, the **Quantitation Method Editor** dialog opens. Data is re-processed and the **Results Table** updates to show the data. Refer to Quantitation Method Editor on page 83 and Results Table Dialogs on page 43. Reapplying the **Quantitation Method** overwrites all manually modified peaks for the specified component and then clears check boxes in the **Modified** column in the Results Table.

Table 3-1 Edit Menu Options (continued)

Menu Option	Description
Project Integration Defaults	Sets the default peak-finding parameters that are used when creating a quantitation method. If there are more than a few components, set the default values based on the chromatography so that they do not need to be adjusted individually for every component. However, no one set of parameters is likely to be ideal for all components, so it might be necessary to adjust some of the parameters individually for some of the components. Refer to Integration Algorithm Parameters on page 122.
Project Units & Calibration Defaults	Sets the default concentration units and regression parameters that are used when creating a quantitation method. The user can also set these parameters when creating the method itself. However if the same settings are used, then it is easier to set the default values after using this command. Refer to Project Units & Calibration Defaults on page 18.
Project Secure Export Settings	If selected, then data in the text file is encrypted during export. Set a password to enable encryption. Refer to Project Secure Export Settings on page 18.
Enable Project Modified Peak Warning	By default not selected. If selected, when a user makes a change to a chromatogram in a **Results Table** and then saves the changes, a warning message opens, indicating that a change has been made. The user has an option to continue saving or to return to the **Results Table**. Refer to Modify Results Table Method on page 17.

Table 3-1 Edit Menu Options (continued)

Menu Option	Description
Cache Chromatograms for Faster Peak Review	When this feature is enabled, each time an extracted ion chromatogram (XIC) is calculated for a particular sample and component, it is saved for future use as long as the associated Results Table remains open. For example, if the user creates a **Results Table** when this feature is enabled, then the chromatograms in the **Peak Review** pane appear quickly because they have been previously cached during the initial integration process to create the **Results Table** and do not need to be recalculated from the information in the wiff file. If the user opens a previously saved **Results Table**, then the individual chromatograms must be calculated the first time they are shown in the **Peak Review** pane. However, returning to a particular previous chromatogram will be faster. There should be sufficient computer memory to cache all chromatograms. However, for very large sample sets with a large number of analytes, this option should be disabled to avoid out-of-memory messages.
Cache all Chomatograms Now	When the Cache **Chromatograms for Faster Peak Review** command is enabled, this command is used to calculate and then cache all chromatograms for the active **Results Table**. For a large data set, this command might take some time to execute. However, after it completes, all chromatograms are cached and the peak review process is faster. The command can be stopped if required. Perform this operation if many chromatograms will be reviewed. If the **Cache Chromatograms for Faster Peak Review** option was initially enabled, this operation does not need to be performed again after creating a **Results Table** because the chromatograms are already cached. This command is useful after opening a previously saved **Results Table**.

Modify Results Table Method

Makes changes to the quantitation method associated with the currently active Results Table. This is useful if the user wants to add or remove components. To modify integration parameters only, use the **Update Quantitation Method for Group** command. Refer to Update Quantitation Method for Group on page 70.

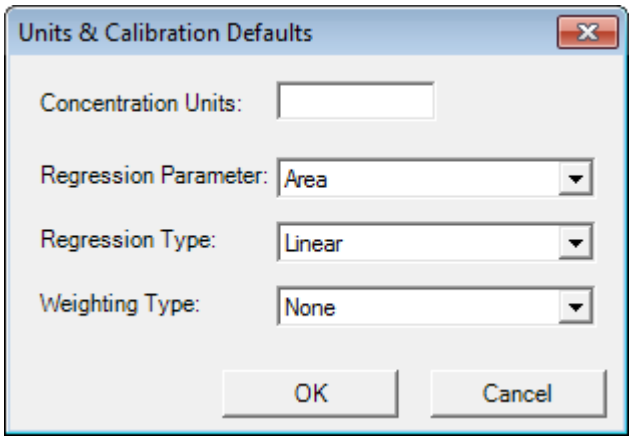
When the command is select, the Quantitation Method Editor dialog opens. Data is re-processed and the Results Table updates to show the new data. Refer to Quantitation Method Editor on page 83.

Reapplying the Quantitation Method overwrites all manually modified peaks for the specified component and then clears check boxes in the **Modified** column in the **Results Table**.

Project Units & Calibration Defaults

Set the **Concentration Units**, **Regression Parameter** (Area or Height), **Regression Type**, and **Weighting Type**. The various regression and weighting types are described in Regression Equations on page 128.

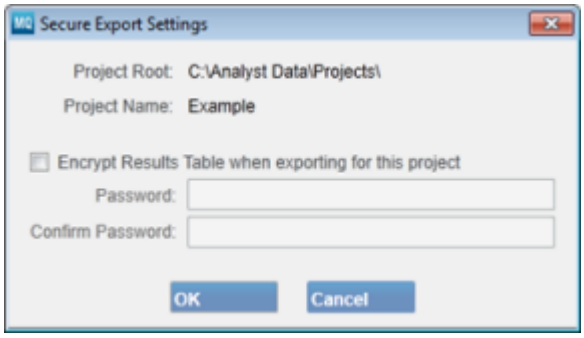
Figure 3-1 Units & Calibration Defaults



Project Secure Export Settings

Data in the text file is encrypted during export. Set a password to enable encryption. Refer to Figure 3-2.

Figure 3-2 Secure Export Settings Dialog



Process Menu 4

Table 4-1 Process Menu Options

Menu Option	Description
Add Samples	Adds additional samples to a currently active **Results Table**. Refer to Select Samples on page 43. A progress bar is shown while the new samples are integrated and added to the existing table. The user must have the **Add samples to Results Table** permission enabled to perform this task.
Remove Selected Samples	Removes selected samples from a currently active **Results Table**. The user must have the **Remove samples from Results Table** permission enabled to perform this task.
Show Only Outliers	Shows the rows that contain outliers. Click **Process > Show Only Outliers.** To show all the rows, click **Process > Show Only Outliers** again.
Go to Next Outlier	Advances to the next outlier in the **Results Table**. Click **Process > Go to Next Outlier.**
Export Calibration and Save Results Table	Saves a copy of the calibration equation for all analytes associated with the active **Results Table** to an external file (*.mqcal). This allows the calibration from one set of standard samples to be applied to other samples that are not part of the same **Results Table**. Refer to Export Calibration on page 20.
Import External Calibration	Applies a previously exported calibration to the active **Results Table**. An alternative to using this command is to specify the external calibration file from the **New Results Table** wizard as described in Define Integration on page 49. Refer to Import External Calibration on page 20.
Remove External Calibration	Removes a previously applied external calibration from an active **Results Table**.

Export Calibration

Saves a copy of the calibration equation for all analytes associated with the active **Results Table** to an external file (*.mqcal). This allows the calibration from one set of standard samples to be applied to other samples that are not part of the same **Results Table**.

The typical workflow is:

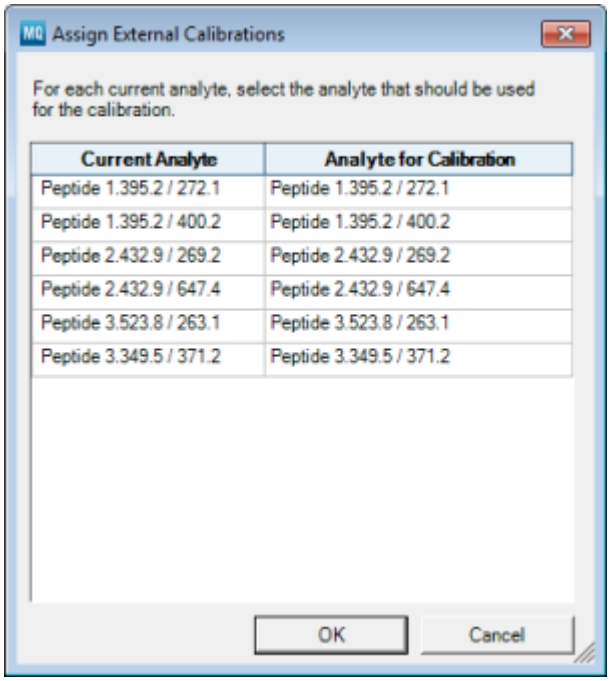
1. Create a new **Results Table** containing only the **Standard**.
2. Use the **Peak Review** pane to make sure that integration was successful.
3. Use the **Export Calibration** command to save a copy of the calibration.
4. Create a new **Results Table** containing samples of unknown concentration.
5. Apply the previously exported calibration to the new table by using the **Import External Calibration** command or by specifying the calibration file.
6. Repeat steps 4 and 5 as required.

If the original **Results Table** (with the **Standard** samples) is changed, then any previously exported calibrations are not automatically updated. The **Results Table** must be exported again.

Import External Calibration

If the same analyte names are used in the current **Results Table** as in the exported calibration, then the dialog is completed automatically and the user can click **OK**. If the analytes in the current **Results Table** are assigned to specific groups and if analytes in the exported calibration are assigned to groups with the same names, then the dialog is completed automatically. If there are more than a few analytes, then use the same analyte names in both cases or use consistent **Group** names.

Figure 4-1 Assign External Calibrations Dialog



Label	Description
Current Analyte	Contains an entry for each analyte from the quantitation method for the current **Results Table**.
Analyte for Calibration	Contains a list of the names of all analytes available in the external calibration file. For each of the current analytes, select the corresponding external analyte from which the calibration is taken.

Audit Trail Menu 5

Note: The audit map is added to the session when the **Results Table** is first created. It cannot be changed after it has been added.

Table 5-1 Audit Trail Menu

Menu Item	Description
Audit Trail Viewer	Opens the **Audit Trail Viewer**.
Audit Map Manager	Selects, modifies, and activates **Audit Maps**.
View Session Audit Map	Opens the current map of the active **Results Table**.

Audit Trail Viewer

The Audit Trail Viewer shows the complete history of a particular sample in the Results Table. Results Tables are saved in the <drive>:\Analyst Data\Projects\<project name>\Results folder.

Note:
The Results Table should not be hidden when performing other actions. For example, as saving an Audit Trial.

To maximize another pane, such as the Peak Review pane, to view the data better, use the **Toggles tab mode** button located on the toolbar.

Using the **Audit Trail Viewer**, users can:

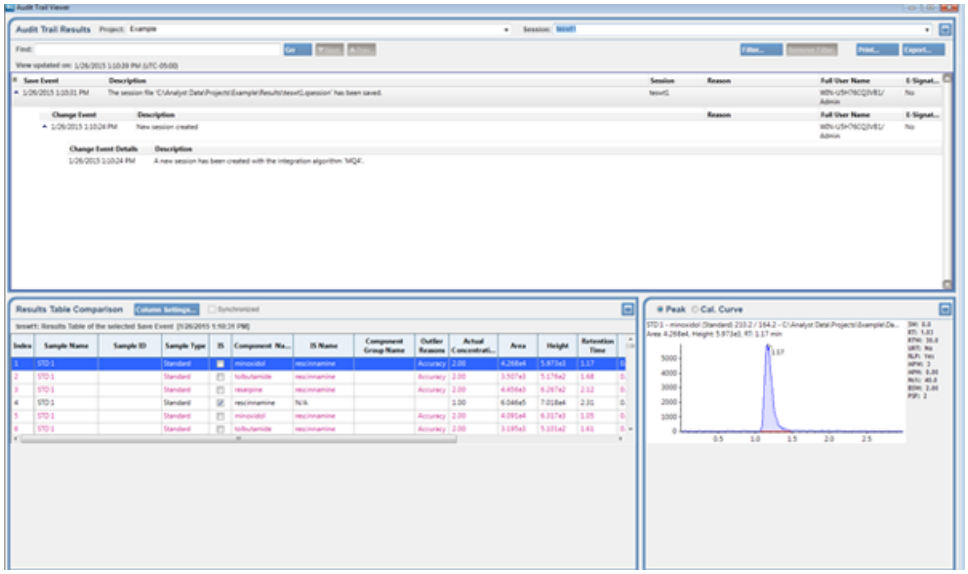
- View the audit trail records for each **Results Table**.
- Perform a keyword search, which highlights every occurrence of the text.
- Filter the audited events in the software audit trail based on a set of specified criteria.
- Export the audit trail records to a txt file. Exported files can be edited.
- Print to a secured PDF.

View the Audit Trail Results in the Audit Trail Viewer

1. Open a Results Table.

2. Click **Audit Trail > Audit Trail Viewer.**
3. To change projects, click the **Projects** list and then select another project.
4. To view other sessions, click the **Sessions** list and then select another session. Users can also select to view all the sessions in the project at the same time.

Figure 5-1 Audit Trail Viewer



Label	Description
Project	Select a project from the list.
Session	Select a session file
Find	A keyword search without filtering. Highlights every occurrence of the text.
Go	Click to start the search.
Next	Click to move to the next word.
Prev	Click to move to the previous word.
Filter	Click to show only the events that match the selected criteria.
Remove Filter	Click to remove the filter.
Print	Click to print the audit trail
Export	Click to export the audit trail.

Label	Description
Save Event	When a session file is saved, a save event is created. The save event captures any changes made from the previous save event as well as every value in the **Results Table**.
Description	Details of the change event.
Session	Shows the name of the session file.
Reason	Shows the reason for the change made to the **Results Table**.
Full User Name	Shows the name of the user who made the change to the **Results Table**.
E-Signature	Indicates if changes to the **Results Table** were accepted.
Column Settings	Click to show or hide columns in the **Results Table**.
Synchronized	Select to have both **Results Tables** scroll horizontally simultaneously.
Previous version	Shows the previous version of the selected session file.
Peak	Click to show the peak of the selected sample.
Cal Curve	Click to show the calibration curve of the selected sample.

Perform a Keyword Search

Users can perform a keyword search, which highlights every occurrence of the text.

1. Open a Results Table.
2. Click **Audit Trail > Audit Trail Viewer.**
3. In the **Find** field, type the word to search for and then click **Go**.

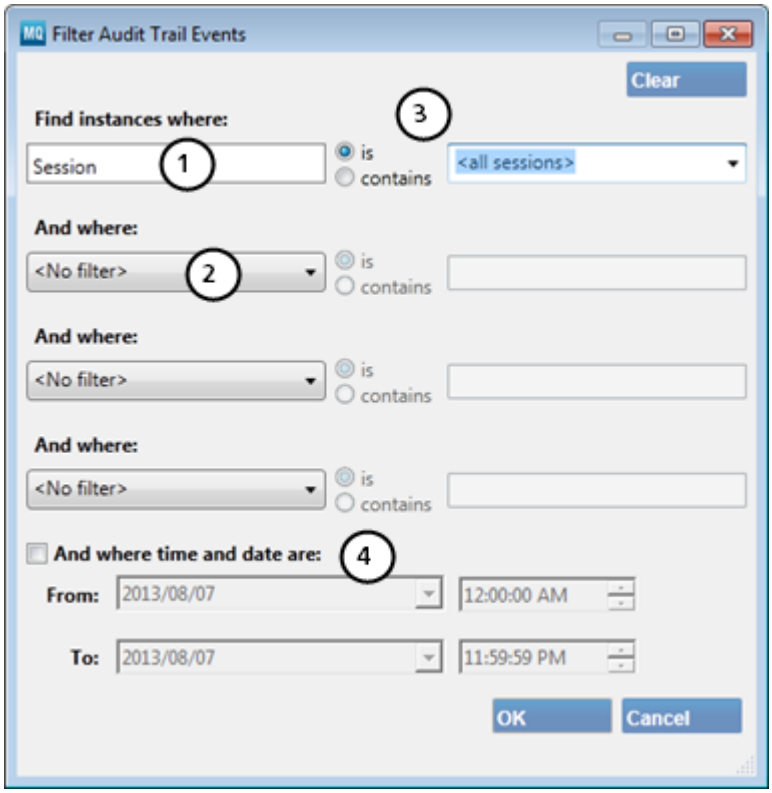
   If matches are found, then the **Find** field turns green, the number of matches is shown, and the word is highlighted in yellow. If matches are not found, then the **Find** field turns pink.
4. Use the **Next** and **Prev** buttons to move between the matches.

Filter Audited Events

Users can filter the audited events in the audit trail based on a set of specified criteria.

1. Open a Results Table.
2. Click **Audit Trail > Audit Trail Viewer.**
3. Click **Filter**.

Figure 5-2 Filter Audit Trail Events Dialog



Item	Description
1	Name of the **Results Table** file. One **Results Table** file or all the **Results Table** files for the active project can be filtered.
2	**Description**: Type the partial or full event type. **Sample Name**: Type the partial or full sample name. **Full User Name**: Type the partial or full name of the user. **E-Signature**: Select Yes or No. **Reason**: Type the partial or full reason.
3	**is**: Use to filter on a specific word or phrase.
4	**contains**: Use to filter on a partial word or phrase.
5	**Date**: Use to filter on events that occurred on a specific date and time.

4. In the **Filter Audit Trail Events dialog**, use the lists to select filter criteria.

Note: The Results Table field cannot be edited.

5. Click **Clear** to reset the filter criteria to **No filter**.
6. Click **OK** to filter the events.

Tip! To remove the filter, in the **Audit Trail Viewer** click **Remove Filter**.

Export the Audit Trail Viewer

1. Open a Results Table.
2. Click **Export** and then type a file name.

   The file is exported as a tab-delimited text file.

Note: Only the saved events portion of the Audit Trail Viewer is exported.

Print the Audit Trail Viewer

1. Open a Results Table.
2. Click **Print** and then select a printer.

   Users can print a secure PDF using pdfFactory.

Note: Only the saved events portion of the Audit Trail Viewer is printed.

Audit Trail Manager

The software groups quantitation audited events into audit trails. Audit trails are files that store records of the audited events. Audit trails, combined with files such as wiff files, quantitation methods, and **Results Table** files, constitute valid electronic records that can be used for compliance purposes.

The **Audit Trail Manager** software maintains all of the events as defined in the audit map. The software captures the electronic signatures and reasons, including the user, date, and details of the changes. It also records additional information, such as comments, according to the audit map.

Tip! A session file contains the **Results Table**, a copy of the quantitation method, a copy of the Audit Map at time of creation, as well as the entire audit trail for the entire session.

When the software creates or modifies a qsession or qmethod file, the event is captured in the **Project Audit Trail** on the **History** tab in the Analyst® MD software. The following events are captured:

- Quantitation method file has been created.
- Quantitation method file has been modified.
- Quantitation **Results Table** has been created.
- Quantitation **Results Table** has been modified.

If the **E-signature** or **Reason Prompt** is selected for creating or modifying the quantitation method file, then the **Audit Trail** dialog generated by the Analyst® MD software opens in the MultiQuant™ MD software.

Table 5-2 Audit Trails

Audit Trail	Examples of Events Recorded
Quantitation Audit Trail (one per Results Table)	Changes to: • Creation and modification of session files. • Sample information. • Peak integration parameters.

About Audit Maps

The MultiQuant™ MD software maintains all of the change history to the processing settings information associated with the quantitation results. The software audits all of the events according to the active project audit map, and it captures all of the electronic signatures and link, to respective records.

Create an Audit Map

The software installs several audit maps. View the audit maps to decide whether modifying one or more of them would be easier than creating a completely new one. Creating or modifying audit maps are audited events in the Analyst® MD software project audit trail.

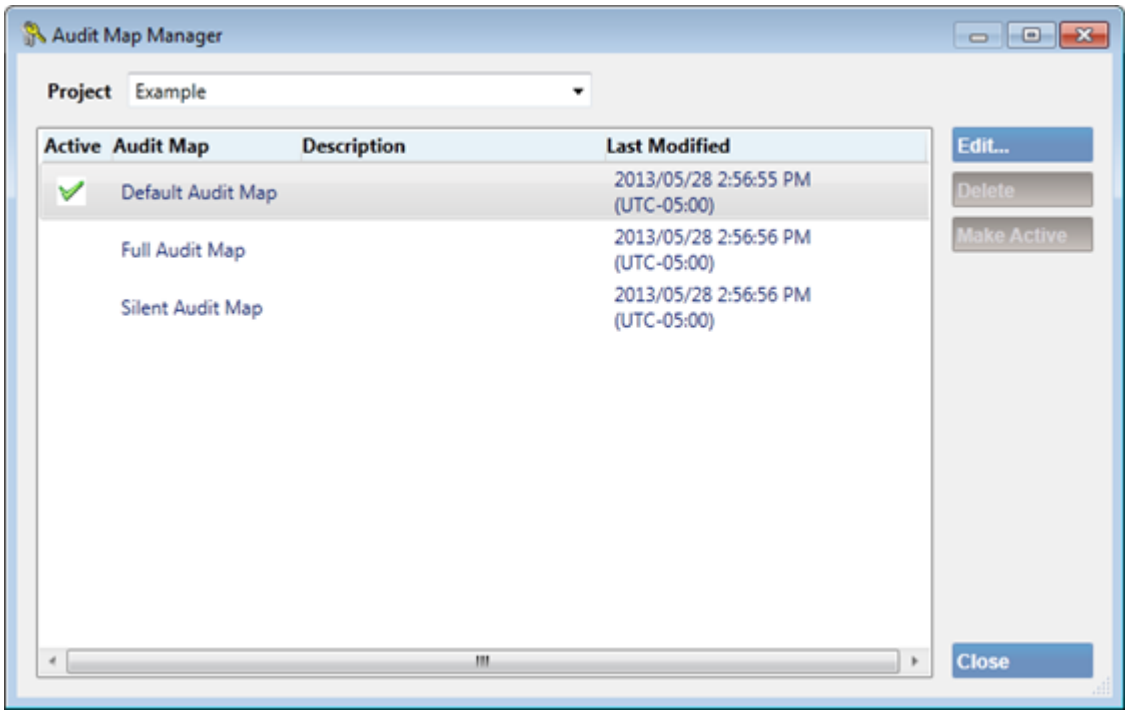
CAUTION: If two users are modifying the same audit map at the same time, then only the changes made by the user who saved the file last are used.

The active audit map for the project determines which events are recorded in the audit trail for any **Results Tables** that are created.

Note: After a **Results Table** is saved, the active audit map is saved with the **Results Table** and the audit map cannot be modified.

1. Click **Audit Trail > Audit Map Manager.**

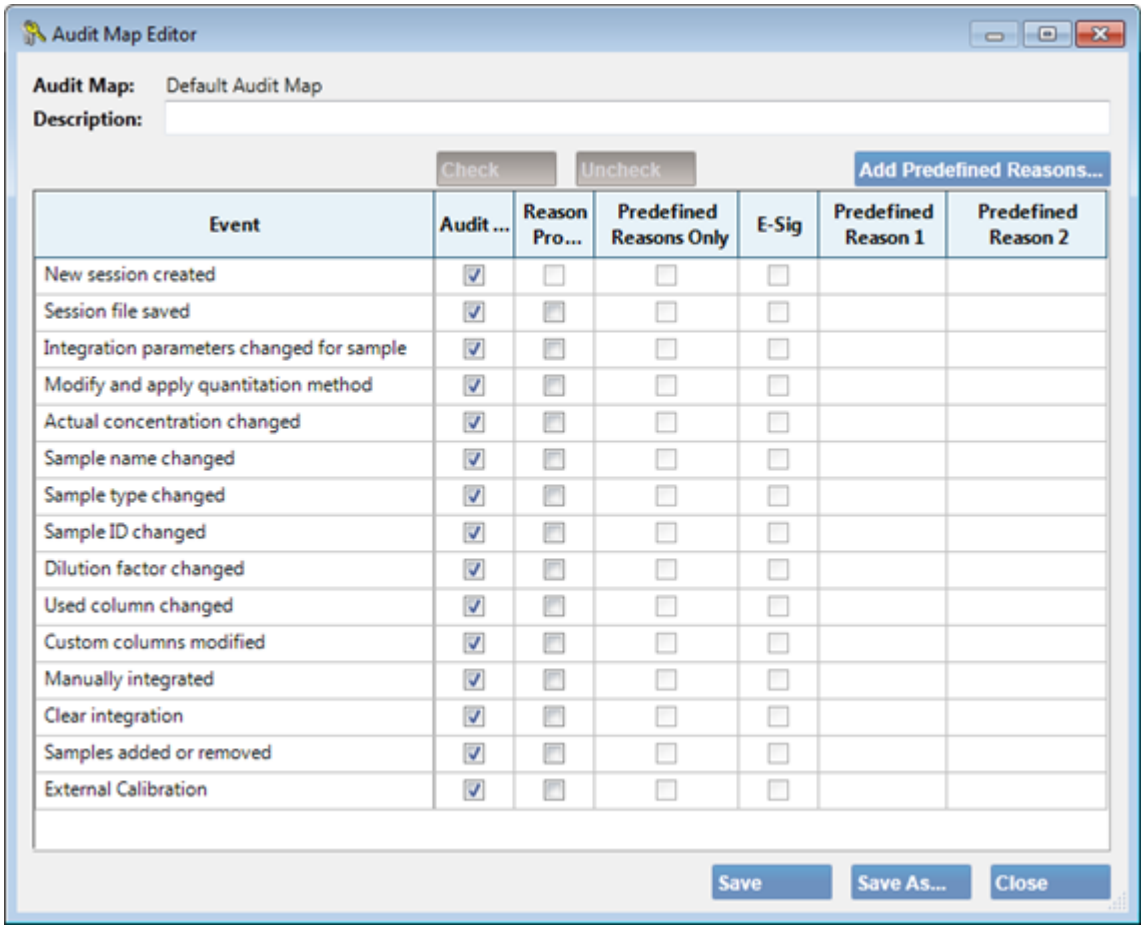
Figure 5-3 Audit Map Manager



Label	Description
Project	Select a project from the list.
Edit	Click to edit the active audit map.
Delete	Click to delete the selected audit map.

2. In the **Project** list, select a project for which to create an audit map.
3. Select an audit map and then click **Edit**.

Figure 5-4 Audit Map Editor



Label	Description
Description	Type a description of the audit map.
Check	Click to select a check box.
Uncheck	Click to clear the check box.
Add Predefined Reasons	Click to add a predefined reason to the list.

4. Type a description of the audit map in the **Description** field if required.
5. In the **Audit Map** table, configure each event as follows:

- To audit the event, select the check box in the **Audited** column.

  Tip! To fill consecutive cells in a column with the check box value, press **Ctrl** or **Shift**, click the cells, and then click **Check**.

- To have the operators type a custom reason or choose a predefined reason, select the check box in the **Reason Prompt** column.
- To have the operators only select a predefined reason for the change when the event occurs, select the check boxes in the **Reason Prompt** and the **Predefined Reasons Only** columns. In the **Predefined Reason** _ columns, select up to ten reasons.

  Tip! To add a predefined reason, click **Add Predefined Reasons**.

- To require electronic signatures for the event, select the check box in the **E-Sig** column.

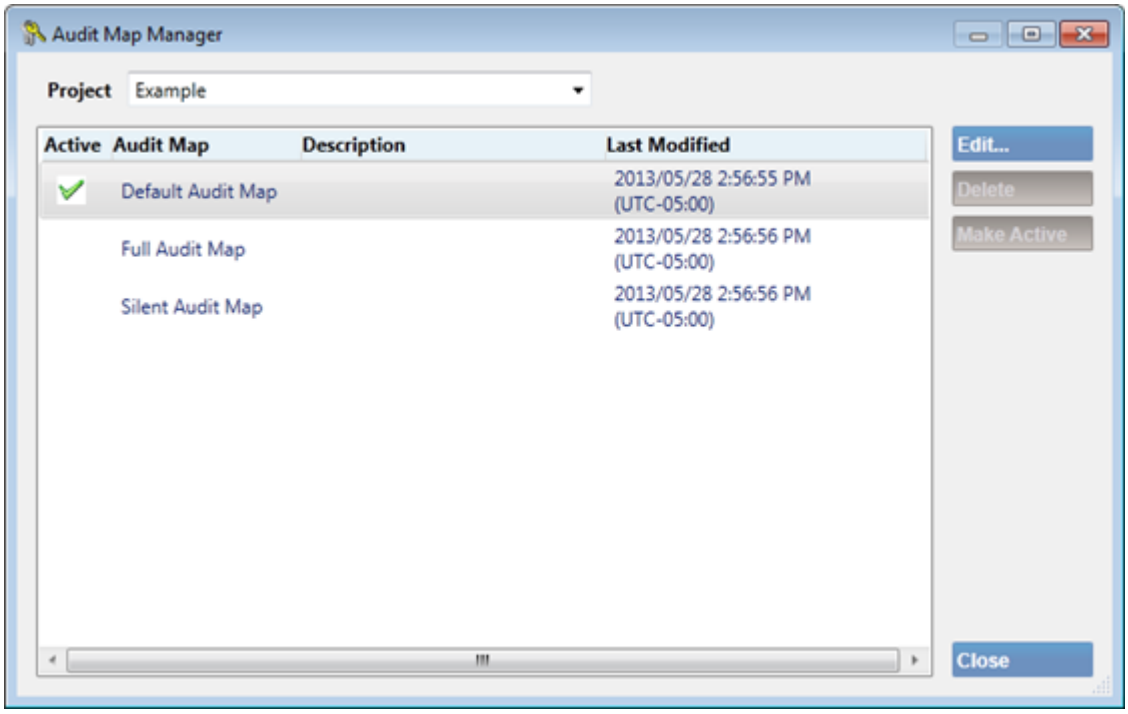
6. Click **Save As** and then type a name in the **Save Audit Map As** dialog.
7. Click **Save**.
8. Click **Close** on the **Audit Map Editor** dialog.
9. Click **Make Active**.

   When an audit map is applied, it becomes the active audit map. The audit configuration in the active audit map determines which events are recorded in the audit trails from this point on.

Change the Audit Map

1. Click **Audit Trail > Audit Map Manager.**

Figure 5-5 Audit Map Manager



Label	Description
Project	Select a project from the list.
Edit	Click to edit the active audit map.
Delete	Click to delete the selected audit map.

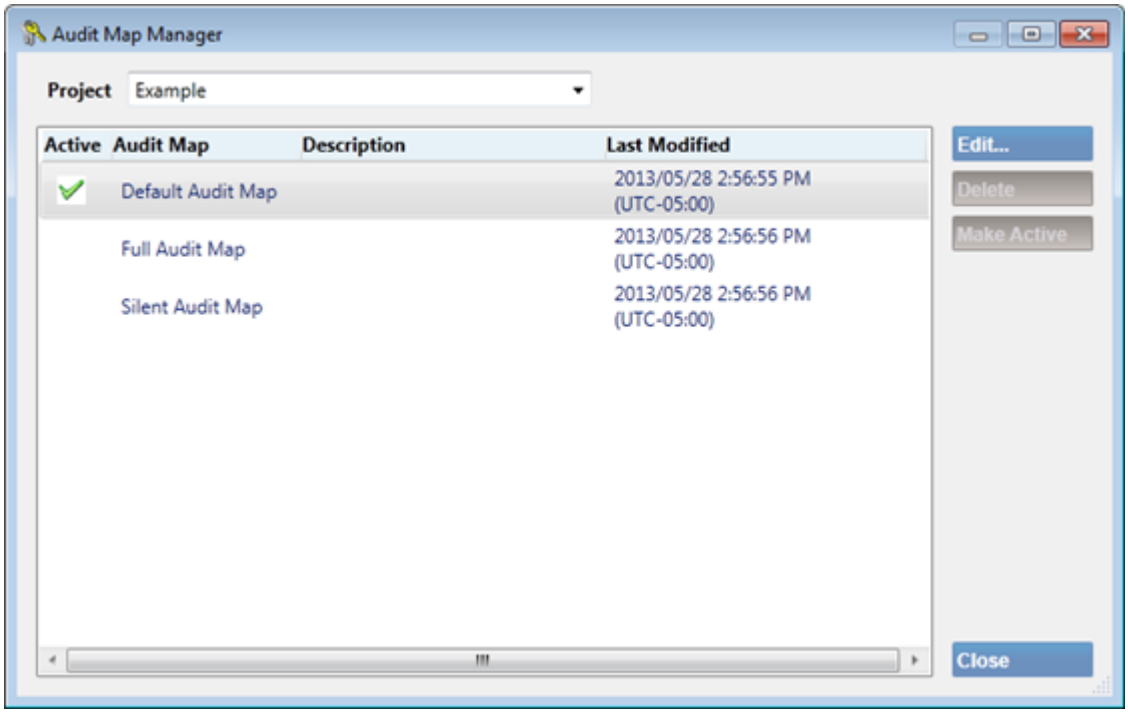
2. In the **Project** list, select a project for which to change the audit map.
3. Select another map and then click **Make Active**.
4. Click **Close**.

Edit the Audit Map

The following audit events are always recorded and are therefore not displayed in the **Audit Map Editor**: Print Report, Export Results Table, and Transfer to LIMS.

1. Click **Audit Trail > Audit Map Manager.**

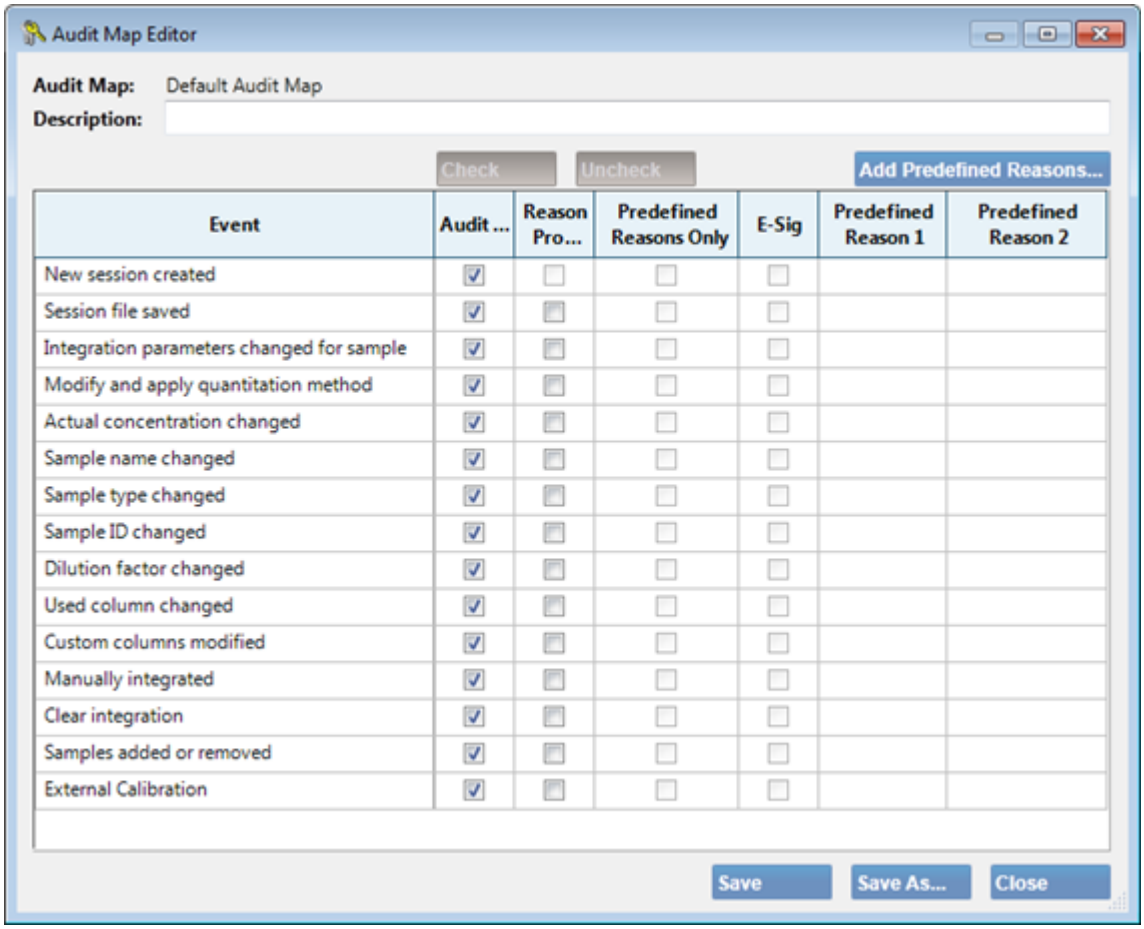
Figure 5-6 Audit Map Manager



Label	Description
Project	Select a project from the list.
Edit	Click to edit the active audit map.
Delete	Click to delete the selected audit map.

2. Select an audit map and then click **Edit**.

Figure 5-7 Audit Map Editor



Label	Description
Description	Type a description of the audit map.
Check	Click to select a check box.
Uncheck	Click to clear the check box.
Add Predefined Reasons	Click to add a predefined reason to the list.

3. Type a description of the audit map in the **Description** field if required.
4. In the **Audit Map** table, configure each event as follows:

- To audit the event, select the check box in the **Audited** column.

  Tip! To fill consecutive cells in a column with the check box value, press **Ctrl** or **Shift**, click the cells, and then click **Check**.

- To have the operators type a custom reason or choose a predefined reason, select the check box in the **Reason Prompt** column.
- To have the operators only select a predefined reason for the change when the event occurs, select the check boxes in the **Reason Prompt** and the **Predefined Reasons Only** columns. In the **Predefined Reason** _ columns, select up to ten reasons.

  Tip! To add a predefined reason, click **Add Predefined Reasons**.

- To require electronic signatures for the event, select the check box in the **E-Sig** column.

5. Click **Save**.
6. Click **Make Active**.

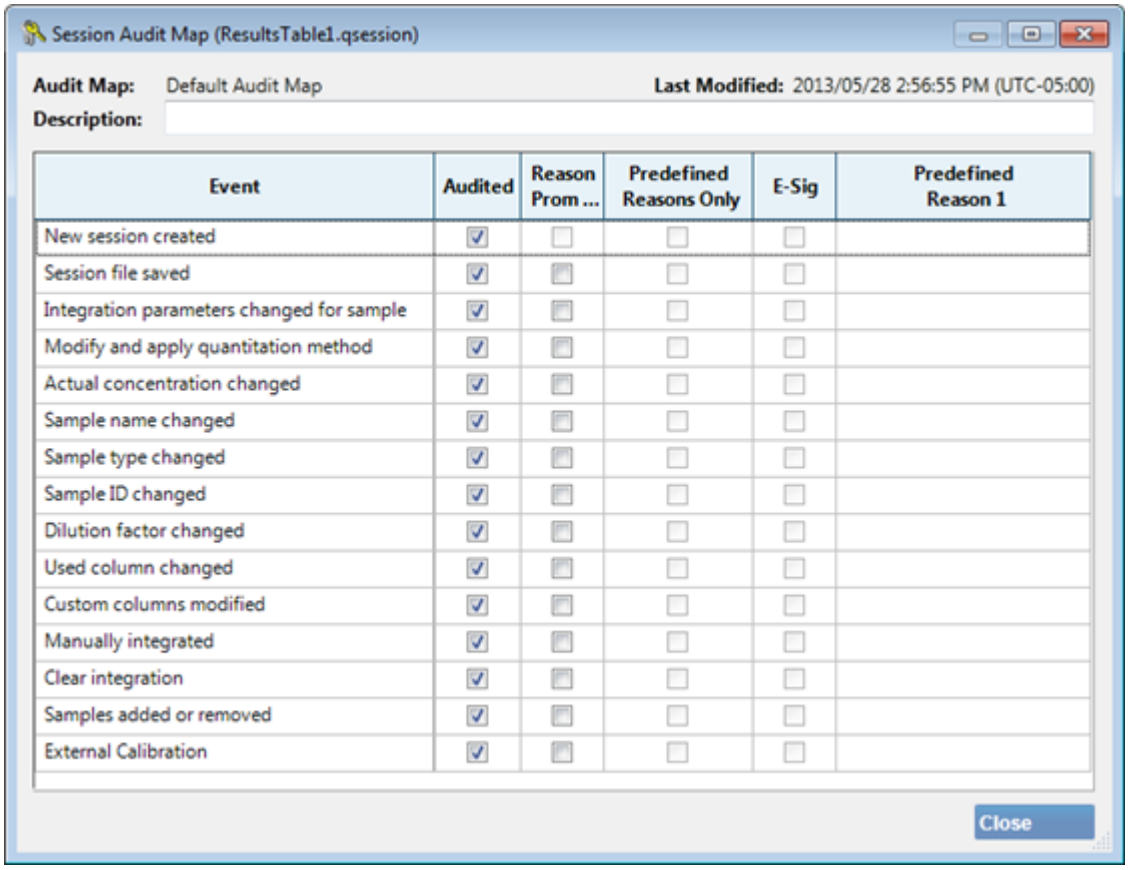
   When an audit map is applied, it becomes the active audit map. The audit configuration in the active audit map determines which events are recorded in the audit trails from this point on.

View the Embedded Audit Configuration

The audit configuration used for a Results Table is embedded in the Results Table file when the Results Table is created. This configuration cannot be changed. The timestamp displayed next to the audit map name indicates when the audit map used to embed the configuration was last saved.

1. Open a Results Table.
2. Click **Audit Trail > View Session Audit Map.**

Figure 5-8 Session Audit Map



Event	Audited	Reason Prom ...	Predefined Reasons Only	E-Sig	Predefined Reason 1
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	☑	☐	☐	☐	

Help Menu 6

With the exception of the **About** item, this menu contains the items listed in Table 6-1. These files are automatically installed and they can also be found in the <drive>:\Program Files\AB SCIEX\MultiQuant 3\Help folder.

Documents or folders (or shortcuts to them) can be copied to this Help folder to have them automatically appear in the menu.

Table 6-1 Help Menu

Menu Item	Description
Install License	Click to open the MultiQuant™ MD Activation dialog.
Verify Installation	Click to verify the files and installation.
Software Reference Guide	Describes the features and functionality of the software.
Software Release Notes	Provides information about the software as well as procedures for installing the software.
About	Shows the version of the program, copyright, and other program information, along with information about which license features are installed.

Results Tables 7

A **Results Table** is the starting point for data review and export. Use the **New Results Table wizard** or click **File > New Results Table** to create a Results Table. Refer to Results Table Dialogs on page 43.

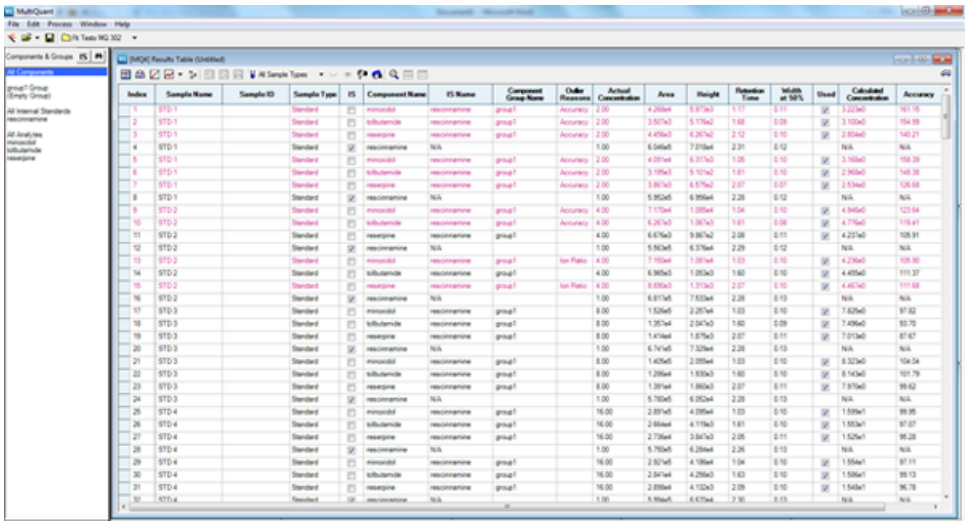
Note: The **Sample Name** and **Sample ID** columns cannot contain: \ / : * ? " < > |=.

The audit configuration used for a **Results Table** is embedded in the **Results Table** file when the **Results Table** is created. This configuration cannot be changed. The timestamp shown next to the audit map name indicates when the audit map used to embed the configuration was last saved.

Note: When moving data, move the whole project to maintain the file structure. If the file and folder structure is not maintained, then a **Results Table** or chromatograms cannot be viewed.

There is a separate row for each component for each of the originally selected samples.

Figure 7-1 Example Results Table



- The **IS**, **Component Name**, and **IS Name** columns contain information about the analytes.
- The selected check box indicates the internal standard for the sample.
- Select which columns are shown in the **Results Table** using the **Column Settings** dialog. Refer to Column Settings on page 40.

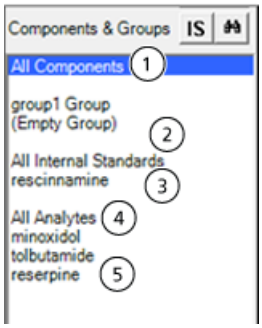
- Change the width of the columns by dragging the line separating the two column headings. This information is automatically saved and is applied when the user opens previously saved **Results Tables**.
- Change the order of the columns by clicking a column header and then dragging it to a new location. This information is automatically saved and is applied when the user opens previously saved **Results Tables**.
- Users can limit the Results Table so that it only shows rows corresponding to particular analytes or internal standards. Use the tool bar to limit the sample types that are shown. Refer to Components & Groups List on page 38 and Sample Type Filter on page 42.
- Certain operations, such as synchronization with the **Peak Review** pane, are applied to the currently selected row or rows. Select rows by clicking the area to the left of the first column.

Components & Groups List

When a **Results Table** is open, a list of the current components and groups is shown on the left side of the main window. Use this list to change which components are visible in the **Results Table** as well as in any linked **Peak Review** pane or **Calibration** plot.

Components are defined as a single transition or mass range. A Group is defined as the name of the group to which the component belongs.

Figure 7-2 Components & Groups List



Item	Label	Description
1	All Components	Click to view all available analytes and internal standards in the **Results Table** as well as the related **Peak Review** and **Calibration** if shown.
2	All Internal Standards	Click to view all internal standards and to hide all analytes. This item is not present if no internal standards are defined.
3	Specific Internal Standards	The name of each separate internal standard is included in the list. Click one of these items to view that internal standard and to hide all other components.

Item	Label	Description
4	All Analytes	Click to view all analytes and to hide all internal standards. This item is not included if no internal standards are defined.
5	Specific Analytes	The name of each separate analyte is included in the list. Click one of these items to view that analyte and to hide all other components.

Click an individual item in the list to display only the components for that item. Press **Shift** or **Ctrl** to select multiple items. This is useful to display, for example, two specific analytes only. Use the up and down arrow keys when the list is active to move through the items.

Tip! Make the list wider or narrower by dragging the right edge of the pane to the left or right.

The actual order of the rows in the Results Table is not affected by filtering. The Results Table is preset to be ordered first by sample and then by component, in the order indicated in the quantitation method. However, the table can also be sorted in a specific order as described in Software Icons on page 156.

Results Table Right-Click Menu

Right-click in the Results Table to access a context menu. The following commands are available.

Table 7-1 Results Table Right-Click Menu Options

Menu Option	Description
Column Settings	Use this command to edit the **Results Table** columns. The changes are only applied to the current **Results Table** unless it is saved as project default.
Add Custom Column	Adds a new editable column to the table. Populate the column by typing directly into the cells or by pasting content. Any text can be entered such as comments or the results of custom calculations.
Rename Custom Column	Renames an existing custom column. Before using this command, click the custom header to select the custom column.
Remove Custom Column	Use to delete an existing custom column. Before using this command, click the column header to select the custom column.
Apply Current Analyte's Actual Concentrations to All	Provides a shortcut for setting the **Actual Concentration** field for all analytes for samples of type **Standard** if there is more than one analyte and all analytes are present in these samples at the same concentration. Refer to Apply Current Analyte's Actual Concentrations to All on page 40.

Table 7-1 Results Table Right-Click Menu Options (continued)

Menu Option	Description
Apply Current IS's Actual Concentrations to All	Similar to the **Apply Current Analyte's Actual Concentrations to All** except that it applies to internal standards rather than analytes.
Set 'Used'	Use this command to perform absolute quantitation to determine whether a particular **Standard** sample should be used in the calculation of the calibration curve for a given analyte. The first two items are used to select or clear the **Used** field for the currently selected rows in the **Results Table**. The third and fourth items are similar except that the operation applies to all analytes for any samples corresponding to a selected row.
Set Peaks to 'Not Found' for Selected Rows	Use this command to clear the peak integration for the currently selected rows.

Apply Current Analyte's Actual Concentrations to All

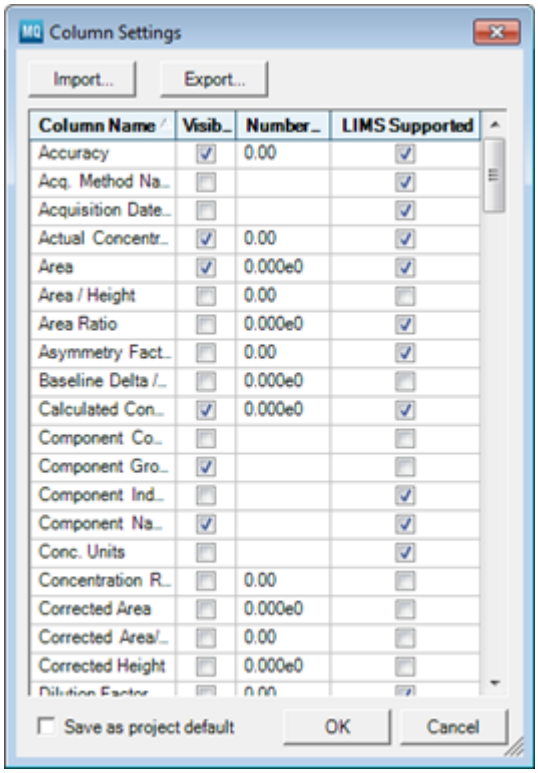
1. Use the Components & Groups List on page 38 to limit the table to only displaying one particular analyte.
2. Optionally use the **Sample Type Filter** to only view **Standard** samples. Refer to Sample Type Filter on page 42.
3. Specify the actual concentrations for the analyte, either by typing directly into the cells or by selecting the column and then selecting **Paste** if the concentrations are available elsewhere in a text format.
4. Click **Apply Current Analyte's Actual Concentrations to All**.
5. Return to viewing all components and all sample types as required.

Column Settings

If column names are truncated, then move the cursor over the field to display the column name in a tool tip.

For numerical fields, use the format 0.00 for non-scientific notations and use the format 0.00e0 for scientific notations. Change the decimal points to indicate the precision of the numbers that are shown. Only a period (.) can be used as a decimal separator. Digit grouping is not supported.

Figure 7-3 Column Settings Dialog



Field	Description
Import	Click to select a column settings file previously saved using **Export**. The dialog fields are updated to use the information from the selected file.
Export	Click to save the current dialog settings to a file. This enables the user to switch between different column settings.
Column Name	Shows the name of the columns in alphabetical order. Refer to Results Table Columns on page 54.
Visible	Select to make the column visible. Otherwise, the column is hidden.
Number Format	For numerical fields, use the format 0.00 for non-scientific notations and use the format 0.00e0 for scientific notations. For displayed precision, change the decimal points.
LIMS Supported	The rows that show LIMS Supported selected are predefined by the LIMS and the column selections cannot be changed.
Save as project default	Select to use the column settings in future Results Tables.

Sample Type Filter

Table 7-2 Sample Type Filter Descriptions

Filter Type	Description
All Sample Types	Shows all sample types.
Unknowns	Shows only Unknown samples, which are normal samples of unknown concentration. When Standard samples are used, their concentration is back-calculated from the calibration curve and reported in the Results Table as the Calculated Concentration. Refer to Regression Equations on page 128.
Standards	Shows only samples of known concentration. These samples are used for the creation of the calibration curve.
Quality Controls	Shows only Quality Control samples. These samples of known concentration are used to check the accuracy of the calibration curve but do not influence its actual construction.
Standards & QCs	Shows both Standard and Quality Control samples.
Unknowns, Standards & QCs	Shows Unknown, Standard, and Quality Control samples.
Blanks	Shows only Blank samples. These are generally samples that contain the internal standard compounds, if used, but no analytes, and that have been through the normal sample preparation procedure. These samples are not used in the construction of the calibration curve. To include them, select the Standard sample type and then set the Actual Concentration at 0.
Double Blanks	Shows only Double Blank samples. These are samples with neither internal standards nor analytes.
Solvents	Shows only Solvent samples. These are double blanks that have not been through the normal sample work-up procedure.
Blanks, Double Blanks & Solvents	Shows all of the blank sample types: Blank, Double Blank, and Solvent samples.

View Hidden Rows

In the **Results Table**, for any given component, rows are only seen for those samples for which the corresponding MRM transition is available. The unused rows, components with transitions not available for a given sample, are present in the table but they are hidden by default.

1. Show the **Peak Comment** column in the **Results Table**, if it is not already visible.

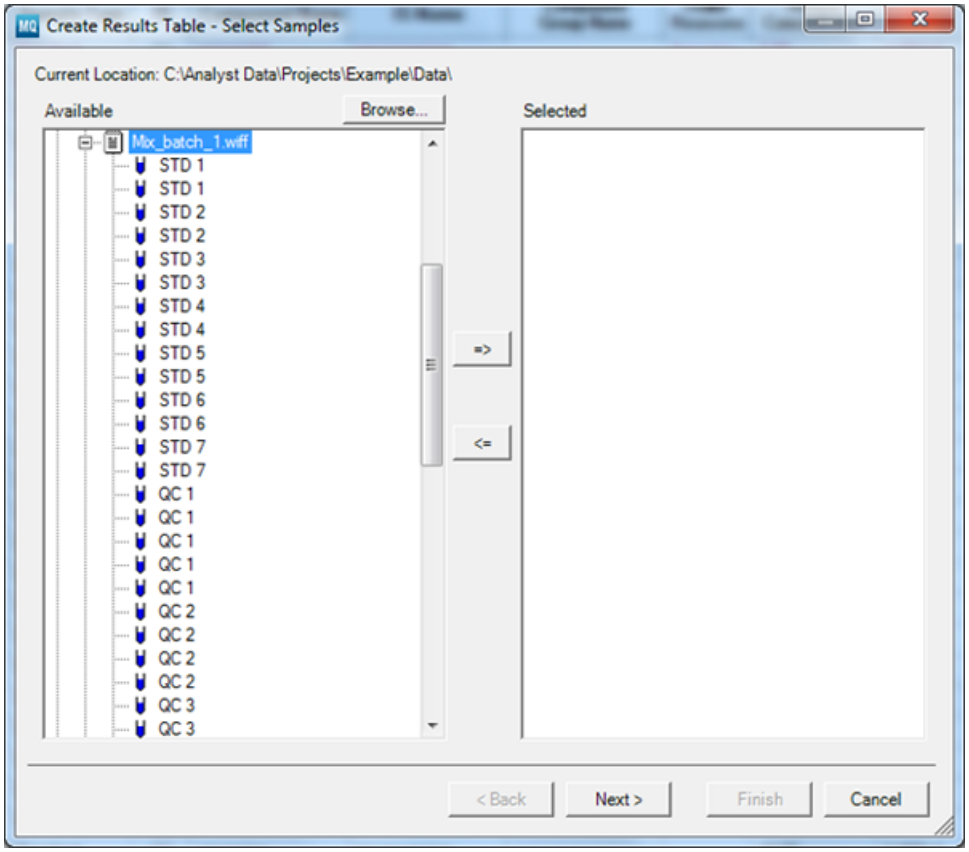
2. Sort the table using this column.
3. Select the (now adjacent) rows with the **Not Present** comment.
4. Click the **Hide selected rows(s)** icon. Refer to Software Icons on page 156.

Results Table Dialogs

Select Samples

Select the samples from the wiff files to be processed.

Figure 7-4 Create Results Table - Select Samples Page



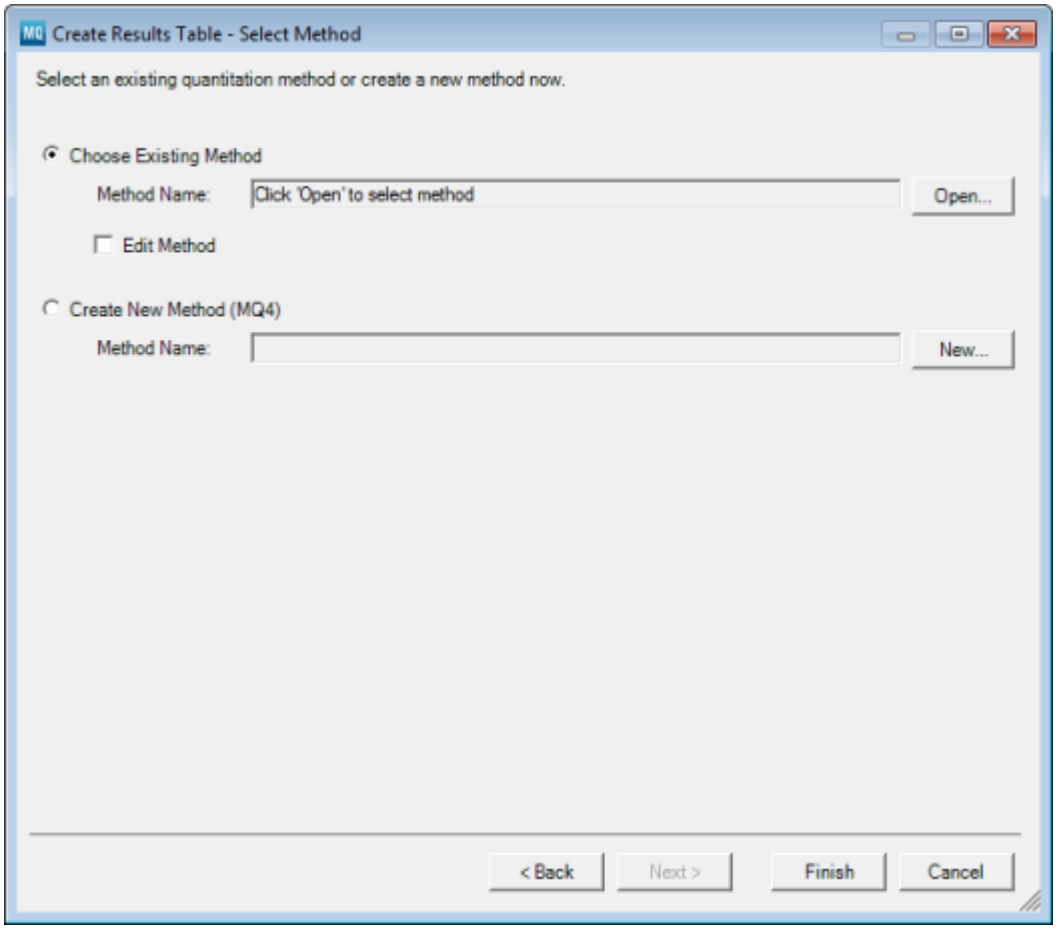
- The **Available** pane shows the subfolders, wiff files, and samples available in the **Data** folder for the selected folder.
- Expand individual folders to see any subfolders or wiff files. If the wiff file is expanded, it opens to show the available samples.

- Use the arrows to add or remove samples.
- Select samples by double-clicking an individual sample, by selecting a sample or data file and then clicking the => button, or by dragging a sample or data file from the left pane to the right one. Press **Shift** or **Ctrl** to select multiple files or samples before moving them.

Select Method

Select the quantitation method. If an existing method is selected but not edited, then a progress bar is shown while the selected samples are processed. At the end of this process, a **Results Table** is created.

Figure 7-5 Create Results Table - Select Method Page



Label	Description
Choose Existing Method	Click **Open** to select an existing quantitation method.
Edit Method	Select this command to edit an existing method. The subsequent pages of the wizard are populated with information from the existing method that can be modified as required.
Create New Method	Click **New** to create a quantitation method. The algorithm in parentheses is the algorithm selected in the **Integration Defaults** dialog.

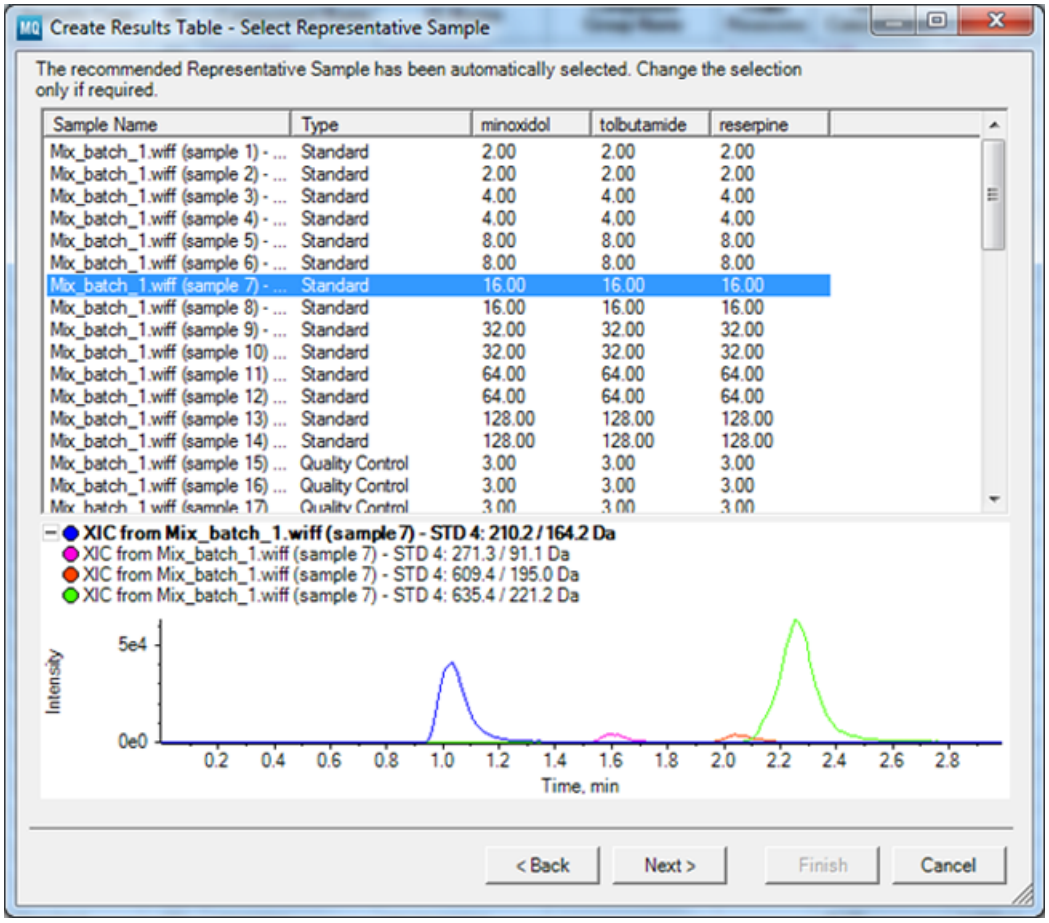
Select Representative Sample

The **Select Representative Sample** page shows the selected representative sample for which chromatograms are shown when visually setting the peak-finding and integration parameters. This sample must contain all of the compounds that will be included in the quantitation method.

If sample types and analyte concentrations were selected using the Analyst® MD software Batch Editor before the samples were acquired, then this information is shown as additional columns.

The software selects a sample by default. If the selected sample is not appropriate, then select another representative sample. If the SignalFinder™ algorithm is selected, to avoid generating an incorrect integration model, no representative sample is recommended by the software if the TIC level is above 1.0e6 in all samples. Users can select a representative sample manually in this scenario.

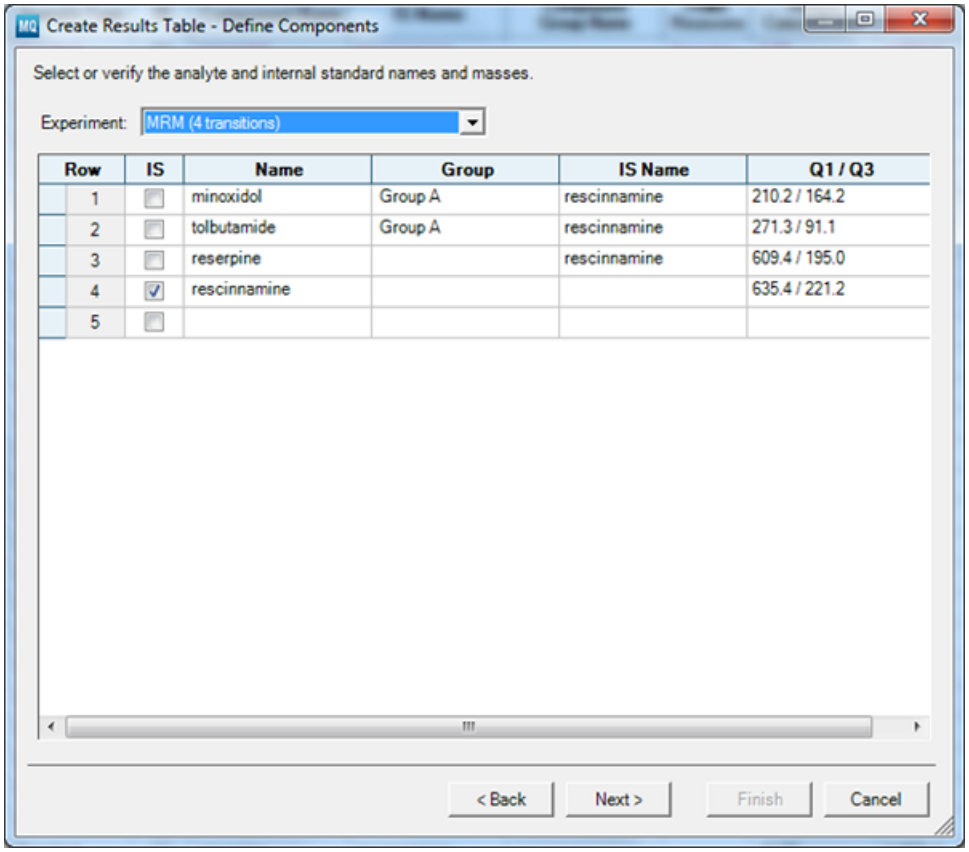
Figure 7-6 Create Results Table - Select Representative Sample Page



Define Components

The **Define Components** page contains a row for each analyte or internal standard. Select the names of the analytes and internal standards, if used. Refer to Define Components Right-Click Menu on page 48.

Figure 7-7 Create Results Table - Define Components Page



Label	Description
Experiment	Select an experiment to process from the list. For multi-period or multi-experiment data, select each of the experiments that must be processed and then fill in the table with the components for the corresponding experiment.
Row	Contains the current row number.
IS	Indicates whether the component defined for the row is an analyte (not selected) or an internal standard (selected).
Name	Contains the name of the component. For MRM experiments, the name is automatically completed using the **Q1/Q3** transition masses. For a more specific name, type a name in the field.

Label	Description
Group	Contains the name of the group to which the component for the row belongs. If analytes or internal standards that are related to one another are placed in the same group, then they can be reviewed and manipulated together more easily. This is true for entities that have the same retention time as one another, for example different MRM transitions for the same compound. Type the group names or populate them automatically. Refer to Define Components Right-Click Menu on page 48.
IS Name	Contains the name of the optional internal standard that should be used for the analyte defined for the row. This field is not applicable to internal standards themselves.
Mass Info	For MRM experiments, this column is entitled **Q1/Q3** and contains the mass pair for the component defined for the row. Select the required transition from the list that shows all of the available transitions for the experiment. Usually, the column is automatically initialized with the available transitions. For profile (scan) experiments this column is entitled **Start - Stop** and contains the mass range used to calculate an XIC (extracted ion chromatogram) for the component defined for the row. Type the mass range with a hyphen separating the two masses. For example, 200-201 or 200-1. For the latter option, the mass range is 199.5-200.5.

Define Components Right-Click Menu

Right-click in the **Define Components** page to access a context menu. The following commands are available.

Table 7-3 Define Components Right-Click Menu Options

Menu Option	Description
Clear	Clears the contents of any selected rows or columns. Rows are selected by clicking or dragging in the area before the row numbers.
Copy	Copies any selected rows or columns to the clipboard.
Paste	Pastes the contents of the clipboard.
Find Component by Name	Selects the component whose **Name** matches the text. The exact text is not required to find a match. This is useful to select a specific component if there are many components. If no row is initially selected in the spreadsheet, the search starts from the first row. Otherwise, the search starts from the row following the selected row and wraps around to the beginning. This is useful if there is more than one component whose **Name** contains the text. If the first search does not find the component, search again, leaving the first component selected, to locate another match in the table.
Insert Row Above	Inserts a single blank row immediately above the currently selected row.

Table 7-3 Define Components Right-Click Menu Options (continued)

Menu Option	Description
Delete Selected Rows	Removes the currently selected rows from the table.
Sum Multiple Ions	Sums chromatograms for multiple MRM transitions or full-scan mass ranges. After the command is selected, additional mass columns are added to the **Components** table. Any masses selected for a given row are used in the construction of the summed XIC for the corresponding analyte or internal standard. It is recommended that this feature is always selected.
Groups	Refer to Groups Submenu on page 84.
Internal Standards	Refer to Internal Standards Submenu on page 86.

Define Integration

Select the expected retention time and other peak finding parameters for each of the components.

The list on the left shows an entry for each component defined on the previous page of the wizard. Click a specific row to view the corresponding chromatogram and the current integration for the representative sample. Scroll through the list by using the up and down arrow keys or by using the scroll wheel. In general, it is recommended that all components be reviewed for correctness of integration. However, if there are many components, then use the **Highlight Components with Uncertain RT** command to limit the number to be reviewed.

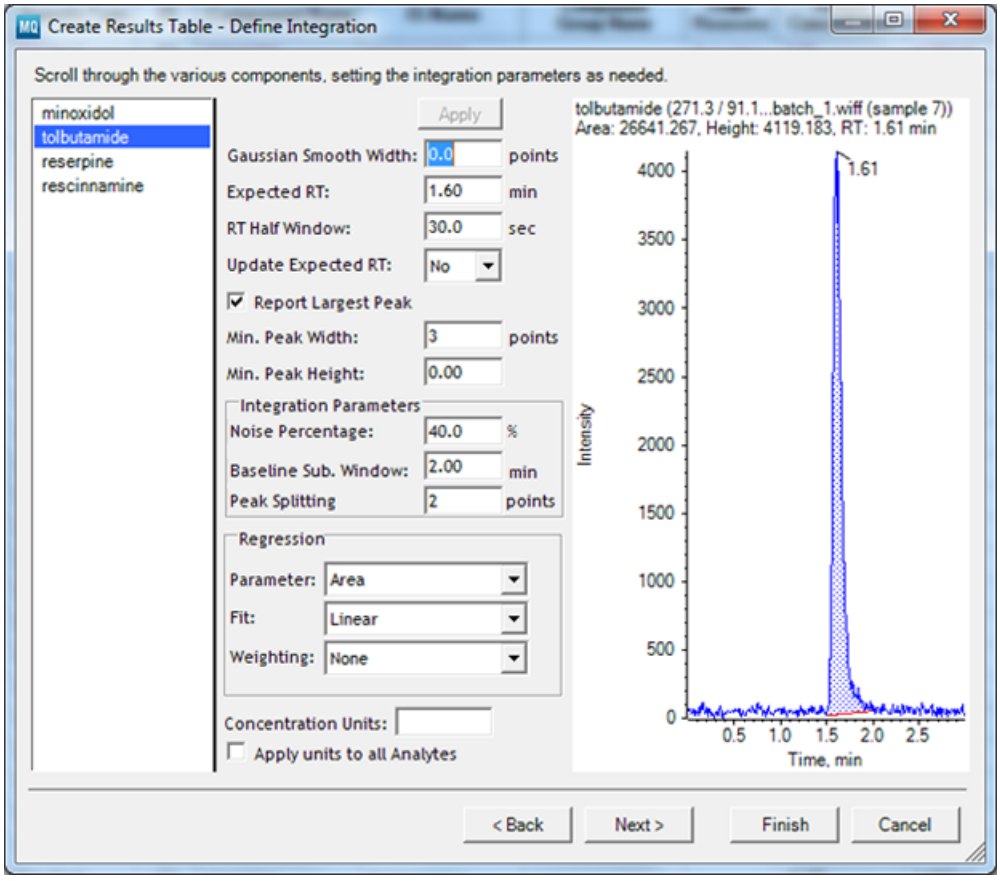
Note: If there are more than a few components, then make sure that the peak-finding parameters are set to reasonable defaults before running the wizard to avoid adjusting the parameters for each component.

Right-click in the page to view the available commands. Refer to Define Integration Right-Click Menu on page 51.

In the **Regression** group, change the calibration options for all or selected components after the Results Table is created. Set the default concentration units and regression parameters so that they do not need to be adjusted each time.

Tip! Zoom in on the graph by dragging the x or y axis regions. Return to the preset view by using the context menu (**Home Graph Axes**) or by double-clicking in the axis region.

Figure 7-8 Create Results Table - Define Integration Page



Label	Description
Apply	Adjusts the peak-finding parameters, if necessary, for a given component. When creating the new Results Table, the specified parameters for a given component are applied to that component for all samples when the data is integrated. Refer to Integration Algorithm Parameters on page 122.
Expected RT	Initially set as the retention time of the point with the largest intensity for the chromatogram. Usually this is the required peak. However, if isomers are present, then this value might need to be adjusted. To adjust the value, type a new value in the **Expected RT** field and then click **Apply**. Alternatively, click in the graph and then drag across the peak of interest. Be careful not to accidentally drag the cursor in the graph and adjust the expected retention time.
Parameter	Select **Area** or **Height**.
Fit	The various fit types are described in Regression Equations on page 128.

Label	Description
Weighting	The various weighting types are described in Weighting Factors on page 129.
Concentration Units	Type the concentration units used for the analytes and any internal standards. If relative quantitation is performed, then leave this field blank. The wizard assumes that the same units are used for all components. If this is not the case, then use the **Quantitation Method Editor**.
Apply units to all Analytes	Users can type a concentration unit for individual components. To apply the same unit to all the components, select this check box. The information should be consistent with the **Concentration Units**.

Define Integration Right-Click Menu

Right-click in the **Define Integration** page to access a context menu. The following commands are available.

Table 7-4 Define Integration Right-Click Menu Options

Menu Option	Description
Find Component by Name	Similar to the command available from the **Define Components** page, except the difference is that instead of selecting rows of the **Components** spreadsheet, individual items in the components list are selected.
Highlight Components with Uncertain RT	Used to highlight those components for which the default expected retention time (taken as the RT of the peak with the largest intensity for each chromatogram) is incorrect. If there are only a few components, then review each one individually and do not use this command. However, if there are many components, then use this command to visually check only those for which there is more than one significant peak present in the chromatogram. Refer to Highlight Components Dialog on page 88.
Home Graph Axes	Returns the zoomed graph to its home view where all data is visible.

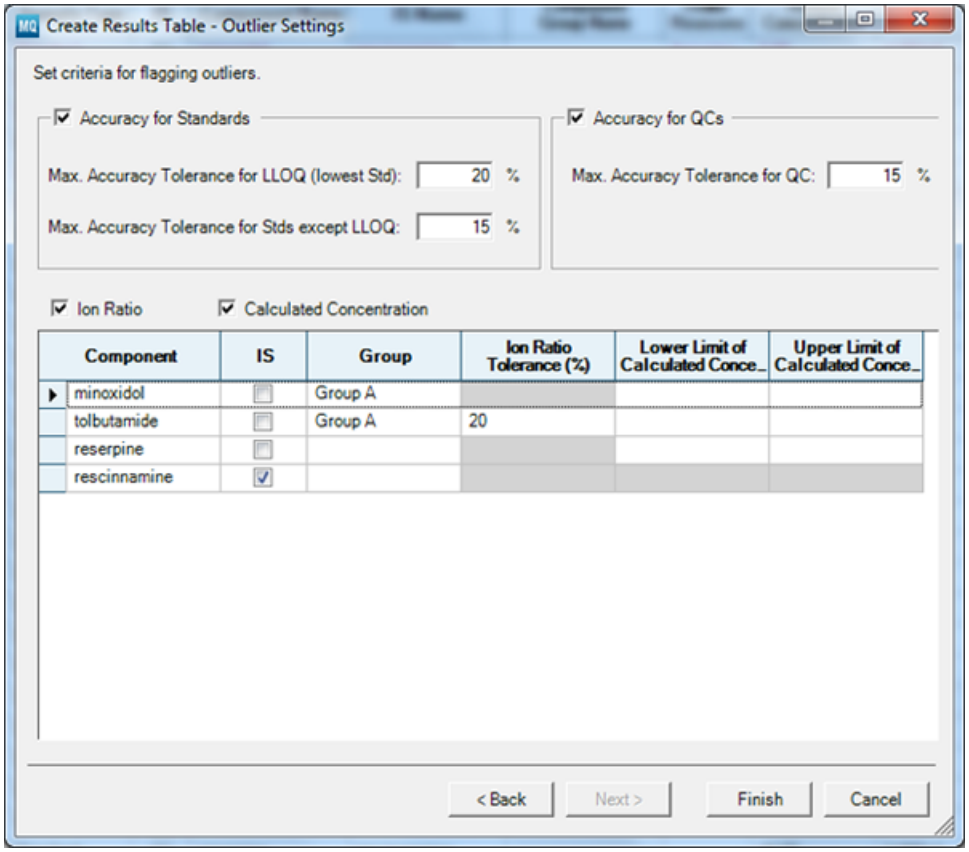
Table 7-4 Define Integration Right-Click Menu Options (continued)

Menu Option	Description
Overlay Other Components for Group	Use this command to overlay chromatograms if various components have been assigned to groups, and if the components assigned to any given group are expected to have the same retention time. For example, if they represent different MRM transitions of the same actual compound. When selected, the chromatogram for the current component, whose integration parameters are being defined, is drawn using a solid blue trace and its integrated peak area is shown. The chromatograms, and not the integrated peak area, for the other components in the same group are overlaid using a dashed line style.
Update Retention Times	Used to reset the expected retention times for a previously created quantitation method. If an existing quantitation method is opened and **Set New Typical Sample** is selected, then the chromatograms shown correspond to the new sample but the expected retention times are left unchanged. For each component, the expected retention time is updated to correspond to the retention time of the peak with the largest intensity within a window of the specified width centered at the original expected retention time. Refer to Update Retention Time Dialog on page 88.

Outlier Settings

Users can flag the outliers of the accuracy for the **Standards**, **QCs**, **Ion Ratio**, and **Calculated Concentration**. The following commands are available.

Figure 7-9 Outlier Settings Dialog



Label	Description
Accuracy for Standards	Edits the accuracy tolerance of the **Standard** samples.
Max. Accuracy Tolerance for Stds except LLOQ%	Edits the accuracy tolerance for the **Standard** samples with a value that is consistent with the laboratory standard operating procedures.
Max. Accuracy Tolerance for LLOQ (lowest Std)%	Edits the accuracy tolerance for the lowest concentration **Standard** if the laboratory standard operating procedure indicates a different tolerance for this **Standard**.
Accuracy for QCs	Edits the accuracy tolerance of the **Quality Control** samples.
Max. Accuracy Tolerance for QC%	Edits the accuracy tolerance for the **Quality Control** samples with a value that is consistent with the laboratory standard operating procedures.
Ion Ratio	Only available if the components are assigned to groups. Select to use the ion ratio of the peak area or peak height. Peak area or peak height is set when selecting the regression parameter during quantitation method development.

Label	Description
Calculated Concentration	When using **Standard** samples of known concentration, this is the back-calculated concentration from the calibration curve. Regression equations describe how the regression is performed for the various regression types and weighting.
Component	The analytes or internal standards for all samples.
IS	The selected internal standard. Only available if the **Ion Ratio** check box is selected.
Group	Components that have the same retention time (that is, different transitions for the same compound) can be grouped. Only available if the **Ion Ratio** check box is selected.
Ion Ratio Tolerance (%)	Use the default setting or edit this setting according to laboratory standard operating procedures. Only available if the **Ion Ratio** check box is selected.
Lower Limit of Calculated Concentration	Type the lower limit of the acceptable concentration range. Any sample with the **Calculated Concentration** lower than this value is flagged as a concentration outlier.
Upper Limit of Calculated Concentration	Type the upper limit of the acceptable concentration range. Any sample with the **Calculated Concentration** higher than this value is flagged as a concentration outlier.

Right-click in the **Outlier Settings** page to access a context menu.

Table 7-5 Outlier Settings Right-Click Menu Options

Label	Description
Apply to all analytes the Lower Limit of Calc. Concentration	Applies the lower limit of the calculated concentration to all of the analytes, if all of the analytes have the same criteria.
Apply to all analytes the Upper Limit of Calc. Concentration	Applies the upper limit of the calculated concentration to all of the analytes, if all of the analytes have the same criteria.

Results Table Columns

Note: Some critical columns of the sample information such as **Sample Name**, **Sample ID**, and so on should not be hidden when users customize the **Results Table** column settings.

For numerical fields, use the format 0.00 for non-scientific notations and use the format 0.00e0 for scientific notations. Change the decimal points to indicate the precision of the numbers that are shown. Only a period (.) can be used as a decimal separator. Digit grouping is not supported.

Table 7-6 Results Table Columns

Label	Description
Accuracy	When using **Standard** samples of known concentration for **Standard** samples and **Quality Control** samples, this is defined as: 100% * (Calculated Concentration) / (Actual Concentration) For other sample types, the value is N/A.
Acq. Method Name	The name of the acquisition method used to acquire the sample.
Acquisition Date & Time	The date and time at which the wiff sample was acquired.
Actual Concentration	For **Standard** samples and **Quality Control** samples, this is the expected known concentration.
Area	The detected peak area. If no peak was detected the value is N/A.
Area / Height	The detected peak area divided by the height. If no peak was detected the value is N/A.
Area Ratio	For analytes using an internal standard, this is the ratio of the **Area** to the **IS Area**. For internal standards or for analytes without an internal standard, the value is N/A.
Asymmetry Factor	The distance from the center line of the peak to the back slope divided by the distance from the center line of the peak to the front slope, with all measurements made at 10% of the maximum peak height.
Baseline Delta / Height	The absolute value of the height difference of the baseline (at the start of the peak and the end of the peak) to the actual peak height. Values greater than approximately 0.1 indicate that the baseline might not have integrated correctly and that the peak should be reviewed.
Calculated Concentration	When using **Standard** samples of known concentration, this is the back-calculated concentration from the calibration curve. Refer to Regression Equations on page 128 for information on how the regression is performed for the various regression types and weighting.
Component Comment	An arbitrary comment that applies for the analyte or internal standard for all samples.
Component Group Name	The group name (if any) associated with the analyte or internal standard.
Component Index	The index of the analyte or internal standard in the original quantitation method. It can be useful to sort the table based on this field.

Table 7-6 Results Table Columns (continued)

Label	Description
Component Name	The name of the analyte or internal standard.
Conc. Units	The concentration units.
Concentration Ratio	For analytes using an internal standard, this is the ratio of the **Actual Concentration** to the **IS Actual Concentration**. For internal standards or for analytes without an internal standard, the value is N/A.
Corrected Area	The detected peak area. If no peak was detected, then the value is N/A.
Corrected Area / Height	The detected peak area divided by the height. If no peak was detected, then the value is N/A.
Corrected Height	The detected peak height. If no peak was detected, then the value is N/A.
Dilution Factor	The factor by which the sample has been diluted. This factor is used in the calculation of the calibration curve. Refer to Regression Equations on page 128.
End Time	The ending retention time of the detected peak, in minutes.
End Time at 10%	The time in minutes along the back side of the peak where the intensity is at 10% of the peak height.
End Time at 5%	The time in minutes along the back side of the peak where the intensity is at 5% of the peak height.
Expected Ion Ratio	The expected ion ratio for all sample types.
Expected RT	The original expected retention time from the quantitation method, in minutes.
Height	The detected peak height. If no peak was detected, then the value is N/A.
Height Ratio	For analytes using an internal standard, this is the ratio of the **Height** to the **IS Height**. For internal standards, or for analytes without an internal standard, the value is N/A.
Index	This is the index of the row in the original, unsorted order. If the table is sorted based on another column, it can be returned to the original order by sorting on this column.
Injection Volume	The volume of sample injected by the autosampler, in mL.

Table 7-6 Results Table Columns (continued)

Label	Description
Integration Type	• A value of **Baseline** indicates that a stand-alone peak was integrated in the usual way. • A value of **Valley** indicates that there were two adjacent peaks and that the signal did not return to the baseline value between them. • A value of **Manual** indicates that the peak was manually integrated. • A value of **N/A** indicates that no peak was detected.

Ion Ratio	• **Ion Ratios** are determined when at least two MRM transitions from a single analyte have been collected into a group.
	• The first component in a subgroup will be used as **Quantifier** ions. The remainder of the components in the subgroup will be used as **Qualifier** ions.
	• Ion Ratio = (Peak Area or Height of Qualifier) / (Peak Area or Height of Quantifier)
	• Subgroups
	  • All analytes of a group constitute an **Analyte** subgroup.
	  • All internal standards of a group constitute an **IS** subgroup.
	• If a component is not a member of a group, then the **Ion Ratio** is N/A.
	• If the peak is not found, then the **Ion Ratio** is N/A.
	• Applied to all components in both **Analyte** and **IS** subgroups, for the **Quantifier**, the **Qualifier** is itself.
	• If the integration changes for either the **Quantifier** or the **Qualifier** peaks, then the **Ion Ratio** is calculated again.
	• Can be calculated for either peak area or peak height. If the **Area** is used in the regression part of a .qmethod for the first component (Component Index is 1) in the **Results Table**, the peak area is used for the calculation of the **Ion Ratio** for the entire **Results Table**. If the **Height** is used in the regression of the first component, then the peak height is used for the calculation.

IS	A selected check box indicates that the component for the row is an internal standard, not an analyte.
IS Actual Concentration	Actual concentration for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Area	Area for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.

Table 7-6 Results Table Columns (continued)

Label	Description
IS Area / Height	The ratio of the **Area** to the **Height** for the internal standard associated with the current analyte, or N/A for internal standards, or for analytes without an internal standard.
IS Baseline Delta / Height	**Baseline Delta / Height** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Comment	An arbitrary comment for the internal standard associated with the current analyte, or N/A for internal standards, or for analytes without an internal standard.
IS Corrected Area	Corrected area for the internal standard associated with the current analyte, or N/A for internal standards, or for analytes without an internal standard.
IS Corrected Area / Height	**Corrected Area** / **Corrected Height** for the internal standard associated with the current analyte, or N/A for internal standards, or for analytes without an internal standard.
IS Corrected Height	**Corrected Height** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS End Time	**End Time** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Expected RT	**Expected RT** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Height	**Height** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Integration Type	**Integration Type** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Mass Info	**Mass Info** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Name	**Component Name** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Peak Comment	**Peak Comment** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Quality	Quality for the internal standard associated with the current analyte, or N/A for internal standards, or for analytes without an internal standard.
IS Region Height	Quality metric for the internal standard associated with the current analyte, or N/A for internal standards, or for analytes without an internal standard.

Table 7-6 Results Table Columns (continued)

Label	Description
IS Retention Time	**Retention Time** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Signal / Noise	**Signal / Noise** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Start Time	**Start Time** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Total Width	**Total Width** for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
IS Width at 50%	Width at 50% for the internal standard associated with the current analyte, or N/A for internal standards or for analytes without an internal standard.
Mass Info	Mass information associated with the component. For MRM experiments this is **Q1/Q3** and for profile (full scan) experiments it is **Start - Stop**.
Modified	A check mark indicates that the peak-finding parameters have been modified, using the **Peak Review** pane, from their original values indicated in the quantitation method.
Operator Name	The name of the instrument operator who acquired the sample.
Original Filename	The name of the wiff file.
Outlier Reasons	When the outlier criteria have been set in the quantitation method, this column indicates which criterion was found to be outside the predetermined limits for the component. The **Outlier Reasons** column is only linked to the **Outlier Settings** in the quantitation method and it is a preset column in the **Results Table**. The reason the outlier is flagged: • **Accuracy** • **Concentration** • **Ion Ratio** If there is a peak for the quantifier but not the qualifier, then the ion ratio will be flagged for both components. If there is a peak for the qualifier but not the quantifier, then the ion ratio will be flagged for both components. If neither have peaks, then there is no flag for either component. • **Cannot calculate the Expected Ion Ratio**.
Peak Comment	An arbitrary comment for the row.

Table 7-6 Results Table Columns (continued)

Label	Description
Plate Number	Autosampler plate number, as originally specified in the **Batch Editor** used to acquire the data.
Points Across Baseline	The number of scans from the start to the stop of the peak.
Points Across Half Height	The number of scans across the peak at approximately 50% of the height.
Quality	This metric attempts to indicate the quality of the integrated peak. • Values near zero indicate that the peak has integrated poorly (or that no actual peak is present). • Values near 1.0 indicate that the peak integrated well and does not need to be reviewed.
Rack Number	Autosampler rack number, as originally specified in **Batch Editor** used to acquire data.
Region Height	The peak height of the largest peak in the vicinity of the actual detected peak. This is useful in conjunction with the **Quality** field. Peaks with a low quality that also have a reasonable **Region Height** need to be reviewed. If the **Region Height** is small, then there is no significant peak present.
Relative RT	For analytes that are using an internal standard, this is the ratio of the **Retention Time** to the **IS Retention Time**. For internal standards, or for analytes without an internal standard, the value is N/A.
Retention Time	The actual retention time of the detected peak, in minutes.
Sample Comment	An arbitrary comment for the sample.
Sample ID	An arbitrary identifier for the sample. It is initialized from the value originally specified in the **Batch Editor** used to acquire the data.
Sample Index	The index of the current sample.
Sample Name	An arbitrary name for the sample. It is initialized from the value originally specified in the **Batch Editor** used to acquire the data.
Sample Type	The type for the sample. Refer to Sample Type Filter on page 42.

Table 7-6 Results Table Columns (continued)

Label	Description
Signal / Noise	An estimate of the ratio of the peak height for the detected peak to the noise present in the chromatogram. When using the SignalFinder integration algorithm, noise is estimated using the calculated relative noise and the baseline at the peak apex position. The MQ4 integration algorithm uses a similar approach, except that the baseline is estimated using the entire chromatogram. Refer to Relative Noise and Signal-to-Noise Calculations on page 151.
Slope of Baseline	Indicates the drift of the baseline.
Start Time	The starting retention time of the detected peak, in minutes.
Start Time at 10%	The time in minutes along the front side of the peak where the intensity is at 10% of the peak height.
Start Time at 5%	The time in minutes along the front side of the peak where the intensity is at 5% of the peak height.
Tailing Factor	The distance from the front slope of the peak to the back slope, divided by twice the distance from the center line of the peak to the front slope, with all measurements made at 5% of the maximum peak height.
Total Width	The chromatographic peak width, in minutes, at the baseline.
Used	For **Standard** samples, a check mark indicates that the corresponding analyte is currently used for construction of the calibration curve. For **Quality Control** samples, a check mark indicates that the analyte is used for the calculation of the **QC** statistics. For other sample types, this field is for informational purposes only.
Vial Number	Autosampler vial number as originally specified in **Batch Editor** used to acquire data.
Width at 10%	The width of the peak measured at 10% of the peak height.
Width at 5%	The width of the peak measured at 5% of the peak height.
Width at 50%	The chromatographic peak width, in minutes, of the detected peak measured at half of its apex intensity.

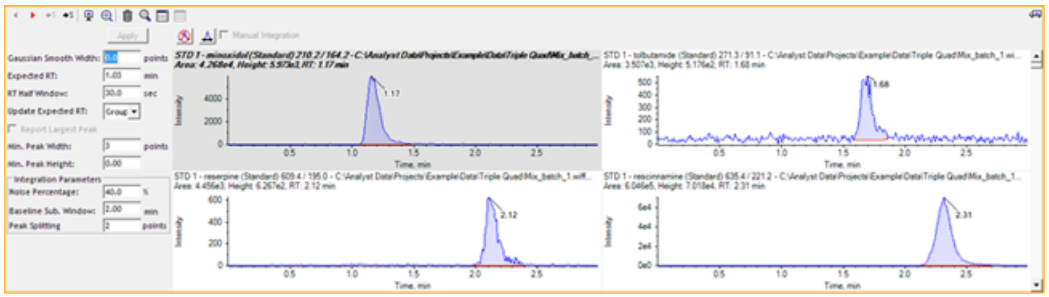
Peak Review 8

Use the **Peak Review** pane to visually inspect the raw chromatograms so that the quality of the peak-finding process can be determined. When a **Results Table** is active, click the **Show Peak Review** icon in the Results Table tool bar to open the Peak Review pane. Reviewers should review the quantitative data according to the criteria of peak integration and data acceptance in their own standard operating procedures (SOPs).

The grouping of numbers is not supported. Users should not group numbers in any text box (for example, integration parameters) and grid (for example, **Results Tables**).

Enhanced **Peak Review** indicates the **Ion Ratio** acceptance on an overlaid chromatogram. Users can also magnify a single chromatogram.

Figure 8-1 Peak Review Pane



Use the **Peak Review** pane to correct chromatograms that did not integrate properly by either adjusting the peak-finding parameters or by manually selecting the starting and ending points for integration. After a chromatogram is integrated, the **Results Table** is automatically updated with the new peak area and other parameters.

Quantitation methods include the criteria used to quantitate the peaks selected for integration. Reviewers should review the quantitative data according to the criteria of peak integration and data acceptance in their own SOPs.

Manual Integration

After a peak in a particular chromatogram is manually integrated, select this check box to indicate that the chromatogram is manually integrated. When in this state, if the user clears the check box, then manual integration for the peak is canceled and the peak is automatically re-integrated using the method parameters.

The difference between this check box and the **Enable Manual Integration Mode** button is that this check box reflects the status of the current peak, whereas the button specifies the behavior when dragging a chromatogram.

Note: After manual integration mode is enabled, it remains enabled for all panes until it is cleared.

Apply

If the user has adjusted any of the peak-finding parameters, then the **Apply** button is enabled. Click the button to apply the modified peak-finding parameters to the active chromatogram.

Except when in manual integration mode, dragging across a particular peak in a chromatogram is equivalent to adjusting the **Expected RT** parameter and then clicking **Apply**.

Note: If the user modifies the peak-finding parameters and then activates a different chromatogram without clicking **Apply**, then the parameters are not applied and the changes are lost.

Tips for Reviewing Peaks

- Sort the **Results Table** on a particular column and review only those chromatograms that sort to the top or bottom of the table.
- The **Peak Review** pane is always synchronized with its corresponding **Results Table** and shows the chromatograms for the same peaks, in the same order, as in the **Results Table**. Any changes (such as sorting rows, filtering sample types, or selecting any components) that are made to the **Results Table** are automatically reflected in the **Peak Review** pane.
- Select the number of chromatograms to view at one time.
- Use the scroll bar at the right of the pane to scroll through the available chromatograms. When the **Peak Review** pane is active, use the up and down arrow keys on the keyboard or the scroll wheel to move through the chromatograms.
- At any one time, one particular chromatogram is considered to be active and is indicated by the title in bold. Make a particular chromatogram active by clicking anywhere within it.
- When a chromatogram becomes active, the integration parameters shown at the left of the pane are updated to reflect the newly active chromatogram. If the user adjusts the peak integration parameters and then clicks **Apply**, this affects the currently active chromatogram.
- Select a row in the **Results Table** by clicking in the gray region to the left of the first column to show the corresponding peak in the **Peak Review** pane. If the user scrolls to a particular chromatogram in the **Peak Review** pane, the **Results Table** highlights the corresponding row and then scrolls it into view.
- If the user drags across a particular peak in a chromatogram, then the **Expected RT** integration parameter is updated with the actual retention time of the peak. The new retention time is then automatically applied and the peak is integrated again, updating the **Results Table**.

- If the user is reviewing peaks in manual integration mode, then dragging across the peak will manually integrate the selected peak.
- The peak review process can be made faster by caching previously calculated chromatograms. Refer to Edit Menu on page 15.

Peak Review Right-Click Menu

These features control the appearance of the integration parameters that are shown to the left of the chromatograms. Right-click in the **Peak Review** pane to access a context menu. The following commands are available.

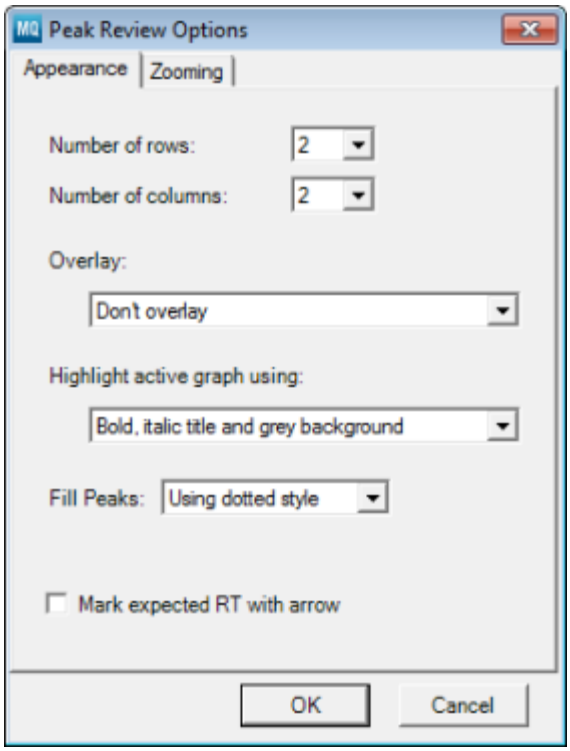
Table 8-1 Peak Review Parameters

Task	Commands
Change the appearance of the **Peak Review** pane.	Peak Review Options Dialog: Appearance Tab on page 65 or Peak Review Options Dialog: Zooming Tab on page 67.
Set the peak review title format.	Set Peak Review Title Format on page 68.
Show the parameters using descriptive names for the individual parameters.	By default, the **Show Parameters-Normal Width** is always set.
Copy the parameters.	Copy Parameters on page 69.
Paste the parameters.	Paste Parameters on page 69.
Set the peak to 'Not Found'.	Set Peak to 'Not Found' on page 70.
Use the peak.	Use Peak on page 70.
Update the quantitation method for the component.	Update Quantitation Method for Component on page 70.
Update the quantitation method for the group.	Update Quantitation Method for Group on page 70.
Apply the integration parameters to a sample within the group.	Apply Integration Parameters to Sample Within Group on page 71.
Revert the peak to the original method.	Revert Peak to Original Method on page 71.
Revert all peaks for the component.	Revert All Peaks for Component on page 71.

Peak Review Options Dialog: Appearance Tab

Right-click in the **Peak Review** pane to select to adjust options affecting the appearance of the **Peak Review** pane. It is recommended that no more than four rows and four columns are set.

Figure 8-2 Peak Review Options Dialog: Appearance Tab

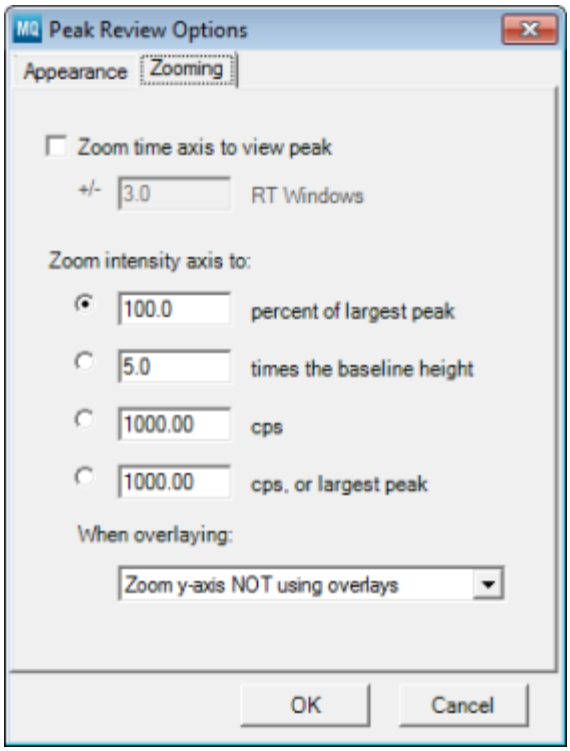


Label	Description
Number of rows and Number of columns	Controls the number of chromatograms that are simultaneously visible. Unless chromatograms have already been cached, it will take longer to scroll between pages if many chromatograms are shown. Refer to Edit Menu on page 15.
Overlay	Determines whether other chromatograms should be overlaid on top of the main chromatogram in each of the sub-panes. • **Don't Overlay**: Prevents overlay of other chromatograms. • **All components for group**: Overlays all chromatograms for components from the same group as the main component (for the current sample). • **Analytes and IS's separately for group**: Similar to the previous option, except that rather than overlaying all components from the same group, analytes and internal standards are kept separate. • **Internal Standard with Analyte**: For analytes, overlays the internal standard used by the analyte (internal standard chromatograms do not have other overlays). • **Qualifier and Quantifier with Ion Ratio Lines**: Shows the ion ratio lines. Select this option to visualize the ion ratio acceptance in the **Results Table**. Users can view the ion ratio acceptance when there are groups defined in the quantitation method. However, the **Ion Ratio Lines** are only an indication of the acceptance and not the final result. The lines are shown in the chromatogram as the peak height but the lines are calculated based on the peak area or height depending on the settings defined in the quantitation method. If there is a discrepancy between the height and area, then the user must confirm the **Ion Ratio** outlier in the **Results Table**.
Highlight active graph using:	Indicates how the currently active chromatogram should be shown. Set to use the bold, italic title, and the grey background.
Fill peaks	Indicates how the integrated area for peaks should be shown. The choices are: • Use a dotted style as used in the screen captures in this document. • Use a solid style. • Use no fill. In all cases the baseline for the peak is also drawn (in red). When the third option is used, only the baseline is drawn and the peak is not filled.
Mark expected RT with arrow	Indicates the **Expected Retention Time** with a blue arrow drawn below the time axis. This can be useful to determine whether the integrated peak is near the expected RT.

Peak Review Options Dialog: Zooming Tab

Right-click in the **Peak Review** pane to select to adjust options affecting the appearance of the **Peak Review** pane. The **Zoom intensity axis to** features are used to automatically adjust the y-axis of the chromatograms.

Figure 8-3 Peak Review Options Dialog: Zooming Tab



Label	Description
Zoom time axis to view peak	When selected, the x-axis of the chromatograms is automatically adjusted so that only a portion of the entire run is visible. This is useful for long LC runs so that the region of interest can be seen more clearly. The window width is expressed in terms of a multiple of the RT Window integration parameter. The total width of the zoomed region is twice the specified number of multiples of the **RT Window**.
Zoom intensity axis to percent of largest peak	Used to automatically adjust the y-axis of the chromatograms. Scales the y-axis to the specified percentage of the largest peak within the visible x-range of the chromatogram. This will be smaller than the total LC run length if the Zoom time axis to view peak feature is used.
Zoom intensity axis to times the baseline height	Used to automatically adjust the y-axis of the chromatograms. Used to focus on the baseline region itself.
Zoom intensity axis to cps	Scales the y-axis directly to the specified value.

Label	Description
Zoom intensity axis to cps, or largest peak	Scales the y-axis to the smaller of the specified value or the largest peak.
When overlaying Zoom y-axis NOT using overlays	Maintains the settings from the Zoom intensity axis to the section using only the main data set. This setting can cause the overlays to be only partially visible if they are more intense than the main data set.
When overlaying Zoom y-axis using overlays	Uses the main data set and all overlays and uses the biggest overall y-value. This feature always keeps the overlays visible.
When overlaying Use a percentage y-axis	Scales the main data set and the overlays separately using a percentage scale. This causes each trace to use the full available height. However, the relative peak heights cannot be directly visually compared.

Tip! Double-click within the y-axis to scale the axis to the most intense peak within the entire data set.

When selected, the chromatogram for the peak currently being reviewed is drawn using a solid blue trace and its integrated peak area is shown. The chromatograms (not the integrated peak area) for the other components (for the same sample) are overlaid using a dashed line.

When the graph is showing overlays in this way, double-click anywhere in the title area to toggle between showing the titles for all chromatograms or just for the active one.

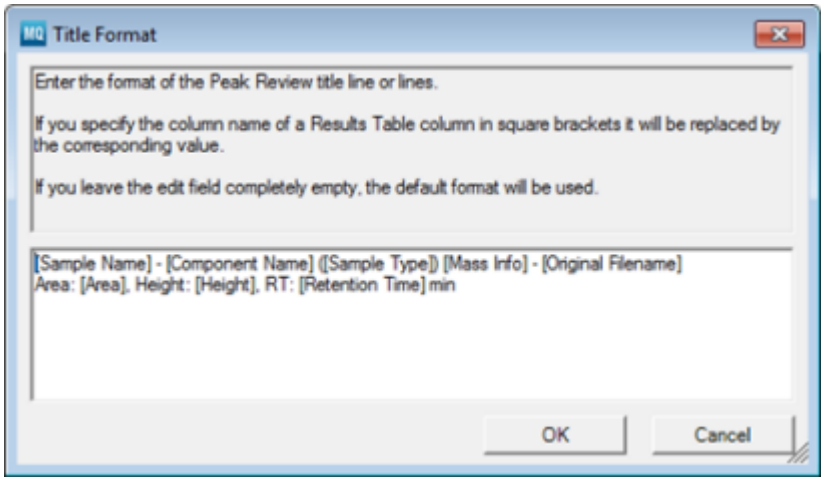
Tip! Double-click within the x-axis to return the graph to its home view in which all data is visible. Zoom in by dragging within the axis to select a time range.

Set Peak Review Title Format

Use the dialog to customize the information that appears in the graph title for each of the chromatograms. If the user types a column name in the **Results Table** in square brackets, then it is replaced by the field value for the current sample and component. The user can also type any additional text that is left as is. It is recommended that the sample name [Sample Name] be included in the peak review title.

- Right-click in the **Peak Review** pane and then click **Set Peak Review Title Format**

Figure 8-4 Title Format Dialog



Copy Parameters

Right-click in the **Peak Review** pane to access this command. Use this command in conjunction with **Paste Parameters** to copy the peak-finding parameters from one chromatogram to another. This command can be used if the same adjustment to the parameters needs to be made for several chromatograms.

1. In a graph with an active chromatogram open, right-click and then click **Copy Parameters**.
2. Use the **Update Quantitation Method for Component** command to apply the change to all chromatograms for the component.

Paste Parameters

1. In a graph with an active chromatogram open, right-click and then click **Copy Parameters**.
2. Right-click in a different chromatogram and then click **Paste Parameters**.

   The previously copied parameters are applied to the new chromatogram.

Set Peak to 'Not Found'

- In a graph with an active chromatogram open, right-click and then click **Set Peak to 'Not Found'** to remove the integration from the selected chromatogram.

Use Peak

- In a graph with an active chromatogram open, right-click and then click **Use Peak** to include or exclude the active peak from the calibration curve.

Update Quantitation Method for Component

After adjusting the peak-finding parameters for a particular chromatogram, select this feature to adjust the copy of the quantitation method saved with the Results Table to use those parameters for the component.

- Adjust the peak-finding parameters, right-click, and then click **Update Quantitation Method for Component**.

  For the particular component, all samples are automatically integrated to use the new parameters and the **Peak Review** pane and **Results Table** are updated. If any peaks have been manually integrated, then the user is asked if the re-integration should apply to all peaks or only to those that were not manually integrated.

Update Quantitation Method for Group

Similar to the **Update Quantitation Method for Component** command, except that the integration applies to all components that belong to the same group as the component for the currently active chromatogram. If the user has assigned the various components to groups, and if the components assigned to any given group are expected to have the same retention time, then this feature is useful so that the user can reset the parameters,

including the expected retention time, for all components for the group at once. This feature is not useful if the components for the groups do not have the same retention times.

- Adjust the peak-finding parameters, right-click, and then click **Update Quantitation Method for Group**.

Apply Integration Parameters to Sample Within Group

After adjusting the peak-finding parameters for a specific chromatogram, use this feature to apply the original parameters from the copy of the quantitation method saved with the Results Table to the chromatogram.

- After adjusting the peak-finding parameters for a specific chromatogram, right-click and then click **Apply Integration Parameters to Sample Within Group**.

Revert Peak to Original Method

After adjusting the peak-finding parameters for a specific chromatogram, use this feature to apply the original parameters from the copy of the quantitation method saved with the **Results Table** to the chromatogram.

- Right-click and then click **Revert Peak to Original Method**.

Revert All Peaks for Component

After adjusting the peak-finding parameters for some chromatograms, use this feature to apply the original parameters from the copy of the quantitation method saved with the **Results Table** to all chromatograms for the same component as the active chromatogram. If any peaks have been manually integrated, then the user is asked if the re-integration should apply to all peaks or only to those that were not manually integrated.

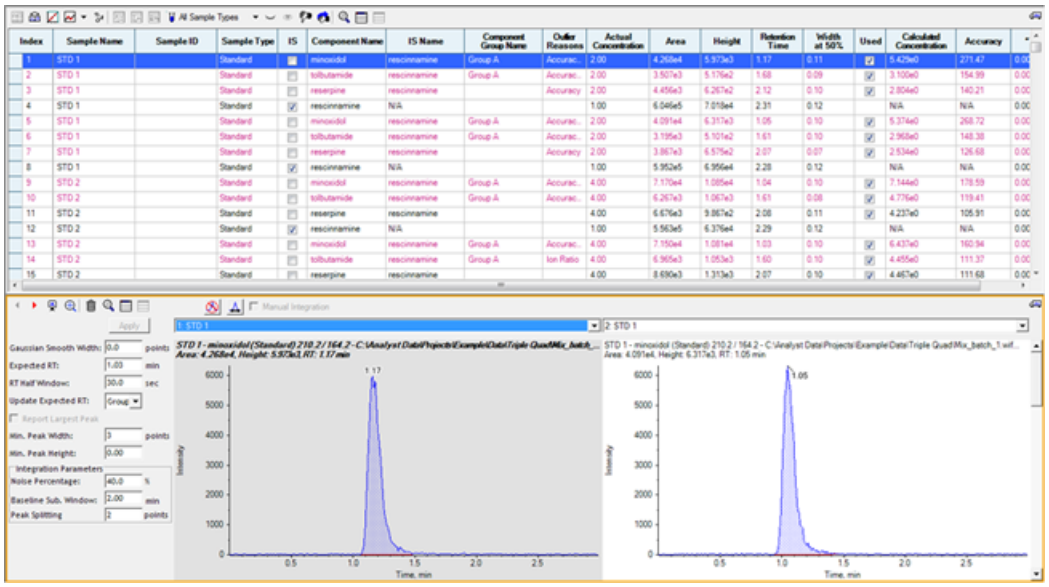
- Right-click and then click **Revert All Peaks for Component**.

Side-by-side Sample Review 9

Use the **Side-by-side Sample Review** feature to screen for particular target compounds. Users can select up to six samples to compare the peak responses across the samples. Reviewers should review the quantitative data according to the criteria of peak integration and data acceptance in their own standard operating procedures (SOPs).

When a **Results Table** is active, click the **Side by Side Sample Review** icon in the **Results Table** tool bar to open the **Side by Side Sample Review** pane.

Figure 9-1 Side by Side Sample Review Pane



Quantitation methods include the criteria used to quantitate the peaks selected for integration. Reviewers should review the quantitative data according to the criteria of peak integration and data acceptance in their own SOPs.

Perform a Side-by-Side Sample Review

1. Open a Results Table.
2. Click the **Side by Side Sample Review** icon.
3. Select a sample from the list in the **Side by Side Sample Review** pane.

   The integration parameters are shown.

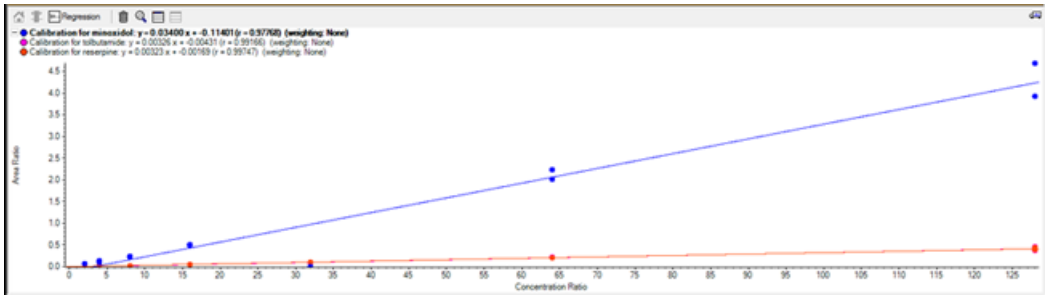
Tip! Right-click in the **Side by Side Sample Review** pane and then click **Options** to change the number of rows or columns in the side-by-side review.

4. Select another sample from the other list.

Calibration Pane 10

Use the **Calibration** pane to visually inspect the regression for each analyte, if **Standard** samples of a known concentration are used. This pane is not applicable if the user is performing relative quantitation and does not have **Standard** samples. When a **Results Table** is active, click **Show Calibration** in the too lbar.

Figure 10-1 Calibration Pane

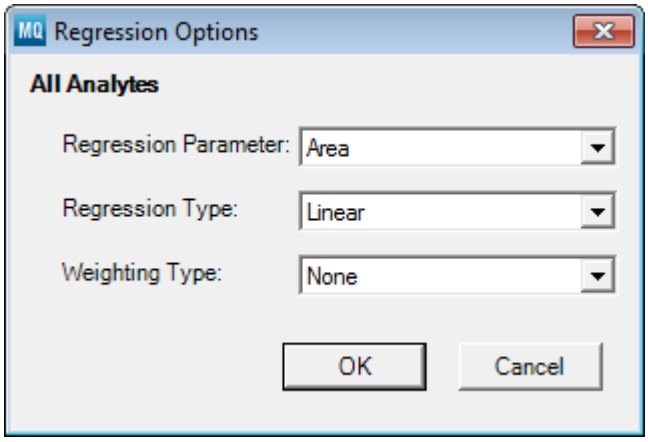


As well as inspecting the regression, the user can exclude **Standard** samples so that they are not used for the regression. After adjustments are made, a new regression is automatically calculated and parameters such as the **Calculated Concentration** and **Accuracy** are recalculated for all samples for the analyte. Refer to Regression Equations on page 128.

Regression Options Dialog

If there are many analytes, then it is easier to apply changes using the **Regression Options** dialog than by changing the regression parameters one-by-one.

Figure 10-2 Regression Options Dialog



Calibration Tips

- For analytes without an associated internal standard, the y-axis is peak **Area** or **Height** as selected in the quantitation method. For analytes with an internal standard, the y-axis is the peak **Area** or **Height** ratio (of the analyte to the internal standard).
- For analytes without an associated internal standard, the x-axis is **Actual Concentration**. Otherwise, it is the **Actual Concentration** ratio (of the analyte to the internal standard).
- If more than one analyte from the **Components & Groups List** is selected, then calibrations for all analytes are overlaid. Otherwise, the calibration for the selected analyte is shown.
- The title region always shows the name of the active analyte and the associated regression equation with the correlation co-efficient. If the regression could not be calculated, for example if there are no **Standard** samples, then the title indicates this. If calibrations for multiple analytes are overlaid, then toggle the title between showing information for all analytes or just the active one by double-clicking anywhere within the title region. If there are many overlaid analytes, then it might not be possible to display all information. In this case, scroll the title by dragging within it.
- The data points for the **Standard** samples that are in use are always plotted as is the calibration equation that uses these points. The user can optionally show data points for excluded **Standard** samples and for **Quality Control** samples.
- If the user clicks a data point, then the corresponding row in the **Results Table** is automatically selected and scrolled into view, provided that the row is currently visible somewhere in the table and has not been hidden.

Calibration Right-Click Menu

Right-click in the **Calibration** pane to access a context menu. The following commands are available.

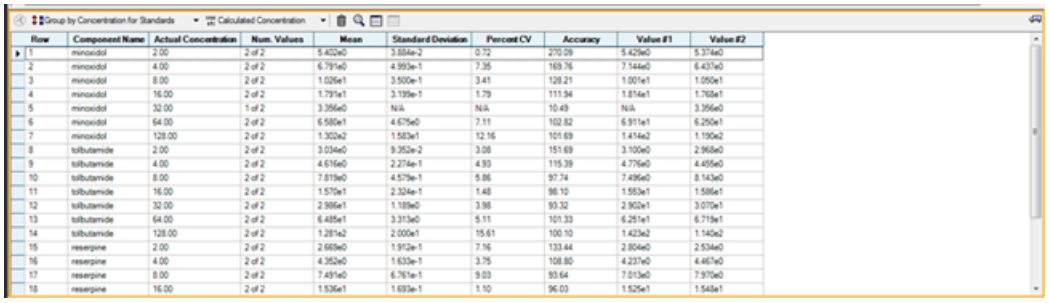
Table 10-1 Calibration Pane Right-Click Menu Options

Menu Option	Description
Exclude (or Include)	If the user right-clicks directly on a data point for a standard that has not been excluded, then this option is used to exclude the sample from the regression calculation (for the sample and analyte for the clicked data point). If the sample has already been excluded, then the text of the menu item reads **Include** and selecting it includes that point. After selection, the regression is calculated and the **Results Table** is updated. This functionality is equivalent to clearing or selecting the **Used** check box in the Results Table for the corresponding row.
Exclude – All Analytes (or Include – All Analytes)	Excludes or includes all analytes, not only the analyte corresponding to a selected data point.
Show Excluded Standards	When selected, data points for excluded standards (if any) are drawn using open circles. When cleared, excluded standards are not shown.
Show QCs	When selected, data points for **Quality Control** (QC) samples are drawn using an open diamond. When cleared, the **QC** samples are not shown.
Show Legend	When selected, a legend is drawn to the right of the plot that shows the point symbols for the various sample types (closed circles for **Standard** samples, open circles for excluded Standards, and open diamonds for **Quality Control** samples). **Note:** If the user is not viewing certain sample types, for example if the **Show QCs** option is not selected, then the entry for those sample types is not present. If neither **QC** samples nor excluded standards are shown, then this option is not available and no legend is drawn.
Use Percent Y-Axis	When not selected, the y-axis for the plot is in units of absolute peak **Area** or **Height** (or the peak **Area** or **Height** ratio if an internal standard is being used). When selected, the y-axis is expressed as a percentage of the data point with the largest y-value for each analyte independently. Using a percentage axis is useful if more than one analyte is overlaid and their absolute responses are fairly different since it allows each trace to be scaled to use the entire available vertical area. Otherwise, analytes with low response lie close to the x-axis and the plot need to be zoomed to see them in detail.
Log-Log Plot	Used to toggle the view between plotting **Area** versus **Concentration** and **Log(Area)** versus **Log(Concentration)**.

Statistics Tables 11

Use the **Statistics Table** to view information related to the reproducibility of an analysis. Each row of the table summarizes information such as the average and standard deviation for a group of related peaks from the same analyte that would ideally be expected to have the same response.

Figure 11-1 Statistics Pane



Label	Description
Row	The row number. Click one of the other column headers to sort the table. Return the table to the original view by clicking this header.
Component Name	The name of the analyte.
Actual Concentration (or Sample Name)	If grouping by actual concentration, then this column shows the concentration. If grouping by sample name, then the title of the column changes and the sample name is shown.
Num. Values	Shows m of n where n is the total number of samples at the actual concentration (or with the same sample name) and m is the number of these samples used for the calculations. Samples are not used if the corresponding peak could not be integrated or if the **Used** field has been manually cleared.
Mean	The average for the used samples.
Standard Deviation	The standard deviation of the used samples.
Percent CV	The co-efficient of variance expressed as a percentage: 100 * (Standard Deviation) / Mean.

Label	Description
Accuracy	The mean value divided by the actual concentration expressed as a percentage: 100 * Mean / (Actual Concentration). This field is shown only when grouping by actual concentration, not when grouping by sample name.
Values	The individual values for the samples appear in additional columns. If the corresponding sample could not be integrated, then the value is N/A. If the **Used** field has been manually cleared, the value is shown with a strike-through line.

Statistics Table Tips

- The **Statistics Table** links to the **Components & Groups List** to show rows corresponding to the selected analytes. If the **All Components** or **All Analytes** items are selected, then there are entries for all analytes. If an individual analyte is selected, then there are entries for that analyte only. If an individual internal standard is selected from the list, then the **Statistics Table** is blank. Refer to Components & Groups List on page 38.
- If the user clicks one of the **Value** cells, then the corresponding row in the **Results Table** for the analyte and sample is selected provided that the row is currently visible in the **Statistics Table**. Only **Unknown** samples in the **Results Table** are shown. If the **Statistics Table** contains information for **Standard** samples, then the corresponding rows are not visible in the **Results Table**. If the **Peak Review** pane is visible, then it links to the **Results Table** and it is updated when the cell is clicked.
- Click one of the column headings to sort the **Statistics Table**.
- The user can copy either the whole **Statistics Table** or just the rows of interest.
  - To copy the whole table, click **Edit > Copy.**
  - To copy just the rows of interest, manually select the rows and then click **Edit > Copy.**
- If the column widths are adjusted, then these widths are restored the next time the **Statistics Table** is shown.
- The format and precision are the same as those in the **Results Table**.
- The **Group by Concentration for Standards and QCs** is based on **Displayed Actual Concentration**, not the **Actual Concentration** stored in the **Results Table**. If the Std 1 concentration is 0.001, the Std 2 concentration is 0.005, and the display format is 0, then Std 1 and Std 2 are grouped together because both of them are treated as 0. To group them separately, in the **Column Settings** dialog, set the precision for **Analyte Concentration** to 0.000. If Std 1 is 0.500 and Std 2 is 0.499, then set the precision to 0.00 to group them together.

Statistics Table Right-Click Menu

Right-click in the **Statistics Table** to access the **Use Peak** command. Use this command to set the **Used** field for the sample and analyte corresponding to the selected cell in one of the **Value** columns. Before right-clicking to obtain the menu, click the appropriate cell in one of the **Value** columns to select it.

Metric Plots 12

Use Metric Plots to plot the values in a Results Table column against either the row number or another column. These plots are a valuable aid for visual data review, especially if users do not want to manually review every chromatogram using the Peak Review pane.

Generate a Metric Plot

1. Select one or two columns in the **Results Table**.
2. Click **Show Metric Plot**.

   If one column is selected, then the resulting plot shows the values from the column as a function of row number in the table. If two columns are selected, then the values from the columns are plotted against one another. The first of the two columns to be selected contains the x values and the second contains the y values.

Save Metric Plot Settings

1. Open a metric plot by selecting a column and then click **Show Metric Plot**.
2. Right-click in the plot and then clicking **Save Setting**.

   This enables the user to quickly generate **Metric Plots** that are frequently used without having to select the corresponding column each time.

Metric Plot Tips

- If users left-click on a data point, then the corresponding row of the Results Table is automatically selected and scrolled into view. If the Peak Review pane is open, then it also updates to show the corresponding chromatogram. This provides a convenient means of performing peak review for outliers.
- If more than one component from the Components & Groups list is selected, then the traces for all of the components are overlaid. Otherwise, the trace for the one selected component is shown.
- The title region always shows the name of the active trace. If traces for multiple components are overlaid, then toggle the title between showing information for all of the traces or just the active one by double-clicking anywhere within the title region. Activate a particular trace by clicking the color spot to the left of the corresponding title.

- Save the settings for the Metric plot to use again. Right-click in the Metric plot and then click **Save Settings As**.

Metric Plot Right-Click Menu

Right-click in the Metric Plot to access a context menu. The following commands are available.

Table 12-1 Metric Plot Right-Click Menu Options

Menu Option	Description
Regression	Shows a regression line on the metric plot. • **Regression Type** • **Weighting Type** • **Include standard deviation lines and Multiplier** Refer to Regression Dialog on page 81.
Display "N/A" as 0.0	When this option is selected, plots values that are not numerical using a y-value of zero. Otherwise, such points are omitted from the plot. For example, the **Retention Time** is reported as N/A for peaks that could not be integrated. For this feature, a point is present for such peaks so that the user can see these potentially problematic samples and then link them to the **Peak Review** pane by clicking the point.
Show Legend	Changes the legend that annotates the point symbols used for the various sample types.
Label Active Series (using sample names)	Changes whether the data points are labeled using the text from the **Sample Name** field of the **Results Table**. If there is more than one overlaid trace, then only the currently active trace is labeled.
Use Percent Y-Axis	Changes whether the y-axis uses absolute units or a percentage of the maximum y-value. When using the percentage feature, the percentage is calculated independently for each overlaid trace. This feature can be used to plot overlaid traces for multiple components and the response for the metric for the components is significantly different.
Start Y-Axis at Zero	Changes whether the y-axis starts at y=0 or at the minimum y-value needing to be plotted.
Connect Points With Lines	Changes whether the data points are connected by lines.
Save Setting	If the plot is currently associated with a setting, then this feature saves the current features. Otherwise, this feature behaves the same as the **Save Setting As** feature.

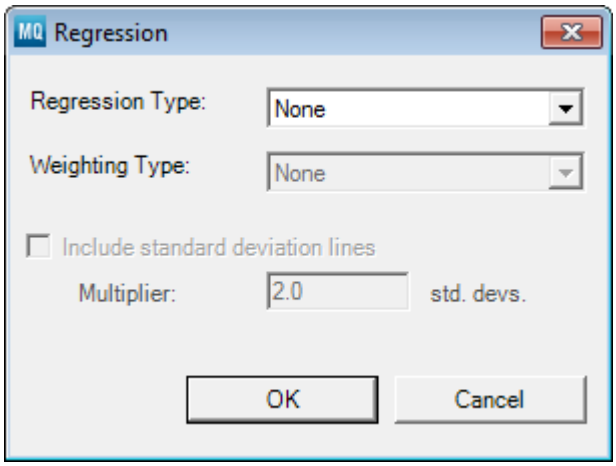
Table 12-1 Metric Plot Right-Click Menu Options (continued)

Menu Option	Description
Save Setting As	If the same columns are frequently plotted, then the user can save the plotting options as a setting. This enables the user to quickly generate a plot even if the required columns are not currently visible in the **Results Table**. In addition to the columns, the various plotting options are saved. After a setting is saved, the name is shown in the **Metric Plot** menu.
Delete Setting	If the current plot is associated with a setting, then use this feature to delete the setting.

Regression Dialog

Click to show a regression line on the metric plot.

Figure 12-1 Regression Dialog



Label	Description
Regression Type	Contains the various regression types (linear, quadratic, and so on). The **Mean** regression type results in a horizontal line at the location of the average y-value for all of the data points and for the **Median** regression type results in a horizontal line at the location of the median y-value for the points. In addition, there is a **None** feature that removes any previous regression.
Weighting Type	The various weighting types are described in Weighting Factors on page 129.
Include standard deviation lines and Multiplier	These options are available when either the **Mean** or **Median** regression type is selected. When selected, additional dashed horizontal lines are added to plot the specified number of standard deviations above and below the main line. Use this option to view points that are, for example, more than two or three standard deviations from the average.

Quantitation Method Editor 13

Use the **Quantitation Method Editor** to create a quantitation method or to edit an existing one.

The typical workflow is to create quantitation methods using the **New Results Table wizard**. However, the user can use the **Quantitation Method Editor** to create a quantitation method that can be used as required.

Components Tab

Right-click in the **Components** tab to access a context menu. The following commands are available.

Table 13-1 Components Right-Click Menu Options

Menu Option	Description
Find Component by Name	Used to select the component whose **Name** matches the text. The exact text is not required to find a match. This is useful to select a specific component if there are many components. If no row is initially selected in the spreadsheet, then the search starts from the first row. Otherwise the search starts from the row following the selected row and wraps around to the beginning. This is useful if there is more than one component whose **Name** contains the text. If the first search does not find the component, search again, leaving the first component selected, to locate another match in the table.
Insert Row Above	Inserts a single empty row immediately above the currently selected row.
Delete Selected Rows	Removes the currently selected rows from the table.
Sum Multiple Ions	Sums chromatograms for multiple MRM transitions or full-scan mass ranges. After the command is selected, additional mass columns are added to the **Components** table. Any masses selected for a given row are used in the construction of the summed XIC for the corresponding analyte or internal standard. It is recommended that this feature is always selected.
Groups	Refer to Groups Submenu on page 84.
Internal Standards	Refer to Internal Standards Submenu on page 86.

Groups Submenu

Table 13-2 Groups Menu Options

Menu Option	Description
Using Constant Group Size	Opens the Set Automatic Groups dialog, which is used to automatically populate the Group column using the name of the first component for each group, assuming that each group contains the same number of components. Refer to Set Automatic Groups Dialog on page 85.
By Filling Down Existing Groups	Automatically completes the same group name for a number of sequential components. To use the command, manually specify the group name for the first component for each separate group and then select the command. The specified group names are filled-down to any subsequent components for which the group name is blank. Only rows for which the Name has been filled in are considered.
Using Q1 Masses	Only available for MRM experiments. Used to populate the Group column using the Q1 mass. This is useful if the same Q1 mass was specified for multiple transitions for the same compound and different fragments were monitored. If there are many components, and if some coincidentally share the same Q1 mass, then they are assigned to the same group.
Using Q3 Masses	Only available for MRM experiments. Used to populate the Group column using the Q3 mass. This is useful if different isotopic forms of a compound were monitored (with different Q1 masses), but a constant Q3 mass was monitored. If there are many components, and if some coincidentally share the same Q3 mass, then they are assigned to the same group.
Using (Q1 – Q3) Mass Differences	Used to populate the Group column using the difference between the Q1 and Q3 masses (only available for MRM experiments). This is useful if different isotopic forms of a compound were monitored (with different Q1 masses), but a consistent Q3 fragment containing all modified isotopes was monitored. If there are many components and if some coincidentally share the same mass difference, then they are assigned to the same group.
Add Group to Start of Component Name	Appends the group name to the beginning of the analyte or internal standard name. This can be useful if the initial names are not unique.

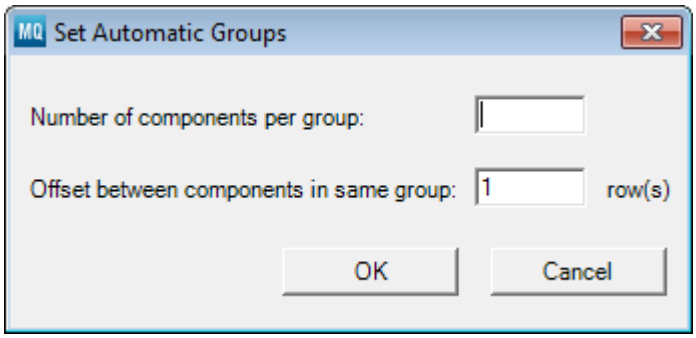
Table 13-2 Groups Menu Options (continued)

Menu Option	Description
Remove Group from Start of Component Name	Removes the group name, if present, from the beginning of the analyte or internal standard name.
Append Summed Ions for Groups	When the Sum Multiple Ions option is enabled, this command appends a new component for each group that uses the summed chromatogram for the group. Separate components are added for analytes and internal standards for the groups, if both are defined. The name for the new analytes defaults to the group name and for internal standards to the group name with .IS appended. If the summed components are required and not the original single-mass components, then the latter can be deleted.

Set Automatic Groups Dialog

Automatically populates the Group column using the name of the first component for each group, assuming that each group contains the same number of components.

Figure 13-1 Set Automatic Groups Dialog



Label	Description
Number of components per group	The total number of components for each group.
Offset between components in same group	The offset in rows between sequential components in the same group. This value is usually 1, but can be larger if the components for the group are not in adjacent rows.

Internal Standards Submenu

Table 13-3 Internal Standards Menu Options

Menu Option	Description
Set IS for All Analytes	Sets the IS Name field for all of the analyte rows. If one internal standard has been defined, then its name is used. Otherwise, select the required internal standard from the dialog that opens.
Set IS for Selected Analytes	If the same internal standard is used for more than one analyte, then provide a shortcut to setting the internal standard separately for each analyte one-by-one. Refer to Set IS for Selected Analytes on page 86.
Set Last Component of Group as IS	Use this command if the various components have been assigned to Groups, either manually or by using the items from the Set Groups submenu. The IS check box for the last component for each group is selected and all of the other components for the group, which are assumed to be analytes, are set to use that last component as an internal standard.
Set for All Groups as for Selected Group	Used to copy the arrangement of internal standards for the group corresponding to the currently selected row to all of the other groups, in a symmetrical way. This is useful if there is more than one internal standard for each of the groups. Refer to Set for All Groups as for Selected Group on page 86.

Set IS for Selected Analytes

1. Make sure that the required internal standard is defined (both the **Name** and the **IS** check box are selected).
2. Select the rows for the analytes for which to use the internal standard.
3. Select the menu item.

   If there is more than one internal standard defined, then a dialog opens prompting the user to select the required one.

Set for All Groups as for Selected Group

1. Assign groups.
2. Manually indicate which components are internal standards by selecting the box in the first column for the first group.
3. Manually indicate the internal standard for each analyte for the first group by selecting from the combo-box in the **IS Name** column.
4. Select any single row corresponding to the first group.
5. Click **Set for All Groups as for Selected Group**.

Integration Tab

Right-click in the **Integration** tab to access a context menu. The following commands are available.

Table 13-4 Integration & Regression Tab Right-Click Menu Options

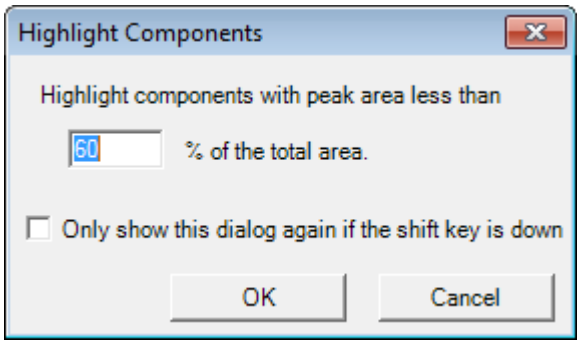
Menu Option	Description
Find Component by Name	Similar to the command available from the **Components** tab, except the difference is that instead of selecting rows of the **Components** spreadsheet, individual items in the components list are selected.
Highlight Components with Uncertain RT	Used to highlight those components for which the default expected retention time (taken as the RT of the peak with the largest intensity for each chromatogram) is incorrect. If there are only a few components, then review each one individually and do not use this command. However, if there are many components, then use this command to visually check only those for which there is more than one significant peak present in the chromatogram. Refer to Highlight Components Dialog on page 88.
Home Graph Axes	Returns the zoomed graph to its home view where all data is visible.
Overlay Other Components for Group	Use this command to overlay chromatograms if various components have been assigned to groups, and if the components assigned to any given group are expected to have the same retention time. For example, if they represent different MRM transitions of the same actual compound. When selected, the chromatogram for the current component, whose integration parameters are being defined, is drawn using a solid blue trace and its integrated peak area is shown. The chromatograms, and not the integrated peak area, for the other components in the same group are overlaid using a dashed line style.
Update Retention Times	Used to reset the expected retention times for a previously created quantitation method. If an existing quantitation method is opened and **Set New Typical Sample** is selected, then the chromatograms shown correspond to the new sample but the expected retention times are left unchanged. For each component, the expected retention time is updated to correspond to the retention time of the peak with the largest intensity within a window of the specified width centered at the original expected retention time. Refer to Update Retention Time Dialog on page 88.
Set New Typical Sample	Used to associate a representative sample with the method. This potentially affects the selections available from the **Q1/Q3** column (for MRM experiments) or **Start - Stop** column (for profile experiments). It also affects the chromatograms that are displayed on the **Integration** tab.

Highlight Components Dialog

The names of any components for which the automatically selected peak does not account for at least the specified percentage of the total peak area in the chromatogram are indicated using bold type. For example, in Figure 13-2, if the default selected peak accounts for 70% to 100% of the total area, then it is not flagged. Review only these peaks by selecting them from the components list.

If the **Only show this dialog again if the shift key is down** check box is selected, then the dialog does not open the next time the command is selected, unless the user presses **Shift**. The previously specified total area percentage parameter is used automatically.

Figure 13-2 Highlight Components Dialog



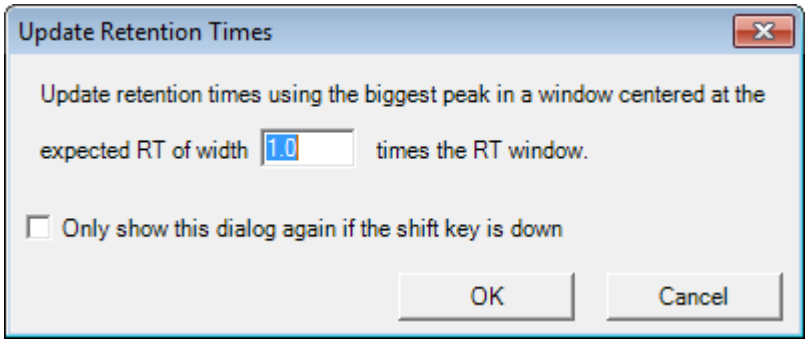
Update Retention Time Dialog

Used to reset the expected retention times for a previously created quantitation method. If an existing quantitation method is opened and Set New Typical Sample is selected, then the chromatograms shown correspond to the new sample but the expected retention times are left unchanged.

For each component, the expected retention time is updated to correspond to the retention time of the peak with the largest intensity within a window of the specified width centered at the original expected retention time.

If the **Only show this dialog again if the shift key is down** check box is selected, then the dialog does not open the next time the command is selected, unless the user presses **Shift**. The previously specified retention time is used automatically.

Figure 13-3 Highlight Components Dialog



Outlier Settings Tab

Right-click in the **Outlier Settings** tab to access a context menu. The following commands are available.

Label	Description
Accuracy for Standards	Edits the accuracy tolerance of the **Standard** samples.
Max. Accuracy Tolerance for Stds except LLOQ%	Edits the accuracy tolerance for the **Standard** samples with a value that is consistent with the laboratory standard operating procedures.
Max. Accuracy Tolerance for LLOQ (lowest Std)%	Edits the accuracy tolerance for the lowest concentration **Standard** if the laboratory standard operating procedure indicates a different tolerance for this **Standard**.
Accuracy for QCs	Edits the accuracy tolerance of the **Quality Control** samples.
Max. Accuracy Tolerance for QC%	Edits the accuracy tolerance for the **Quality Control** samples with a value that is consistent with the laboratory standard operating procedures.
Ion Ratio	Only available if the components are assigned to groups. Select to use the ion ratio of the peak area or peak height. Peak area or peak height is set when selecting the regression parameter during quantitation method development.
Calculated Concentration	When using **Standard** samples of known concentration, this is the back-calculated concentration from the calibration curve. Regression equations describe how the regression is performed for the various regression types and weighting.
Component	The analytes or internal standards for all samples.
IS	The selected internal standard. Only available if the **Ion Ratio** check box is selected.
Group	Components that have the same retention time (that is, different transitions for the same compound) can be grouped. Only available if the **Ion Ratio** check box is selected.

Label	Description
Ion Ratio Tolerance (%)	Use the default setting or edit this setting according to laboratory standard operating procedures. Only available if the **Ion Ratio** check box is selected.
Lower Limit of Calculated Concentration	Type the lower limit of the acceptable concentration range. Any sample with the **Calculated Concentration** lower than this value is flagged as a concentration outlier.
Upper Limit of Calculated Concentration	Type the upper limit of the acceptable concentration range. Any sample with the **Calculated Concentration** higher than this value is flagged as a concentration outlier.

Table 13-5 Outlier Settings Right-Click Menu Options

Label	Description
Apply to all analytes the Lower Limit of Calc. Concentration	Applies the lower limit of the calculated concentration to all of the analytes, if all of the analytes have the same criteria.
Apply to all analytes the Upper Limit of Calc. Concentration	Applies the upper limit of the calculated concentration to all of the analytes, if all of the analytes have the same criteria.

Quantitation Analysis Workflow Tutorial 14

Objectives:

- Learn how to process data using the SignalFinder™ algorithm.
- Learn how to process data using the MQ4 integration algorithm.
- Learn how to use the MQ4 and SignalFinder™ integration algorithm parameters.

Quantitation methods include a set of instructions on how to quantitate the peaks selected for integration. In this tutorial, a quantitation method is created at the same time as the Results Table.

Also included are additional tasks that can be used to manipulate the data in the **Results Table**, as well as information about the available software icons.

Note: Audit Trail and Security edition users are restricted to using the Analyst Data folder structure. Users can only process data files that are in the Analyst® MD software file structure. If the file and folder structure are not maintained, then the user might not be able to view the chromatograms.

About Calibration Curves

A calibration curve (also know as a standard concentration curve) is a method for determining the concentration of a substance in an **Unknown** sample by comparing the **Unknown** sample to a set of **Standard** samples of known concentration. The calibration curve is a plot of how the instrument responds (the analytical signal) to changes to the concentration of the analyte (the substance to be measured). The user prepares a series of **Standard** samples across a range of concentrations near the expected concentration of the analyte in the **Unknown** sample.

Prerequisites

In the Analyst® MD software, select the **Example** project.

The Mix_batch_1. Wiff file can be found in the Analyst Data\Projects\Example\Data\Triple Quad folder.

Modify the Columns Shown in the Results Table

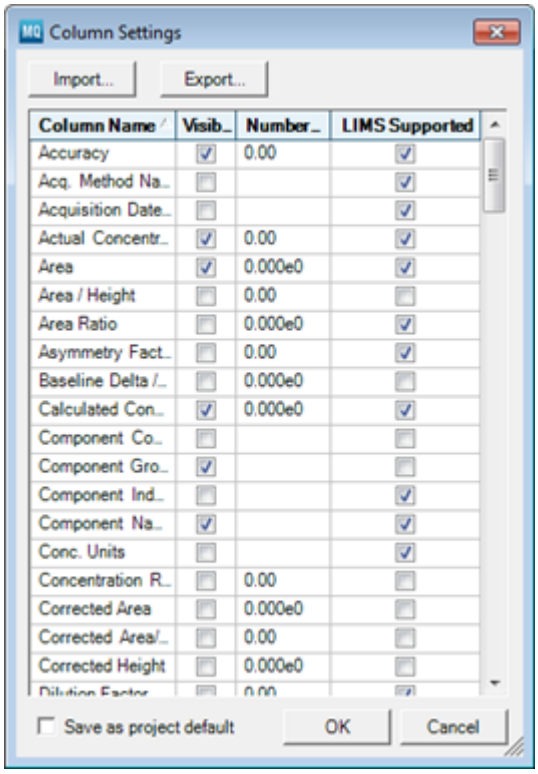
Use this procedure to show or hide columns in the **Results Table** or change the precision of the number format. For numerical fields, use the format 0.00 for non-scientific notations and use the format 0.00e0 for scientific

notations. Change the decimal points to indicate the precision of the numbers that are shown. Only a period (.) can be used as a decimal separator. Digit grouping is not supported.

Note: Some critical columns of the sample information such as **Sample Name**, **Sample ID**, and so on should not be hidden when users customize the **Results Table** column settings.

1. Right-click in the **Results Table** and then click **Column Settings**.

Figure 14-1 Column Settings Dialog



2. Select or clear the check box in the **Visible** column as required.
3. In the **Number Format** column, change the format to integer or scientific notation. The number of decimal points to be shown can also be changed.

Tip! To apply the column settings to all **Results Tables** in the project, select the **Save as project default** check box.

4. Click **OK**.

Process Data Using the SignalFinder™ Integration Algorithm

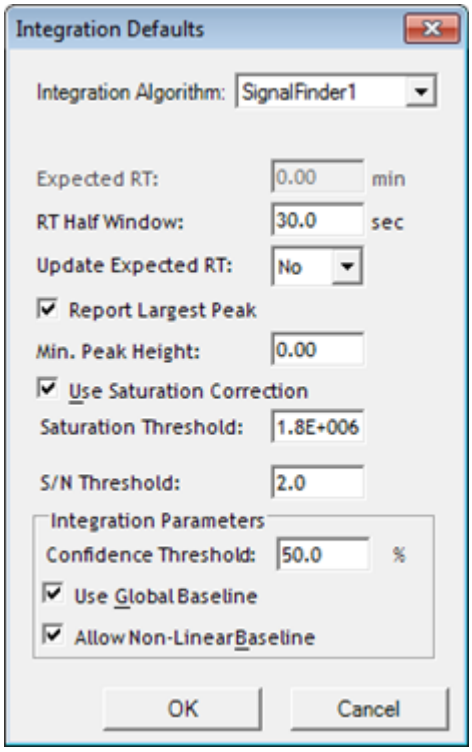
Unlike the MQ4 integration algorithm or the algorithms available in the Analyst® MD software, the SignalFinder™ builds a peak model using the selected sample when creating a quantitation method. This model describes the shape of the selected peak used by the algorithm. At integration time, the SignalFinder integration algorithm applies this model to the other samples, stretching or skewing the sample. This allows for the fact that the peak shape is similar, but not identical, for a given analyte or internal standard for multiple samples.

Set the Peak Integration Parameters

Use the following procedure to check or set the integration algorithm processing the data. Refer to About the SignalFinder Integration Algorithm on page 110.

1. In the Analyst® MD software, on the **Navigation** bar, under **Companion Software**, double-click **MultiQuant 3.0.3**.
2. Click **Edit > Project Integration Defaults.**
3. In the **Integration Defaults** dialog, select **SignalFinder1** from the **Integration Algorithm** list.
4. Select the **Use Saturation Correction** check box and then set the **Saturation Threshold** to **1.8E+006**.

Figure 14-2 Integration Defaults Dialog



Note: Peaks above the **Saturation Threshold** are considered saturated. This value is detector-dependent.

5. Click **OK**.

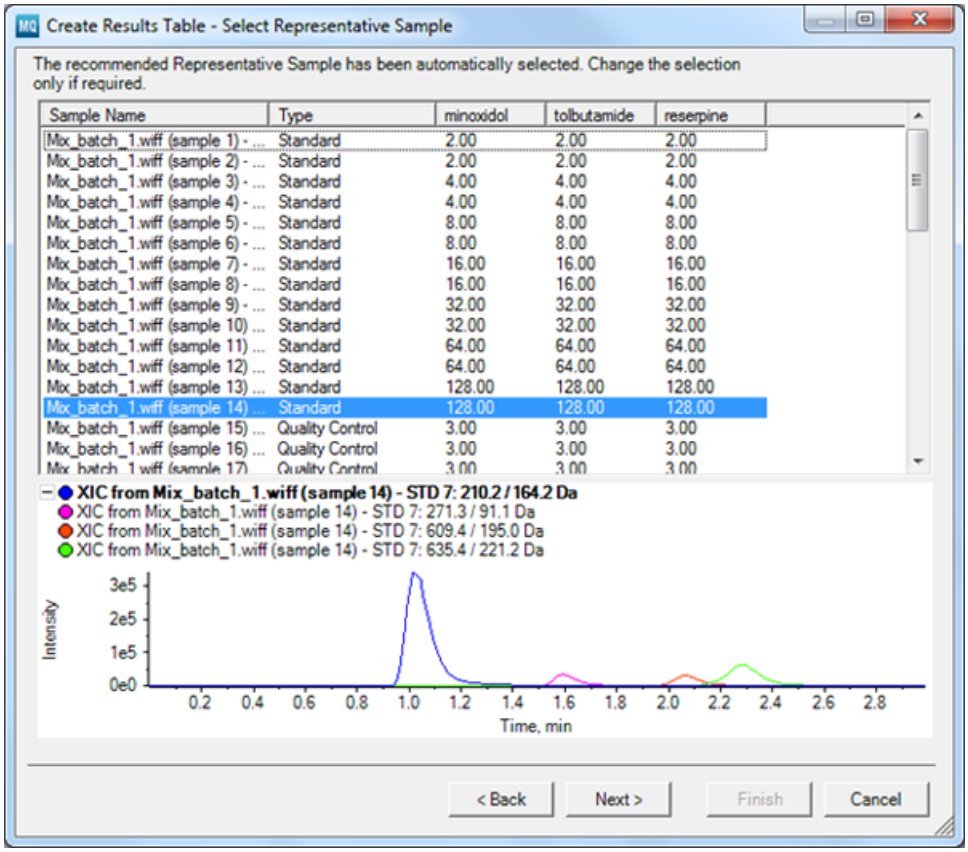
Create a Results Table

1. Click **File > New Results Table.**
2. On the **Create Results Table - Select Samples** page, expand the **Example Data** folder and then drag the **Mix_batch_1.wiff** file into the **Selected** pane.
3. Click **Next**.
4. Click the **Create New Method (SignalFinder1)** option.
5. Click **New**.
6. Type a name for the method in the **Save Quantitation Method As** dialog and then click **Save**.
7. Click **Next**.

On the **Create Results Table - Select Representative Sample** page a representative sample has been selected. The software recommends a representative sample based on selecting a chromatogram that provides the best opportunity to select integration parameters that fit the entire batch. It is recommended to select a non-saturated, high concentration standard or **QC** sample (TIC below 1E+006 cps).

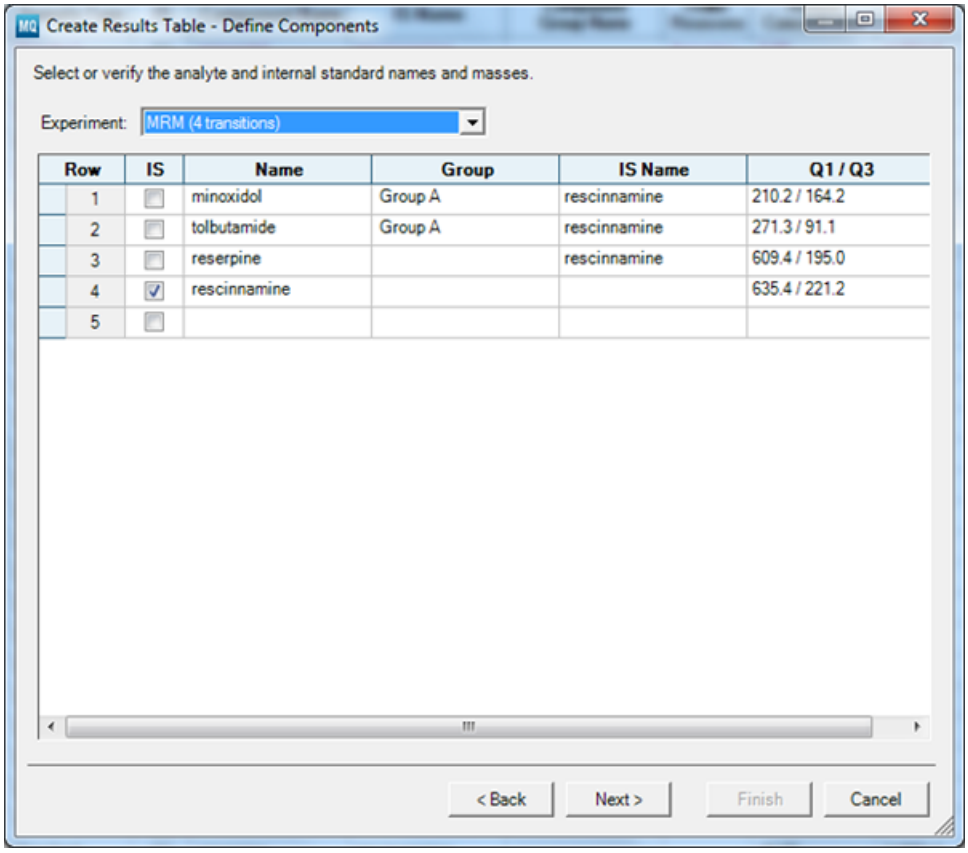
Tip! During peak review, another sample from which to build a peak model during peak review can be selected.

Figure 14-3 Create Results Table - Select Representative Sample Page



8. On the **Create Results Table - Define Components page**, confirm the analytes and internal standards.
9. Click **Next**.

Figure 14-4 Create Results Table - Define Components Page

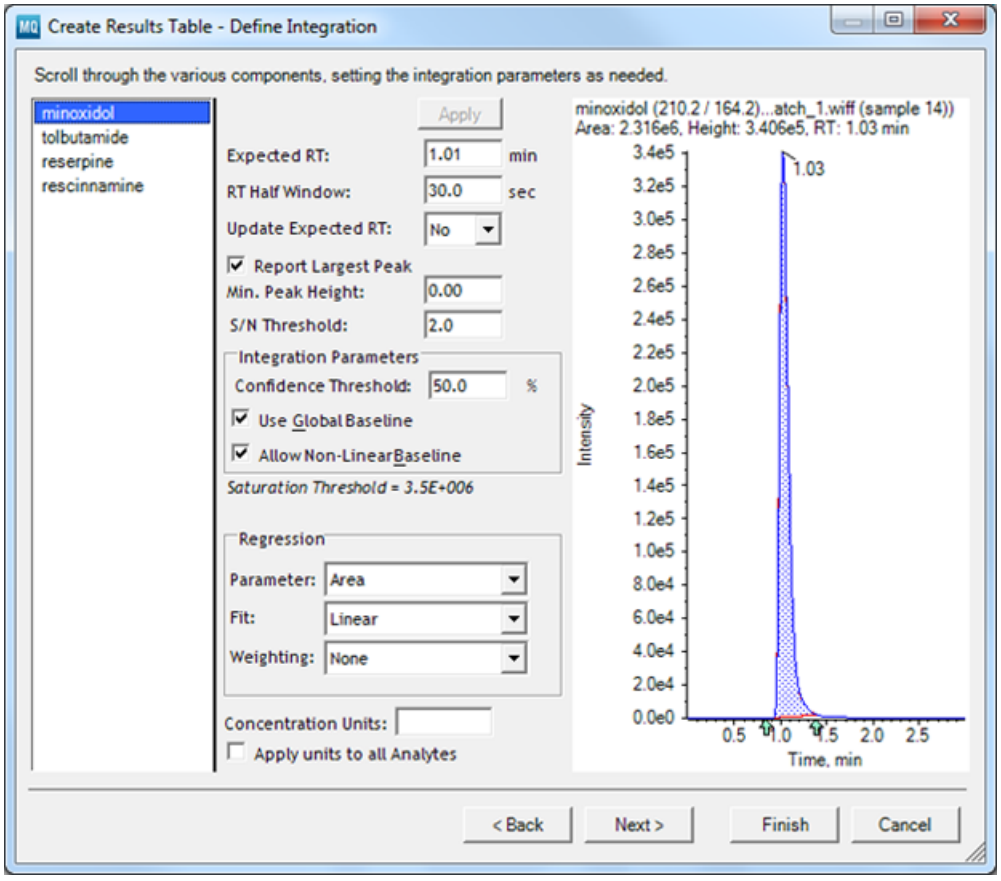


Note: When an acquisition method is created, if the component name is included in the **ID** column in the mass ranges table, then that name is populated automatically in the **Define Components** page. If the component name was not included, then manually update the table with the component name.

On the **Create Results Table - Define Integration** page, the analytes and internal standards are shown on the left side. The current integration parameters have been applied to the representative sample and the chromatogram is shown.

The components of the representative sample previously selected are shown in the **Integration** pane. Peaks in this representative sample are found and integrated using the parameters that were set in the **Integration Defaults** dialog.

Figure 14-5 Create Results Table - Define Integration Page



If required, adjust the peak-finding parameters and the positions of the green arrows in the x-axis of the chromatograms. This enables the user to more precisely set the required starting and ending position of peak integration. Effectively, this is a visual way of adjusting two peak-finding parameters that are saved with the quantitation method and applied to all peaks to be integrated. The software constrains the limits of these parameters within what it considers to be reasonable limits for the extent of the peak.

If there is more than one peak in the chromatogram and the correct peak has not been selected automatically, then drag across a peak to set the expected retention time. Drag from the actual start to the actual end of the peak and do not select a very wide or very narrow region. The reason is that the algorithm assumes that there is just one peak within the selection. For example, if the data set is noisy and the algorithm finds two merged peaks when there is only one peak present, then select a region containing both peaks to cause the algorithm to adjust its internal parameters so that only one peak is found. Alternatively, if the algorithm has found one peak when it is believed that there are two or more adjacent peaks present, then select a region spanning just the peak of interest.

10. In the **Integration Parameters** group, select the **Global Baseline** check box to use the entire chromatogram as the baseline.

If this option is not selected, then the software considers only a narrow area around the peak of interest.

11. Select the **Allow Non-Linear Baseline** check box select between a linear or non-linear baseline. A non-linear baseline estimates the baseline under each peak. A linear baseline fits a line between the points at the beginning and end of that specific group of peaks.
12. Review the peak integration for each component by clicking the component name in the left pane. Adjust the integration parameters to get the representative peak integrated properly.
13. For the components **Minoxidol**, **Tolbutamide**, and **Reserpine**, use the **Regression** group parameters to set the following and then click **Apply**:

    - **Parameter**: Area
    - **Fit**: Linear
    - **Weighting**: None

14. Set **Concentration Units** to **ng/mL** and then select the **Apply units to all Analytes** check box.
15. Click **Apply**.
16. Click **Finish**.

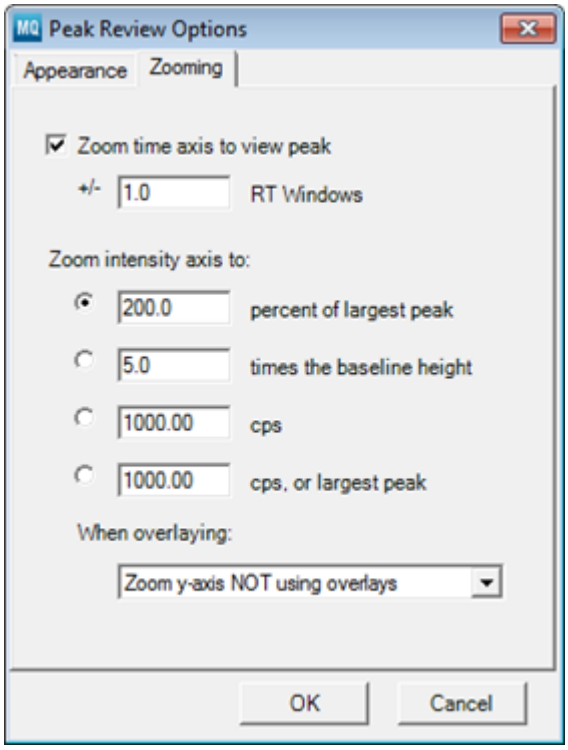
    The sample files are automatically integrated and a **Results Table** is generated.

    Refer to Review Peaks on page 98 to manage the data in the **Results Table**. Refer to Reports on page 134 for information on creating reports.

Review Peaks

1. Click the **Peak Review** icon.
2. Right-click in the table and then click **Column Settings.**
3. Make the **SF Saturated** column visible.
4. Right-click in the **Peak Review** pane and then click **Options.**
5. In the **Zooming** tab, change the **Zoom time axis to view peak** to **1**.
6. Set the **Zoom intensity axis** to **200 percent of largest peak**.

Figure 14-6 Peak Review Options



7. Use the red arrows to scroll through the peaks.

   If the detector is saturated, then the peak appears flatter than normal. For example, this peak would have a red profile around the peak and **Yes** appears in the **SF Saturated** column because the peak intensity is above the saturation threshold of 1.8^6 cps.

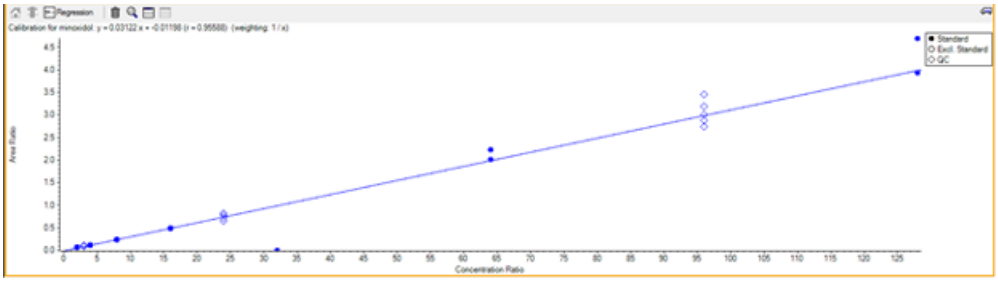
   Note: The representative sample might not be suitable for all components. A new representative sample can be selected during peak review and a new model generated.

8. To create a new model, select a new peak and then click the **Update Peak Model** icon. Select a peak that is similar in shape to the other peaks and is not saturated.
9. Right-click and then click **Update Quantitation Method for Component** to apply changes to all of the samples in the component.

Modify the Calibration Curve

1. Click the **Show Calibration Curve** icon to view the calibration curve.
2. To add a legend, right-click in the **Calibration** pane and then click **Show Legend**.

Figure 14-7 Calibration Curve



3. To add the QCs to the curve, right-click in the **Calibration** pane again and then click **Show QCs**.

Tip! To exclude a point from the curve, right-click a point on the curve and then click **Exclude**.

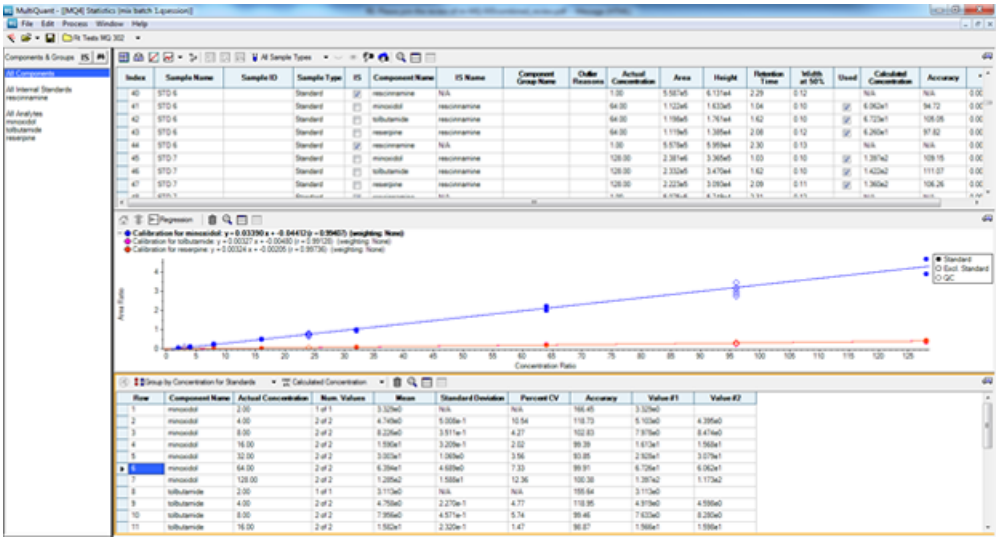
4. To confirm or edit the regression parameters for an individual analyte, select the analyte in the **Components and Group** list and then click the **Regression** button on the tool bar.

Review Sample Statistics

Users can review statistics for a single Results Table. Reviewing the peak integration, the calibration curve, and the sample statistics is an iterative process.

1. With a Results Table open, click the **Show Statistics Table** icon.
2. From the **Sample Grouping** list, click an item to specify how the sample (for a given analyte) should be grouped for the calculation of the statistics.

Figure 14-8 Statistics Pane



3. From the **Metric** list, click an item to specify the actual metric that is used for the calculation of the statistics.
4. Review the **Value** columns. The struck out points indicate excluded data points.

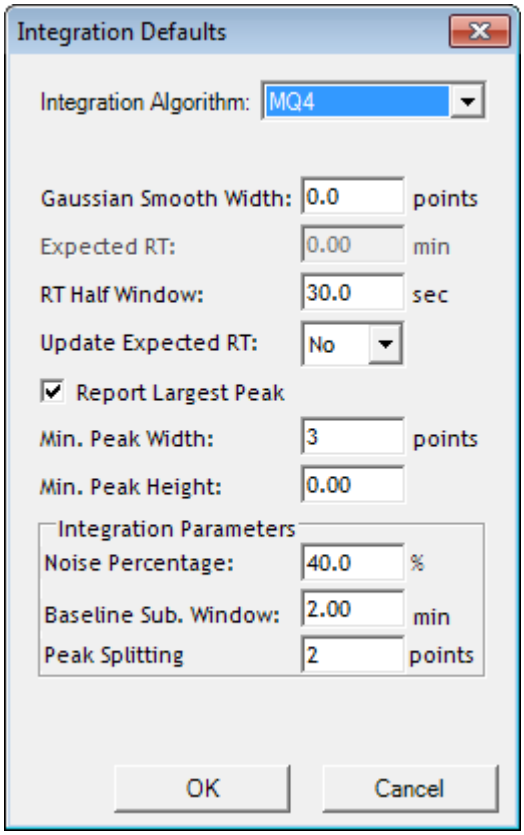
Process Data Using the MQ4 Integration Algorithm

Set the Peak Integration Parameters

Use the following procedure to check or set the integration algorithm before processing the data. Refer to MQ4 Integration Algorithm Parameters on page 117.

1. In the Analyst® MD software, on the **Navigation** bar, under **Companion Software**, double-click **MultiQuant 3.0.3**.
2. Click **Edit > Project Integration Defaults.**
3. In the **Integration Defaults** dialog, in the **Integration Algorithm** list, select **MQ4**.

Figure 14-9 Integration Defaults Dialog



4. If required, change the parameters for the project and then click **OK**.

   The MQ4 integration algorithm and parameter settings are used for any new methods created in this **Example** project folder. These default settings are project-based. To change the default settings for other projects, repeat this procedure for the selected project.

Create a Results Table

1. Click **File > New Results Table.**
2. On the **Create Results Table - Select Samples** page, expand the **Example Data** folder and then drag the **Mix_batch_1.wiff** file into the **Selected** pane.
3. Click **Next**.
4. Click the **Create New Method (MQ4)** option.
5. Click **New**.

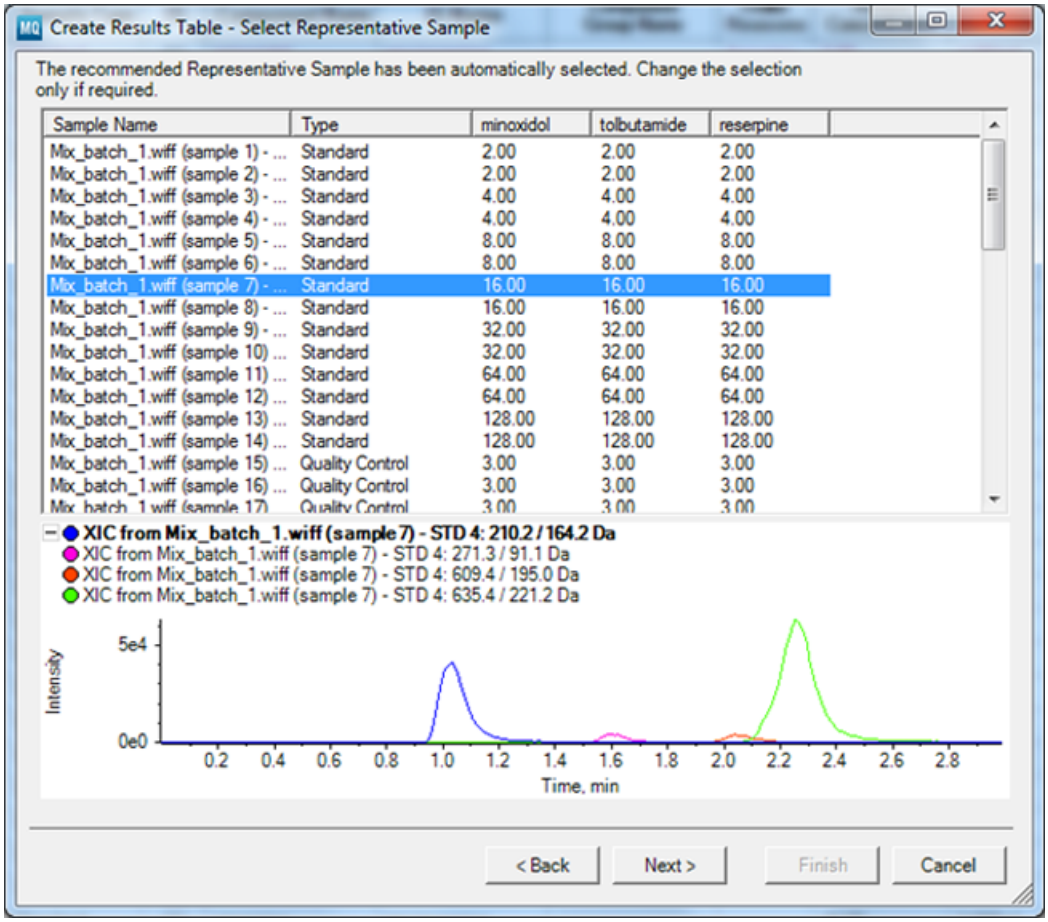
6. Type a name for the method in the **Save Quantitation Method As** dialog and then click **Save**.

   In this tutorial, a method is created. Creating methods provides an opportunity to review and apply different parameters for the integration of the data.

   If there is an existing method, then select the **Choose Existing Method** option and then select the **Edit Method** check box to review and apply different parameters to the method. If the **Edit Method** check box is not selected, then the wizard will create the **Results Table** using the existing method.

7. On the **Create Results Table - Select Representative Sample** page, a representative sample has been recommended and is selected.

Figure 14-10 Create Results Table - Select Representative Sample Page



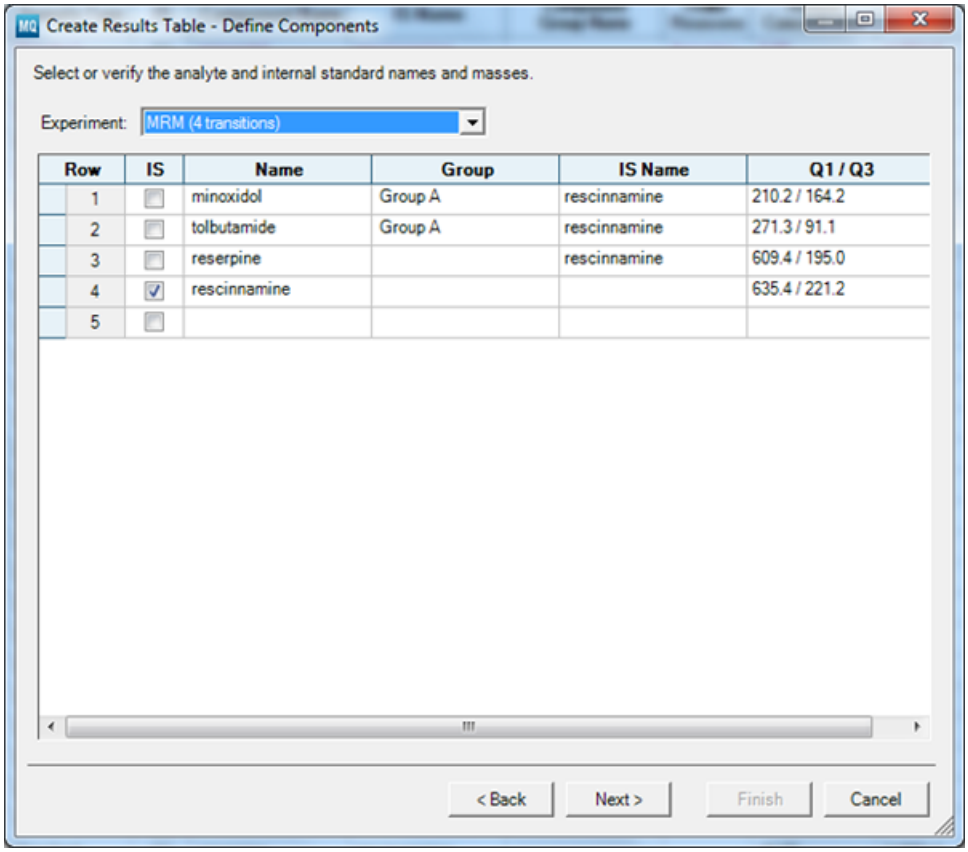
8. Click **Next**.

   The software recommends a representative sample based on selecting a chromatogram that provides the best opportunity to select integration parameters that fit the entire batch. It is recommended that the second lowest concentration standard or QC sample for the MQ4 integration algorithm is selected if the analyte concentration

information is embedded in the .wiff file. For example, if the concentration range is from one to eight, then the second lowest is two. If the default representative sample is not intense enough, then select another representative sample by clicking the **Back** button in the wizard and then selecting another sample. Another sample can be selected during peak review. Refer to Review Peaks on page 106.

9. On the **Create Results Table - Define Components page**, confirm the analytes and internal standards.

Figure 14-11 Create Results Table - Define Components Page



10. Click **Next**.

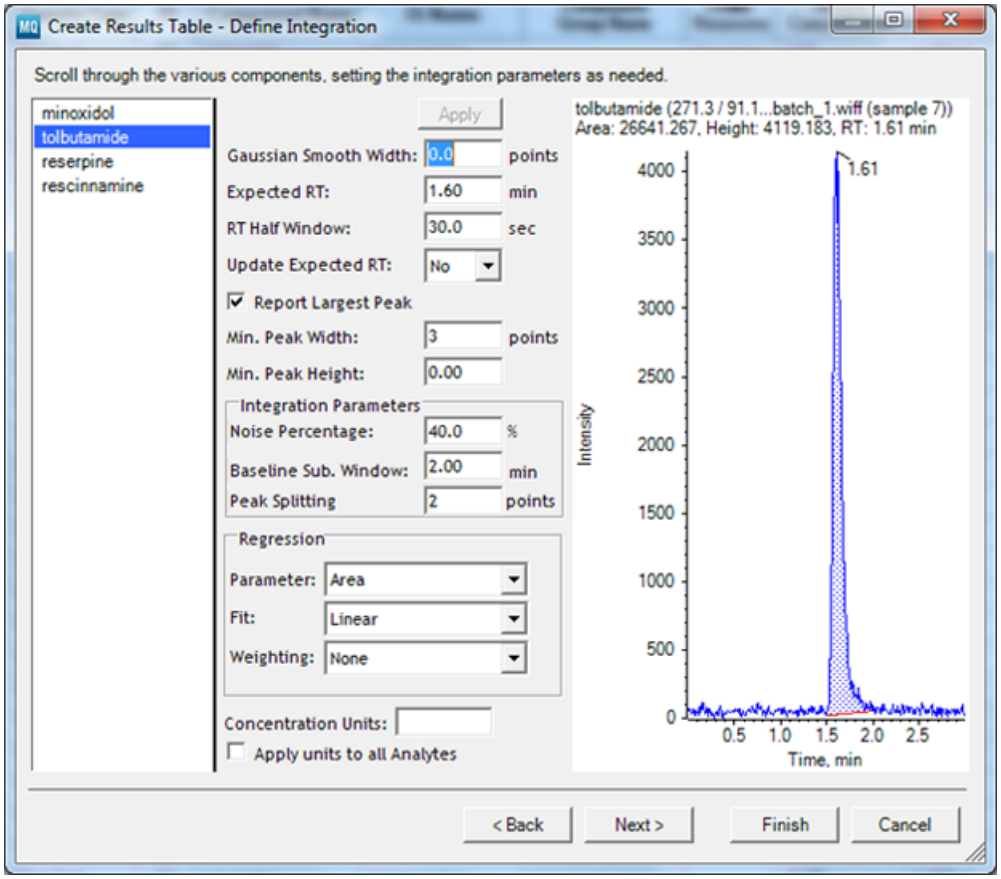
Note: When an acquisition method is created, if the component name is included in the **ID** column in the mass ranges table, then that name is populated automatically in the **Define Components** page. If the component name was not included, then manually update the table with the component name. If an .IS extension is added to a component name, the software identifies the component as an internal standard and assigns the .IS component as the internal standard to its matching analyte.

On the **Create Results Table - Define Integration** page, the analytes and internal standards are shown on the left side. The current integration parameters have been applied to the representative sample and the chromatogram is shown.

The components of the representative sample previously selected are shown in the **Integration** pane. Peaks in this representative sample are found and integrated using the parameters that were set in the **Integration Defaults** dialog.

11. Review the peak integration for each component by clicking the component name in the left pane. Adjust the integration parameters to get the representative peak integrated properly. Refer to Set the Peak Integration Parameters on page 101.

Figure 14-12 Create Results Table - Define Integration Page



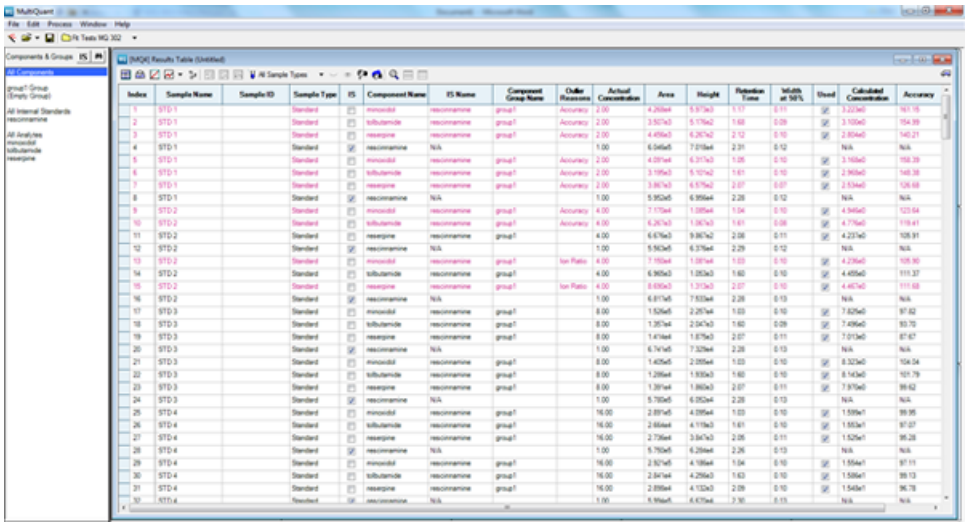
12. For the components **Minoxidol**, **Tolbutamide**, and **Reserpine**, use the **Regression** group parameters to set the following and then click **Apply**:

    - **Parameter**: Area
    - **Fit**: Linear
    - **Weighting**: None

13. Set **Concentration Units** to **ng/mL** and then select the **Apply units to all Analytes** check box.
14. Click **Apply**.
15. Click **Finish**.

    The sample files are automatically integrated and a Results Table is generated.

Figure 14-13 Results Table

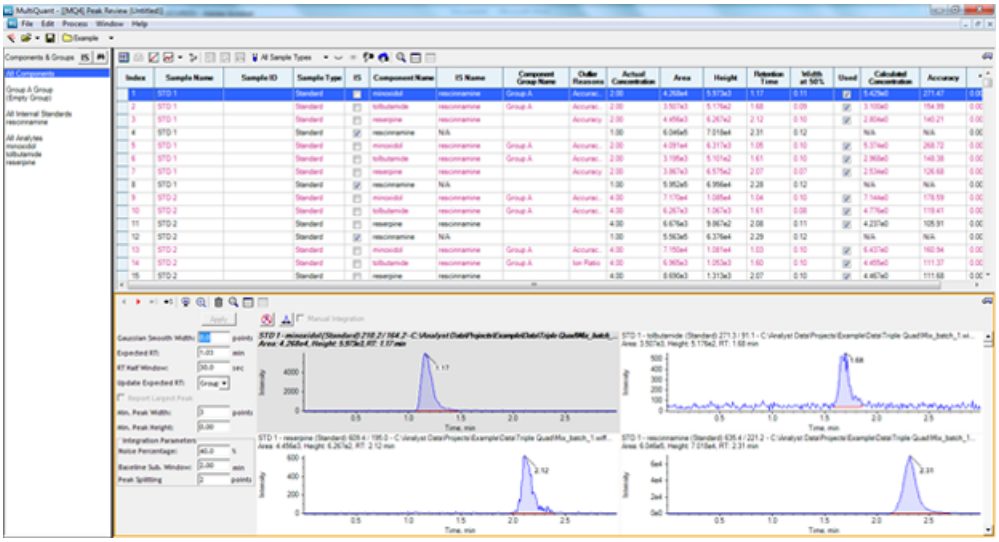


Refer to Review Peaks on page 98 to manage the data in the Results Table. Refer to Reports on page 134 for information on creating reports.

Review Peaks

1. Click the **Peak Review** icon.

Figure 14-14 Peak Review Pane



2. Right-click in the table and then click **Column Settings.**
3. Right-click in the **Peak Review** pane and then click **Options.**
4. In the **Zooming** tab, change the **Zoom time axis to view peak** to **3 RT Windows**.
5. If a chromatogram contains multiple peaks and an incorrect peak is integrated, then drag across the correct peak to set a new **Expected RT**. If required, adjust the peak finding and integration parameters. Refer to Integration Algorithms on page 109.
6. To apply the new parameters to all other samples, for the same component, right-click in the chromatogram and then click **Update Quantitation Method for Component**.
7. The embedded quantitation method can be modified while viewing the **Results Table** by clicking **Edit > Modify Results Table Method.** The user can change the integration parameter regression options and component information for each component.

   If the integration parameter regression options and component information for each component is changed, then only the quantitation method embedded in the **Results Table** is modified. The actual quantitation method file used to create the **Results Table** is not modified. To use this embedded quantitation method to process other data files, export this embedded method to a method file using the **Export** function.

   Note: Clear the integration by clicking **Set Peak to Not Found** to view the raw data before manually integrating the peak.

8. To use the manual integration mode, click the **Enable Manual Integration Mode** icon in the **Peak Review** pane. Drag the cursor from the base of one side of the peak of interest to the other. The peak is now manually integrated and the integration parameters used previously are unavailable.

Tip! If the peak has just been modified, then revert the peak to the original method by right-clicking and then clicking **Revert Peak to Original Method**.

Note: The **Calculated Concentration** field in the **Results Table** reflects any changes resulting from the fit of the curve to the points of the standard.

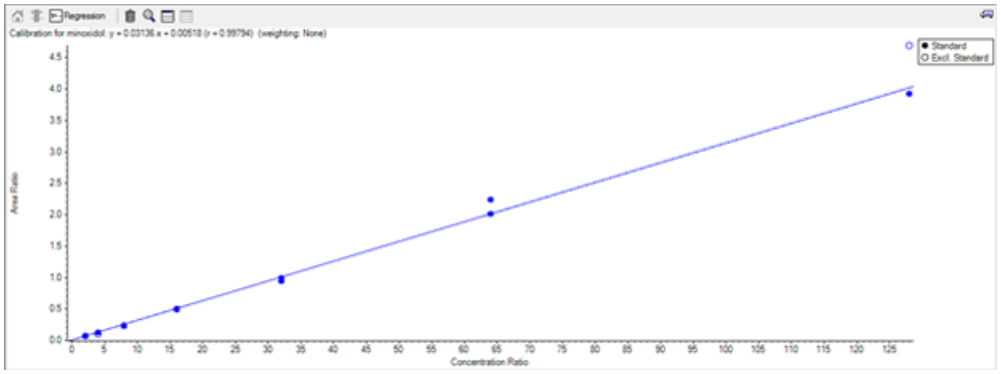
Modify the Calibration Curve

1. Click the **Show Calibration Curve** icon to view the calibration curve.
2. To add a legend, right-click in the **Calibration** pane and then click **Show Legend**.
3. To add the QCs to the curve, right-click in the **Calibration** pane again and then click **Show QCs**.

Tip! To exclude a point from the curve, right-click a point on the curve and then click **Exclude**.

4. To confirm or edit the regression parameters for an individual analyte, select the analyte in the **Components and Group** pane and then click the **Regression** button on the tool bar.
5. To make the calibration curve fit better, exclude the second STD 2 sample (concentration 4.00 ng/mL) and the first STD 7 sample (concentration 128.00 ng/mL). To do this, use the **Actual Concentration** column and the **Used** column to remove the samples. Clear the check box in the Used column to remove the point from the curve. The calibration curve should now look like the one shown in Figure 14-15.

Figure 14-15 Calibration Curve with Excluded Samples

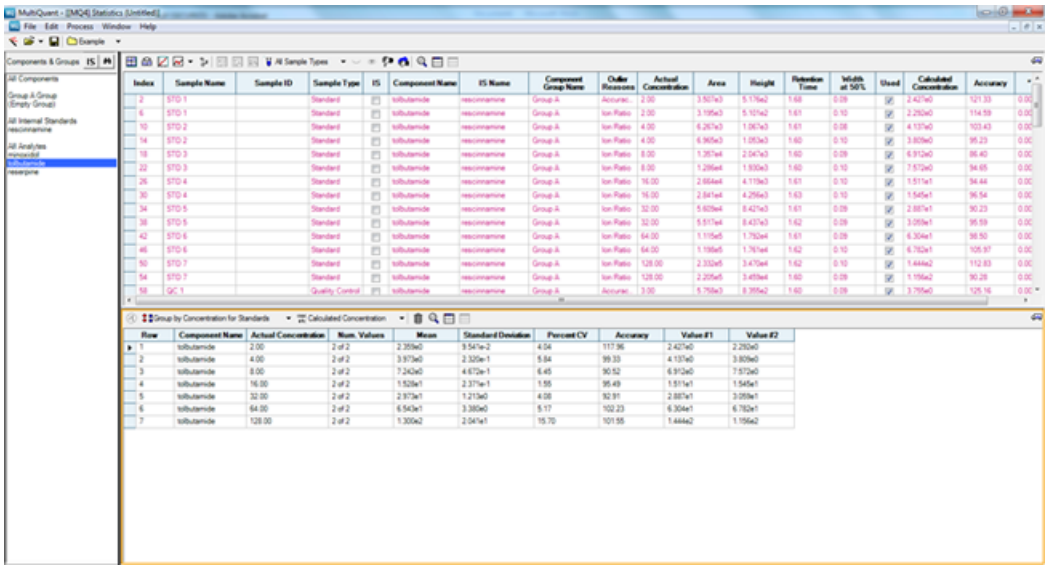


Review Sample Statistics

Users can review statistics for a single Results Table. Reviewing the peak integration, the calibration curve, and the sample statistics is an iterative process.

1. With a Results Table open, click the **Show Statistics Table** icon.

Figure 14-16 Statistics Table



2. From the **Sample Grouping** list, click an item to specify how the sample (for a given analyte) should be grouped for the calculation of the statistics
3. Click the **Value #1** column.

> **Note:** The **Group by Concentration for Standards and QCs** are actually based on **Displayed Actual Concentration**, not the **Actual Concentration** stored in the Results Table. If the Std 1 concentration is 0.001, Std 2 concentration is 0.005, and the display format is 0, then Std 1 and Std 2 are grouped together because both of them are treated as 0. To group them separately, in the **Column Settings** dialog, set the precision for **Analyte Concentration** to 0.000. If Std 1 is 0.500 and Std 2 is 0.499, then to group them together, set the precision to 0.00. Refer to Modify the Columns Shown in the Results Table on page 91.

4. Click an item from the **Metric** list to specify the actual metric that is used for the calculation of the statistics.
5. Review the **Value** columns. The struck out points indicate excluded data points.

Integration Algorithms

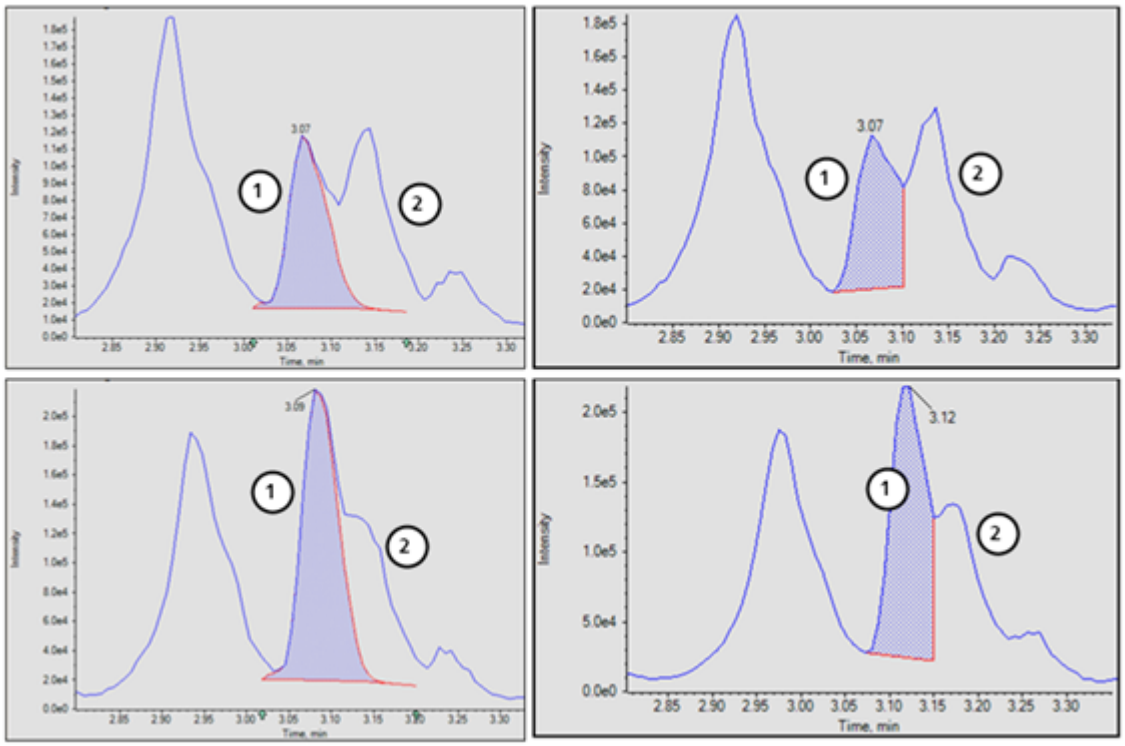
This section describes the different parameters available for each algorithm.

About the SignalFinder Integration Algorithm

Closely Eluting Peaks

The SignalFinder™ gives a more accurate representation of the peak area of closely eluting peaks. Figure 14-17 shows an example of how the MQ4 (graph on the right) and SignalFinder (graph on the left) integration algorithms handle closely eluting peaks. In this example, the background peak (item 2) is interfering with the peak of interest (item1). Because the interference peak comes from either the LC or the matrix, it is fairly constant throughout the entire batch. However, the analyte peak intensity increases as the analyte concentration increases, which results in the combined peak shapes changing dramatically. The SignalFinder integration algorithm, based on a peak model that is user defined, can consistently identify the peak of interest at all concentration levels while the MQ4 integration algorithm can only draw a vertical line from the valley to the baseline. This only integrates a partial peak, which introduces errors into the peak area.

Figure 14-17 Closely Eluting Peaks



Item	Description
1	Peak of interest
2	Co-eluting background peak

Tailing Peaks

For tailing peaks, previous algorithms are often inconsistent in selecting the retention time at which the peak ends. Depending on the exact nature of the noise in this region, two peaks that look similar might have different reported peak ends. The integration can usually be made more consistent by adjusting the peak-finding parameters. However, this is at the expense of time and effort. With a modeling approach, the integration is cut off when the model drops below a threshold, so it is much less affected by noise.

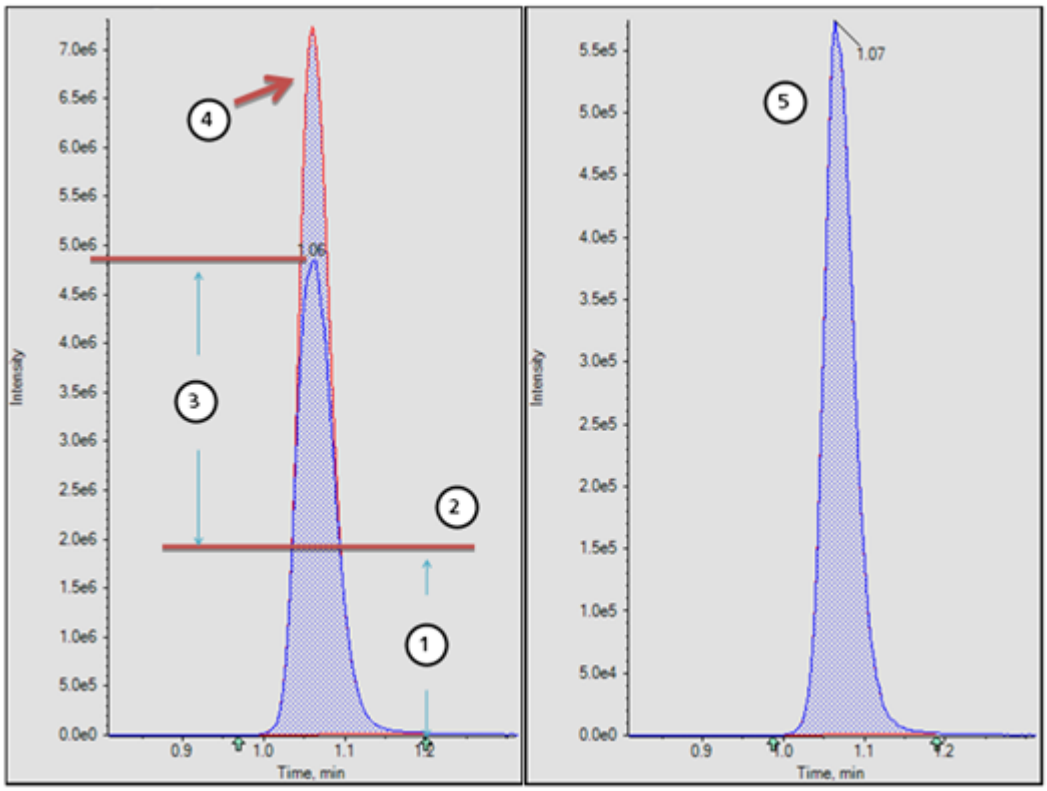
Saturated Peaks

When the algorithm detects that a peak is saturated, it uses a model to predict how the peak might look if the detector is not saturated. This is shown as a red profile extending above the peak to approximate the response that would have been obtained if the detector had not been saturated. This feature only corrects detector saturation and not ion source saturation or column saturation. Figure 14-18 shows an example of saturation correction.

Before using the SignalFinder™ algorithm, select an unsaturated sample to use for building the peak model, and then set the saturation threshold to a value that is appropriate for the detector. In this example, a saturation threshold of 1.8E+006 cps is used. The algorithm matches the unsaturated portion of the peak that remains, the peak below 1.8E+006 cps, to the peak model. The algorithm then predicts the rest of the peak indicated by the red trace based on the peak model selected.

Note: The saturation threshold is dependent on a number of factors including the type of detector, the age of the detector, and the compound of interest. For optimum results, the saturation threshold must be adjusted appropriately.

Figure 14-18 Detector Saturation Correction



Item	Description
1	Unsaturated portion (match peak model)
2	Threshold 1.8e6 cps
3	Saturated portion
4	Corrected peak profile
5	Peak model

Notes on Use

Some workflows do not have a typical sample that contains all the components of interest. For example, in drug discovery work, users might search for oxidation metabolites by adding +16 to the Q1 mass of the parent drug and either +0 or +16 to the Q3 mass. These metabolites are usually present for some samples, but not necessarily in the sample chosen as the model used to create the quantitation method. In this situation, the SignalFinder™ algorithm will use a default model if, for a given MRM transition, a reasonable peak does not exist in the typical sample. In many cases this default model will be sufficiently accurate. However, it is also possible to create a new model during subsequent peak review using a sample that does contain the peak of interest.

SignalFinder™ Integration Algorithm Parameters

The following parameters are used to identify and report the peak of interest. Refer to Integration Algorithm Parameters on page 122 for a complete list of available parameters.

Use Saturation Correction

This option is only available when setting the overall algorithm default values and not during quantitation method creation or individual peak review, because it is not useful to use this setting for only some peaks.

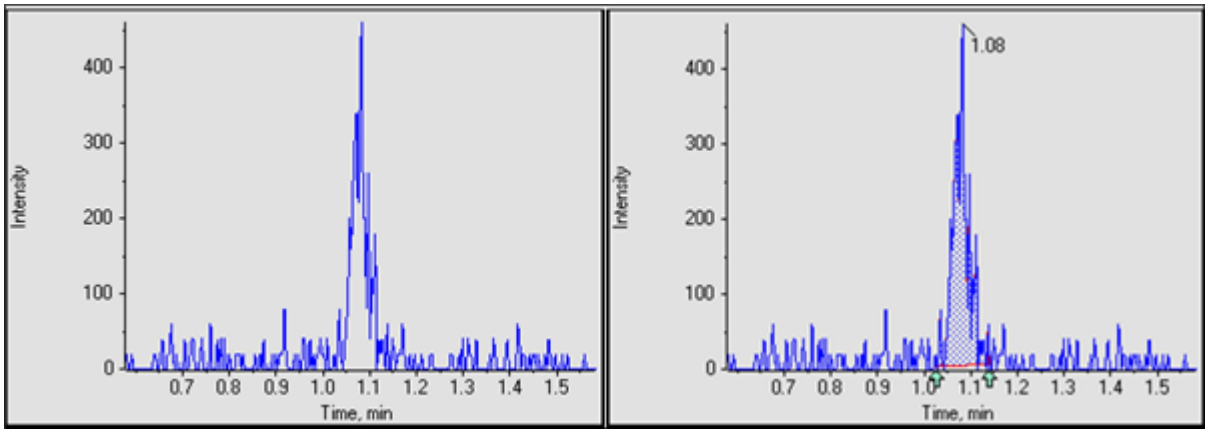
Saturation Threshold

Peaks above this threshold are considered saturated. This value is detector-dependent.

S/N Threshold

In Figure 14-19, if the S/N Threshold is set to seven (the graph on the left), then the peak is not reported. If the S/N Threshold is set to two (the graph on the right), then the peak is reported. This parameter does not affect integration.

Figure 14-19 S/N Threshold



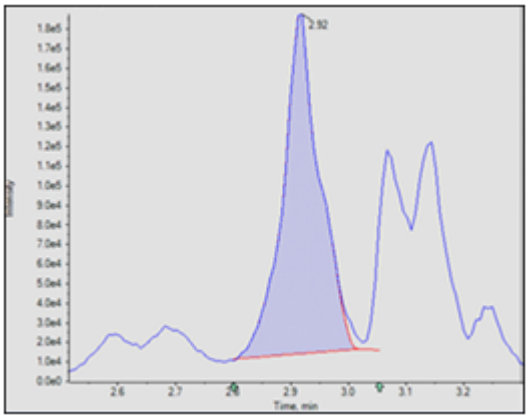
Confidence Threshold

This parameter is used to filter potential peaks that are false positives. The default value is 50%, which is usually suitable. However, the user might want to use a larger value for very noisy data or for data for which the peak width has considerable variation from sample-to-sample.

Figure 14-20 and Figure 14-21 show how the **Confidence Threshold** affects the number of peaks identified. When the **Confidence Threshold** is set to 50%, the peak with a little shoulder is identified as one peak. When the **Confidence Threshold** is lowered to 16%, the SignalFinder™ algorithm finds two peaks. Drag across the two peak regions to view the two peaks.

To determine which other peaks are potentially present in this single peak, and if the correct **Confidence Threshold** is not known, press **Ctrl** and then drag across the peak region of interest. This automatically lowers the **Confidence Threshold** to reveal the second peak of interest that is not present when the **Confidence Threshold** is set to 50%.

Figure 14-20 50% Confidence



At 16% confidence, two peaks are found. Drag across the peak area to identify the two peaks

Figure 14-21 16% Confidence

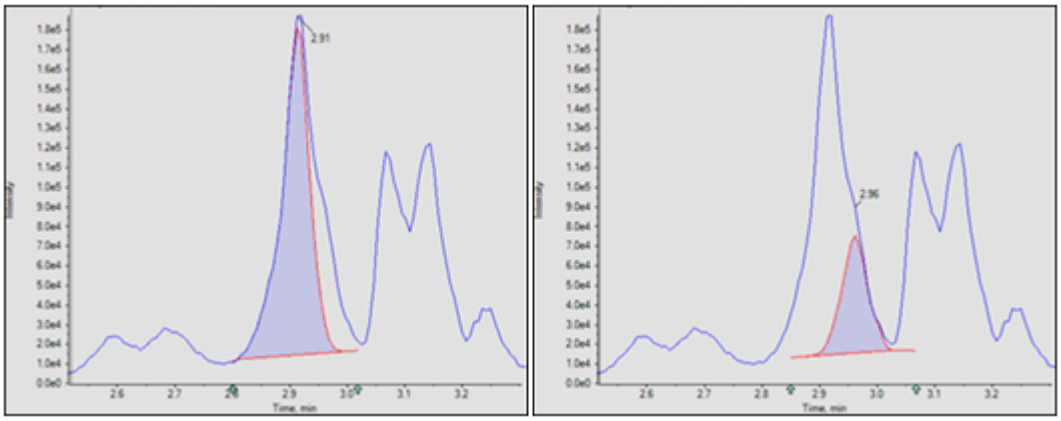
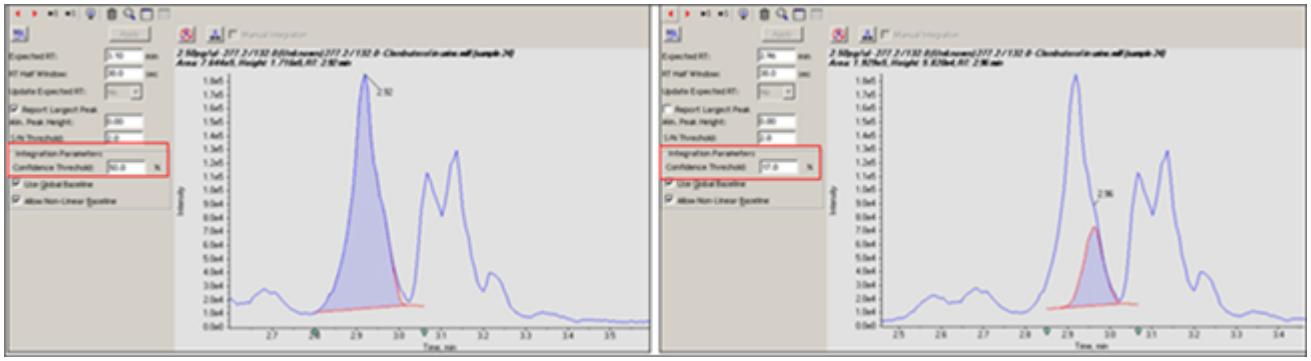


Figure 14-22 Confidence Threshold Parameter

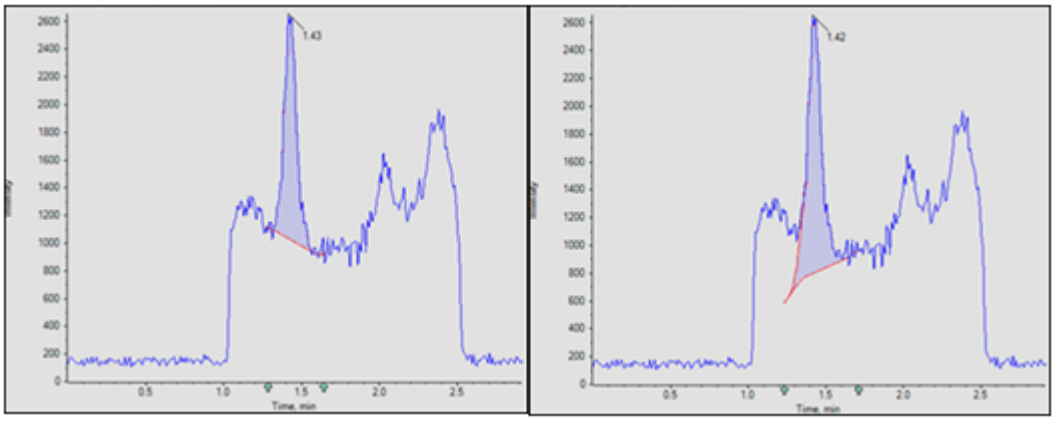


Use Global Baseline

Select this option to use the entire chromatogram as the baseline. If the option is not selected, then the quantitation software assesses changes to the baseline locally. Figure 14-23 shows an example of when the local baseline should be used.

The left graph shows a chromatogram that was properly integrated using the local baseline. The right graph shows the same chromatogram, improperly integrated using the global baseline.

Figure 14-23 Use Global Baseline



Allow Non-Linear Baseline

Use this option to select between a linear or non-linear baseline. A non-linear baseline estimates the baseline under each peak. The linear option fits a line between the points at the beginning and end of that specific group of peaks. Figure 14-24 and Figure 14-25 show examples of linear and non-linear baselines for co-eluting peaks. Items 1 to 4 are convolved peaks.

A non-linear baseline is recommended for multiple peaks. For a single peak, the difference between linear and non-linear is insignificant.

Figure 14-24 Example of a Linear Baseline

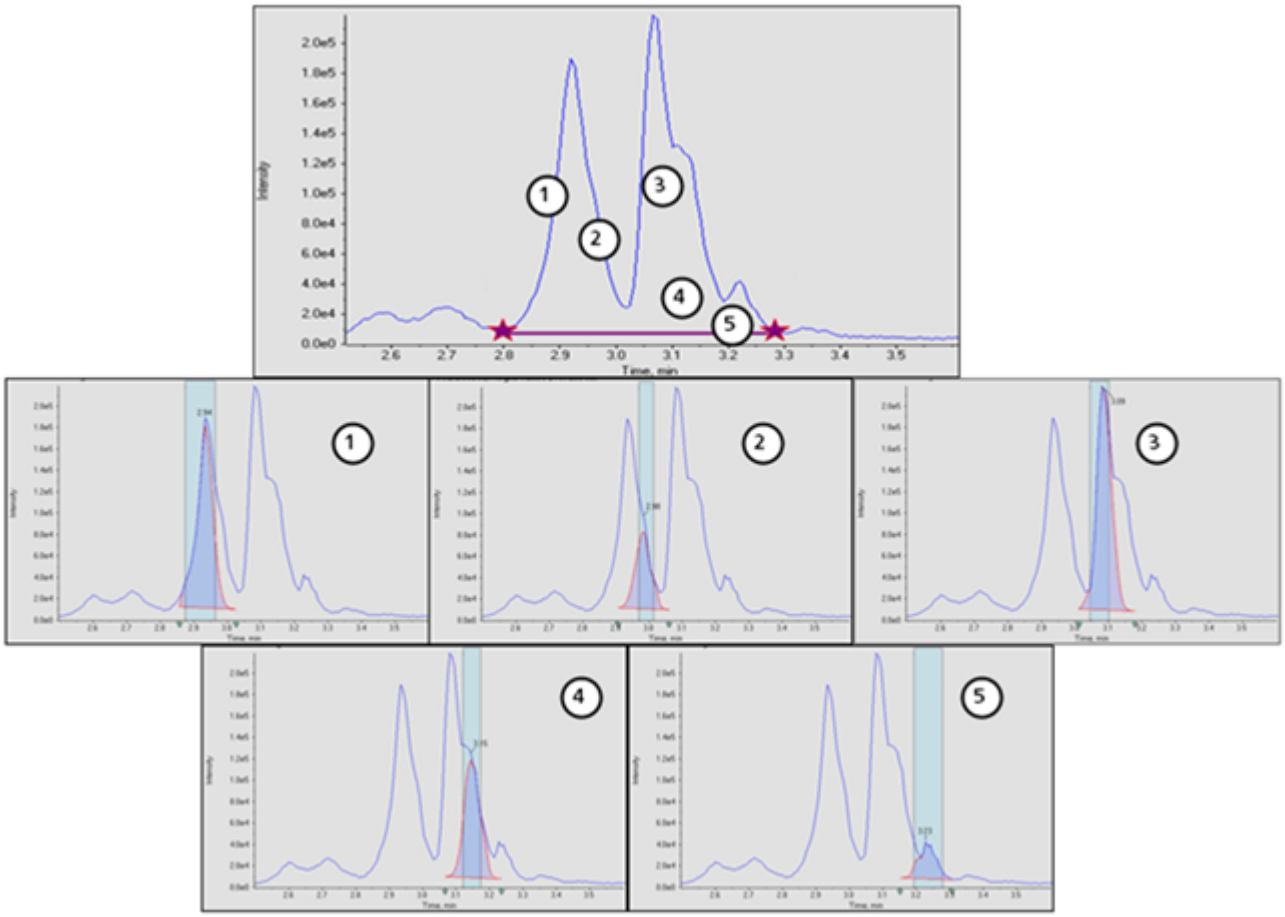
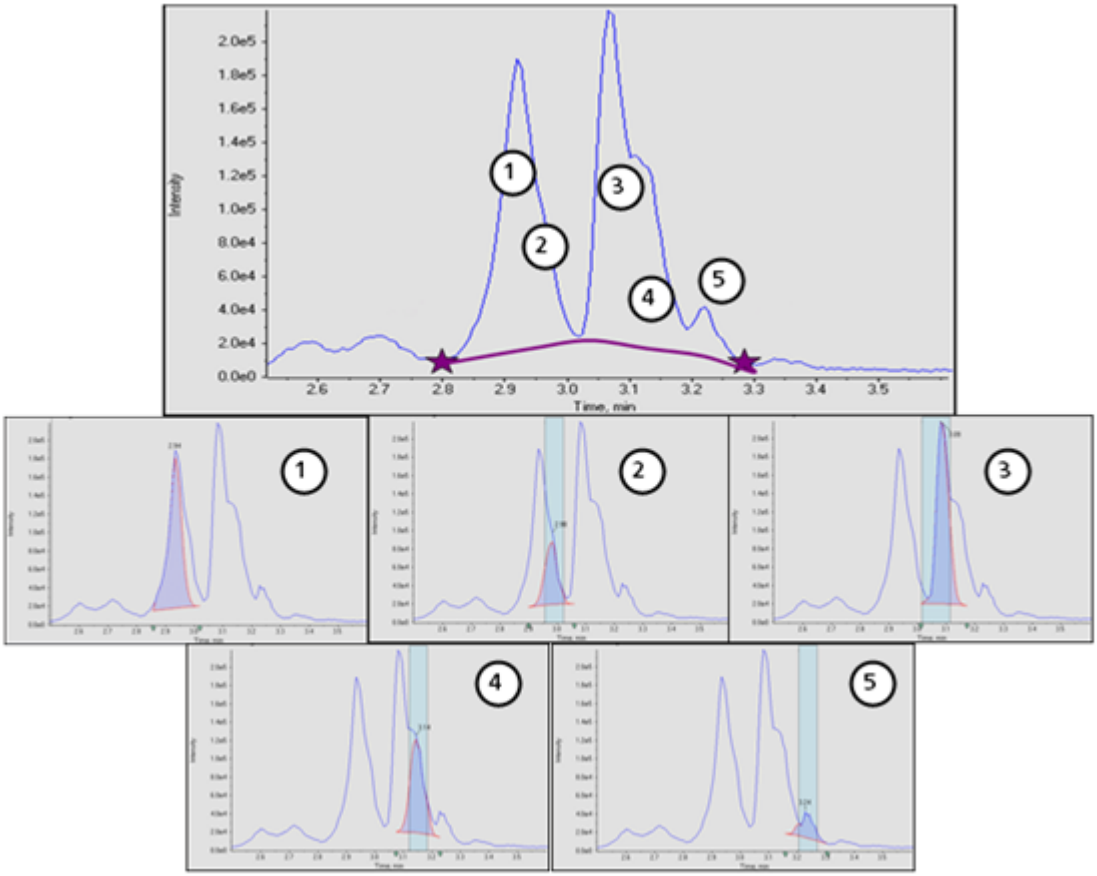


Figure 14-25 Example of a Non-linear Baseline



Tips for Using the SignalFinder™ Integration Algorithm

- Merge two peaks: Occasionally, the SignalFinder integration algorithm detects two peaks. To merge the two peaks, press **Ctrl** and then drag across the two peaks. The software tries to merge the peaks by reducing the convolution sensitivity unless the two peaks are too far apart.
- Change the peak start and end times: To change the peak start and end times either while creating a **Results Table** or during peak review, drag the peak start and end arrows.

> **Note:** The user can only change the start and end arrows within reasonable limits.

MQ4 Integration Algorithm Parameters

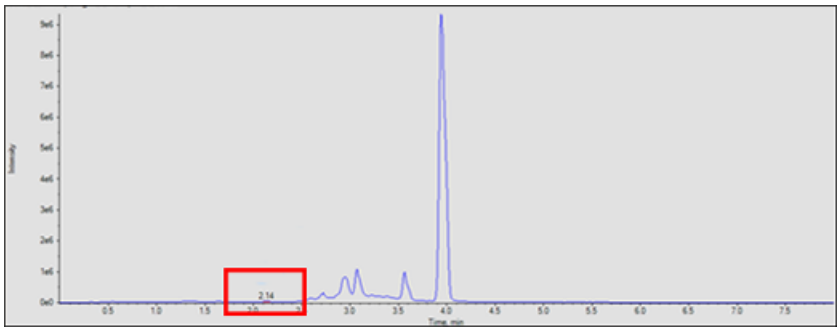
The following parameters are used to identify and report the peak of interest. Refer to Integration Algorithm Parameters on page 122 for a complete list of available parameters.

Noise Percentage

This parameter is used to estimate the noise level in the chromatograms. The specified percentage of the data points with the smallest intensity are assumed to be noise.

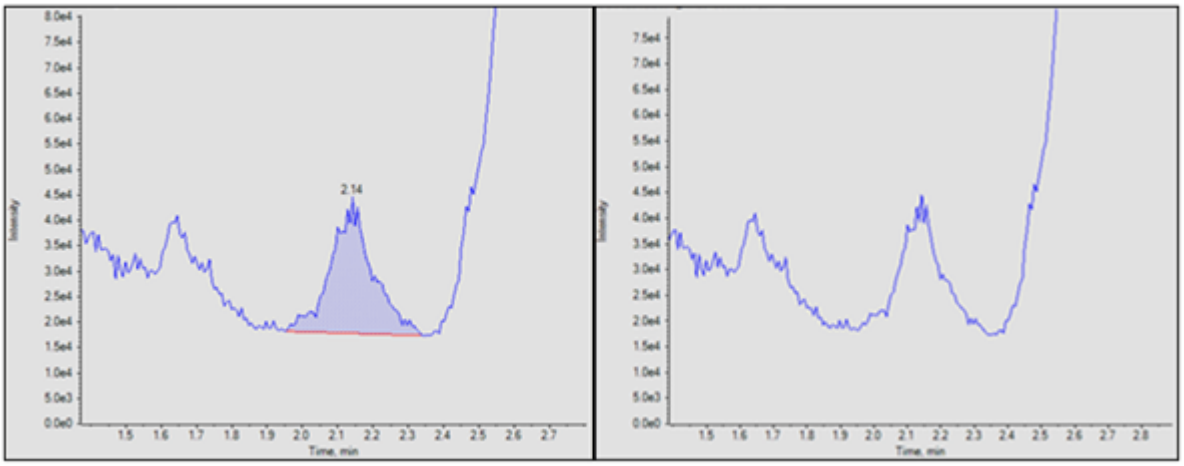
Typical values range from 20% to 60%. If small peaks in the presence of larger peaks are not being found, then the noise percentage should be lowered. Figure 14-26 is an example of a small peak in the presence of an extremely large peak. This peak is not found when the noise percentage is set to 90% but is found when the noise percentage is set to 40%.

Figure 14-26 Peak of Interest



In Figure 14-27, the left graph shows the noise percentage set to 40%. The right graph is set to 90%.

Figure 14-27 Noise Levels

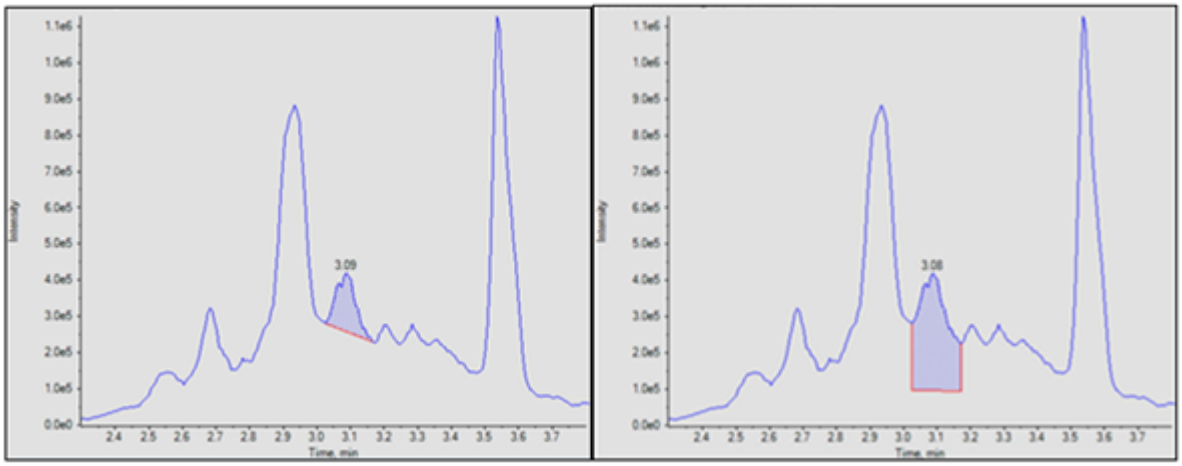


Baseline Sub. Window

After smoothing, but before other processing, chromatograms are baseline subtracted to remove humps in the data. For each data point, the baseline is calculated using the data points on both the left and right side of the current point with minimum intensity (within the subtraction window).

The exact value of this parameter is not critical, provided that it is set at least a few times larger than the expected peak width.

Figure 14-28 Baseline Subtraction Window



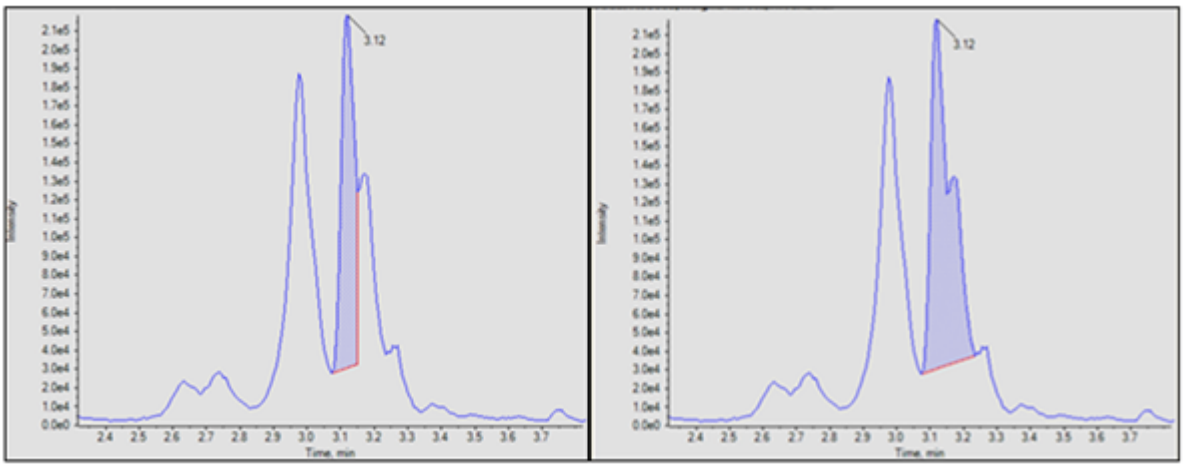
Peak Splitting

This parameter controls whether a potentially noisy peak is found as one single peak or as two (or more) separate peaks. If the dip between two potential peaks is less than the specified value, then a single peak is found. Otherwise, two peaks are found.

Setting this parameter to a large value will prevent noisy peaks from being split and found as two separate peaks. However, a smaller value needs to be used if there are two closely eluting (overlapping) distinct peaks.

The graph on the left shows Peak Splitting set to two points. The graph on the right shows Peak Splitting set to three points.

Figure 14-29 Peak Splitting



Optional Tasks

This section contains optional tasks that can be used to enhance data analysis.

Create Metric Plots

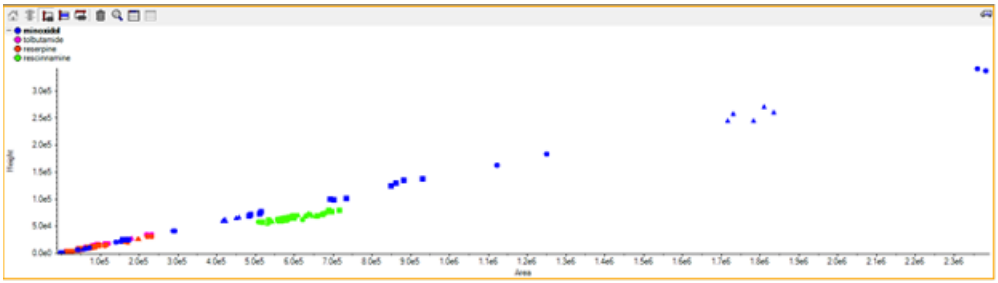
Use a **Metric Plot** to plot the values in a **Results Table** column against either the row number or another column. These plots are a valuable aid for visual data review, especially if every chromatogram does not have to be reviewed manually using the **Peak Review** pane.

Note: Metric plots use the same regression formulas as the calibration curves. For metric plots there are two additional formulas, mean and median.

1. Open a **Results Table**.
2. Select one or two columns and then click the **Metric Plot** icon. For this example, select the **IS Area** column.

   If one column is selected, then the resulting plot displays the values from the column as a function of the row number in the table. If two columns are selected, then the values from the columns are plotted against one another. The first of the two columns to be selected contains the x values and the second contains the y values.
3. Right-click in the plot pane and then click **Show Legend** to view an explanation of the symbols used by the plot.

Figure 14-30 Metric Plot



Create Custom Columns

1. With a **Results Table** open and active, right-click and then click **Add Custom Column**.

   A column is added to the end of the table.
2. Type the name of the column in the **Custom Column Name** dialog.
3. Click **OK**.

About Quantitation Method Files and Embedded Methods

Quantitation methods can be created using one of the following options:

- Use the **Quantitation wizard**.
- Edit an existing method in the **Quantitation wizard** with the **Edit** check box selected.
- Open and edit an existing quantitation method.

Quantitation methods are saved in the **Quantitation Method** folder.

When a **Results Table** is created, the quantitation method used to create the **Results Table** is embedded in the **Results Table**. Edit the embedded quantitation method, however, any changes to the quantitation method apply only to the **Results Table** embedded method and not to the methods in the **Quantitation Method** folder.

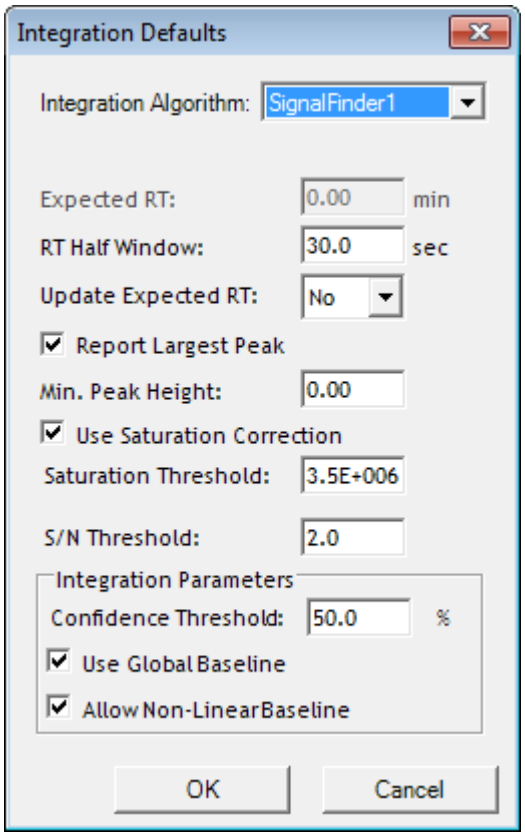
Tip! This modified embedded method can be exported for future use.

Integration Algorithm Parameters A

SignalFinder Integration Algorithm Parameters

The SignalFinder™ integration algorithm builds a peak model using the selected sample when creating a new quantitation method. This model describes the shape of the selected peak used to train the algorithm.

Figure A-1 Integration Defaults Dialog

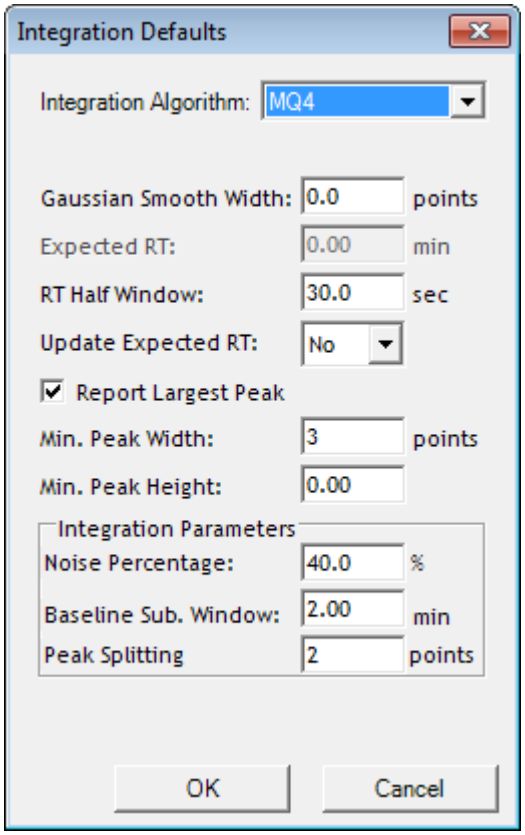


Label	Description
Integration Algorithm	The selected integration algorithm.
Expected RT	The expected retention time in minutes. This is initially set to the retention time of the largest peak in the chromatogram for the representative sample used to build the quantitation method. This field is not editable. It is updated depending on the compound in the quantitation method.
RT Half Window	Half of the total retention time window in seconds. In order for a peak to be detected and reported, the difference between the apex and the expected retention time must be less than or equal to this value.
Update Expected RT	Indicates whether the expected retention time should be adjusted on-the-fly by using other components. Makes use of additional information to compensate for shifts in retention time from sample-to-sample. The choices are: • **No**: The expected retention time is used as is. • **Group**: Applicable for components that have been assigned to groups for which all components for a given group have the same retention time (that is, different transitions for the same compound). The expected retention time is updated using the position of maximum overlap of the individual chromatograms for the group (for a given sample) within the RT window. The idea is to set the expected RT to the probable RT for the actual component of interest (where a peak is expected in each chromatogram.) If there are at least two internal standards defined for a group, then only their chromatograms are used to determine the new retention time. Otherwise, all chromatograms for the group are used. The intention is to only use those chromatograms for which the component is most likely to be present at a reasonable level. • **IS**: For analytes using an internal standard, the actual retention time of the internal standard peak (for the corresponding sample) is first determined. The expected RT for the analyte is determined by multiplying the specified expected RT by the ratio of the actual to the expected RT for the internal standard. This option is sometimes referred to as relative retention time. **Note:** This option does not apply to internal standards or to analytes that do not use an internal standard.
Report Largest Peak	If more than one peak is found in a chromatogram, then within the retention time window and satisfying the minimum width and height, this parameter controls which peak is reported. When the check box is selected, the peak with the largest area is reported. When the check box is cleared, the peak with retention time closest to the expected time is reported. Enabling this option is recommended unless the retention times are very reproducible.

Label	Description
Min. Peak Height	This parameter does not affect integration. It is used for reporting only. Any potential peaks that are less intense than this value are assumed to be not-of-interest and are not used.
Use Saturation Correction	When the algorithm detects that a peak is saturated, it uses the model to predict how the peak might look if the detector is not saturated. This causes the profile to extend above the top of the peak to approximate the response that would have been obtained if the detector had not saturated. This can extend the linear dynamic range of calibration curves. This option is only available when setting the overall algorithm default values and not during quantitation method creation or individual peak review, because it is not useful to use this setting for only some peaks.
Saturation Threshold	Peaks above this threshold are considered saturated. This value is detector-dependent.
S/N Threshold	This parameter does not affect integration. It is used for reporting only. Peaks that are below the threshold are not reported.
Confidence Threshold	Used to filter potential peaks that are false positives. The default value is 50%, which is usually suitable. However, a larger value can be used for very noisy data or for data for which the peak width has considerable variation from sample-to-sample.
Use Global Baseline	Select to use the entire chromatogram as the baseline. If the check box is not selected, then the software assesses changes to the baseline locally.
Allow Non-Linear Baseline	Select between a linear or non-linear baseline. A non-linear baseline estimates the baseline under each peak. A linear baseline fits a line between the points at the beginning and end of that specific group of peaks.

MQ4 Integration Algorithm Parameters

Figure A-2 Integration Defaults Dialog



Label	Description
Integration Algorithm	The selected integration algorithm.
Gaussian Smoothing Width	A standard Gaussian smoothing algorithm with a half-width equal to the specified value (in points) is applied. For noisy chromatograms, a value close to the actual peak width (at half height) is a good choice. For less noisy data, a smaller value can be used.
Expected RT	The expected retention time, in minutes. This is initially set to the retention time of the largest peak in the chromatogram for the representative sample used to build the quantitation method.
RT Half Window	Half of the total retention time window in seconds. In order for a peak to be detected and reported, the difference between the apex and the expected retention time must be less than or equal to this value.

Label	Description
Update Expected RT	Indicates whether the expected retention time should be adjusted on-the-fly by using other components. Makes use of additional information to compensate for shifts in retention time from sample-to-sample. The choices are: • **No**: The expected retention time is used as is. • **Group**: Applicable for components that have been assigned to groups for which all components for a given group have the same retention time (that is, different transitions for the same compound). The expected retention time is updated using the position of maximum overlap of the individual chromatograms for the group (for a given sample) within the RT window. The idea is to set the expected RT to the probable RT for the actual component of interest (where a peak is expected in each chromatogram.) If there are at least two internal standards defined for a group, then only their chromatograms are used to determine the new retention time. Otherwise, all chromatograms for the group are used. The intention is to only use those chromatograms for which the component is most likely to be present at a reasonable level. • **IS**: For analytes using an internal standard, the actual retention time of the internal standard peak (for the corresponding sample) is first determined. The expected RT for the analyte is determined by multiplying the specified expected RT by the ratio of the actual to the expected RT for the internal standard. This option is sometimes referred to as relative retention time.
Report Largest Peak	If more than one peak is found in a chromatogram, within the retention time window and satisfying the minimum width and height, then this parameter controls which peak is reported. When the check box is selected, the peak with the largest area is reported. When the check box is cleared, then the peak with retention time closest to the expected time is reported. Enabling this option is recommended unless the retention times are very reproducible.
Min. Peak Height	This parameter does not affect integration. It is used for reporting only. Any potential peaks that are less intense than this value are assumed to be not-of-interest and are not used.
Min. Peak Width	Any potential peaks that are narrower than this value are assumed to be noise and are not used.
Noise Percentage	This parameter is used to estimate the noise level in the chromatograms. The specified percentage of the data points with the smallest intensity are assumed to be noise. Typical values range from 20% to 60%. If small peaks in the presence of larger peaks are not being found, then this value should be lowered.

Label	Description
Baseline Sub. Window	After smoothing, but before other processing, chromatograms are baseline subtracted to remove humps in the data. For each data point, the baseline is calculated using the data points on both the left and right side of the current point with minimum intensity (within the subtraction window). The exact value of this parameter is not critical, provided that it is set at least a few times larger than the expected peak width.
Peak Splitting	This parameter controls whether a potentially noisy peak is found as one single peak or as two (or more) separate peaks. If the dip between two potential peaks is less than the specified value, then a single peak is found. Otherwise, two peaks are found. Setting this parameter to a large value prevents noisy peaks from being split and found as two separate peaks. However, a smaller value needs to be used if there are two closely eluting (overlapping) distinct peaks.

Regression Equations B

This section describes the equations used to calculate the regression curves. In the following equations, x represents the analyte concentration for **Standard** samples and y represents the corresponding peak area or height. The exact variables used for the regression depend on whether an internal standard is being used and whether the peak area or the peak height is used as shown in Table B-1.

Table B-1 Regression Variables

Internal Standard Used?	Area Used?	x	y
Yes	Yes	C_a / C_{is} / DF	A_a / A_{is}
Yes	No	C_a / C_{is} / DF	H_a / H_{is}
No	Yes	C_a/ DF	A_a
No	No	C_a/ DF	H_a

where:

- C_a = actual analyte concentration
- C_{is} = internal standard concentration
- DF = dilution factor
- A_a = analyte peak area
- A_{is} = internal standard peak area
- H_a = analyte peak height
- H_{is} = internal standard peak height

Weighting Factors

Table B-2 shows how the weighting factor (w in the equations) is calculated for each of the seven weighting types.

Table B-2 Weighting Factors

Weighting Type	Weight (w)
None	Always 1.0.
1 / x	If $\|x\| < 10^{-5}$, then $w = 10^{5}$. Otherwise, $w = 1 / \|x\|$.
$1 / x^2$	If $\|x\| < 10^{-5}$, then $w = 10^{10}$. Otherwise, $w = 1 / x^2$.
1 / y	If $\|y\| < 10^{-8}$, then $w = 10^{8}$. Otherwise, $w = 1 / \|y\|$.
$1 / y^2$	If $\|y\| < 10^{-8}$, then $w = 10^{16}$. Otherwise, $w = 1 / y^2$.
ln x	If $x < 0$, then an error is generated. If $x < 10^{-5}$, then $w = \ln 10^{5}$. Otherwise, $w = \|\ln x\|$.
ln y	If $y < 0$, then an error is generated. If $y < 10^{-8}$, then $w = \ln 10^{8}$. Otherwise, $w = \|\ln y\|$.

Regressions

This section provides the equations for each of the regression types. In the following equations, x, y, and w are as defined previously. All sums are calculated over all **Standard** samples, with the exception of those **Standard** samples that are marked as not used.

The correlation co-efficient is calculated as:

$$r = \left(\sum w \sum wyy_c - \sum wy \sum wy_c\right) / \sqrt{\left(D_y D_{yc}\right)}$$

where:

$$D_y = \sum w \sum wy^2 - \left(\sum wy\right)^2$$

yc = Calculated y-value using the appropriate equation below

$$D_{yc} = \sum w \sum wy_c^{\,2} - \left(\sum wy_c\right)^2$$

Linear

The linear calibration equation is:

y = mx + b

The slope and intercept are calculated as:

$$m = \left(\sum w \sum wxy - \sum wx \sum wy\right) / D_x$$

$$b = \left(\sum wx^2 \sum wy - \sum wx \sum wxy\right) / D_x$$

where:

$$D_x = \sum w \sum wx^2 - \left(\sum wx\right)^2$$

Linear Through Zero

The linear through zero calibration equation is:

y = mx

The slope is calculated as:

$$m = \sum wxy / \sum wx^2$$

Mean Response Factor

The mean response factor calibration is:

y = mx

This is the same equation as for the linear though zero case. However, the slope is calculated differently as:

$$m = \sum w(y/x) / \sum w$$

and the standard deviation of the response factor as:

$$\sigma = \sqrt{(nD/(n-1))} / \sum w$$

where:

$$D = \sum w^* \sum wy^2/x^2 - \left(\sum wy/x\right)^2$$

Note: Points whose x value is zero are excluded from the sums.

If there is some linearity and some curvature in the line of points, then use power regression instead of linear or quadratic regression to produce a line somewhere between these fits.

Quadratic

The quadratic calibration equation is:

$y = a_2x^2 + a_1x + a_0$

The polynomial co-efficients are calculated as:

$a_2 = (b_2/b_0 - b_5/b_3) / (b_1/b_0 - b_4/b_3)$

$a_1 = b_5/b_3 - a_2b_4/b_3$

$$a_0 = \left(\sum wy - a_1\sum wx - a_2\sum wx^2\right)/\sum w$$

where:

$$b_0 = \sum wx / \sum w - \sum wx^2 / \sum wx$$

$$b_1 = \sum wx^2 / \sum w - \sum wx^3 / \sum wx$$

$$b_2 = \sum wx / \sum w - \sum wxy / \sum wx$$

$$b_3 = \sum wx^2 / \sum wx - \sum wx^3 / \sum wx^2$$

$$b_4 = \sum wx^3 / \sum wx - \sum wx^4 / \sum wx^2$$

$$b_5 = \sum wxy / \sum wx - \sum wx^2 y / \sum wx^2$$

Power

The power function calibration equation is:

$y = ax^p$

The equations for the linear calibration are used as described above to calculate the slope (m) and intercept (b), except that x in those equations is replaced by ln x and y is replaced by ln y. When this is done, a and p are calculated as:

$a = e^b$

$p = m$

If any of the x or y values are negative or zero, then an error is reported.

Wagner

The Wagner calibration equation is:

$\ln y = a_2 (\ln x)^2 + a_1 (\ln x) + a_0$

The equations for the quadratic calibration are used as described above to calculate a_0, a_1, and a_2, except that x in those equations is replaced by ln x and y is replaced by ln y.

If any of the x or y values are negative or zero, then an error is reported.

Hill

The Hill calibration equation is:

$y = (a + bx^n) / (c + x^n)$

It is not possible to provide an analytical function for solving for a, b, c, and n. Instead, the co-efficients are determined using the iterative Levenberg-Marquardt method.

Calculating Final Concentrations

This section explains how to calculate the final concentration from the resultant regression equations, using the IS concentration and dilution factor used in the original concentration.

Linear

$x = (y – b) / m$

Linear Through Zero and Mean Response Factor

$x = y / m$

Quadratic

$x = (–a_1 \pm (a_1^2 – 4 \times a_2 \times (a_0 – y))^{0.5}) / (2 \times a^2)$

- If both the + and – roots are within the range of the standards, then an error is generated since there is no unique solution.
- If exactly one of the two roots is within the concentration range of the standards, then that value is reported.
- If both roots are below the lowest concentration standard, then the + root is reported.
- If both roots are above the highest concentration standard, then the – root is reported.
- If the – root is below the lowest standard and the + root is above the highest standard, then the – root is reported if the difference from the lowest concentration standard is less than the difference of the + root from the highest concentration. Otherwise, the + root is reported.

Power

$x = (y / a)^{(1 / p)}$

Wagner

The same equation for the quadratic case is used for the main calculation, except that x is replaced by ln x and y is replaced by ln y.

Hill

$x = ((a - y \times c) / (y - b))^{(1 / n)}$

Reports C

This section describes how to use the report functionality in the software to create formatted reports from **Results Tables**.

Create Reports

This software uses Microsoft Word documents as predefined templates. When a report is created, values are extracted from the most current Results Table and associated files.

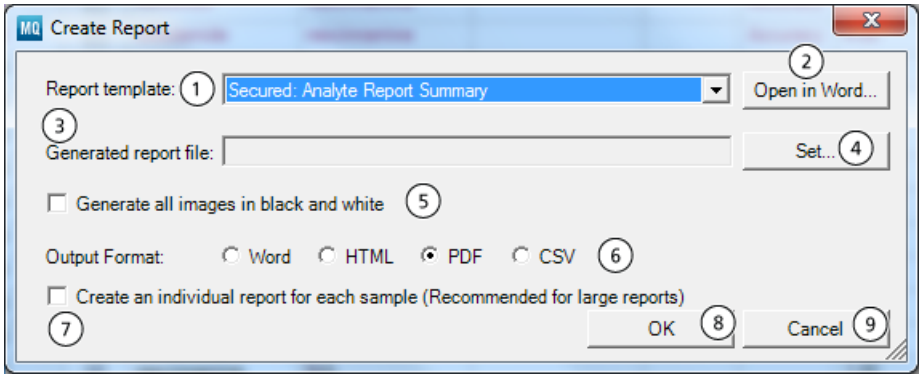
Users are responsible for validating custom templates. The user can edit the number format in the report template editor. If the number format is not specified in the template, then the format in the **Results Table Column Setting** is used in the report. Make sure that the correct number of decimal places are used.

The controlled ways to output data from the software are exporting **Results Tables**, transferring to LIMS, and reporting. The other sources of output data such as copying and pasting from **Results Tables** are not controlled. Users should not use those uncontrolled output methods for regulated purposes.

Browse to any folder to access and store data. The previous locations that templates were opened from and reports saved to are opened by default.

1. Open a **Results Table**.
2. Click **File > Create Report and Save Results Table.**

Figure C-1 Create Report Dialog



Item	Description
1	Report template: Select a template from the list..
2	Open in Word: Click to open the specified report template directly in Microsoft Word to verify or edit it.
3	Generated report file: Shows the name of the report file.
4	Set: Click to specify the filename of the report to generate.
5	Generate all images in black and white: Select the check box to print in black and white.
6	Output Format: Word, HTML, PDF, or CSV. PDF is the most secure method of output because the report cannot be edited.
7	Create an individual report for each sample (Recommended for large reports)
8	Click **OK** to print the report.
9	Click **Cancel** to close the dialog without creating a report.

3. Select a template from the Report template list. The report templates are stored in the following locations:

   - For Windows 7 and 10: C:\ProgramData\AB SCIEX\MultiQuant\Reporter.

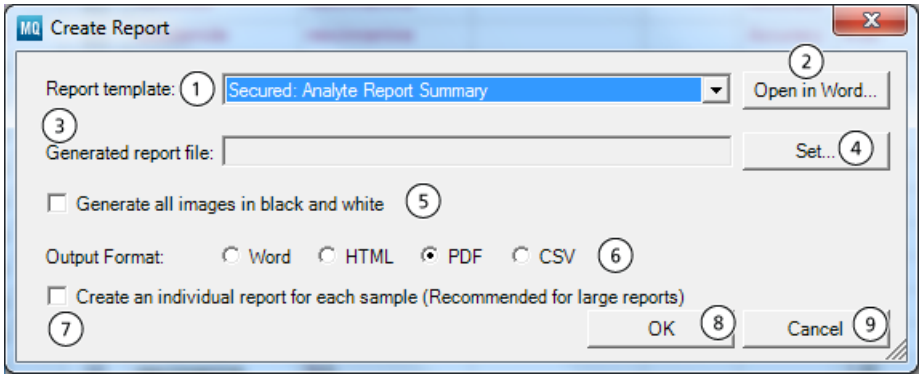
   Refer to Report Templates on page 137 for a description of the templates.
4. Click **Set** to create the name and location of the report.
5. Click **OK** to generate the report.

Create Custom Report Templates

The controlled ways to output data from the software are exporting **Results Tables**, transferring to LIMS, and reporting. The other sources of output data such as copying and pasting from **Results Tables** are not controlled. Users should not use those uncontrolled output methods for regulated purposes.

1. Open or create a **Results Table**.
2. Click **File > Create Report and Save Results Table**.

Figure C-2 Create Report Dialog



Item	Description
1	Report template: Select a template from the list..
2	Open in Word: Click to open the specified report template directly in Microsoft Word to verify or edit it.
3	Generated report file: Shows the name of the report file.
4	Set: Click to specify the filename of the report to generate.
5	Generate all images in black and white: Select the check box to print in black and white.
6	Output Format: Word, HTML, PDF, or CSV. PDF is the most secure method of output because the report cannot be edited.
7	Create an individual report for each sample (Recommended for large reports)
8	Click **OK** to print the report.
9	Click **Cancel** to close the dialog without creating a report.

3. Select a template from the **Report template** list.
4. Click **Open in Word**.

   The docx template opens and the Reporter template editor is shown on the right. The template editor is automatically populated with the tag information.
5. Edit the template as required.
6. Save the template.

Report Templates

The following table describes the available templates found in <drive>:\ProgramData\AB SCIEX\MultiQuant\Reporter.

In the event of creating a custom template, the user is responsible for validating the template. The user can edit the number format in the Report Template editor. If the number format is not specified in the template, the format in the **Results Table Column Settings** dialog will be used in the report. It is the responsibility of the user to validate the custom report template.

Some report templates use queries. Users can create queries using Microsoft Excel-based formulae to evaluate, manipulate, and present the data from the Results Table in a report. The Metafield tag in the report template tells the report the name of the query file that it should use. To use queries, the name of the query file must be specified in the MetaField tag in the report template. Queries must also have the extension ".query" to be recognized as a query. The queries must be stored in the Reporter folder where the report templates are stored.

We recommend that the user validate the generated results when a Reporter template is used, especially when queries are used in a template. If any modifications are made to the report template after validation, then the report template should be re-validated. Changes to the report template include any modification to reporter tags or queries.

Table C-1 Report Template Descriptions

Template	Description
Analyte Report Summary	Secure report showing a Samples Summary Table for each analyte. This report template is suitable for a Results Table with defined groups.
Calibration Curves Template	Report showing File Information, Statistics Table (standards) and Calibration Curve for analytes, one page per analyte.
Metric Plot_IS Area	Secure report showing, for each internal standard, a section including File Information and metric plot of IS peak area.
Per Analyte Ion Ratio Report	Secure report showing, for each analyte, a section including File Information, Results Table, Calibration Curves for each analyte, and chromatograms including IS and each analyte. This template is suitable for a Results Table with defined groups.
Per Analyte Report	Secure report showing, for each analyte, a section including File Information, Results Table, Calibration Curves for each analyte, and chromatograms including IS and each analyte. This template is suitable for a Results Table with no defined groups.
Per Sample Ion Ratio Report	Secure report showing, for each sample, a section including File Information, Sample Information, Analyte Results Table, Calibration Curves for each analyte, and chromatograms including IS and each analyte. This template is suitable for a Results Table with defined groups.

Table C-1 Report Template Descriptions (continued)

Template	Description
Per Sample Report	Secure report showing, for each sample, a section including File Information, Sample Information, Analyte Results Table, Calibration Curves for each analyte, and chromatograms including IS and each analyte. This template is suitable for a Results Table with no defined groups.
Sample Report Summary	Secure report showing an Analytes Summary Table for each sample. This report template is suitable for a Results Table with defined groups.
Sample Report with Concentration Threshold.docx	Report showing File Information, Sample Information, and Results Summary Table for each unknown sample. The Results Summary Table includes analyte-specific concentration thresholds. Analytes are flagged as positive if the concentration is above the threshold. This template references the Sample Report With Concentration Threshold.query file. The user can edit the query file to specify the analyte names, analyte groups (for example, compound class), and analyte concentration thresholds.

Report Template Tags

Table C-2 Report Template Tags

Type	Field Type	Tag Description
Tags from the Analyst® MD software data provider schema		
Analyte	ForEach	Loops over all the analytes, in the order they are defined in the Results Table.
AnalyteGroup	ForEach	Loops over the various analyte groups only. TextField or PictureField tags retrieve values for the Quantifier ion. If tags of this type contain an additional For_Each tag specifying the RatioIons attribute, then the inner loop is only for Qualifier ions that are part of the current group.
InternalStandard	ForEach	Loops over all internal standards.
QCStatistics	ForEach	Loops over all Quality Control statistics.
RatioIons	ForEach	Refer to AnalyteGroup.
Sample	ForEach	Loops over each of the individual samples. This is used, for example, in conjunction with a TextField tag setup to insert the Sample Name.

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
Statistics	ForEach	Loops over all Standards statistics.
MQ_Group	ForEach	Loops over the various groups, including IS groups or subgroups. TextField or PictureField tags retrieve values for the Quantifier ion. If tags of this type contain an additional For_Each tag specifying the RationIons attribute, then the inner loop is only for Qualifier ions that are part of the current group.
MQ_AnalyteRatioIons	ForEach	Refer to MQ_Group for Analyte qualifier only.
MQ_ISRatioIons	ForEach	Refer to MQ_Group for IS qualifier only.
AnalyteRatio	PictureField	Shows the overlays of chromatograms of Quantifier and Qualifier of the analyte subgroup. Shows the solid line in the middle to indicate the Expected Ion Ratio. The middle line = the peak height of the Quantifier x Expected Ion ratio. Shows the lower and upper bounds of the acceptable Ion Ratio range with dotted lines. Lower Bound = Peak Height of Quantifier x Expected Ion Ratio x ((100-tolerance)/100). Upper Bound = Peak Height of Quantifier x Expected Ion Ratio x ((100+tolerance)/100).
AnalyteRatioNoLines	PictureField	Shows the overlays of chromatograms of Quantifier and Qualifier of analyte subgroup without the lines.
Calibration	PictureField	Shows the calibration curve of the analyte.
IS_AnalyteRatio	PictureField	Shows the overlays of chromatograms of Quantifier and Qualifier of internal standard subgroup. Shows the solid line in the middle to indicate the Expected Ion Ratio. The middle line = the peak height of the Quantifier x Expected Ion ratio. Shows the lower and upper bounds of the acceptable Ion Ratio range with dot lines. Lower Bound = Peak Height of Quantifier x Expected Ion Ratio x ((100-tolerance)/100) Upper Bound = Peak Height of Quantifier x Expected Ion Ratio x ((100+tolerance)/100)

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
IS_AnalyteRatioNoLines	PictureField	Shows the overlays of chromatograms of Quantifier and Qualifier of internal standard subgroup without the lines.
IS_PeakReview	PictureField	Shows the chromatogram of the internal standard.
Overlay_All_XIC	PictureField	Shows the overlay of the chromatograms of all the analytes in the sample.
Overlay_All_XIC_with_IntStds	PictureField	Shows the overlay of the chromatograms of all the analytes and internal standards in the sample.
Overlay_All_XIC_with_IntStds_NoLegend	PictureField	Shows the overlay of the chromatograms of all the analytes and internal standards in the sample, without the legend.
Overlay_All_XIC_NoLegend	PictureField	Shows the overlay of the chromatograms of all the analytes in the sample, without the legend.
PeakReview	PictureField	Shows the chromatogram of the analyte.
TIC	PictureField	Shows the TIC of the sample.
Acquisition_Date	TextField	The date on which the sample was acquired. Shows the "Acquisition Date & Time".
Acquisition_Duration_Minutes	TextField	Shows the time period of data acquired of the sample, reported in minutes.
Acquisition_Method	TextField	The acquisition method that was used to acquired the sample data. Shows the "Acq. Method Name".
Analyte_AnalyteAnnotation	TextField	Shows the "Component Comment".
Analyte_AnalyteCorrelation	TextField	Shows the R value of regression.
Analyte_AnalyteRegression	TextField	Shows the regression equation, including the R value and weighting.
Analyte_Concentration	TextField	The actual concentration of the analyte, as defined by the user in the Results Table. Shows the "Actual Concentration".

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
Analyte_Expected_RT	TextField	The expected retention time for a specific analyte, in minutes. Shows the "Expected RT".
Analyte_Integration_Type	TextField	The type of integration used for specific analyte peaks. Peaks can be manually integrated or can be integrated using the available parameters. Shows the "Integration Type".
Analyte_IS_Area_Ratio	TextField	The ratio of the area of the analyte peak to the area of the peak from an internal standard solution. Calculated as Analyte Peak Area / IS Peak Area. Shows the "Area Ratio".
Analyte_IS_Height_Ratio	TextField	The ratio of the height in counts per second (cps) of the analyte peak to the height of the peak from an internal standard solution. Calculated as Analyte Peak Height / IS Peak Height. Shows the "Height Ratio".
Analyte_Mass_Ranges	TextField	The user-defined MRM transition for an analyte, defined in the acquisition method used. Shows the "Mass Info".
Analyte_Peak_Area	TextField	The peak area for an analyte in a chromatogram. Shows the "Area".
Analyte_Peak_Height	TextField	The height for the analyte peak, in counts per second (cps). Shows the "Height".
Analyte_Peak_Name	TextField	The user-defined name assigned to specific samples when creating the Results Table. Shows the "Component Name".
Analyte_Peak_Width	TextField	The width of an analyte peak, in minutes. Shows the "Total Width".

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
Analyte_Peak_Width_at_50%_Height	TextField	The width at 50% of the peak height for an analyte peak, in minutes. Shows the "Width at 50%".
AnalyteQuantPeak_info	TextField	Shows the integration information including algorithm and parameters.
Analyte_QTY	TextField	The Analyte Quantity, calculated from the analyte calculated concentration and weight-to-volume ratio (for example, ng of analyte per gram of sample). Shows the "Quality".
isCurrentAnalyteQuantifier	TextField	Is the first analyte in the group.
Analyte_Processing_Alg	TextField	Shows the integration algorithm.
Analyte_Retention_Time	TextField	The actual retention time for an analyte in a chromatogram used to generate a Results Table. Shows the "Retention Time".
Analyte_R_Squared	TextField	Shows the R^2 value of regression.
Analyte_RT_Window	TextField	The range of time, in seconds, in which an analyte peak is expected to appear. The center of this range is the expected retention time for the analyte. Shows the value of "RT Half Window" of the integration parameters.
Analyte_Signal_To_Noise	TextField	The signal-to-noise ratio for a specific analyte peak. Shows the "Signal/Noise".
Analyte_Slope_of_Baseline	TextField	The slope of the baseline for an analyte, taken in terms of % Intensity/minutes. Shows the "Slope of Baseline" for the analyte.
Analyte_Start_Scan	TextField	Analyte Start Scan.
Analyte_Start_Time	TextField	The time where the analyte peak begins, in minutes. Shows the "Start Time".

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
Analyte_Stop_Scan	TextField	Analyte Stop Scan.
Analyte_Stop_Time	TextField	The time where the analyte peak ends, in minutes. Shows the "End Time".
Analyte_Unit	TextField	The units used to represent the concentration for analytes. The standard unit for Results Tables is ng/mL. Shows the "Conc. Units".
Analyte_Use_Record	TextField	A selection box which determines whether a specified record will be used for subsequent analysis such as calibration curves. Shows the "Used".
Analyte_Count	TextField	Shows the total number of analytes.
Analyte_Index	TextField	Shows the order number of the analyte in sample, starting from 0.
Calculated_Accuracy	TextField	The accuracy for the analyte peak, derived by comparing the actual analyte concentration to the calculated analyte concentration. Shows the "Accuracy".
Calculated_Concentration	TextField	The calculated concentration for the analyte peak performed by the Analyst® MD software using the peak area. Shows the "Calculated Concentration".
Calculated_Relative_Retention_Time	TextField	The retention time for an analyte or internal standard specific record in a Results Table. Shows the "Relative RT".
IS_Concentration	TextField	The actual concentration of an internal standard, as defined by the user in the Results Table. Shows the "IS Actual Concentration".
IS_Expected_RT	TextField	The expected retention time of an internal standard peak, in minutes. Shows the "IS Expected RT".

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
IS_Integration_Type	TextField	The type of integration used for specific internal standard peaks. Peaks can be manually integrated or can be integrated using the available parameters. Shows the "IS Integration Type".
IS_Mass_Ranges	TextField	The user-defined MRM transition for an internal standard, defined in the acquisition method used. Shows the "IS Mass Info".
IS_Peak_Area	TextField	The peak area for an internal standard. Shows the "IS Area".
IS_Peak_Height	TextField	The height for the internal standard peak, in counts per second (cps). Shows the "IS Height".
IS_Peak_Name	TextField	The user-defined name given to a specific internal standard, when creating the Results Table. Shows the "IS Name".
IS_Peak_Width	TextField	The width of an analyte peak, in minutes. Shows the "IS Total Width".
IS_Peak_Width_at_50%_Height	TextField	The peak width, in minutes, for an internal standard peak at half of its height, in counts per second (cps). Shows the "IS Width at 50%".
IS_Retention_Time	TextField	The actual retention time for an internal standard. Shows the "IS Retention Time".
IS_RT_Window	TextField	The range of time, in seconds, in which an internal standard peak is expected to appear. The center of this range is the expected retention time for the internal standard. Shows the value of "RT Half Window" of the integration parameters for IS.
ISQuantPeak_Info	TextField	Shows the integration information including algorithm and parameters.

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
IS_Signal_To_Noise	TextField	The signal-to-noise ratio of an internal standard peak. Shows the "IS Signal/Noise".
IS_Slope_of_Baseline	TextField	The slope of the baseline for an internal standard, taken in terms of % Intensity/minutes. Shows the "Slope of Baseline" for the Internal Standard.
IS_Start_Scan	TextField	Internal Standard Start Scan.
IS_Start_Time	TextField	The time where the internal standard peak begins, in minutes. Shows the "IS Start Time".
IS_Stop_Scan	TextField	Internal Standard Stop Time.
IS_Stop_Time	TextField	The time where the internal standard peak ends, in minutes. Shows the "IS End Time".
IS_Units	TextField	The units used to represent the concentration for internal standards. The standard unit for Results Tables is ng/mL. Shows the "Conc. Units" for IS.
MQ_Accuracy_Tolerance_LLOQ	TextField	Shows the value of the Max. Accuracy Tolerance for LLOQ in the Outlier Setting dialog of the Quantitation Method.
MQ_Accuracy_Tolerance_STD	TextField	Shows the value of the Max. Accuracy Tolerance for Standards in the Outlier Setting dialog of the Quantitation Method.
MQ_Accuracy_Tolerance_QC	TextField	Shows the value of the Max. Accuracy Tolerance for QCs in the Outlier Setting dialog of the Quantitation Method.
MQ_Analyte_Group_Name	TextField	Shows the name of the analyte group name.
MQ_Created_With	TextField	Shows the name of the product that is used to generate the report.
MQ_Expected_Ion_Ratio	TextField	Shows the "Expected Ion Ratio".

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
MQ_Group_Index	TextField	Shows the order number of the group in sample, starting from 1. Use with ForEach MQ_Group loop.
MQ_Group_Name	TextField	Shows the name of the group. Use with ForEach MQ_Group loop.
MQ_Ion_Ratio	TextField	Shows the "Ion Ratio".
MQ_IonRatio_Tolerance	TextField	Shows the value of the Max. Ion Ratio Tolerance for the analyte in the Outlier Setting dialog of the Quantitation Method.
MQ_IS_Group_Name	TextField	Shows the name of the internal standard group.
MQ_IsRowHidden	TextField	Shows the row hidden in Results Table.
MQ_Lower_Limit_Concentration	TextField	Shows the value of the Lower Limit of Calculated Concentration in the Outlier Setting dialog of the Quantitation Method.
MQ_Outlier_Reasons	TextField	Shows the "Outlier Reasons".
MQ_Peak_Asymmetry_Factor	TextField	Shows the "Asymmetry Factor".
MQ_Peak_BaselineDelta_to_Height	TextField	Shows the "Baseline Delta/Height".
MQ_Peak_End_at_10pct	TextField	Shows the "End Time at 10%".
MQ_Peak_End_at_5pct	TextField	Shows the "End Time at 5%".
MQ_Peak_Points_Across_Baseline	TextField	Shows the "Points Across Baseline".
MQ_Peak_Points_Across_Half_Height	TextField	Shows the "Points Across Half Height".
MQ_Peak_Start_at_10pct	TextField	Shows the "Start Time at 10%".
MQ_Peak_Start_at_5pct	TextField	Shows the "Start Time at 5%".
MQ_Peak_Tailing_Factor	TextField	Shows the "Tailing Factor".
MQ_Peak_Width_at_10pct	TextField	Shows the "Width at 10%".
MQ_Peak_Width_at_5pct	TextField	Shows the "Width at 5%".
MQ_Quantifier_Mass_Ranges	TextField	Shows the "Mass Range" for the quantifier in the analyte group.
MQ_Quantifier_Peak_Area	TextField	Shows the "Area" for the quantifier in the analyte group.

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
MQ_Quantifier_Calculated_Concentration	TextField	Shows the "Calculated Concentration" for the quantifier in the analyte group.
MQ_Report_Generation_Date	TextField	Shows the date of the report generation, reflecting the culture settings from the software.
MQ_Upper_Limit_Concentration	TextField	Shows the value of the Upper Limit of Calculated Concentration in the Outlier Setting dialog of the Quantitation Method.
Query_Name	TextField	The name of the query referenced in the report template (if applicable).
Record_Modified	TextField	Shows the "Modified".
Reporter_Template_Name	TextField	The name of the report template used to create the report.
ResultTbl_CreateDate	TextField	Shows the date the Results Table was created.
ResultTbl_IntegrAlgorithm	TextField	Shows the processing algorithm used to process the Results Table (for example, MQ4, SignalFinder1).
ResultTbl_Name	TextField	Shows the filename for the Results Table.
ResultTbl_ProjName	TextField	Shows the project name in which the Results Table saved.
Sample_Comment	TextField	A comment related to the sample. Shows the "Sample Comment".
Sample_Dilution_Factor	TextField	The total number of unit volumes in which the sample is dissolved. Shows the "Dilution Factor".
Sample_File_Name	TextField	The name of the data file where the raw data for the specific sample is stored. Shows the "Original Filename".
Sample_ID	TextField	A user-defined value for listing specific IDs for each sample or analyte in the Results Table. Shows the "Sample ID".
Sample_Index	TextField	Shows the "Index".

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
Sample_Count	TextField	Shows the the total number of analytes.
Sample_InjectionVolume	TextField	The injection volume used in the autosampler used when the original sample was injected, as defined in the acquisition method. Shows the "Injection Volume".
Sample_Instrument	TextField	Shows the type of instrument used to acquire the sample, which is extracted from the wiff file.
Sample_InstrumentSerialNumber	TextField	Shows the serial number of the instrument used to acquire the sample, which is extracted from the wiff file.
Sample_Name	TextField	The user-defined name assigned to the specific sample when creating the Results Table. Shows the "Sample Name".
Sample_Operator	TextField	The logged in user at the time of the acquisition. Shows the "Operator Name".
Sample_Plate_Number	TextField	The position of the sample plate in the autosampler used when acquiring the samples. Shows the "Plate Number".
Sample_Rack_Number	TextField	The position of the sample rack in the autosampler used when acquiring the samples. Shows the "Rack Number".
Sample_Type	TextField	The user-defined value indicating what type of sample each specific injection is from. For example, Blank, Standard, and so on. Shows the "Sample Type".
Sample_Vial_Position	TextField	The vial position defined in the acquisition batch used in the autosampler to determine which vial holds the sample. Shows the "Vial Number".
Sample_File_Full_Name	TextField	Shows the file name with the full path.
Sample_Index_In_Wiff	TextField	Shows the order number of the sample in the wiff file, starting from 0.

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
Sta_Accuracy	TextField	The accuracy for the analyte peak, determined by comparing the actual analyte concentration to the calculated analyte concentration. Shows the "Accuracy".
Sta_CV	TextField	Shows the conditional variance percent that dictates how close or far in terms of percent a calculated concentration value deviates from the mean concentration value. Calculated by taking standard deviation/mean.
Sta_ExpectedConcent	TextField	The expected concentration for an analyte calculated by the Analyst® MD software, using the peak area. Shows the "Actual Concentration".
Sta_Mean	TextField	Shows the mean value (average) for the calculated concentrations that are calculated by the Analyst® MD software.
Sta_NumVal	TextField	Shows the number of values that make the statistic. How many samples are taken into account when an average is performed.
Sta_QCAccuracy	TextField	The accuracy determined by comparing the expected concentration to the actual concentration for a quality control sample as defined by the user in the sample type column. Shows the "Accuracy".
Sta_QCCV	TextField	Shows the conditional variance percent that dictates how close or far in terms of percent a calculated concentration value deviates from the mean concentration value. Calculated by taking standard deviation/mean. Applies to a Quality Control sample.
Sta_QCExpectedConcent	TextField	The expected concentration for a Quality Control sample, as defined by the user. Shows the "Actual Concentration" for the Quality Control sample.

Table C-2 Report Template Tags (continued)

Type	Field Type	Tag Description
Sta_QCMean	TextField	Shows the mean value (average) for the calculated concentrations that are calculated by the Analyst® MD software for a Quality Control sample.
Sta_QCNumVal	TextField	Shows the number of values taken into account for a quality control sample concentration mean when performing the average.
Sta_QCStdDev	TextField	Shows the standard deviation for the concentration values for each sample. The standard deviation represents a measure of the spread of a set of values from the mean value.
Sta_StdDev	TextField	Shows the standard deviation for a standard sample. The standard deviation represents a measure of the spread of a set of values from the mean value.
CUSTOM	TextField	Shows the value of Results Table custom columns.

Relative Noise and Signal-to-Noise Calculations D

When performing quantitative mass spectrometry data processing, it is important to determine whether a given peak is significant or not, where 'significant' typically means 'does this signal exceed background noise?'

Usually the peak height is compared to background noise measured in a peak-free region where the noise is typically estimated as either one or three times the standard deviation of the data points in this range. This approach is less than ideal for the following reasons:

- It is subjective, as the noise region is selected manually.
- A background region without a peak might not exist or the region might be too narrow for an accurate estimate of the noise.
- The noise at the peak position might be quite different from that in the selected noise region.
- The factor of 'one or three' is also subjective and different authorities have different recommendations.
- The apparent noise can be altered if the data have been pre-processed. For example, smoothed, or thresholded.

By using the concept of Relative Noise (Rn), it is easy to develop a simple method to calculate the expected noise at any point in the data, to compare against the measured signal. This is a robust, objective metric that can be used to calculate signal-to-noise (S/N) and to evaluate and compare instrument and assay performance. There are many applications of the relative noise concept, one of which is the calculation of S/N.

The basic algorithm works as follows:

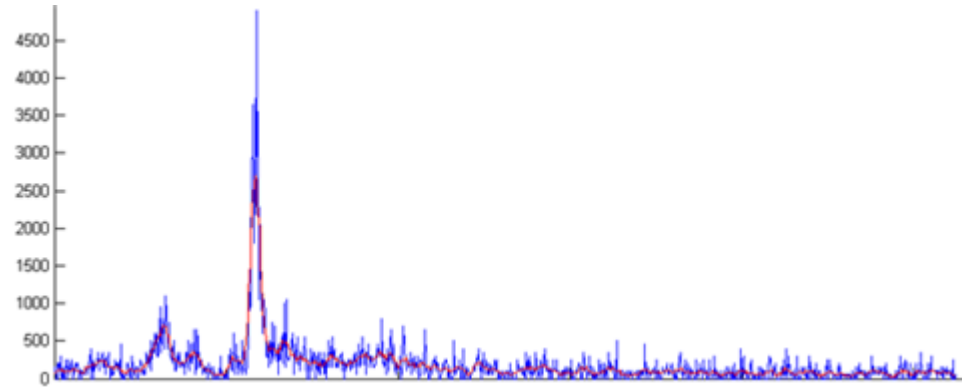
1. Devise a noise model that will allow the user to calculate the expected noise at any point in the data record, given the level of the underlying signal at that point.

   The noise model can be determined from theoretical considerations or can be modeled from real measurements for a particular system. For pulse counting detectors, the standard deviation of a signal, and therefore the expected noise, is proportional to the square root of the signal and therefore varies with the signal. In other systems there will be a constant 'white noise' component, possibly combined with an intensity-dependent component.

2. Estimate the underlying signal from the measured signal.

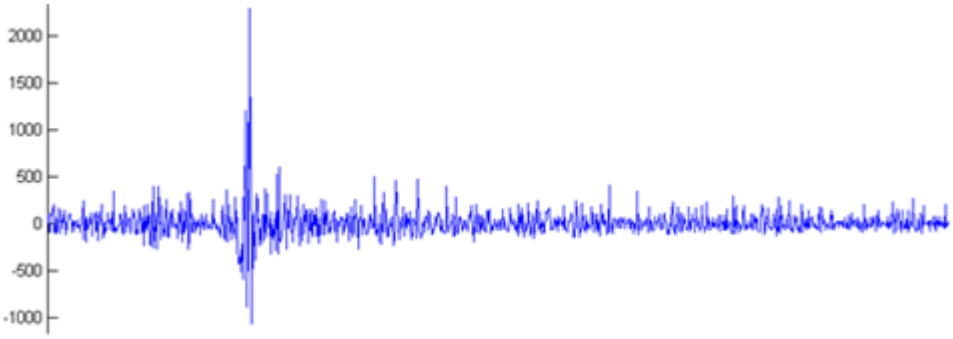
   This can be achieved in many ways, but the simplest is to generate a smoothed version of the data as shown in Figure D-1.

Figure D-1 Overlay of Raw and Smoothed Data



3. Measure the actual noise across the data using all points (peaks and background).
   This is achieved by subtracting the underlying signal estimate from the measured signal at each point in the data where the smoothed signal has been subtracted from the original. This is known as the delta noise. The range of the delta noise is reasonably constant, except where there are large peaks because the noise is dependent on the signal and therefore greater where the signal is larger. Refer to Figure D-2.

Figure D-2 Plot of the Delta Noise Values of Each Data Point



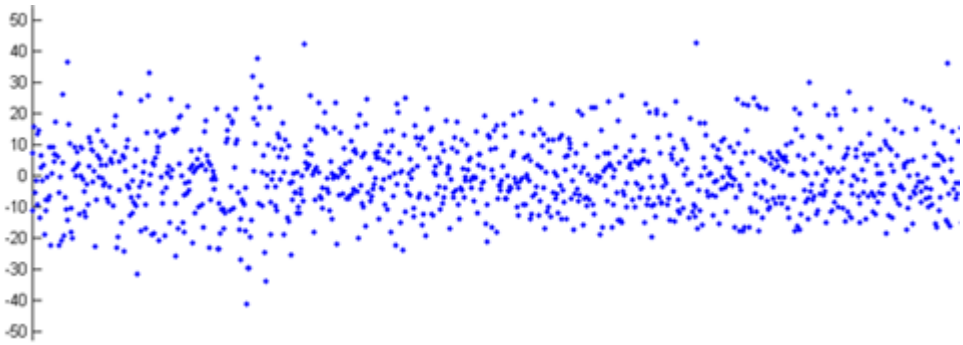
4. At each data point, calculate the ratio of the measured noise to the expected noise.

   That is, at every data point we divide the noise we measured in step 3 by the value our noise model predicts (in our case the square root of the intensity). If the noise model is good, then generates a series of values that mostly remain bounded by some limits as shown Figure D-3. Figure D-3 also shows the plot of

$$\Delta noise / \sqrt{intensity}$$

Note: This reduces the large variation in the delta noise and results in a well constrained set of values.

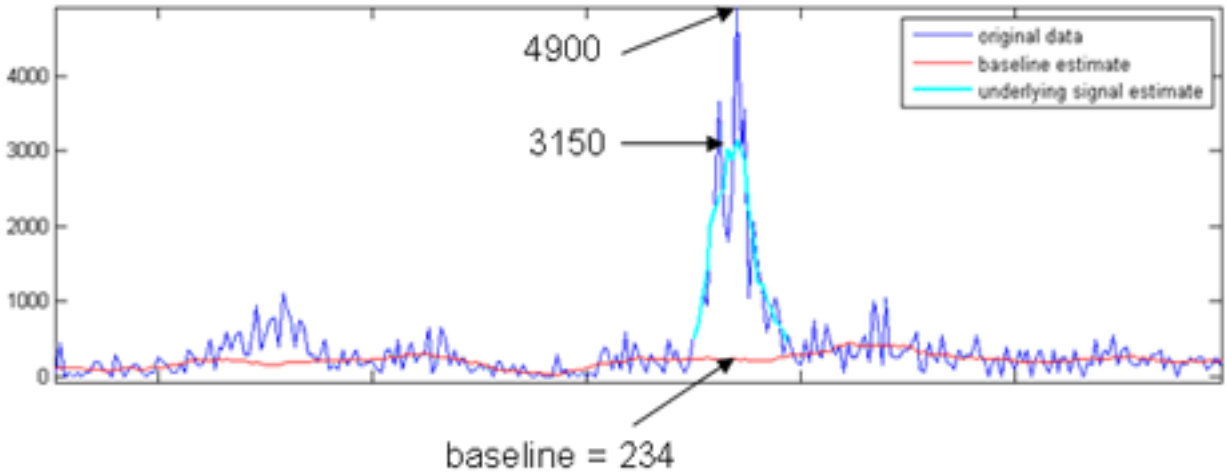
Figure D-3 Noise Model



5. Calculate the standard deviation of the ratio values. This is the Rn, an estimate of the most likely relationship between the actual delta noise and that predicted by the model. In Figure D-3, this results in a value of 9.5.

   Figure D-4 shows an example of how relative noise can be used to calculate S/N.

Figure D-4 Overlay of Raw Data, Underlying Signal Estimates, and Baseline Estimates



As described previously:

$$noise = R_n \times \sqrt{(baseline)}$$

in this particular example:

$$noise = 9.5 \times \sqrt{234} = 145$$

If the apex of the peak is used as the signal, then this gives a S/N of 34 (4900/145) and if the height of the smoothed signal is used, then this gives a S/N of 22 (3150/145).

When reporting the S/N, the MQ4 integration algorithm uses the procedure described here and the peak apex as the signal. Because the SignalFinder™ integration algorithm is fitting a model to the peak, it uses the height of the fitted profile. This results in a smaller reported S/N. However, it is a more accurate value because it is less affected by possible noise spikes. The SignalFinder integration algorithm also has a more sophisticated approach to baseline estimation, so for these two reasons, the S/N values reported by the two algorithms are not identical although they will usually be similar.

In summary, compared to the usual approach of estimating the noise as the standard deviation of a background region, the relative noise approach to calculating S/N has the following advantages:

- It is much less subjective because a background region does not need to be selected manually.
- An accurate S/N can be predicted even if no peak-free regions of the chromatogram exists.

- The baseline and therefore the noise is estimated near the peak of interest. This can make a large difference to the reported S/N value because the background region selected for the usual approach might be much quieter than the background near the peak. As described previously, the S/N calculated using the **Relative Noise** approach might give smaller values than the usual approach. However, they are more accurate and useful values. Refer to Figure D-4.

To make the **Signal / Noise** column visible in the **Results Table**, refer Modify the Columns Shown in the Results Table on page 91.

Note on Signal-to-Noise when Using the SignalFinder Integration Algorithm

Because the SignalFinder™ integration algorithm calculates signal-to-noise more accurately (and thefore more accurately predicts CVs), if the 1-sigma signal-to-noise approach is used, then consider decreasing the minimum acceptable signal-to-noise value on any standard operating procedures (SOPs), based on empirical data from the laboratory.

Software Icons E

Only one pane is active at a time. Active panes have an orange border and the user can activate a pane by clicking anywhere within it. Many menu commands operate on the active pane.

The tool bar icons described in this section appear in the pane-specific tool bar for all pane types. Additional icons specific to each pane type are also available.

Table E-1 Tool Bar Icons

Icon	Name	Description
	New Results Table	Opens the **New Results Table wizard**.
	Open	Opens a **Results Table**.
	Save	Saves any open files.
	Select Analyst Project	Selects a project folder.
	Screen Lock	Locks the screen. This feature in available only when the Analyst® MD software is in Mixed Mode and the screen lock feature is enabled.
	Show Internal Standard with Analyte	Shows the rows in the **Results Table** for both the currently selected analyte and the corresponding internal standard. When this option is selected, the user can click an analyte name and view it with the internal standard. This is equivalent to clicking the analyte and then clicking the internal standard while pressing **Ctrl** (so that both are selected).
	Find Component or Group	Selects the items in the list that match the specified text.
	Arranging Panes	Changes the relative positions of the panes. Click the icon in one pane and then drag it to the top, bottom, left, or right portion of a second pane. Depending on where the cursor is released, the first pane changes positions relative to the second. As the cursor is dragged, one side of the second pane is highlighted in red to indicate where the first pane will be drawn.
	Delete Pane	Deletes the pane. If a **Results Table** is deleted, then other related panes (**Peak Review** and **Calibration**) are also deleted and the entire window is closed.

Table E-1 Tool Bar Icons (continued)

Icon	Name	Description
	Toggles tab mode	Maximizes the pane to fill the entire window (or vice versa). This is useful if there are several panes in the window so that the user can temporarily focus on one. In zoomed mode, a separate tab appears at the top of the window for each pane. Switch between panes by clicking the appropriate tab. From zoomed mode, return to the original view showing all panes by clicking **Zoom Pane** a second time. Clicking the icon toggles between the two states.
	Hide Pane	Hides the pane so that other panes in the window fill the available space.
	Show Hidden Panes	Shows all panes that have been previously hidden.

Table E-2 Peak Review Tool Bar Icons

Icon	Name	Description
	Display Previous Page	Shows the previous set of chromatograms. This is equivalent to pressing the up or left arrow key, or clicking the upper arrow on the scroll bar.
	Display Next Page	Shows the next set of chromatograms. This is equivalent to pressing the down or right arrow key, or clicking the lower arrow on the scroll bar.
	Display Previous Sample	Scrolls backwards in the **Peak Review** pane. This is equivalent to clicking the up arrow on the scroll bar until the first sample that is different from the first currently visible chromatogram is shown.
	Display Next Sample	Scrolls to the next sample.
	Starts Slide Show Peak Review mode	Starts the slide show. On first use, the **Slide Show Options** dialog opens. Set the delay time in seconds between peaks. To prevent the dialog from opening again, select the **Only show this dialog again if the shift key is down** check box. Click anywhere in the **Peak Review** pane to stop the slide show.
	Peak Magnifier	Enlarges the selected peak.
	Peak Demagnifier	Returns the magnified peak to its original size.

Table E-2 Peak Review Tool Bar Icons (continued)

Icon	Name	Description
	Set Peak to 'Not Found'	Click to indicate that no peak is present in the active chromatogram. In some cases when no significant peak is actually present, small noise peaks might be integrated and reported. Click this icon to override that behavior. The peak area shows in the **Results Table** as N/A. After the user marks the peak as **Not Found**, the peak-finding parameters at the left of the pane are not available for the chromatogram because they are not being used. Click the icon again to return to automatic mode.
	Enable Manual Integration Mode	Click to enter manual integration mode. When the software is in manual integration mode, drag in a chromatogram plot to specify the exact region to be integrated. Integration starts from the (time, intensity) point at which the cursor is first clicked and proceeds to the point at which the cursor is released. Click the icon again to exit manual integration mode. After the user manually integrates the peak, the peak-finding parameters at the left of the pane are not available for the chromatogram because they are not being used. Click the icon again to return to automatic mode.
	Recalculate Peak Model	Recalculates the peak model using the active chromatogram and applies it to that chromatogram (SignalFinder™ integration algorithm only).

Table E-3 Calibration Tool Bar Icons

Icon	Name	Description
	Edit Regression and Weighting	Used to change the calibration parameters. This includes both the actual parameter used for the regression (Area or Height) as well as the regression type and weighting. Refer to Regression Equations on page 128.

Table E-4 Statistics Tool Bar Icons

Icon	Name	Description
	Remove Trailing Index from Sample Name	The **Statistics Table** can be arranged so that samples (for a given analyte) are grouped by actual concentration or by sample name. When grouping by sample name, the **Remove Trailing Index from Sample Name** option controls whether sample names must match exactly in order to be grouped or whether a trailing numerical index following a dash (-) should be removed. For example two samples with names of Sample 1 - 001 and Sample 1 - 002 would be grouped together if this option were selected, but not otherwise.
	Sample Grouping	The items in this list specify how the sample for a given analyte should be grouped for the calculation of the statistics. The following choices are available: • **Group by Concentration for Standards**: **Standard** samples are grouped by actual concentration. • **Group by Concentration for QCs**: **Quality Control** samples are grouped by actual concentration. • **Group by Sample Name for Standards**: Replicate **Standard** samples are grouped by the **Sample Name** field. As described previously, if the **Remove Trailing Index from Sample Name** option is not used, then the sample names must match exactly. Otherwise, the names can differ by a trailing number (following a dash). • **Group by Sample Name for QCs**: Similar to the previous option, except that only **Quality Control** samples are used. • **Group by Sample Name for All Samples**: Similar to the previous option, except that all samples are used.

Table E-4 Statistics Tool Bar Icons (continued)

Icon	Name	Description
	Metric	The items in this list specify the actual metric that is used for the calculation of the statistics. The following choices are available: • **Calculated Concentration**: The **Calculated Concentration** field of the **Results Table** is used. • **Area**: The **Area** field of the **Results Table** is used. • **Height**: The **Height** field of the **Results Table** is used. • **Calibration Y-Value**: The regression parameter specified for the analyte is used. This is either **Area** or **Height** for an analyte that does not have a corresponding internal standard, or **Area Ratio** or **Height Ratio** for an analyte that does use an internal standard.

Table E-5 Results Table Tool Bar Icons

Icon	Tool Tip	Description
	Displays the peak review	Shows the **Peak Review** pane so that the quality of the peak integrations can be checked and modified if necessary.
	Displays the side by side sample review	Shows two sample lists so that users can select up to six samples to compare the peak responses across the samples.
	Displays the calibration curve	Shows the calibration curve (this is only applicable if **Standard** samples of known concentration are used). This pane enables the user to review the calibration and adjust the regression type and weighting.
	Creates a metric plot	Shows a metric plot for the currently selected column or columns. These plots can be very useful for finding outliers. The menu to the immediate right of the button lists any saved plot settings.
	Displays the statistics pane	Shows the **Statistics** pane. This table shows the average calculated concentration, standard deviation, and CV for each concentration level.

Table E-5 Results Table Tool Bar Icons (continued)

Icon	Tool Tip	Description
	Sort selected column from smallest to largest	Sorts the **Results Table** so that the values in the selected column are in ascending order. This icon is available only after the column header is clicked.
	Sort selected column from largest to smallest	Sorts the **Results Table** so that the values in the selected column are in descending order. This icon is available only after after the column header is clicked.
	Removes any previous sorting	If the table has been sorted, returns the **Results Table** to the default order.
	Shows only the selected sample type(s)	Filters the **Results Table** so that only samples of a specific type are visible. This is only useful if there are **Standard** samples of known concentration and not all samples are **Unknowns**.
	Hide selected row(s)	Hides the selected rows in the **Results Table**. Select the rows to hide and then click the icon. Because the **Peak Review** pane synchronizes with the **Results Table**, hiding rows for those peaks that do not need to be reviewed makes the review process faster. For example, the user can sort the table on the **Quality** column and hide all rows with a quality greater than some value (for example 0.8). The table can then be sorted on the **Region Height** column and all rows with a low value hidden (to hide rows for which the peak is definitely not present). The result is that only peaks with a low quality, but for which a peak is actually present, are visible. The user can then step through these visible rows from the **Peak Review** pane in less time than it would take to review all possible peaks.
	Show previously hidden row(s)	Shows all of the rows. The shown rows might still be constrained by the **Sample Type Filter** and the **Components & Groups List** selection.
	Show only outliers	Shows the rows that contain outliers.
	Go to next outlier	Advances to the next outlier in the **Results Table**.

Table E-5 Results Table Tool Bar Icons (continued)

Icon	Tool Tip	Description
	Lock and Save	Locks the **Results Table** after it has been saved. Changes to the **Results Table** are not saved unless the file is unlocked.
	Review and Save	Click to save the **Results Table** after it has been reviewed. The icon is unavailable if the **Results Table** is read-only.

MultiQuant™ MD Software Access F

Note: When the MultiQuant™ MD software is removed, the MultiQuant™ MD software security items in the Analyst® MD software remain. Security permissions are found on the **Roles** tab in the **Security Configuration** dialog.

Preset Access	Description
Create session file	Allows users to create a **Results Table**.
Create quantitation method	Allows users to create quantitation methods.
Modify quantitation method files	Allows users to modify the quantitation methods located in the **Quantitation Methods** folder in the **Analyst Data** folder.
Allow Export and Create Report of unlocked Results Table	Allows users to export or create reports of unlocked **Results Tables**.
Replace existing Results Table when saved	Allows users to update existing **Results Tables** but does not allow them to create a new **Results Table** using an existing **Results Table** name. For example, if a **Results Table** called RT1 is created, then users can update it but they cannot create a new **Results Table** using the name RT1. Users cannot name an untitled **Results Table** using an existing **Results Table** name.
Change default quantitation method integration algorithm	In the **Integration Default** dialog, allows users to change the algorithm. Click **Edit > Project Integration Defaults.**
Change default quantitation method integration parameters	In the **Integration Default** dialog, allows users to change the algorithm default parameters. **Edit > Project Integration Defaults.**
Allow Enable Project Modified Peak Warning	Allows users to activate or deactivate the flag that enables the **Project Modified Peak Warning** option on the **Edit** menu.
Allow Project Secure Export Settings	If enabled, then data in the text file is encrypted during export. Set a password to enable encryption.
Add samples to Results Table	Allows users to add samples. Click **Process > Add Samples.**
Remove samples from Results Table	Allows users to remove selected samples. Click **Process > Remove Selected Samples.**

Preset Access	Description
Export, import, or remove External Calibration	Allows users to export, import, or remove an external calibration using one of the following options: • Click **Process > Export Calibration.** • Click **Process > Import External Calibration.** • Click **Process > Remove External Calibration.**
Change Audit Map settings	Allows users to modify the project audit map and modify the audit map definition. Click **Audit Trail > Audit Map Manager.**
Modify Sample Name	Allows users to modify the sample name in the **Results Table**.
Modify Sample Type	Allows users to modify the sample type (**Standard**, **QC**, **Unknown**) in the **Results Table**.
Modify Sample ID	Allows users to modify the sample **ID** in the **Results Table**.
Modify Actual Concentration	Allows users to modify the actual concentration of the **Standard** and **QC** in the **Results Table**.
Modify Dilution Factor	Allows users to modify the dilution factor in the Results Table.
Modify Comment Fields	Allows users to modify comment fields: • **Component Comment** • **IS Comment** • **IS Peak Comment** • **Peak Comment** • **Sample Comments**
Allow manual integration	Allows users to enable manual integration mode in the **Peak Review** pane. If this permission is enabled, then the **Modify Results Table integration parameters for a single chromatogram** permission must also be enabled. The **Allow manual integration** command can be disabled if the **Modify Results Table integration parameters** is enabled.
Allow set to Peak Not Found	Allows users to use the **Set peak to not found** . To perform this action, right-click in the **Peak Review** pane.
Include or exclude a peak from the Results Table	Allows users to include or exclude peaks from **Results Tables**, **Statistics Tables**, and calibration curves.
Modify regression settings for fit and weight	Allows user to modify the regression settings in the calibration curve pane when using the **Modify Results Table Method** functionality and when using the **New Quantitation Method wizard**.

Preset Access	Description
Modify Results Table integration parameters for a single chromatogram	Allows user to modify a single chromatogram.
Modify quantitation method for the Results Table component	Allows user to apply the modifications from the single chromatograms to the component. Users must have this permission and the **Modify Results Table integration parameters for a single chromatogram** permission enabled if they want to update and then apply single modifications to components.
Create, use, or export Metric Plots in Results Tables	Allows users to create and use metric plots in the **Results Table** (**Metric Plot** button is enabled) or export metric plots. Click **File > Export.**
Set Peak Review Title Format	Allows users to modify the **Peak Review Title Format in Peak Review**. To perform this action, right-click in the **Peak Review** pane.
Add, Rename, or Modify custom column	Allows users to add, rename, or modify a custom column. Even without this permission, users can run queries that will automatically create custom columns. If this permission is disabled, then the **Remove custom column** permission must also be disabled. The **Remove custom column** can be disabled if the **Add, Rename, or Modify custom column** permission is enabled.
Remove custom column	Allows users to delete a custom column in the **Results Table**.
Modify Results Table column settings	Allows users to modify **Results Table** column settings within a **Results Table**.
Save Column Settings as Project Default	Allows users to apply the column settings to the project.
Lock and save Results Table	Allows users to lock and save a **Results Table**.
Unlock and save Results Table	Allows users to unlock and save a **Results Table**.
Review and save Results Table	Allows users to review and save the **Results Table**.
Edit Report Template	Allows users to edit the Report templates.
Transfer to LIMS	Allows users to transfer saved and locked **Results Table** to a LIMS. The event is recorded in the audit trail.

Security Settings

Table F-1 contains the recommended security settings for the user roles.

Table F-1 Security Settings Based on User Roles

Security Setting	Administrator	Supervisor	Analyst	Reviewer
Create session file	Access	Access	Access	No Access
Create quantitation methods	Access	Access	No Access	No Access
Modify quantitation method files	Access	Access	No Access	No Access
Allow Export and Create Report of unlocked Results Table	Access	Access	No Access	No Access
Replace existing Results Table when saved	Access	Access	No Access	Access
Change default quantitation method integration algorithm	Access	Access	No Access	No Access
Change default quantitation method integration parameters	Access	Access	No Access	No Access
Allow Enable Project Modified Peak Warning	Access	No Access	No Access	No Access
Allow Project Secure Export Settings	Access	No Access	No Access	No Access
Add samples to Results Table	Access	Access	Access	No Access
Remove samples from Results Table	Access	Access	Access	No Access
Modify Sample Name	Access	Access	No Access	No Access
Modify Sample Type	Access	Access	Access	No Access
Modify Sample ID	Access	Access	No Access	No Access

Table F-1 Security Settings Based on User Roles (continued)

Security Setting	Administrator	Supervisor	Analyst	Reviewer
Modify Actual Concentration	Access	Access	Access	No Access
Modify Dilution Factor	Access	Access	Access	No Access
Modify Comment Fields	Access	Access	No Access	No Access
Allow manual integration	Access	Access	Access	No Access
Allow set to Peak Not Found	Access	Access	Access	No Access
Include or exclude a peak from the Results Table	Access	Access	Access	No Access
Modify regression settings for fit and weight	Access	Access	No Access	No Access
Modify Results Table integration parameters for a single chromatogram	Access	Access	Access	No Access
Modify quantitation method for the Results Table component	Access	Access	Access	No Access
Create, use, or export Metric Plots in Results Tables	Access	Access	Access	Access
Set Peak Review Title Format	Access	No Access	No Access	No Access
Add, Rename, or Modify custom column	Access	Access	No Access	No Access
Remove custom column	Access	Access	No Access	No Access
Modify Results Table column settings	Access	Access	No Access	No Access
Save Column Settings as Project Default	Access	Access	No Access	No Access

Table F-1 Security Settings Based on User Roles (continued)

Security Setting	Administrator	Supervisor	Analyst	Reviewer
Lock and save Results Table	Access	Access	Access	Access
Unlock and save Results Table	Access	Access	No Access	No Access
Review and save Results Table	Access	Access	No Access	Access
Modify Report Template	Access	Access	No Access	No Access
Transfer to LIMS (Controls Initiate Transfer to Watson LIMS as well)	Access	Access	No Access	Access
Export, import, or remove External Calibration	Access	Access	No Access	No Access
Change Audit Map Setting	Access	Access	No Access	No Access

Revision History

Revision	Reason for Change	Date
A	First release of document.	September 2013
B	Updated File Menu section. Updated Audit Trail Menu section. Updated Results Table Columns table. Updated Reports section.	January 2015
C	Changed AB SCIEX logo to SCIEX Diagnostics on the cover page. Updated the copyright page and changed AB Sciex to SCIEX where required. Added Windows 10 to the Introduction to the Software chapter. Updated the Contact Us section. Changed Topic title Audit Map Manager to About Audit Maps. Updated the description of the Set Last Component of Group as IS menu option in the Internal Standards Submenu section. Replaced "total area percentage parameter" with the "retention time" in the Update Retention Time Dialog section. Updated the description of Expected RT in the SignalFinder Integration Algorithm Parameters section. Added Windows 10 to the Create Reports section. Updated the content in the Report Template Tags section. Changed the screenshot in Figure 7-3. New templates were applied to the content, which has led to some edit changes in the content. Removed all references to Windows XP.	June 2017