User Guide

Reporter Software

TPUB-CUST-16110-A

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Contents

Introduction 1

Use the Reporter software to do these tasks:

- Create reports in `docx`, `txt`, `html`, `csv`, and `pdf` format. The reports contain information from Results Tables and data files that were created by the SCIEX OS software.
- Create and edit report templates. Report templates are `docx` files.

  The template files are installed in the `C:\Program Data\SCIEX\Analytics\Reporter` folder.

This guide supplies instructions to create and edit report templates. To create reports, refer to the document: *Help*.

Note: The Reporter software is the same as in the previous version of the SCIEX OS software, but the documentation is updated.

Note: After the installation of the SCIEX OS software is completed, save a backup copy of the installed report templates in a safe location.

CAUTION: Potential Data Loss. To prevent the modification of templates, make sure that the templates for the Reporter software are kept in secured, read-only folders to which only system administrators have write access.

Edit a Report Template 2

If the default templates are not satisfactory, then custom templates can be created. This section gives a description of the procedure to edit templates. For other options to create customized report templates, contact a SCIEX representative.

Note: When users create or edit a report template, they are responsible for template validation.

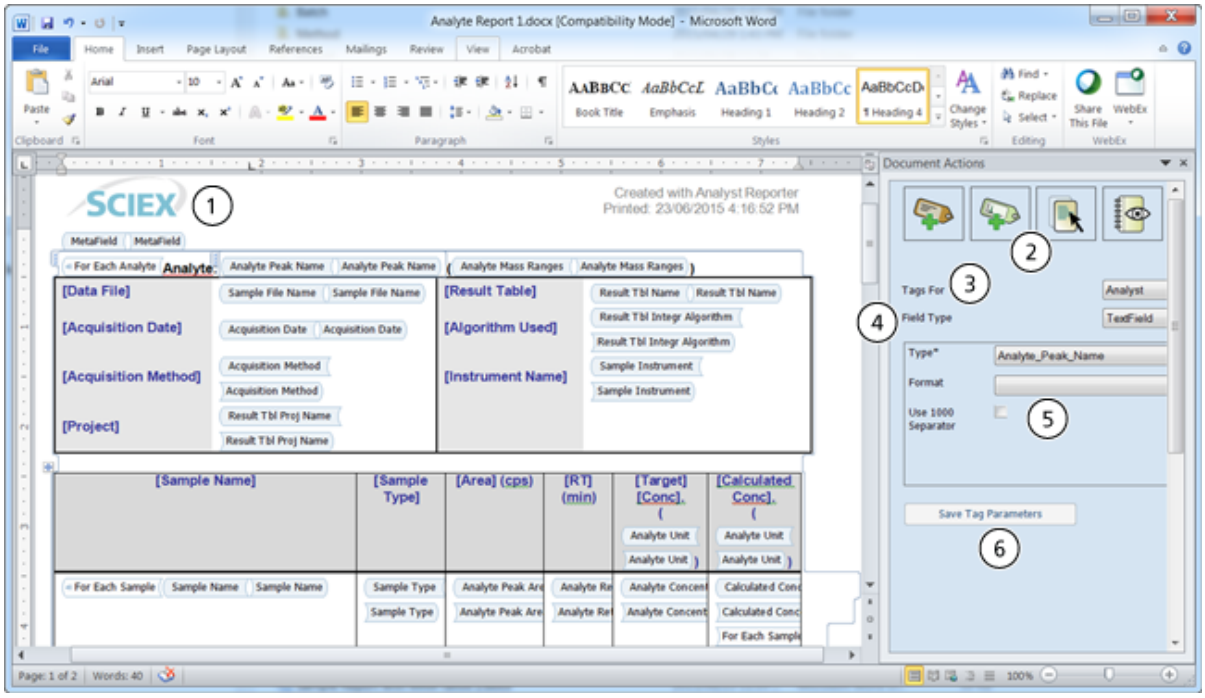
Note: To prevent issues with the default templates, do not edit them. Make a copy of the default template, and then edit the copy.

1. Browse to the folder that contains the templates, and then double-click the applicable `docx` file.

   The template opens in Microsoft Word. The template editor is shown on the right.

Note: If the template folder is in a trusted location, and the correct version of Microsoft Office is installed, then the tags that are used in the template are shown. For more information about trusted locations, go to http://sciex.com/support/knowledge-base-articles/reporter-error-not-in-your-trusted-location_en_us.

Figure 2-1 User Interface for the Report Template Editor



Item	Description
1	Report template with the tags shown.

Item	Description
2	Icons: •  **(Add new tag)** •  **(Add picture tag)** •  **(Show content area)** •  **(View document change log)**
3	**Tags For**: Shows the name of the software that supplies the tag information.
4	**Field Type**: Shows a software-specific name.
5	Shows a list of attributes that can be used with the **Type*** field: • **Type***: Shows a list of available tags. Different tags are available for different software applications. Refer to the section: Reporter Tags. • **Format**: Shows the format of the field that is selected in the **Type*** field, as set in the Results Table. To use a different value, select a value from the list. • **Use 1000 Separator**: Gives the option to use a comma to separate digits by 1000. For example, if **Use 1000 Separator** is selected, then the number 1234567.89 is shown as 1,234,567.89. To use the value that is set in the Results Table, keep this field empty.
6	**Save Tag Parameters**: Click to save changes. If changes are not saved, then a prompt to save the changes is shown.

2. Add, edit, or delete tags as required.

Table 2-1 Reporter Functions

To do this...	Do this...
Change the field type	Click inside the tag, select a new field type, and then select the attributes.
Change the attributes of the field type	Click inside the tab, and then change the attributes as required.
Add a tag	Click  **(Add new tag)**, select the **Field Type**, and then select the attributes.
Add a picture	Click  **(Add picture tag)**, and then select the attributes.
Show where a tag starts and ends	Click  **(Show content area)**.
Show the document audit log	Click  **(View document change log)**.
Copy tags	Copy the selected tags, paste them in the new location, and then update the attributes. **Note:** The attributes are not copied and must be selected.
Move between the tags	Use the left and right arrow keys to move between the tags.
Delete tags	Do one of these steps: • If the cursor is to the left of the tag, then push **Delete**. • If the cursor is to the right of the tag, then push **Backspace**.

3. Click **Save Tag Parameters**.

Tip! To the left of the field, a red exclamation mark flashes to show where information is mandatory.

4. Save the template file.

Reporter Tags

A

Table A-1 ForEach Tags

Column Tag	Description	SCIEX OS Software	MultiQuant Software
`Analyte`	Shows an iteration of the information in the loop for each analyte	Y	Y
`AnalyteGroup`	Shows an iteration of the information in the loop for each quantifier	Y	Y
`InternalStandard`	Shows an iteration of the information in the loop for each internal standard (IS)	Y	Y
`QCStatistics`	Shows an iteration of the information in the loop for each quality control (QC) statistic	Y	Y
`RatioIons`	Shows an iteration of the information in the loop for each qualifier[1]	Y	Y
`Sample`	Shows an iteration of the information in the loop for each sample	Y	Y
`Statistics`	Shows an iteration of the information in the loop for each statistic	Y	Y

[1] This tag must be included in a **ForEach** `AnalyteGroup` tag.

Table A-1 ForEach Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
`MQ_Group`	Shows an iteration of the information in the loop for each component group, with ISs	Y	Y
`MQ_AnalyteRatioIons`	Shows an iteration of the information in the loop for each quantifier[2]	Y	Y
`MQ_ISRatioIons`	Shows an iteration of the information in the loop for each analyte group	Y	Y
`VisibleAnalyte`	Shows an iteration of the information in the loop for each analyte that can be seen in the Results Table	Y	N
`VisibleSample`	Shows an iteration of the information in the loop for each sample that can be seen in the Results Table	Y	N
`Statistics_Custom`	Shows an iteration of the values in a customized statistics table[3]	Y	N

[2] This tag must be included in a **ForEach** `MQ_Group` tag.
[3] This tag is available for the SCIEX OS software 3.4 and later.

Table A-2 Picture Tags

Column Tag	Description	SCIEX OS Software	MultiQuant Software
AnalyteRatio	A chromatogram for each qualifier with an overlay of the quantifier, with horizontal (upper limit and lower limit) lines	Y	Y
AnalyteRatioNoLines	A chromatogram for each qualifier with an overlay of the quantifier, without horizontal (upper limit and lower limit) lines	Y	Y
Calibration	Calibration curve image	Y	Y
FormulaFinderTrafficLight_xcm	Traffic light image for Formula Finder confidence	Y	N
MassTrafficLight_xcm	Traffic light image for mass error confidence	Y	N
LibraryTrafficLight_xcm	Traffic light image for library match confidence	Y	N
FragMassTrafficLight_xcm	Traffic light image for fragment mass error confidence	Y	N
MsPeak	Mass spectrum image	Y	N
MsMsPeak	MS/MS spectrum image	Y	N
ISMsMsPeak	MS/MS spectrum image for each IS		
IonRatioConfidenceTrafficLight_xcm	Traffic light image for ion ratio confidence	Y	N

Table A-2 Picture Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Ms1SpectrumWithTheory_xcm	MS theory spectrum (shown in gray in the MS pane for comparison with the MS spectrum)	Y	N
MsMsSpectrumWithLibrary_xcm	MS/MS spectrum with library	Y	N
IQ_AverageSpectrum	Intact quant workflow: Averaged spectrum image	Y	N
IQ_ReconstructionSpectrum	Intact quant workflow: Reconstruction spectrum image	Y	N
IQ_IS_AverageSpectrum	Intact quant workflow: Averaged spectrum for an IS	Y	N
IQ_IS_ReconstructionSpectrum	Intact quant workflow: Reconstruction spectrum for an IS	Y	N
IS_AnalyteRatio	A chromatogram for each IS qualifier with an overlay of the quantifier, with horizontal (upper limit and lower limit) lines	Y	Y
IS_AnalyteRatioNoLines	A chromatogram for each IS qualifier with an overlay of the quantifier, without horizontal (upper limit and lower limit) lines	Y	Y
IsotopeTrafficLight_xcm	Traffic light image for isotope confidence	Y	N

Table A-2 Picture Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
IS_PeakReview	Extracted ion chromatogram (XIC) for each IS	Y	Y
Overlay_All_XIC	XICs for all of the analytes in one graph, with a legend	Y	Y
Overlay_All_XIC_NoLegend	XICs for all of the analytes in one graph, without a legend	Y	Y
Overlay_All_XIC_with_IntStds	XICs for all of the analytes with ISs on one graph, with a legend	Y	Y
Overlay_All_XIC_with_IntStds_NoLegend	XICs for all of the analytes with ISs on one graph, without a legend	Y	Y
PeakReview	XICs for analytes	Y	Y
RetentionTimeTrafficLight_xcm	Traffic light image for retention time (RT) confidence	Y	N
TIC	Total ion chromatogram (TIC) image	Y	Y
Xic_xcm	XIC image	Y	N

Table A-3 Text Tags

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Acquisition_Date	Date that the data was acquired	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Acquisition_Duration_Minutes	Time that was required for the acquisition	Y	Y
Acquisition_Method	Acquisition method that was used to acquire the data in the Analyst software	Y	Y
Analyte_AnalyteAnnotation	Component comment for the analyte	Y	Y
Analyte_AnalyteCorrelation	Correlation coefficient for the analyte	Y	Y
Analyte_AnalyteRegression	Regression equation with the correlation coefficient and weight	Y	Y
Analyte_Concentration	Actual concentration of the analyte	Y	Y
Analyte_Expected_RT	Expected RT of the analyte	Y	Y
Analyte_Integration_Type	Integration type for the analyte	Y	Y
Analyte_IS_Area_Ratio	Ratio of the analyte area to the IS area	Y	Y
Analyte_IS_Height_Ratio	Ratio of the analyte height to the IS height	Y	Y
Analyte_Mass_Ranges	Mass information for the analyte	Y	Y
Analyte_MSMS_Fragmentation	Fragmentation mode for the analyte: EAD, CID, or N/A	Y	N
Analyte_Peak_Area	Peak area for the analyte	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Analyte_Peak_Height	Peak height for the analyte	Y	Y
Analyte_Peak_Name	Name of the analyte	Y	Y
Analyte_Peak_Width	Peak width for the analyte	Y	Y
Analyte_Peak_Width_at_50%_Height	Peak width at half height for the analyte	Y	Y
AnalyteQuantPeak_Info	The integration parameters for the analyte	Y	Y
Analyte_QTY	—	Y	Y
isCurrentAnalyteQuantifier	Shows **true** or **false**, to identify the analyte as a quantifier	Y	Y
Analyte_Processing_Alg	Integration algorithm that was used	Y	Y
Analyte_Retention_Time	RT for an analyte	Y	Y
Analyte_R_Squared	Squared correlation coefficient	Y	Y
Analyte_RT_Window	RT window for the analyte	Y	Y
Analyte_Formula	—	Y	N
Analyte_Precursor_Mass	Mass of the precursor ion	Y	N
Analyte_Accuracy_Acceptance	Shows if the result of the Accuracy Acceptance test was **Pass** or **Fail**	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Analyte_Concentration_ Acceptance	Shows if the result of the Concentration Acceptance test was **Pass** or **Fail**	Y	N
Analyte_Integration_ Acceptance	Shows if the result of the Integration Acceptance test was **Pass** or **Fail**	Y	N
Analyte_Signal_To_Noise	Signal-to-noise ratio for the analyte	Y	Y
Analyte_Slope_of_Baseline	Slope of the baseline for the analyte	Y	Y
Analyte_Start_Scan	Experiments with the Scheduled MRM (sMRM) algorithm: The time that acquisition starts for an analyte	Y	Y
Analyte_Start_Time	Time that peak integration starts for an analyte	Y	Y
Analyte_Stop_Scan	Experiments with the Scheduled MRM (sMRM) algorithm: The time that acquisition stops for an analyte	Y	Y
Analyte_Stop_Time	Time that peak integration stops for an analyte	Y	Y
Analyte_Unit	Concentration units for an analyte	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Analyte_Use_Record	Shows **true** or **false**, to identify if the **Used** check box is selected for the analyte	Y	Y
Analyte_Count	—	Y	Y
Analyte_Index	Number of the analyte in the processing method	Y	Y
Area_Height	Ratio of the peak area to peak height	Y	N
AutoPeak_Asymmetry	AutoPeak algorithm: Asymmetry factor for the analyte	Y	N
AutoPeak_Candidate_Model_Quality	AutoPeak algorithm: Quality of the candidate model for the analyte	Y	N
AutoPeak_Group_Confidence	AutoPeak algorithm: Group confidence value for the analyte	Y	N
AutoPeak_Integration_Quality	AutoPeak algorithm: Integration quality for the analyte	Y	N
AutoPeak_Model_Source	AutoPeak algorithm: Sample and component that were used to create the model for the analyte	Y	N
AutoPeak_Num_Peaks	AutoPeak algorithm: Number of peaks	Y	N
AutoPeak_Peak_Width_Confidence	AutoPeak algorithm: Confidence value for the peak width	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
AutoPeak_Saturated	—	Y	N
Calculated_Accuracy	Calculated accuracy for the analyte	Y	Y
Calculated_Concentration	Calculated concentration for the analyte	Y	Y
Calculated_Relative_Retention_Time	Calculated relative RT for the analyte	Y	Y
Component_Type	Component type for the analyte	Y	N
Component_Group_Name	Group name for the analyte	Y	N
Difference_From_Average_Sample_Time_Seconds	—	Y	N
Fragment_Mass	Information about the fragment mass	Y	N
IQ_ExpectedMW	Intact quant workflow: Expected molecular weight of the analyte	Y	N
IQ_MW	Intact quant workflow: Actual molecular weight of the analyte	Y	N
IQ_MWDeltaDa	Intact quant workflow: Difference between the expected and actual molecular weight of the analyte, in Da	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
IQ_MWDeltaPpm	Intact quant workflow: Difference between the expected and actual molecular weight of the analyte, in ppm	Y	N
IQ_IS_ExpectedMW	Intact quant workflow: Expected molecular weight of the IS	Y	N
IQ_IS_MW	Intact quant workflow: Actual molecular weight of the IS	Y	N
IQ_IS_MWDeltaDa	Intact quant workflow: Difference between the expected and actual molecular weight of the IS, in Da	Y	N
IQ_IS_MWDeltaPpm	Intact quant workflow: Difference between the expected and actual molecular weight of the IS, in ppm	Y	N
IS_Concentration	Concentration of the IS	N	Y
IS_Expected_RT	Expected RT for the IS	Y	Y
IS_Integration_Type	Integration type for the IS	Y	Y
IS_Mass_Ranges	Mass ranges for the IS	Y	Y
IS_Peak_Area	Peak area for the IS	Y	Y
IS_Peak_Height	Peak height for the IS	Y	Y
IS_Peak_Name	Peak name for the IS	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
IS_Peak_Width	Peak width for the IS	Y	Y
IS_Peak_Width_at_50%_Height	Peak width at half height for the IS	Y	Y
IS_Retention_Time	RT for the IS	Y	Y
IS_RT_Window	RT window for the IS	Y	Y
ISQuantPeak_Info	Concatenation of integration parameters for the IS for the peak in one string	Y	Y
IS_Signal_To_Noise	Signal-to-noise ratio for the IS	Y	Y
IS_Slope_of_Baseline	Slope of the baseline for the IS	Y	Y
IS_Start_Scan	Start time of the scan for the IS	Y	Y
IS_Start_Time	Start time for the IS peak	Y	Y
IS_Stop_Scan	Stop time of the scan for the IS	Y	Y
IS_Stop_Time	Stop time for the IS peak	Y	N
IS_Units	Concentration units for the IS	Y	Y
Is_Area_Height	Ratio of peak area to peak height for the IS	Y	N
Is_Baseline_Delta_To_Height	Absolute value of the difference between the baseline and peak height for the IS	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Is_Comment	Component comment for the IS	Y	N
Is_Peak_Comment	Comment for the IS peak	Y	N
Is_Quality	Quality of the IS related to the analyte	Y	N
Is_Region_Height	Height of the IS region	Y	N
MQ_Accuracy_Tolerance_LLOQ	Tolerance limit for accuracy acceptance for standards at the lower limit of quantitation (LLOQ)	Y	Y
MQ_Accuracy_Tolerance_STD	Tolerance limit for accuracy acceptance for standards that are not at the LLOQ	Y	Y
MQ_Accuracy_Tolerance_QC	Tolerance level for accuracy acceptance for QCs	Y	Y
MQ_Analyte_Group_Name	Group name for the analyte	Y	Y
MQ_Barcode	Barcode number for the sample	Y	N
MQ_Created_With	Software version that was used to create the Results Table	Y	Y
MQ_Expected_Ion_Ratio	Expected ion ratio for the analyte	Y	Y
MQ_FitPercentage	—	Y	N
MQ_ExtractionMass	—	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
MQ_Group_Index	Number of the group in the processing method	Y	Y
MQ_Group_Name	Group name for the component, ISs included	Y	Y
MQ_Ion_Ratio	Actual ion ratio for the analyte	Y	Y
MQ_IonRatio_Tolerance	Tolerance value for the ion ratio	Y	Y
MQ_IS_Group_Name	Group name for the IS	Y	Y
MQ_IsRowHidden	Shows **true** if the IS row can be seen or **false** if it cannot	Y	Y
MQ_Libraryhit_KE	Kinetic energy (KE) value of the library match	Y	N
MQ_Libraryhit_MSMS_Fragmentation	Fragmentation mode for the library match: CID, EAD, or N/A	Y	N
MQ_Lower_Limit_Concentration	Lower limit for the Concentration Acceptance test	Y	Y
MQ_Outlier_Reasons	Automatic removal of outliers: Shows the criterion that was outside the limits for the component	Y	Y
MQ_Outlier	Automatic removal of outliers: Shows **true** if the component is an outlier or **false** if it is not	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
MQ_Peak_Asymmetry_Factor	Peak asymmetry factor for the analyte	Y	Y
MQ_Peak_BaselineDelta_to_Height	Absolute value of the difference between the baseline and peak height	Y	Y
MQ_Peak_End_at_10pct	Time, in minutes, along the back side of the peak where the intensity is 10% of the peak height	Y	Y
MQ_Peak_End_at_5pct	Time, in minutes, along the back side of the peak where the intensity is 5% of the peak height	Y	Y
MQ_Peak_Points_Across_Baseline	Number of scans across the peak	Y	Y
MQ_Peak_Points_Across_Half_Height	Number of scans across the peak at approximately half of the peak height	Y	Y
MQ_Peak_Start_at_10pct	Time, in minutes, along the front side of the peak where the intensity is 10% of the peak height	Y	Y
MQ_Peak_Start_at_5pct	Time, in minutes, along the front side of the peak where the intensity is 5% of the peak height	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
MQ_Peak_Tailing_Factor	Distance from the front slope of the peak to the back slope, divided by two times the distance from the center line of the peak to the front slope, measured at 5% of the maximum peak height	Y	Y
MQ_Peak_Width_at_10pct	Width of the peak, measured at 10% of the peak height	Y	Y
MQ_Peak_Width_at_5pct	Width of the peak, measured at 5% of the peak height	Y	Y
MQ_Quantifier_Mass_Ranges	Mass ranges for the quantifier	Y	Y
MQ_Quantifier_Peak_Area	Peak area for the quantifier	Y	Y
MQ_Quantifier_Calculated_Concentration	Calculated concentration for the quantifier	Y	Y
MQ_Report_Generation_Date	Date that the report was created	Y	Y
MQ_XICProfile	List of time and height data points for the XIC	Y	N
MQ_MS1Profile	List of mass and height data points for the MS spectrum	Y	N
MQ_MS1PeakList	—	Y	N
MQ_MSMSPeakList	—	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
MQ_MSMSDeconvPeakList	—	Y	N
MQ_LibraryHitPeakList	—	Y	N
MQ_ScannedBarcode	Barcode that was scanned before the injection	Y	N
MQ_ReverseFit	Reverse fit score	Y	N
MQ_Upper_Limit_Concentration	Upper limit of the acceptable calculated concentration	Y	Y
Peak_Comment	—	Y	N
Polarity	Polarity used for acquisition	Y	N
Processing_Method	Name of the processing method	Y	N
Query_Name	Name of the query in the Reporter software	Y	N
Record_Modified	Shows **true** if the integration was changed or **false** if it was not	Y	Y
Region_Height	—	Y	N
Report_Created_by	Name of the user who created the report	Y	N
Reporter_Template_Name	Name of the template that was used for the report	Y	N
ResultTbl_CreateDate	Date that the report was created	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
ResultTbl_IntegrAlgorithm	Integration algorithm that was used for the Results Table	Y	Y
ResultTbl_Name	Name of the Results Table	Y	Y
ResultTbl_ProjName	Name of the project that contains the Results Table	Y	Y
Sample_Comment	Comment for the sample	Y	Y
Sample_Dilution_Factor	Dilution factor for the sample	Y	Y
Sample_File_Name	Name of the data file that contains the sample acquisition data	Y	Y
Sample_ID	The identifier for the sample	Y	Y
Sample_Index	Number of the sample in the Results Table	Y	Y
Sample_Count	Number of samples in the Results Table	Y	Y
Sample_InjectionVolume	Injection volume that was used to acquire the sample	Y	Y
Sample_Instrument	Mass spectrometer that acquired the sample	Y	Y
Sample_InstrumentSerial Number	Serial number of the mass spectrometer that acquired the sample	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Sample_Name	Name of the sample	Y	Y
Sample_Operator	User who was logged on when acquisition of the sample started	Y	Y
Sample_Plate_Number	Number of the plate from which the sample was acquired	Y	Y
Sample_Rack_Number	Number of the rack from which the sample was acquired	Y	Y
Sample_Type	Sample type: Standard, Blank, Double Blank, Quality Control, Unknown, or Solvent	Y	Y
Sample_Vial_Position	Position of the vial from which the sample data was acquired	Y	Y
Sample_File_Full_Name	File name and folder path of the file to which the sample data was acquired	Y	Y
Sample_Index_In_Wiff	Number of the sample in the data file	Y	Y
Sample_LC_Method	LC method that was used to acquire the sample data with the SCIEX OS software	Y	N
Sample_MS_Method	MS method that was used to acquire the sample data with the SCIEX OS software	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Sample_WeightToVolumeRatio	Ratio of weight to volume for the sample	Y	N
Sta_Accuracy	Accuracy, from the Statistics table, for Standard samples	Y	Y
Sta_CV	%CV, from the Statistics table, for Standard samples	Y	Y
Sta_ExpectedConcent	Expected concentration, from the Statistics table, for Standard samples	Y	Y
Sta_Mean	Mean value, from the Statistics table, for Standard samples	Y	Y
Sta_NumVal	Number of values in the Statistics table for Standard samples	Y	Y
Sta_QCAccuracy	Accuracy, from the Statistics table, for QC samples	Y	Y
Sta_QCCV	%CV, from the Statistics table, for QC samples	Y	Y
Sta_QCExpectedConcent	Expected concentration, from the Statistics table, for QC samples	Y	Y
Sta_QCMean	Mean value, from the Statistics table, for QC samples	Y	Y
Sta_QCNumVal	Number of values in the Statistics table for QC samples	Y	Y

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
Sta_QCStdDev	Standard deviation, from the Statistics table, for QC samples	Y	Y
Sta_StdDDev	Standard deviation, from the Statistics table, for Standard samples	Y	Y
Sta_Accuracy_Custom	Accuracy for a customized Statistics table[3]	Y	N
Sta_CV_Custom	%CV for a customized Statistics table[3]	Y	N
Sta_Mean_Custom	Mean value for a customized Statistics table[3]	Y	N
Sta_NumVal_Custom	Number of values in a customized Statistics table[3]	Y	N
Sta_StdDev_Custom	Standard deviation for a customized Statistics table[3]	Y	N
StdAddn_Accuracy	Standard addition: The accuracy for the component	Y	N
StdAddn_ActualConcentration	Standard addition: The actual concentration for the component	Y	N
StdAddn_Calculated Concentration	Standard addition: The calculated concentration for the component	Y	N
Time_Since_First_Sample_ Seconds	Time since the acquisition of the first sample, in seconds	Y	N

Table A-3 Text Tags (continued)

Column Tag	Description	SCIEX OS Software	MultiQuant Software
`Time_Since_Last_Sample_Seconds`	Time since the acquisition of the last sample, in seconds	Y	N
`XIC_Width_Ppm`	XIC width, in ppm	Y	N
`XIC-Width_Da`	XIC width, in Da	Y	N
`CUSTOM`	Custom calculation or column to be exported	Y	N

Reporter Templates 3

It is the responsibility of the user to validate the custom report template.

CAUTION: Potential Data Loss. To prevent users from modifying templates, make sure that the Reporter templates are located in secured, read-only folders that are accessible for writing only by system administrators.

Some report templates use queries. Users can use Microsoft Excel-based formulas to create queries to analyze and do calculations on data in a Results Table, and show the data in a report. To use a query, add the name of the query file in the `MetaField` tag in the report template. Query files must have the extension `query` and must be saved in the `Reporter` folder where the report templates are kept.

It is always a good practice to validate the results when a Reporter template is used, but if a query is used, then we recommend the validation of the results. If changes are made to the report template, for example, to tags or queries, after validation, then the report template should be validated again.

Table 3-1 Default Templates

Template	Template Description[4]	Additional Notes
All Peaks Qual	A report showing, for each sample, a section including the File Information, Sample Information, Analyte Results Table, and overlaid chromatograms of all of the analytes and internal standard. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	N/A
Analyte 20 percent Report	A report showing, for each analyte, a section including File Information, and an XIC table for each Blank, Standard, QC, and 20% of all Unknowns.	This is an example report template that has a Query attached: Analyte20percent.Query.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
Analyte summary	Table of results showing Sample Name, Calculated Concentrations and Outliers for all samples in the batch for the specific analyte and the related Internal Standard.	N/A
Calibration Curve	A report showing the File Information, Statistics Table (standards), and Calibration Curve for analytes, one page per analyte.	• Standards for which the Reportable check box is cleared will not be reported in the data table. Statistics will not be affected by the Reportable status. • The report will show the regression equation and graph, as shown and calculated in the Calibration Curve pane in the Analytics workspace, based on the status of the **Used** column.
Intact Quant All Peaks and Graphs	A report showing the Results Table entries for each sample. All columns visible in the Results Table are shown in the report. The report also includes the XIC chromatograph, average spectrum, and reconstruction spectrum, for each sample and analyte.	This report is specific to the Mass Reconstruction workflow.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
Intact Quant Analyte Summary and Calibration Curve	A report showing the Results Table entries, the calibration curve, and the statistics data for each analyte. The Results Table includes Sample Name, Sample Type, Analyte name, Actual Concentration, Area, Height, Expected MW, MW, MW Delta, Calculated Concentration, and Accuracy.	This report is specific to the Mass Reconstruction workflow.
Intact Quant Sample Summary	A report showing Results Table entries for all samples. The Results Table includes Sample Name, Sample Type, Analyte Name, Actual Concentration, Area, Height, Expected MW, MW, MW Delta, Calculated Concentration, Accuracy and Accuracy acceptance.	This report is specific to the Mass Reconstruction workflow.
Metric Plot	A report showing, for each analyte, a section including the File Information and a metric plot of the analyte peak area.	The state of the **Reportable** check box does not affect the report content. All data points are included even if the check boxes are cleared.
MQ Analyte Report 1	A report showing, for each analyte, a section including File Information, Sample Results Table, and XIC table for each sample - WILL GENERALLY PRINT 2 PAGES PER ANALYTE FOR < 8 SAMPLES	N/A
MQ Analyte Report 2	A report showing, for each analyte, a section including File Information and XIC table for each unknown sample - WILL GENERALLY PRINT 2 PAGES PER ANALYTE FOR < 8 SAMPLES	Only unknowns are reported.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
MQ Analyte Report 3	A report showing, for each analyte, a section including File Information, and Unknown Samples Summary Table.	Only unknowns are reported.
MQ Analyte Report condensed table	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. The table is shown as 2 columns to fit more samples per page.	Only unknowns are reported.
MQ Analyte Report with chromatograms	A report showing, for each analyte, a section including File Information, Sample Results Table, and a small chromatogram for each sample.	Only unknowns are reported.
MQ Blank Template	N/A	Only header information, the logo, and page numbers are shown in the report.
MQ Pep Quant	N/A	For use with the Peptide Quantitation dataset. Refer to the absolute quantitation example in the document: *MultiQuant Software Peptide Quantitation Tutorial*.
MQ QC Summary 1 with flags	A report showing File Information, QC Summary Table per analyte (values with a CV higher than 20% are highlighted), and QC Detailed Results Table (values with an accuracy outside of 80-120% are highlighted).	Quality Controls that have the **Reportable** check box cleared will not be included in the report, nor will they be used in the calculations.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
MQ Sample Report 1	A report showing, for each sample, a section including File Information, Sample info, IS info, Analyte Results Table, XIC table including IS and each analyte - WILL GENERALLY PRINT 2 PAGES PER SAMPLE FOR < 8 SAMPLES	N/A
MQ Sample Report 2	A report showing, for each unknown sample, a section including File Information, TIC, Sample Details, Analyte XIC, and results in table form - WILL GENERALLY PRINT 2 PAGES PER SAMPLE FOR < 8 SAMPLES	Only unknowns are reported.
MQ Sample Report 3	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table.	Only unknowns are reported.
MQ Sample Report condensed table	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. The table is shown as 2 columns to fit more analytes per page.	Only unknowns are reported.
MQ Sample Report with chromatograms	A report showing, for each sample, a section including File Information, Sample info, Analyte Results Table, and a small chromatogram for each analyte.	Only unknowns are reported.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
MQ Sample Report with Concentration Threshold	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Sum	• The related query file is Sample Report with Concentration Threshold.query. • Components must be named "Cmpd *X*#", where *X* is any character from A to F, and # is any numeric value. **Example:** In the report, a component named "Cmpd A 1" will be shown under the heading **Compound Group A**; a component named "Cmpd B 1" will be shown under **Compound Group B**, and so on. • If components are in the same group, then only the first component, alphabetically, in the group will be included in the report. **Example 1:** If "Cmpd B 25" and "Cmpd C 1" both belong to the group "Grp", then "Cmpd C 1" will not be in the report. **Example 2:** If "Cmpd A 1", "Cmpd A 2", and Cmpd A 3" are not assigned to groups, then "Cmpd A 2" and "Cmpd A 3" will not be in the report. **Example 3:** If "Cmpd A 1", "Cmpd A 2", and Cmpd A 3" are assigned to groups 1, 2, and 3, respectively, then

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
		all 3 components will be in the report under the heading **Compound Group A**.
MQ Sample Report with MRM ratios 2	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table, overlay of all XIC. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns in the Results Table. Any values outside 20% of expected are flagged. Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	N/A

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
MQ Sample Report with MRM ratios EU	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns in the Results Table. Any values outside of expected are flagged (using EU guidelines for ratio tolerances). Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	The related query file is `MRM ratios EU.query`.
MQ Sample Report with MRM ratios MQ EFAB 03	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns in the Results Table. Any values outside 20% of expected are flagged. Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	N/A

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
MQ Sample Report with MRM ratios	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns in the Results Table. Any values outside 20% of expected are flagged. Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	The related query file is `MRM ratios.query`.
MQ Sample Report with standards, QC, and blanks	A report showing, for each sample, a section including File Information, Standards Summary Table, QC Summary Table, Blanks Results Table; then for each unknown sample a section including File Information, Sample info, IS info, Analyte Results Table, XIC table including IS and each analyte - WILL GENERALLY PRINT 2 PAGES PER SAMPLE FOR < 8 ANALYTES.	Standards and Quality Controls that have the **Reportable** check box cleared will not be shown in their respective summary tables in the report, nor will they be used in the statistical calculations.
MQ Tutorial Dataset Heavy Light	N/A	This report is intended for use with the Tutorial Dataset Heavy Light dataset. Refer to the second example, the relative quantitation example, in the *User Guide* for the MultiQuant Software.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
Per Analyte Quant-Qual	A report showing, for each analyte, a section including the File Information, Results Table, Calibration Curves, and chromatograms including the internal standard and each analyte. This template is suitable for a Results Table with a group.	N/A
Per sample Quant-Qual with statistics	A report showing components for each sample with a WYSIWYG table. XIC, MS, and MS/MS are shown. A statistics summary table for area is shown at the end of the report.	• If the component table has UV components, then the UV trace is reported under XIC graph in the report. **Note:** If the name of the UV component is in the format [*compound_name*uv] or [uv], then no UV traces are reported, because the uv suffix is related to the UV MS Qual report. • If a sample is labeled as a QC and there are 2 or more samples, then the mean, STDEV, and %CV will be calculated and included in a QC summary table at the end of the report. • If the **Reportable** check box is cleared for a QC row, then that row will not be used for any calculations in the QC summary table.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
Per Sample Quant-Qual	A report showing, for each selected sample, a section including the File Information, Sample Information, and Analyte Results Table for the selected analytes. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	N/A
Per Sample Quant-Qual Visible Rows Using Visible Analyte	A report showing, for each selected sample, a section including the File Information, Sample Information, and Analyte Results Table for the selected analytes. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	The hidden state of a row takes precedence over the state of the **Reportable** check box. If the **Reportable** check box is selected but the row is hidden, then the row is not reported.
Positive Hits Qual	A report showing, for each selected sample, a section including the File Information; Sample Information; Analyte Results Table for the selected analytes; overlaid chromatograms of all of the analytes, internal standard, and the XIC; the Acquired/ Theoretical MS spectra; and the Acquired/Library MS/MS spectra for each selected analyte. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	N/A

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
Qual CSV report	A report in a csv format showing, for each sample, a section including the File Information, Sample Information, and Analyte Results Table.	Recommended to use CSV option for Report format.
Sample summary	A report showing, for each sample, a section of Analytes Summary Table. This report template is suitable for a Results Table with groups.	N/A
SCIEX OS LIMS Template A	A template that exports a Results Table for use in third-party systems, for example, a LIMS or LIS.	The analytes are shown vertically.
SCIEX OS LIMS Template Export as from Analyst with regr and ion ratio	A template that exports a Results Table for use in third-party systems, for example, a LIMS or LIS.	This template can be used for data that was acquired with the Analyst software.
SCIEX OS LIMS Template_Displaying Analytes Horizontally	A template that exports a Results Table for use in third-party systems, for example, a LIMS or LIS.	The analytes are shown horizontally.

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
UV MS Qual report	A report showing, for each sample, the components of that sample and their corresponding UV component with a WYSIWYG table. XIC, MS, and MS/MS are shown along with UV data. A statistics summary table for area is shown at the end of the report.	• UVMS data should be processed with the naming convention *compound 1* (any string) for the mass spectrometer (MS) component and *compound 1*uv (any string plus uv) for the corresponding UV component. • Only the Mass error, Fragment Mass Error, RT confidence, Istotope confidence and Library confidence traffic lights are shown. • A graph table is created to shown the individual components of the Results Table, including the XIC, MS1 trace, MS/MS trace, and header information from compound 1, and the UV trace from compound 1uv. Refer to Figure 3-1. • Analyte graphs are only repeated for the MS experiments, not for the not the UV experiments. • If a sample is labeled as a QC and there are 2 or more samples, then the mean, STDEV, and %CV are calculated and included in a QC summary table at the end

[4] As shown in the Create Report dialog

Table 3-1 Default Templates (continued)

Template	Template Description[4]	Additional Notes
		of the report. Refer to Figure 3-2. • If the **Reportable** check box is cleared for a QC row, then that row in not used for any calculations in the QC summary table.

Figure 3-1 Graph Table

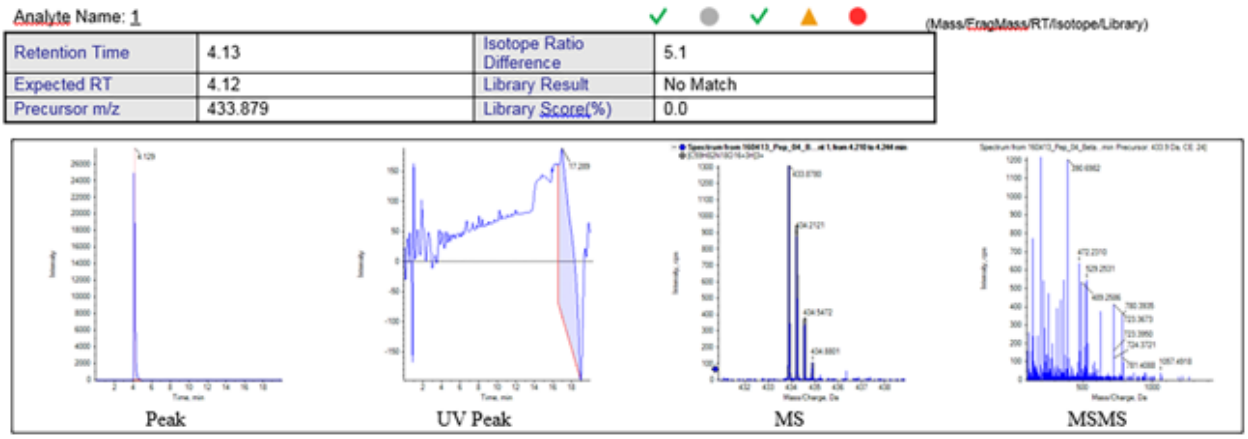


Figure 3-2 Statistics Table

Statistics (Grouped by Concentration for QCs - Area)

Analyte Peak Name (MRM Transition)	Mean	Std. Deviation	% CV	Number of Values Used
1 (723.3573 - 723.3773)	1.062e4	7.367e2	6.93	2 of 2
2 (753.3091 - 753.3291)	2.215e4	6.858e2	3.10	2 of 2
3 (760.3353 - 760.3553)	9.332e3	1.955e1	0.21	2 of 2
4 (631.3450 - 631.3650)	3.244e4	1.110e3	3.42	2 of 2
5 (636.3373 - 636.3573)	1.144e5	3.962e2	0.35	2 of 2
6 (871.4354 - 871.4554)	6.479e4	1.198e3	1.85	2 of 2
7 (932.4493 - 932.4693)	2.183e4	7.301e2	3.34	2 of 2
8 (1000.5743 - 1000.5943)	2.553e4	5.007e2	1.96	2 of 2
9 (755.4352 - 755.4552)	1.127e5	8.422e3	7.48	2 of 2
10 (1184.5929 - 1184.6129)	3.576e4	7.231e2	2.02	2 of 2
11 (884.4871 - 884.5071)	5.183e4	1.512e3	2.92	2 of 2
12 (1176.5468 - 1176.5668)	1.670e4	1.848e2	1.11	2 of 2
13 (871.9418 - 871.9618)	1.597e5	5.501e2	0.34	2 of 2
14 (879.4236 - 879.4436)	1.868e5	5.182e3	2.77	2 of 2

[4] As shown in the Create Report dialog

Contact Us

Addresses

EC REP	Leica Microsystems CMS GmbH Ernst-Leitz-Strasse 17-37 35578 Wetzlar Germany
UKRP	Leica Microsystems (UK) Ltd 19 Jessops Riverside 800 Brightside Lane, Sheffield S9 2RX, England
	AB Sciex Pte. Ltd. Blk33, #04-06 Marsiling Industrial Estate Road 3 Woodlands Central Industrial Estate, Singapore 739256
SCIEX Headquarters	AB Sciex LLC 250 Forest Street Marlborough, MA 01752 USA

Customer Training

- Global: sciex.com/contact-us

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